



## Fall 2009 All Hands Meeting

**Wednesday September 23, 2009**

SURAGrid members were invited to participate in the Coalition for Academic Scientific Computation (CASC) 20th Anniversary Symposium. Notes, presentations, and photos from the CASC meeting and Symposium are available at <http://www.casc.org/meetings1.html>.

**Thursday September 24, 2009**

### **9:00AM - State of SURAGrid**

The "State of SURAGrid" review was accompanied by extended discussion of Membership growth, SGC's Working Group rankings and metrics. There was good discussion generated around the ideas and concepts from the panel presentations of the CASC (Coalition for Academic Scientific Computation <http://www.casc.org/>) 20th Anniversary Symposium, held 9/23 and to which SURAGrid attendees were welcomed.

[http://www.sura.org/programs/docs/State\\_Of\\_SURAGrid.pdf](http://www.sura.org/programs/docs/State_Of_SURAGrid.pdf)

### **9:30 AM - Community Site Reports**

Twelve site reports were submitted for this All Hands. There were several points of common interest and discussion:

- SURAGrid member sites supporting SURAGrid users – but outside the Globus/SURAGrid portal. We discussed how we might consider expanding the SURAGrid Portal so as to capture this activity (which is not necessarily being represented by the "pure" Globus Grid access implied for the current SURAGrid portal resources). That is, if a SURAGrid member site is supporting other participants (even if by providing direct login/SSH access), should we not recognize the value of that community collaboration?
- Several sites are investigating fee-for-service models and are interested in experiences of other sites in this area.
- There is interest in Virtual Computing initiatives (including such as North Carolina State University's Virtual Computing Lab (see <http://vcl.ncsu.edu/>))
- Sites are reporting expansions or end of warranty periods for some systems, as is expected from the dynamic nature of our SURAGrid resources.

[http://sura.org/programs/docs/Fall09\\_Site\\_Reports.pdf](http://sura.org/programs/docs/Fall09_Site_Reports.pdf)

### **11:00 AM – SURAGrid Sustainability**

All Hands participants (in person and remote attendees) considered the topic of SURAGrid Sustainability, as introduced in a short document drafted by the SURAGrid Governance Committee. In particular, the SGC noted that *Key elements to creating a sustainable model for SURAGrid* include:

- An easy to use operational infrastructure
- Users seeking access to SURAGrid services
- A diverse, multi-year funding stream

There was an extensive discussion that continued through lunch with a general agreement that our SURAGrid working groups should be charged to focus on:

- Operations – as in production environment, making easier to use
- User Base – as in growing base, encouraging ease of use
- Funding – any opportunities

[http://sura.org/programs/docs/Sustainability\\_Challenge.pdf](http://sura.org/programs/docs/Sustainability_Challenge.pdf)

[http://sura.org/programs/docs/Production\\_SURAgrid.pdf](http://sura.org/programs/docs/Production_SURAgrid.pdf)

### **1:00 – 5 PM - SURAgrid Working Group Meetings**

The All Hands Participants reviewed all extant SURAgrid working groups. The outcome of the process was:

1. Summary of key focus areas for each Working Group
2. Reprioritization, specifically noting Working Groups actively engaged at this time
3. Reconfirming SGC Oversight of all working groups

#### Access Management Working Group

1. Define an access management process for the SURAgrid CA
2. Propose a level of assurance that involves in-person vetting
3. Define an operational model for the proposed access management process
4. Address accounting data requirements
5. Emphasize the ease of use and responsive
6. Leverage LDAP groups for project tracking

#### Funding Working Group

1. Improve Funding Agency Interaction – Communicate more frequently with Program Officers
2. 3<sup>rd</sup> Party review of declined proposals with the reviewer comments; resubmit if appropriate
3. Obtain input from broader SG community early in proposal process; circulate abstract
4. Expand proposals to more agencies such as DARPA, NASA, Industry others . . .
5. Align proposals to strategic strengths (SURAgrid; Institution; PIs)
6. Develop the proposals around the Science and not the infrastructure
7. Broaden our community – HBCU, MSI, et al . . .

#### Packaged Stack Working Group

1. Evaluate packaged stack options across SURAgrid
2. Evaluate OSG stack usefulness within SURAgrid
3. Define support model for stack, including bug fixes
4. Incorporate new platforms (e.g. AIX)

#### Accounting Data Working Group

1. Simplify accounting uploads from sites
2. Have consistent tracking of machine domain and user domain attributes
3. Establish regular accounting period and notification
4. Define standard analytics
5. Address access management requirements

#### SGC (Working Group)

1. Produce operations plan and assignments to working groups
2. Coordinate and prioritize working group alignments with strategic plan
3. Strategic Grid Relationships – SG-OSG: not a working group but should be coordinated through the SGC point of contact for SG-OSG agreement (JPR)

#### Reduced number of working groups to help focus limited resources

The bolded Working Groups below are those that are active and which will receive *Flywheel* support at this time. (Condor continues due to Jerry Perez volunteering to continue as flywheel. Four other active working groups are supported by SURA staff as flywheels.

Note that underlined entries below are determined not to be working groups per se, but are managed as part of domain and activities of the SURAgrid Governance Committee.

Bottom line, we agreed that this provided a more practical, sustainable and realistic basis for Working Group activities – with **focus on operations, user base and funding**.

| <i>Rank</i> | <i>RANKING based on input from 7 of 9 SGC Members</i>     | <i>Flywheel</i>    |
|-------------|---|--------------------|
| 2.1         | <b>Access Management Working Group</b>                    | Dai Wang           |
| 4.5         | <b>Funding Review Working Group</b>                       | Gary Crane         |
| 5.7         | <b>Packaged Stack Working Group</b>                       | TTU                |
| 6.3         | <b>Accounting (Data) Working Group</b>                    | Dai Wang           |
| 4.5         | <del>Strategic Grid Relationships Working Group</del>     | SGC domain         |
| 8.0         | <del>Collaboration Infrastructure Working Group</del>     | SGC domain         |
| 9.5         | <del>SURAggrid Membership Development Working Group</del> | SGC domain         |
| 9.0         | <del>Minority Outreach Working Group</del>                | part of membership |
| 9.8         | <b>Condor Working Group</b>                               | Jerry Perez        |
| 6.8         | Metascheduler Working Group                               | not active         |
| 11.0        | Teaching Environment Working Group                        | not active         |

### **5 - 6 PM - Open Mike**

Our day wrapped up with Open Mike. Several topics were carried forward from the Working Groups discussion and we wrapped up with a Big Picture (below). But first we recognized several SURAggrid community persons\_with a cake.

**Sue Fratkin** was recognized for her skills with the politics of federal agencies, funding and research and thanked for her service to SURA and SURAggrid. As Sue continues in her role with CASC, we hope that our SURAggrid/CASC relationship means we'll continue seeing Sue!

**Mary Fran Yafchak** was honored by the SGC for her over 7 years services to SURAggrid, from its origins in NMI Testbed site discussions in November 2002. We certainly could say we have "**Sure, a grid**" but with Mary Fran's dedication and tireless efforts we say "**SURAggrid!**" The SGC is presenting Mary Fran with **Recognition of Service**. Thank you Mary Fran!

**Nicole Geiger** stopped in to join us as she begins her new work at the U.S. Naval Observatory, leaving Georgia State University where she began in 2003 as an REU student under the original NMI Integration Testbed Award. Good luck to Nicole - maybe SURAggrid and USNO will find points of common interest.

### **Big Picture [bottom line!]**

After wrapping up working group discussions, we closed with a suggestion from Steve Johnson about our SURAggrid big picture focus. We need to make compelling case for SURAggrid use: Specifically, client access and usability needs to be accomplished quickly – on the order of a day from request to access granted.

We discussed the somewhat complex workflow that Account requests may have:

- Local registration authority practice impacts a Level of Assurance and thereby a SURAggrid-wide consensus on access levels.
- It is preferred that we have in-person validation of user request for credential. How accomplish this well in a heterogeneous community like SURAggrid? Can using SURAggrid CA be a solution?
- Once account created, how ensure the user can access that account on each of SURAggrid systems? In fact, local systems now have autonomy and do not have common practice for adding accounts.

**BIG PICTURE GOAL:** Within 3-6 months have a solution for simple, fast user access to SURAggrid. User request should result in prompt fulfillment and active use of SURAggrid resource.

**Friday September 25, 2009 – SURAgri Meeting (continued)**  
**SURA Offices, 1201 New York Avenue, NW, Washington, DC 20005**

**8:30 AM - Applications Panel with Core Insights**

Linda Akli organized an Applications Panel of six researchers who presented their research with specific insights for SURAgri. These insights ranged from researchers who are using SURAgri for their research, who may have used SURAgri and graduated on to other resources (such as TeraGrid or other national resources), or who were not using SURAgri but whose experience was informative. Below are the presenters, with links to their presentations and some brief comments on their insights.

- *Eric Schnetter, Center for Computation & Technology, LSU*  
 Access Management Maze – Based on experience trying to deploy Cactus on SURAgri, the challenges researchers face trying to sort out access via “grid” certificates. Cactus is an open source problem solving environment to enable parallel computation across different architectures and collaborative code development between different groups.

Why are grid certificates (valuable for access to compute resources) so complex to use? We need easy introduction, simple install, and one-step mode for loading needed certificates. Especially important to have better way to debug rather opaque error messages (typically have to Google message and hope for best.) <http://sura.org/programs/docs/Cactus.pdf>

- *Li-Shi Luo, Department of Mathematics and Statistics, ODU*  
Non-Stop Flight to Miami - Dr. Luo’s direct access to the University of Miami P5 for running turbulence studies represents an all too common scenario on how users access resources contributed by SURAgri member institutions. Mathematical modeling of micro/nanoscale phenomenology and metrology, with the overall objective to develop a multi-scale multi-physics simulation methodology based on the Boltzmann equation (BE) and molecular dynamics (MD) for micro- and nano-scale flows of engineering interest.

Basically, Dr. Luo is always looking for a more cores. AIX requires recompiling of code – which means additional work is required. [http://sura.org/programs/docs/Luo\\_SURA09.pdf](http://sura.org/programs/docs/Luo_SURA09.pdf)

- *Yaohang Li, Department of Computer Science, North Carolina A&T State University*  
SURAgri the On-Ramp – NCAT researchers are benchmarking Protein Loop Structure Prediction software. Before porting the application to SURAgri, the researcher received allocations on TeraGrid and is now running on TeraGrid. What role does or can SURAgri play in assisting researchers in taking moving from the campus, to regional, and national CI resources?

Went direct to Kraken (National Institute for Computational Sciences (NICS)) since had allocation and was “easy to use.” Kraken required one software install (compared to needing multiple “installs” for multi-system grids?) Additionally, lack of sufficient student support (funding) is a limitation in looking to deploy to other clusters/grids. <http://sura.org/programs/docs/YaohangLi.pdf>

- *Tarynn M Witten, Center for the Study of Biological Complexity, VCU*  
Scaling Up Applications - The focus of the Virtual Parasite Project is to understand host-parasite dynamics which is intrinsic to the study of infection at all organismal scales. The VCU research team is scaling their application to model the behavior of over a million parasites and comparing the performance of the model in several HPC environments including Linux, IBM AIX, and Microsoft HPC2008.

Did “graduate” from SURAgri (Georgia State IBM p575), to Argonne National Labs, and now has account request pending at Blue Waters. Challenges include finding sufficient technical support for debugging, just getting an account (cf. Argonne account request experience...) and student support (funding.) Future work will require graphics resources, real-time results (vs. batch), large memory and IO for processing video results and interactive options to manipulate model. [http://sura.org/programs/docs/Virtual\\_%20Parasite%20Project.pdf](http://sura.org/programs/docs/Virtual_%20Parasite%20Project.pdf)

Jaroslav (Jarek) Pillardy, Cornell Center for Advanced Computing, Cornell University

Simplifying User Interfaces - BioHPC is a suite of computational biology applications that allows researchers from biological laboratories to submit their jobs to a parallel cluster through an easy-to-use web interface manage HPC hardware and software infrastructure and integrate distributed HPC resources.

Computational biology suite has user base that is international. bioHPC provides a relatively robust portal interface for user submission, monitoring and results; and administrative interfaces. "Open applications" do not require login. <http://www.sura.org/programs/docs/BioHPC.pdf>

- Eduardo A. Socolovsky, Center for Biotechnology and Biomedical Sciences, NSU  
Transition or Integration - The NSU Center for Biotechnology and Biomedical Sciences (CBBS) runs SYBYL, commercial an expert molecular modeling environment and has recognized the need to bring HPC to their campus and research programs. SURAgrid and the SURA-MS Distributed HPC test bed offer different applications Dock and bioHPC.

NSU's CBBC is using SYBYL suite of pharmaceutical workflows for protein modeling, as well as other tools (NCBI, etc.) Also uses some BioHPC. CBBS submitted a funding proposal for a BladeServer (NIH pending). SYBYL has sophisticated graphical interface. Biologists usually prefer to leave technical infrastructure to others - hence BioHPC is popular for its graphical interface, etc. Some modules of SYBYL are not parallelized. There is some complexity of spreading workflow over systems. Docking function is not currently in BioHPC.  
<http://www.sura.org/programs/docs/NSUCBBS.pdf>

### **10:30 AM - Access Management Policies**

Jim Jokl, Chair Access Management Working Group, presented a policy document for review and potential approval. His presentation provided guidance to best practices as relates how an organization would process policy documents - effectively a life-cycle management recommendation. Such life-cycle management includes aspects from policy Meta-data (Title, Contact, Version Number/Date, WG name, Status...) to Process aspects (document ownership and approval process...)

**Action:** Document submitted for SURAgrid Governance Committee approval: "SURAgrid User CA X.509 Certification Authority Policy & Practices Higher Education PKI-Lite," Version 1.0: March 2009  
(<https://www.pki.virginia.edu/sura-bridge/doc/SURAGRIDCA-CP-CPS-v1.doc>)

Jim noted that the Access Management Working Group has identified additional documents likely requiring review, approval, adoption:

- SURAgrid iKey credential process
- Designation of SURAgrid site admin
- Operation of SURAgrid LDAP authorization infrastructure

We discussed a number of other aspects of access management including in-person vetting (consider InCommon (<http://www.incommonfederation.org/>) Silver?), having multiple levels of assurance (low for development and trials versus higher for site/resources requiring more secure/stable environments to be maintained), operations support for access management and the role of SGC in the adoption of policy.  
[http://www.sura.org/programs/docs/SURA\\_IdM.pdf](http://www.sura.org/programs/docs/SURA_IdM.pdf)

### **Noon - Adjournment and Acknowledgement**

We agreed that this SURAgrid All Hands benefited from our presenters, from our member sites' continued support, from participation from in-person and remote attends, and made valuable contributions to the continued sustainability of our SURAgrid community.