We have virtual CPUs and move things around but storage isn’t like this. Fundamental change is needed.

– Miron Livny

In the 60s, we had to share machines because it was so expensive. The PC became popular for a reason: because it was mine. Then we started stitching together the cluster, but computers were still not large enough. In 30 years, we have come full circle. What was old is new, what was new is old.

– James Cuff

The social engineering of working cross institutions and campuses in the future— that is our larger issue.

– John Towns

If we think of the cyber infrastructure as an ecosystem, species diversity is a predictor of resilience: making sure there is diversity in the types, sizes, roles, content, and recognizing all the pieces of the ecosystem.

– Irene Qualters

The business model should never drive the science, but it has to be factored into the 5th inning, not the 9th inning.

– Dave Richardson

More students in our universities are going back to their country after studying. In order for the US research capability to be as competitive as possible, we must collaborate in other countries.

– John Towns

The technical problems on campus are being defined as “cultural issues,” more than “technical issues.”

– Irene Qualters

2014 ARCC

http://www.ncsa.illinois.edu/Conferences/ARCC/index.html

January 15-17, 2014

Best Practices Workshop Summary

Closets at biological labs have things much worse than energy-draining computers.

– Miron Livny
Welcome
Thursday, January 16, 2014

John Towns

The goal of this conference is for campus computing groups and national computing centers to collaborate productively together to come up with ways to support computational science on campus and the tremendous amount of resources required to sustain it. The next ARCC conference is currently scheduled for Feb 10-12, 2015 at Clemson University.

Opening
Thursday, January 16, 2014

Ed Seidel

University of Illinois – National Center for Supercomputing Applications

The last decade has seen major changes in the way research is done across all disciplines. From NSF’s perspective, there are two significant ways in which research is changing:

- Everything has become digitized, from networking to data services to access to HPC resources. “Big data” is probably the most significant aspect, on which an enormous amount of discussion is focused and which will have the greatest impact both on education and future infrastructure development.
- Research has become a much more collaborative process. As research problems become more complex, outcomes no longer depend so much on the efforts of individual researchers working in isolation as on collaborative teams, often consisting of researchers from around the world—including both massive collaborations (e.g., the Large Hadron Collider, the Dark Energy Survey, and LIGO.)

Large or small, these collaborations depend on sharing data. Constructing scientific instruments and experimental apparatus is no longer the sole point of a project; data services (collecting data and making it accessible to users) are absolutely critical to these efforts.

User communities tend to be located at universities: one important challenge is to connect campus computing efforts to the national cyberinfrastructure (“campus bridging”) in order to facilitate sharing of data both locally and globally. Specific issues that need to be addressed include, for instance, usability, reliability, and identity management.

Funding and budget limitations are always an issue. Often campus bridging falls into a funding gap between NSF and other funding agencies and the campus itself; self-funding is usually a necessity.

- Limiting research to specific major problems and interdisciplinary centers for complex problem-solving. This is the model used by the Skolkovo Institute of Science and Technology, where Dr. Seidel was affiliated until late last year. Enabling this approach required a redesign of local cyberinfrastructure, which needed to happen at all levels.
• The condo cluster model, which is becoming more and more common, is usually self-funding. Locally, NCSA has been leading the charge on organizing compute resources.
• XSEDE, which brings HPC centers together from across the country, might provide a model for connecting campus clusters to the national infrastructure.
• Feedback is critical. Research communities need to tell NSF what they need and what NSF should be doing. NCSA, for instance, which is approaching 30, was originally the result of an unsolicited proposal.
“Hotel or Condo? The Evolution of Research Computing Services at USC”

Richard Moore
San Diego Supercomputing Center

Triton began as a pay-as-you-go “hotel” model only. Its successor, the Triton Shared Compute Cluster (TSCC), has been in production for less than a year, and has a hybrid model where the bulk of the systems are condo nodes but time can be purchased on hotel nodes by the hour to smaller or bursty users.

Currently, Triton has ~425 users (~150 users across 15 condo owners; ~275 hotel users), and an additional ~100 temporary student accounts. The campus aims to cover fixed costs while users cover incremental costs. Condo owners purchase a node and pay a supplemented operating fee; hotel users pay a supplemented core-hour fee.

| 2013 Costs for UCSD & UC users |
|-----------------|-----------------|-----------------|-----------------|
| ITEM            | PURCHASE COST (ONE-TIME) | INFRASTRUCTURE FEE (ONE-TIME) | OPS FEE (ANNUAL) |
| Standard Node   | $3,934            | $939             | $495            |
| 128 GB Option   | $75              |                  |                 |
| InfiniBand Option | $0              | $200             |                 |
| GPU Node        | $8,310            | $399             | $495            |
| Titan GPU Upgrade | $1,960          | $939             | $495            |
| InfiniBand      | $495             | $200             |                 |
| Hotel Nodes     | $0.025 per core-hour UCSD users; $0.03 per core-hour other UC campuses | |

Notes:
1. Infrastructure Fee covers racks, switches, cabling, etc.
2. Ops Fee is subsidized for UCSD users; full Ops Fee is $1,805 per node

Currently, Triton faces four challenges:

- Adoption. On a distributed campus with many independent research groups, getting the word out about the cluster’s availability can be a challenge.
- Marketing. It’s both reaching researchers about the program and convincing them that buying into the condo model is preferable to being one’s own system administrator and having control of one’s compute facilities.
- Potentially stumbling out of the blocks. Early lapses can leave bad impressions -- reputations are hard to build and easy to lose.
• Sustainability. Is this a sustainable business model, and will there be enough adoption to provide the desired impact from the campus investment?

Pros and cons of program

<table>
<thead>
<tr>
<th>Advantages</th>
<th>Disadvantages</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flexibility in condo/hotel, nodes and interconnect allows us to tailor our services to user needs</td>
<td>More sys admin/support/business costs</td>
</tr>
<tr>
<td>Users nominally pay incremental costs; keeps campus supplement fixed</td>
<td>May hurt adoption by passing on more costs to PIs</td>
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<tr>
<td>User support partially handled by email list crowdsourcing</td>
<td>User email list can substitute for individual tickets — may moderate list</td>
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<tr>
<td>Modest and fixed campus investment—leveraging existing expertise (~3 FTES)</td>
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<tr>
<td>Persistent storage options</td>
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TSCC’s acknowledged successes include the availability of both condo and hotel access for different types of users; close to 24/7 availability of user support, in part thanks to crowdsourcing (despite some need for moderation) and support for educational users (classes of students).

Areas in which Triton could improve include more widespread adoption on campus; an increase in the number of staff available to manage basic operations, user support, and business; the addition of computational expertise, and an upgrade in the persistent storage offerings.

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Shared Cluster Program, Institute for Digital Research and Education, University of California, Los Angeles

**Tajendra Vir Singh**  
*UCLA IDRE*

RC Infrastructure at UCLA – History. In 2002, the Math Sciences Datacenter had ~2500 square feet of floor space and built a 16-node cluster. By 2006, there were 16 clusters ranging from 16 nodes up to 267 nodes; one even broke into the Top 500. Networking infrastructures were GigE, Myrinet, and Infiniband; CPUs were AMD, Xeon/Itanium, and IBM Power PC; OS were mainly Linux with some MacOS; clusters used multiple disk arrays. Power, cooling, storage, and physical space were issues; use of Beowulf clusters was spreading across campus.

In 2007, the IDRE data center added another ~2500 square feet of space and a shared cluster/shared storage program was initiated; cooling and weight were issues in the new space.

The current IDRE Shared cluster program enables a PI to buy nodes and/or storage with a 3-year warranty from a program-specified vendor; IDRE provides the storage at an annual rate of $500/TB with backup. PIs can sponsor users (i.e., students or members of their research groups); each one gets a 20 GB home directory and can share (if any) extra disk the PI purchases.
Group members have access to high-priority queues on the PI’s compute nodes, which guarantee that jobs will start running within 24 hours and can run for up to 14 days. When not in use by PI, “owned” compute resources are available to common users from across campus. Anyone at UCLA can get a “common user” cluster account, which comes with a 20 GB home directory and access to the 24-hour shared or low-priority queue.

The shared cluster program has grown from 64 initial nodes in 2007 to 1219+ nodes, or from 256 initial cores to 12,316 cores, and from 200 TB storage to ~1.5 PB (including the parallel file system). It has approximately 100 PIs and 1500 users and currently running at ~90% utilization.

The program has not been without “hiccups,” node-level and networking are minor issues. Persistent issues include physical space (the main data center shares its floor space with ITS) and, in the case of the second data center, cooling (enough for maximum capacity of 400 nodes), and weight (beam-level floor reinforcement is needed). The cost of addressing these problems is rather enormous.

Fortunately, POD’s installation in 2011 provided great relief when it became the third data center. All three centers are connected by multiple Longbow and 10Gbps links.

Other ongoing issues include I/O (there is no single solution for all types of I/O patterns) and storage, which was initially NAS (Blue Arc) until it was outgrown. Now IDRE uses integrated parallel storage and cooperates with the vendor to fix issues as they arise. Daily backups are no longer daily basis. Scheduling is also a persistent issue, particularly with regard to integrating shared cluster’s policies. Upgrading versions of scheduler is risky once we have one that is up and running. Upgrades that were successful during test have failed multiple times in production. It requires constant monitoring.

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**Should We Restart the LCI Workshops?**

**John Towns**  
*NCSA*

The emergence of condo-style campus clusters has created a serious training need for both users and administrators, many of whom have had no experience using/running HPC clusters, let alone operating condo-style campus resources. While some training is available for users of HPC systems, it is focused mostly on homogeneous resources with respect to funding, policy, and operation; whereas most condo-style resources are not homogeneous.

LCI emerged as response to a similar problem in late 1990s, when HPC clusters first emerged and created a serious need to train both system operators and users. It began when a small group of folks at the leading edge of this emerging new platform banded together to provide training opportunities for our own users and administrators and, over the course of ten years, expanded to provide 3x/year workshops and an annual meeting that attracted 100-125 attendees on average.

Is a new effort needed, one tailored for those operating and using condo-style campus shared research computing resources? LCI operated on a volunteer basis, but there was enough interest in the community to sustain it. Does that community support exist today, and are there community members
who are willing to provide leadership? There is a small amount of leftover funding from LCI to seed the effort.

If interested, email jtowns@ncsa.illinois.edu.

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**Implementing Campus Bridging: Laying the Foundations on Both Sides of the Divide**

*Richard Knepper  
*Indiana University*

XSEDE Campus Bridging came about as a result of two messages received from the XSEDE community: that there were not enough compute resources, and that it was hard to transition to existing ones. The aim of campus bridging is to facilitate movement of researchers from labs to campus resources to regional cyberinfrastructure. It focuses on tools that make data management and job submission easier for all users, such as Globus Online, Unicore 6, and Genesis II; and tools and can be implemented on multiple levels that allow campus resources to look more like XSEDE resources, such as Rocks Rolls and rpms of XSEDE software packages, so that no matter where users are in the system (campus, regional, or national infrastructure) the environment always looks the same. An additional aim is unified documentation and training that apply to both local and national resources.

In conjunction with the campuses, XSEDE is confronting a number of challenges at various levels in implementing Campus Bridging. At the campus level, a major challenge is identifying researchers whose research requires scaling and big data requirements, who can be flexible, and who have the time to engage in an adaptive process.

For XSEDE, the goals of Campus Bridging will stretch the XSEDE concept and require accommodation; there are also a number of technical challenges (access, shared compute facilities) and user management challenges (access, conventions, and permissions). Finally, there are cultural challenges, as users with a broad variety of needs must be accommodated, including new users who are not traditional users of HPC facilities and their projects.

Those directly involved in Campus Bridging face a different set of challenges: figuring out how the program aligns with other programs like Campus Champions and Extended Collaborative Support, identifying optimal users (who are typically not novices and may already have significant workflows at the regional level), and identifying tools that will fit users’ needs and can fit into an integrative environment.

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**A Business Model for Affordable, Sustainable Archival Storage**

*Henry Neeman  
*University of Oklahoma  
*Oklahoma PetaStore*

The OK PetaStore consists of a mix of tape and disk, with many media slots and few media. These slots are available on a first come/first serve basis. Persistent storage is archival, rather than live (i.e., “Write Once, Read Seldom if Ever”) and is NOT a substitute for backup.
The PetaStore’s business model shares costs among the NSF, the offices of the OU Chief Information Officer and the Vice President for Research, and the researchers themselves. The NSF Major Research Instrumentation grant provides hardware, software, and 3-year warranties on everything. CIO and VPR provide space, power, cooling, labor, and maintenance after the 3-year warranty period, with one MRI proposal slot every five years. Researchers provide their own media (i.e., tape cartridges and disk drives).

For researchers, compared to roll-your-own disk, PetaStore LTO tape is cheaper, more reliable, requires less labor and training, and potentially faster (~200 MB/sec to write, ~140 MB/sec to read). While PetaStore disk is more expensive than roll-your-own disk, it is otherwise like tape.

Expanding the disk system would be too expensive; once all the slots are filled, that’s it. However, the tape library is expandable to over 22,600 tape cartridge slots (up to 18 total cabinets, 17 with 1320 slots each). Currently, there is over 34 PB of storage at LTO-5 (current), which is expected to increase over 56 PB at LTO-6 in the coming year. (We don’t expect ever to get to that point, but could go beyond our current 2889 tape cartridge slots.)

Data retention is a major challenge. A typical research grants runs between 2-5 years, rarely longer than 10 years; however, data generated by a grant may be needed well beyond the end of the grant period.

Continuing to fund archival storage after the grant runs out thus becomes problematic: it may not be possible to fund new storage media on later grants, if those grants won’t use the data being retained. Cloud storage is one possible solution, but monthly charges can be very challenging for a typical researcher, specifically after the end of the grant period.

The current PetaStore can retain files for its entire lifetime. The rated lifetime for LTO tape cartridges is 30 years or 200 full read/writes or 1,000 load/unloads. Because this is “write once, read seldom if ever,” the rate at which tape cartridges are traversed is quite low. But what about the next generation PetaStore?

As part of the current grant’s proposal, OU’s VPR committed that we can have one NSF MRI acquisition proposal slot every 5 years. The current PetaStore is LTO-5, with LTO-6 to be added. The next generation PetaStore will still be LTO (announced through Gen 8), expecting LTO-7 and LTO-8. LTO-N drives can write LTO-(N-1) and read LTO-(N-2).

The strategy for the next generation PetaStore involves requiring all participating vendors to accept the old tapes; purchasing two LTO-6 drives and four or more LTO-7 drives, and later, two or more x LTO-8 drives; and purchasing a modest number of LTO-7 tape cartridges. All files from the old PetaStore will then be copied to the new PetaStore. As old cartridges get copied, they will be emptied and moved into the new PetaStore, where they will be kept for up to 12 years.

For the next NSF MRI proposal, the plan is to buy one tape library at the beginning, which is expected to last more than ten years. Two disk systems and two sets of servers would also be purchased—one at the very beginning of the grant period and one at the very end. Each disk system and server is expected to last 4-5 years, meaning that the next generation PetaStore’s tape library will last 8-9 years; thus, the lifetime of a PetaStore tape cartridge can approach 15 years, depending on when it has been bought. After 15 years, the current price per TB would likely be somewhere between 10% and 1% of the price per TB of LTO-5, which would make replacing old media affordable for data owners, assuming they still
require the data. Although no one really knows what storage technology will look like in 15 years, it is reasonably likely that data stored on this media will still be readable.

A Negative View of Research Computing at KSU
Daniel Andresen
Kansas State University
Beocat

- We don’t exist. We’re not on the organization chart, which gives us a lot of flexibility and freedom that we would not otherwise have if we were an official unit.
- We aren’t central IT. Researchers are sometimes burned by central IT—metrics are different for central IT than they are for researchers. Central IT believes in cost recovery, for instance; also, in upgrading and shuttering working equipment that for researchers would have a longer life in production mode.
- We have no administrative authority. No stick; more give-and-take, which encourages cooperation from researchers.
- We have no budget. Funding comes directly from the president and the provost.
- We don’t charge. HPC is as vital as labs and office space and should be free for everyone; researchers who get grants pay for higher priority.
- We don’t spend money on software. Other than Intel compilers, everything is free and open-source or self-provided by researchers.
- We aren’t homogeneous. Consequently, we always have something that is nearly state-of-the-art. This does, however, create some problems on the backend.
- We aren’t bored.
- Lots of outreach.

HPC Environment at Yale University
Andrew Sherman and Kiran Keshav
Yale University

Yale’s HPC environment, which is grant-funded, consists of two logical HPC centers: one in the Arts & Sciences, which consists of 1,300 nodes, 11,000 cores, and 1.5 PB usable storage, and one dedicated to biomedical research, which consists of 500 nodes, 6,100 cores, and more than 3 PB usable storage.

There have been over 800 active users in the past year and millions of jobs, which include for instance, a lot of small high-energy physics jobs, and sequencer data which the genomic center feeds directly to HPC storage. Other major scientific application areas include astrophysics, geology and geosciences (climatology), chemistry, engineering, and HPC.

The current HPC architecture is very traditional and very heterogeneous. In terms of operations and planning, storage and processor lifecycles are tied closely together, and cluster “islands” lead to technology divergence and heterogeneity, making it difficult to manage condo-style facilities.
Data management consists of cluster-specific scratch/project storage (same physical hardware), which is slow and hard to get to; a workable solution would be expensive. Because every cluster is different, current storage solutions are necessarily heterogeneous, resulting in chaotic data replication as users move around and making quota management difficult. Archive storage is also cluster-specific and tied to specific archive nodes. Consequently, data is accessible only on the cluster on which it was stored; users who exceed their storage quotas on one cluster often have to leave their data behind. Users can archive data manually as well, but this is a slow, error-prone process that is inconsistently used.

Because the capacity tier is very slow, users don’t utilize it, asking instead for expensive scratch/project storage.

Collaboration and data sharing require cluster accounts and manual processes, which are slow as a result of network performance. Because most systems don’t support ACLs, file access control tends to be inconsistent. Users guess where to run jobs, which are prioritized locally (on a per-cluster basis).
The new architecture will improve on the current architecture in several ways. In terms of operations and planning, it will facilitate global policy and administration for an HPC “commons”. It will also be more expandable and easier to upgrade, because condos are easier to deploy and modify—short-term “sandboxes” allow for testing. Finally, node and storage life cycles are independent, which enables more flexible planning and purchase cycles, more choice in terms of vendors, and thus more leverage with vendors.

As far as data management is concerned, the clearly delineated storage tiers of the new architecture will make all storage accessible everywhere, which is simpler for users and reduces undesirable data replication. Hierarchical Storage Management will also be automated. Storage is mounted on the external data transfer server, which eliminates network bottlenecks and makes data sharing and collaboration less cumbersome. Additionally, the new Globus Online Institutional Server allows data sharing between individual users, both internally and externally, without the need for external collaborators to have local user accounts and Yale credentials.

Job management will also be improved in that the new architecture has both a single point of entry for jobs and a single place for job status queries. This enables uniform global job prioritization and management and potentially permits automatic job scheduling with just-in-time data routing.

HPC Sustainability at the University of Arkansas: Contributions from the Condo Model

Jeff Pummill
Manager, Cyberinfrastructure Enablement, Arkansas High Performance Computing Center

In condo computing, rather than buying homes in a building, users buy nodes in a cluster as a way of increasing capacity between large allocations. The concept originated at institutions such as Purdue, Clemson, and others to address the needs of researchers who often write grants without planning ahead for computing needs.
There are, however, some problems that result from implementing a condo cluster. Researchers see the nodes they’ve purchased as their tangible property. Not only do they want high-priority access to their own nodes, which requires more high-priority queues, but they also often want to use non-approved equipment, which makes hardware management difficult. Additionally, moving funds between cost centers can be problematic.

So far the AHPCC Condo Project, which made its first actual purchases in 2010, has installed 8% of the hardware that will eventually make up the cluster; this, should rise to 12% soon. An MOU is available for complete purchases (located at [http://hpc.uark.edu/hpc/support/condo.html](http://hpc.uark.edu/hpc/support/condo.html)). The project has recruited many new faculty who are currently considering condo purchases and who have been given computational startup money by the Office of the Vice-Chancellor for Research. Currently, the Condo Project is undergoing seamless integration into AHPCC’s existing system, and has succeeded in creating an environment for users that is no different from the traditional HPC environment.

Areas that the AHPCC Condo Project is still working on include creating long-term data storage, negotiating a more sustainable purchase agreement from vendors, making more data migration options available for Condo members, and coming up with a “greener” way of disposing of old hardware.

**Service Platforms for Advancing Scientific Computation on Campus**

**Rob Gardner**

*University of Chicago*

This cluster setup, considered a Tier 2 center, consists of distributed high throughput clusters located at the Universities of Chicago, Indiana, and Illinois, funded by high-energy physics (NSF Cooperative Agreements PHY06-12811, PHY11-19200). The clusters are integrated as one logical center (job scheduling and storage) by a distributed team (“The Midwest Tier2 Center”) and are part of the Open Science Grid and the CERN LHC computing grid (WLCG). The setup consists of 8861 cores, 3.7 petabytes (globally federated) and as such is a leading ATLAS computing facility in WLCG – in 2012-13, it was ranked second only to Brookhaven Lab.

The clusters are connected by a 100 Gbps Science DMZ (NSF CC-NIE), LHCONE network, peering at CIC OmniPoP with Inernet2 & ESnet, with local and wide area, regional, national, and transatlantic direct access and high throughput transfers. However, connection speeds to each cluster have not yet reached 100 Gbps.

The system leverages the campus computing cooperative at UChicago (UC3), the campus cluster at NCSA/Illinois (ICC), and Campus Bridging & Research Infrastructure group (CBRI) at Indiana University in a manner similar to the Beocat cluster. In addition to leveraging the clusters themselves, it also leverages Illinois Campus Cluster expertise.

The cluster is shared in that spare cycles are given the VO’s and research projects affiliated with the OSG and local campus grid users.

Operationally speaking, core services are no longer much of an issue—OSG and LHC grid services have teams ensuring their security and stability while investigating new, cutting-edge technologies to keep
current. However, data management is a major issue—the platform has a 300-petabyte global catalog that currently stores around 20 million files in 100,000 datasets, with user data resident in many different physical locations. I/O is also an issue, with I/O-intensive applications from a diverse and distributed user community of around 300 active users.

Aside from hardware, performance, and storage, engagement with research communities, campus integration, and distribution of applications are ongoing concerns, particularly in making the setup useful for small non-physics science domains which do not have advanced, fault tolerant workload and data services or which have little distributed HTC experience. The overall objective is a model with less management overhead and more local computing, even though resources are located elsewhere. Resources are transparently provisioned from local environments to global ones, thereby giving resource-strapped users the experience of running locally (/home, low latency, reliability, control), but computing “globally” (to use opportunistic cycles) is a particular challenge.

So far, the project’s most important success has been to demonstrate the effectiveness of leveraging already-existing resources and community expertise. Other VO-specific successes include:

- ATLAS: Built a distributed Tier2 infrastructure for ATLAS which is open to Campus and the 115 virtual organizations and 59 Projects of the OSG (http://www.mwt2.org);
- UC: Built a campus grid system that integrates diverse research clusters with campus identity management and job and data services at UChicago (http://uc3.uchicago.edu);
- OSG: Built a campus researcher-centric job submission platform for the OSG using HTCondor for job management and Globus for reliable file transfer (http://osgconnect.net);
- Duke University+UC: Built a platform service template to bridge between the Duke HTCondor grid, UChicago UC3 grid, and the OSG (http://duke.ci-connect.net); and
- The construction of ATLAS Connect, a community-centric job submission and data platform to connect LHC Tier 1/2/3 centers and the 44 campuses of the US ATLAS collaboration (http://connect.usatlas.org), as well as TACC Stampede, an XSEDE resource. Users experience a virtually unified high throughput computing environment, aided by technology such as CCTools from the University of Notre Dame which allows mounting remote file systems containing application-specific software repositories too large to “carry with” the job.

The last three of these (OSG, Duke University+UC, and ATLAS Connect) are service platforms that leverage globus.org, htcondor, and ci-connect.net.

Areas which have been identified as needing improvement include getting scientists on-board to use the infrastructure we built; addition of versatile, generic portals/gateways to quickly engage user communities and bring advanced capabilities to their work; distributed storage systems and access (technically, the most difficult part); implementation of a flexible provisioning infrastructure (IT Infrastructure, platforms, software) to reduce operational cost; installation of intelligent, high capacity networks; implementation of services that break CPU-data locality constraints; and other improvements to enhance the science data lifecycle, including preserving data and execution environments (c-f. daspos.org).

Research Computing at Notre Dame: Past Challenges and Ideas for the Future
Jarek Nabrzyski and Paul Brenner
CRC Director and Associate Director
Notre Dame University

In 2009, the Center for Research Computing was a modest-sized effort with 7 FTEs focused on HPC/HTC and Storage Support, operating on a tight budget. It consisted of one centrally funded cluster along with several faculty-funded clusters in a collocation facility hosting 1200 servers (up from 600 in 2007). Many small clusters were still located on campus, and 80% of the computational resources were centrally funded.

By 2014, the CRC's staff has grown to include 7 computational scientists (65% soft money), 18 research programmers (funded on 100% soft money), 9 HPC engineers (funded on 20% soft money) plus administrative staff, grad students, postdocs, and interns. The CRC now hosts ~20,000 computing cores (1700+ servers) and > 1PB of storage. Only 30% of computational resources are now centrally funded; ~50% of the budget comes from grants and re-charge services. The CRC serves 1450 active users (350 faculty, 700 grad/postdoc, + undergrad)—five times the number of users in 2009—and has supported dozens of CI projects of various size the over last two years.

The CRC’s successful growth is due to a number of different factors. Making user satisfaction the #1 priority was followed by a focus on internally generated research. Two specialized but integrated teams were created, one to focus on cyberinfrastructure development, one to focus on HPC. Computational scientists were hired in key areas to devote 50% of their time to service and the other 50% to research, not in order to compete with academic departments but to partner with them, while research programmers were hired for CI development, funded entirely on soft money.

At the same time, the Center’s computational infrastructure was consolidated to provide an enterprise data center facility at same or lower cost as that required to retrofit campus closets. If faculty-funded software and hardware meets CRC specifications, the CRC provides them with free administration; if it must be customized to meet research requirements, an administration fee is charged. While the faculty owns the resources, they do not own the allocations of cpu hours in the queue; when these resources are idle, they can be scavenged as resources for campus.

The CRC has not completely consolidated all compute resources, however. There are still a variety of systems (e.g., GPU, storage, multipurpose, low power, secure) running in departments/offices as a result of logical scale, capability and personality factors.

There are several issues that the CRC faces currently and expects to face in the future. Staff members are funded by soft money and thus their responsibilities are project-dependent. Determining which items to fund centrally and which to recharge and creating effective system consolidation policies that take into account faculty requests for “no-cost tweaks” of the template are also current issues. Future challenges that the CRC anticipates include how to best leverage cloud resources as pricing and capability improve from year to year, continuous shifting of computational scientists between staff/faculty and support/research roles (not to mention teaching) and, as always, recalcitrant faculty who dislike the notion of consolidated compute resources.
Managing Programs of Condo-style Resources
Thursday, January 16, 2014
Moderator: Jim Pepin

Session Two focused on research, condominiums, and sharing on campuses and featured speakers from four different campuses who discussed their condo models—traditional or non-traditional, and supporting cyberinfrastructure—why they chose that particular model, who their users are, the effect of cultural factors campus politics and the user community, and what has worked well and what hasn’t.

Research Computing at Purdue

**Preston Smith, Purdue University**

Preston Smith is the manager of Purdue University’s HPC User Support Group, which provides campus faculty with support for Purdue’s cluster computing program.

Research Computing (RCAC) is a unit of ITaP (Information Technology at Purdue), Purdue’s central IT organization, which is led by Purdue’s CIO, who reports to the president of the university.

Purdue has done central research computing in some capacity for a long time, beginning in 1967 with the CDC 6500, one of the first supercomputers. Purdue’s CDC 6500 has actually been moved to Paul Allen’s Living Computer Museum in Seattle, where engineers are attempting to restore it to life.¹

The CDC 6500 was succeeded by a Cyber 205 in 1983, then an Intel Paragon in the 1990s, and finally an IBM SP. Purdue’s campus computing had an impressive refresh policy in which 1/3 of the computers in the student labs would be replaced every year, after which they would be turned into cluster nodes. While they were free, however, because they were not designed for HPC, their capabilities were not as good as could be desired.

Since 2004, HPC at Purdue has been provided by the community cluster program. The early clusters were heterogeneous and made up of different processors and interconnect nodes, which tended to limit usability; storage was centralized and was difficult to make scalable. Another major difference between then and now was that faculty members physically owned the hardware and could point to a node and say, “This is mine.”

Now, ITaP centrally funds the basic elements of cluster computing, including support and application staff; system administration staff who manage and maintain the hardware, operating systems, and storage; the hardware itself, including data centers, racks, cooling, headnodes, and servers; the networking, mass storage, and scratch storage; some software (such as a user management app available to faculty members) and schedulers. Instead of owning the hardware outright, faculty members pay only the cost of a node, which provides them with five years of computing services, on which Purdue does not charge facilities and administrative costs.

Each year, RCAC builds a new 8-10k core system with a 5-year lifespan. Providing a new system annually enables faculty to count on there being a build soon before or after they arrive at Purdue (if they’re new) or their grant period begins. Selection of a new system is accomplished in a few different ways.

One method involves putting out an RFP and holding meetings with faculty to provide input on the proposed systems and select one—usually, cost turns out to be the most important criterion. One of the requirements of the RFP is a guaranteed five-year warranty, which generally proves satisfactory to both faculty and vendors. Another is a six-month price guarantee, which ensures that faculty can get the same hardware for the same price and enables six months of purchase and growth. Another method of acquiring a new cluster is to partner with vendors to design the system, which the University then purchases upfront and sells, as nodes, to faculty.

Faculty members get a dedicated queue equivalent to the number of nodes they have purchased and can authorize users. They also get access to a standby queue that allows them to run up to four hours on nodes that are idle. The queues are handled by the TORQUE Resource Manager and the Moab Workload Manager.

Each system usually provides several different node types, both GPU and non-GPU, with varying amounts of RAM. The latest system is named “Conte,” currently ranked #33 in the list of Top500 Supercomputer sites. Each node has 16 Sandy Bridge cores on two 8-core Intel Xeon-E5 processors and 64 GB of memory, a 40 Gbps FDR10 Infiniband connection (no oversubscription), 1.4 PB of scratch storage and a 100TB/user quota (with a purge after each 90 days) and a maximum job runtime of two weeks. The system was bought with University funds and the nodes sold off; its users consist of 22 faculty and their groups in 14 different departments. The faculty on Conte also get a queue/user management application, a usage reporting tool, and access to web-based node/storage purchase, and self-service quota management.

RCAC also provides condo-based purchasable storage (condo-based), persistent group storage available at a reasonable rate per TB per year. This is useful for source code, applications, and data, but because it is shared by the enterprise side, it’s not appropriate for running jobs, which would hinder enterprise services such as SMTP. A more robust solution is expected in 2014; centrally-provided archive storage has grown 272% since 2011.

RCAC is, however, still in the process of addressing a number of challenges. For example, when a system is ready to be taken offline, the faculty users have the option to take the hardware with them, but that’s not really desirable, so instead, they have been offered trades, which are always accepted. There is also the issue of faculty who don’t need an entire node and would prefer to pay for compute resources by the hour; RCAC is exploring various “hotel” models in response. And there are other user requests that are not quite compatible with the Purdue condo model, such as faculty who want to use the Hadoop framework for processing datasets on clusters, or who want root access to their nodes (generally, the CS faculty). Finally, there is the ongoing challenge of managing to stay ahead of demand—having five major systems and a few smaller ones could require that staff spend all their time just in maintenance mode.

So far, the cluster program as a whole has been used to run 12.4 million jobs over a total of 238 million hours of runtime. It has been used by 146 faculty groups in 34 departments on all three campuses, a significant portion of whom have purchased nodes on more than one system at a time, with 50 group spaces purchased. Significantly, a full one-third of external funding coming into Purdue has gone to
community cluster users, demonstrating that the faculty partnering with RCAC are themselves making significant impacts in their fields.

Finally, engagement with faculty has also been important and productive. Every fall, HPC User Support staff meet face-to-face with new faculty in their offices to learn about their research and their potential computation needs. Some faculty are intent on building their own clusters, but the cluster program has become a successful part of faculty recruitment at Purdue.

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**USC Condo Model**

*Maureen Dougherty*

*University of Southern California*

A division of the Information Technology Services (ITS) department, HPCC is a central resource headed by the CIO funded by the Office of the Provost to provide cluster computing cycles and limited storage at no cost to all USC researchers and graduate students. HPCC began as a way to get rid of smaller clusters distributed around campus and make resources available that wouldn't generally leverage central IT staff for networking and storage support. HPCC’s business model is to purchase cluster computing hardware upfront, which it then presents to users. It currently supports a diverse set of researchers, many of whose work falls outside the usual areas of HPC research, via both general and condo cluster resources.

HPCC shares its professional staff with ITS; it has a core group of about 7 FTEs, who are involved primarily in system administration and leverages ITS for network and hardware support. Storage is available for labs and the cluster, as well as internal cluster storage; for archival storage, USC has a digital repository that provides 20 years of storage to tape.

With regard to the general resources, HPCC provides all resources at no cost to its users (who must apply for accounts and follow HPCC’s user policies). This includes the compute nodes and the infrastructure necessary to create the cluster, including ethernet switches, low latency bandwidth switches, cards, cables, and boards, interconnect cables, head nodes, racks, power, and cooling, in addition to a 350TB/staging OrangeFS file system for multiple job workflow and a Science DMZ, which provide the core of the Ethernet network.

Other resources provided by HPCC include heterogeneous compute node clusters; a full-time professional staff to install and configure hardware and manage and maintain the cluster; limited storage (up to 1TB) with tape backup to store data sets and results (restricted to HPCC cluster and head nodes, with data transfer through head nodes); tape backups of general storage; and general software applications, including some licensed applications (e.g., compilers, message passing, MATLAB, and Globus).

HPCC is advantageous to USC researchers in a number of ways. It eliminates the cost of data center infrastructure, including electricity, cooling, networking, and data center support, the last of which is available 24 hours a day, seven days a week and receives no funding from researchers or their departments. HPCC’s professional staff handles all cluster management and maintenance, which eliminates the problem of “brain drain” that occurs when the graduate student managing a lab cluster leaves, or the need for research staff to devote work time to hardware, OS, or software installation
issues. HPCC actually provides assistance with software installation into a faculty member’s working directory, even if the application is not supported by HPCC. All of this means that, for faculty, funds and personnel saved by using HPCC, rather than running one’s own cluster, can be focused on one’s research, which gives them an advantage when applying for grants and recruiting new staff in that it demonstrates that USC, by providing this central resource at no cost, is committed to its researchers.

However, for USC researchers centralized HPC is not without its drawbacks—mainly with regard to its queuing system. To provide resources to USC’s diverse research community, with its various deadlines and compute needs, four different queues were created with the following limits:

<table>
<thead>
<tr>
<th>Queue</th>
<th>Maximum nodes per job</th>
<th>Maximum compute time (hours)</th>
<th>Maximum number of simultaneous running jobs/user</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quick queue</td>
<td>4</td>
<td>1</td>
<td>10</td>
</tr>
<tr>
<td>Main queue</td>
<td>99</td>
<td>24</td>
<td>10</td>
</tr>
<tr>
<td>Large queue</td>
<td>256</td>
<td>24</td>
<td>1</td>
</tr>
<tr>
<td>Large memory queue</td>
<td>1 (1 TB, 40-core node)</td>
<td>336</td>
<td>1</td>
</tr>
</tbody>
</table>

Only one job at a time can be run on a node, and there is no possibility of sharing with other jobs, which wastes resource potential, as well as time. All jobs are run on a first come first serve basis, depending on resource availability. However, HPCC queues are set up for back filling, so that if a job waiting for a large number of nodes is ahead of a job waiting for fewer nodes, and the fewer node job will finish with the available nodes before the larger job has enough resources to launch, the smaller job will be allowed to run first.

Other disadvantages to faculty include lack of root access, lack of HIPAA compliance, and maintenance downtime, which occurs twice a year (usually once in the spring and in the fall) and can take up to a week, although not without a minimum of 30 days’ written notice (hence the maximum of 336 runtime hours for the large memory queue). Many researchers don’t realize that there are two separate clusters which use different technologies and therefore don’t communicate with each other, which is why jobs that are inadvertently split between nodes on different clusters don’t finish. It’s not “one size fits all,” but HPCC does try to make resources as useful as possible to the widest possible user community.

Some researchers would prefer to have exclusive access to compute cycles and/or larger storage, and have the funds to pay for it; these researchers are better served by the condo cluster. In the condo model, researchers pay for compute nodes, storage, and in some cases head nodes at cost, while HPCC both pay for the infrastructure and installs, manages and maintains these resources at no cost to the researcher. Vendor support is required for three years on compute nodes and for the life of the storage arrays. The researcher is given exclusive access to these resources and can create their own policies for their compute nodes (maximum 336 compute hours). The Memorandum of Understanding (MOU) is valid for three years, after which HPCC continues to support compute and head node hardware until either spare parts are no longer available or a cluster upgrade results in the old nodes being decommissioned. Typically, new storage is acquired every three years.
For USC researchers, the condo clusters are advantageous in several ways. Because HPCC purchases in volume and has vendors compete for the best price, the price is typically much better than what the researcher could obtain on his/her own. Researchers receive the same support as they would for general resources, also at no cost, and they have exclusive access to condo resources, can set their own policies, and even share resources, if they are using a single processor. In addition, they have access to the USC Digital Repository, a storage system available both to the condo cluster and to lab clusters, as well as an archival option.

One major disadvantage of the condo model for USC researchers is that changes in technology can split a condo into separate clusters and prevent nodes from communicating with one another, which reduces investment-based potential compute power. Another is that condo nodes are not always in use; idle nodes mean wasted resources. There are also several storage-related issues: for instance, if a user’s storage directory is too large or not part of the condo cluster’s standard configuration, HPCC does not back up to tape at no cost. Further, some file systems cannot back up to tape, and those that can must work seamlessly with existing infrastructure, because within ITS, tape drives and silos are shared resources. However, the biggest storage issue for users is that if vendor support is lost, storage is decommissioned and users are forced to migrate their data.

At first, it was hard to get people to see the value of the general and condo clusters--there are many who want to "hug" their clusters close. But over time they've come to see the value of not having to pay for the infrastructure or spend valuable research time on administration and maintenance, and we have letters of support to this effect. It has also been an effective tool for faculty recruitment. A recent Nobel Prize winner was one of the first users on the system, which has also been used by faculty to test codes before porting them to national resources.

Until recently, there has not been a lot of training available, but we've recently started doing more outreach, which we hope to expand via some upcoming NSF proposals. Some of our current training offerings include tutorials on Linux, how to use the cluster, and Parallel MATLAB.

**Q & A**

Q. Why did you move from Maui to Moab?
A. With Maui, we had issues with a large number of queues and with general vendor support.

Q. What are users buying in the way of condo storage?
A. We vet the hardware, which includes storage arrays with a minimum of 15 TB usable storage. They pay for the storage and support, while we provide the infrastructure and operations. Full storage is only available through CHPC, although the campus digital repository allows buying fractional amounts of storage on a contract basis.

Q. What resources are condo users able to leverage?
A. They don't have to spend funds on operations and they have access to the general queue.
Q. Are there any service level agreements?
A. No, because they make a one-time hardware purchase and they don’t pay for service.

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**The CHPC Condo Model at Utah**

*Brian Haymore*

*Center for High Performance Computing (CHPC), University of Utah*

The University of Utah’s Center for High Performance Computing provides large-scale computer systems, storage, networking, and the expertise to optimize the use of these high-end computer technologies. CHPC supports faculty and research groups whose main focus requires computing, storage, and advanced networking as core instruments central to their research.

CHPC provides core infrastructure and general resources to campus, while faculty, usually through research overhead, pay at cost, or at a marginal cost, for “owner” hardware resources. We are currently being steered to diversify our funding sources and are increasingly relying on staff support through inclusion of partial FTE on grants.

Our downtown data center came online in the spring of 2012. We provide all the infrastructure, common applications and licenses, hpc scratch space, high-speed network, and virtual machines for users whose needs are more customized. We also support dedicated personnel for security and compliance.

We set resource usage policies via consensus by CHPC and the user advisory council, who also determine the warranty duration and best effort life cycle. The allocation process is very similar to that used by XSEDE, with a kind of secondary “freecycle” queue for users who have run out of allocation. Storage is sold whole and in slices. Owners set usage policies within reasonable limits and have the option to allow guest jobs to run in pre-emptible mode. When possible, we are able to leverage existing software licenses as well as contribute to them to meet user needs.

Handling sensitive data is an important responsibility for which CHPC has dedicated, protected resources. Initially, this applied to HIPAA data but now includes FISMA and FERPA data as well. For these projects and needs we maintain similar general and “owner” HPC-style resources with VM resources as well. The condo model’s advantage with regard to sensitive data is that it allows for more consistent and better vetting, and therefore better visibility and oversight, all while leveraging common processes and controls. This is a significant area in which CHPC expects to grow in coming years, one which we have described in a recent paper (Bradford et al., [http://www.ncbi.nlm.nih.gov/pubmed/23911553](http://www.ncbi.nlm.nih.gov/pubmed/23911553)).

User support also includes documentation and training—these include web- and wiki-based application/tools documentation (i.e., getting started and how-to guides), training in the form of quarterly hands-on sessions and online archived recordings, one-on-one and on-site visits with faculty and their groups, and individual consulting. Other user support initiatives aim to look ahead to new developments on the technology horizon, introduce users to new resource options as they become available, and evaluate/demonstrate new solutions that could reach beyond research computing. A particularly important initiative is in the area of big data, supporting research in areas like genomics and astronomy (i.e. astrophysical data management site for the Sloan Digital Sky Survey IV).
Q. Could you talk a little more about your approach to HIPAA compliance?
A. For HIPAA data, we have resources that are physically isolated. What measures are taken depends on the project itself and the nature of the data—data security policies are customized for each project.
Q. Do you use the same credentials to authenticate?
A. Everything is shadowed, but a separate password and two-factor authorization are required.
Q. How do you collaborate with the visualization center?
A. This is a more recent trend—initially, the two centers had operated independently. Right now we want to see how we can leverage each other’s resources— their expertise, our research, etc.
Q. Why require a different password for HIPAA data?
A. In order to address risks—our intention is to move forward and try to leverage things like InCommon.
Q. Is the protected environment truly separate?
A. Yes. While it is located in the same data center, it occupies separate racks, and there is no physical connection between it and the other resources.

Research Computing at Stanford

Ruth Marinshaw
Stanford Research Computing Center

The SRCC was originally the Stanford Research Computing Facility, but because names matter, it has since become a center. Our staff has grown from an initial three or four to a total of eight so far; we’ve just posted a ninth position and will soon be posting a tenth as well. SRCC reports jointly to the Vice-Chancellor for Research and the Chief Information Officer; while SRCC staff interact more with the CIO, Ruth Marinshaw (director) has more interaction with the VCR.

What SRCC provides is very similar to the other centers represented at this conference: HPC and HTC services (i.e. clusters, parallel processing, GPUs/accelerators, cloud computing services) and storage and data management, which are ever-increasing in scale, from gigabytes in the 1990s to petabytes currently. We provide hosting and physical facilities, system administration, training, support (i.e. codes, tools, methods) as well as encouraging collaboration and community building across campus and linking to national resources.

The SRCC has a new space (the building is known as the Stanford Research Computing Facility) funded in part by faculty purchases of space and leasing part of it to DOE SLAC. $1.4 million in funding for a new cluster was provided by the Office of the Provost; it will be a condo-style cluster along the lines of the one at USC. It has only just arrived, has yet to be installed, and is as of yet unnamed.

With the new facilities come new opportunities. As of Tuesday, we will be involved in a protected clinical sequencing project—a great opportunity that takes advantage of the abundance of healthcare funding available. Data analytics is another big opportunity for SRCC; in this instance Stanford is partnering closely with SAP and will be deploying some HANA clusters. Finally, we are talking with the XSEDE gateway folks about building a science gateway at Stanford for the biophysics community.

One major challenge for SRCC is negotiating the alphabet-soup of compliance—not just with federal regulations, but with university rules and regulations, all of which can make it challenging to maintain productivity for both computing and research. Funding is another challenge. The Provost provided the center with a one-time grant of $1.4 million for a cluster, and while the potential exists for future one-
time grants, in the meantime SRCC must prove itself in order to be eligible for them as well as for continued funding of the FTEs.

On the technical side, other challenges include keeping up with new technologies and managing complex scheduling policies in a way that meets everyone’s demands and requests, using a variety of scheduling software—all of which must be accomplished while remaining flexible, nimble, and stable enough to convince Stanford PIs that SRCC can meet their needs with a minimum of downtime. What helps us to meet these challenges includes having a diverse team with different interests and skills; building and maintaining relationships with PIs (whose relationships with Central IT often range from suspicion to outright hatred); starting small (with five clusters) and scaling up gradually and successfully to 15 clusters; providing plenty of training opportunities; collaborating with others on campus on new initiatives; and, last but not least, telling our story over and over and over to everyone, including the Dean of Research: explaining why HPC matters, talking about the research successes of SRCC’s faculty partners, all the time making it possible for others at the University to tell the story as well in ways that could prove more powerful.

General Q & A From the Panel

Q. When a center offers both free and condo-style resources, what can be done to minimize their misuse?
Smith (Purdue): Many of our systems are scheduled at core level so that if one user is tying up a node, the job can be overridden. We accurately provision memory per node and ensure that people aren’t using more memory than they are allocated.
Dougherty (USC): We restrict the user’s usage to a single node.
Haymore (Utah): Users are prevented from misusing resources by the limits of their allocations, although we are starting to look at cgroups to do more provisioning of memory.

Q. How do you monitor clusters to find out whether one condo user is affecting another’s usage?
Smith (Purdue): We use system-level monitoring (e.g. Nagios), but we don’t do much in the way of monitoring queue activity.

Q. Is anyone trying to use soft condo boundaries?
Haymore (Utah): We ran a previous cluster that way for a year, where one group owned two-thirds of the cluster and the other one-third was available as a general resource and tried to let affinity work. In the end, it may have been a technical win, but it was a political failure—the queueing system confused a lot of users, and the burden of that confusion wasn’t worth it.

Q. What effort, if any, do you give to helping users use non-local resources?
Marinshaw (Stanford): We help people with XSEDE, Campus Champions, AWS, and Google. It’s a work in progress.
Purdue: Our user support group also assists with resources like XSEDE.

Q. Is there any way for faculty to contribute grant funds to common nodes?
USC: No, setup funds go to dedicated nodes for a given researcher.
Clemson: We backfill onto them.
Purdue: We have faculty in general purpose and also in an island for export controlled computing.
Common: Write into letter to NSF stating that funding will be used for general pool computing purchase.

Q. (addressed primarily to Smith (Purdue)): With regard to your model in which you first design a system, buy it upfront, and then have faculty purchase shares, what percentage has to be sold to cover costs?
Smith (Purdue): We assume a 100% sell-out in 12-18 months, but we also use unsold nodes to replace other nodes that fail to make commitments.

Q. (addressed to Smith (Purdue)): Why do you purchase a new cluster every year?
Smith (Purdue): We've determined that as a result of what we've observed demand to be. It’s typically tied to the start of the academic year, when new faculty arrive.

Q. (addressed to Marinshaw (Stanford)): Can you tell us whether you’ll be using the dedicated cluster for clinical work?
Marinshaw (Stanford): No, for that we’ll have a separate, dedicated cluster, due in part to security breaches last year on campus that were related to protected health information.

Q. (addressed to Haymore (Utah)): Who does your compliance work?
Haymore (Utah): We did it ourselves – we don’t hire anyone to fill those roles specifically. We found that the compliance office was not prepared to do what was needed on their side to ensure that the dedicated resource was compliant. It took more than 16 months to work through iteratively.

Q. If you had the flexibility to provision your infrastructure so all condos just look like pure silicon and run schedulers on top of that, could you convince faculty to share cycles?
Haymore (Utah): On the non-protected side, I think we’re achieving that. We try not to let a cycle go to waste.
Increasingly, researchers are outgrowing their desktops and needing access to advanced computing resources; however, while some are experienced HPC users who simply need access to the resource, others are new to computational research and have no experience in building and/or administering such systems. Although both research communities and technology undergo rapid and dramatic changes over time, the support process should not.

The Dell Scalable Unit (DSU) is introduced as a “complete HPC/RC solution” that provides all the components required to solve specific problems, including compute and storage hardware, software (such as MPI, Math, other libraries, etc.), networking (protocols, interconnect hardware), infrastructure, installation, deployment (scalability, device drivers, etc.), training, and service and support (including provisioning, patching, and updating). The applications and workloads of a given machine can be tailored to the needs of a specific user, department, or industry and can be used to manage workloads across systems. The intention is to provide a solution that is complete, scalable, flexible, and sustainable, as well as “move-in”-ready—researchers should be able to begin using the system right away.

An underlying assumption of the DSU is that most researchers using HPC are not computer scientists and should not be expected to think like computer scientists—after all, for example, no one expects a computer scientist to think like a geneticist and to be familiar with the intimate details of RNA sequence processing—to the computer scientist, it’s a “black box.” Similarly, geneticists should be able to consider HPC to be a “black box” as well.

An example deployment of a DSU is SANGER, which is specifically built to solve genetic analysis problems associated with pediatric cancer research. System specifics (RedHat OS, Intel Xeon, Phi cores, Mellanox Infiniband, NVIDIA K20X and other features) which would be essential to CS researchers and everyone at ARCC are not relevant to the researchers (for whom the machine might as well be powered by thousands of hamster wheels); the applications installed on the machine (Bowtie, Tophat, Cufflinks, IGV, etc.) and the results obtained, however, are critical: an RNA sequencing data analysis problem that once took five days to run now takes four hours, and the analysis of a complete human genome takes eight hours.

Fernandez offers three recommendations to centers implementing the condo model. First, a common observation of DSU users begins thus: “Most importantly, I have been able to focus on science, rather than...” and it’s important to work on making the “rather than” invisible to the researcher, whatever his or her discipline—materials science or quantum chromo dynamics.

Second, where the system is located matters, and the value of that location to the researcher should be prioritized. It should be in good proximity to sensors, instruments, and access points; a cloud computing solution should “extend” the desktop and/or instruments.
Third, the system’s “amenities” – bells and whistles such as visualization capabilities, business systems, network, etc – are of far lesser importance than the science being done and should be de-emphasized.

Q: suggesting putting these sequencers around campus, what we used to do 15 years ago that ran buildings out of power and cooling

Q extended: what about adding networks that are capable of extending these to the needed locations

A: this is in data center, in the cloud

just don't start by stating that it needs to be in the cloud

Q: but need really fast networking

A: runs on 1Gb/s today and not even saturated

Q: nice model for a certain set of researchers, what about other communities

A: yes, 3-4 others in works prioritized by marketing and sales.
A Genomics Perspective on Advancing Research Computing on Campuses

F. Alex Feltus
Associate Professor, Clemson Department of Genetics and Biochemistry
Faculty Consultant, Clemson University Genomics Institute
CEO, Allele Systems LLC ffeltus@clemson.edu

One of the most important pieces of the discussion is the reason for building all this infrastructure: to support researchers and help them do their work. This panel consists of three researchers from different universities who will give their perspectives on using centralized campus computing.

I’m a genomics guy, originally trained as a cell biologist to do biomedical work. Primarily, I’m a biology person at heart. I’ve always been interested in technology and done this kind of work for quite a while, but I also work with people—undergraduates, graduates, postdocs, and colleagues—who may share a lot of my research interests but don’t share the desire to do things the same way. Getting them on the machines, running jobs, processing and analyzing data is a challenge.

I’ve done HPC for a long time, but talking with engineering-type people, I get the sense that they have a different concept of big data. To them, genomics is not big data, because big data is Tier 1/Tier 2-type projects like the LHC, where the amount of potential data could be infinite.

But genomics is at least approximately big data. The graph below shows that 655,000 human genomes have been deposited in the last five years, and once the sequencing technology catches up, we’ll be able to sequence chromosomes efficiently. Genomes usually have to be sequenced a couple of times—once as it is now, then later, when it’s at the genetic state. When you sequence a tumor to see what changes are taking place, you’re generating a good 10GB of data at a time. If you multiply that by 655,000, keeping in mind that you need access to this data over the next 20 years or so—that’s big data.

And humans are only one of millions of organisms on this planet—there’s going to be a tremendous amount of data associated with genomics for lots of different kinds of research.
When you're trying to get someone else to use HPC for the first time, you get a sense of who they are. My transition to an HPC guy began in high school, when I got a Commodore 64 for Christmas (best Christmas ever!). I was learning how to do some basic programming, reading manuals cover to cover, along with a lot of friends in high school—I started at an early age. At Vanderbilt, I learned how to pipette data. After that, I did a postdoc at Emory at a time when the human genome had just come online and was dealing with a large data set for the first time, so I had to learn Linux skills to do basic bioinformatics work and had to approach it bioinformatically. I transitioned from biomedical work to plants because it was an opportunity to do genomics. One of the cool things about that transition was that I learned bioinformatics skills, and I was able to use my rudimentary programming skills to process datasets on HPC clusters.

At Clemson, I do plant genomics and consulting, working with clients who don't do HPC. My work involves building gene interaction networks by downloading from repositories all the genes that have been turned on in an organism (in our case rice plants and other grasses like maize) and constructing networks of those genes that interact. This further involves constructing sub-networks of co-functional genes, for which we need to do tons of correlation analysis for every given gene pair—and there are 40,000 genes. We then align the networks together and look for groups of genes that make grass grass and rice plants rice plants.

As a biologist, I want to reach out to other people like computer and cyberinfrastructure engineers to help me optimize the algorithms we use and look for particular genetic events and traits. The figure below shows the relationship of genomics with genetics in rice chromosomes -- where genes are expressed together. We look for particular genetic events, such as much rice we have, etc. We need to be able to optimize for doing huge genome sequences with more data -- there's a lot of opportunity in agriculture to analyze for things like rice, which is a very important grain and represents 50% of the calories consumed by humans.

I can approach problems like these from an agricultural perspective and build a bioinformatics pipeline, but not every researcher is going to care about rice. So a lot of what I do is to build workflows, optimize them, and get them on the cluster. I work with CI people to look at ways to optimize algorithms and run through more data faster. For example, in collaborating with Melissa Smith at Clemson, I've found that optimizing correlations between all the genes in an organism can be as simple as going from Perl to C – there is lots of opportunity to do this kind of work.
Working with network engineers on a grant we have opened up possibilities of doing things I had never before considered doing. I can take my research to a new level by listening to people outside of my field about networked software, piping data from public repositories via Internet2 into our systems, getting data from sequencers on campus or from other campuses, pumping it into our system, then sharing what we've processed with other universities, to solve problems like how to increase the grain yield of rice and develop bioenergy crops.

For ten years, I’ve been learning that the power to get things done opens doors -- that’s what researchers want, especially grad students. Once you get the job done, you think about scaling up to two genes. I try to introduce bioinformatics and HPC to others in my field, from undergrads all the way up to colleagues, by teaching undergraduate and graduate-level courses and workshops on topics such as how to use the cluster to sequence, how to build workflows. It’s especially important to train grad students and get them on the clusters, or they won’t end up becoming successful collaborators.
There are some impediments to folding LS researchers into CI. For example, there’s the common response – “I’m successful, I publish -- why change?” But in genomics, the sooner researchers realize that they need to be working from a global perspective to get funding, the better. Another issue is that biology has always been reductionist, but we are now shifting to a systems-level perspective where, instead of looking at a single gene, you look at five genes. For students accustomed to working with graphical interfaces, there’s the hurdle of learning to work with the command line. We need to get students doing Linux as soon as possible, ideally in high school. And finally, if the code works fine, why optimize? However, if you show them how much more quickly optimized code runs, they start to become interested.

Researchers are like genomes – there are dozens of different subfields, each with a different archetype of a researcher whose methods are different. If you want to get them to buy into using HPC, you need to find out who they are, get to know their field and their archetype, know how they do research. A good way to do this with life scientists is by holding an intramural workshop in which someone who shares their background, knows their language, and can talk with them about their experience, and have all kinds of HPC people there as well.

And it’s great to put researchers on CI grants, but it’s better to build research aims directly into grants instead of simply citing application examples. Researchers and technologists need to be writing NSF reports together to cover both technology rollout and science.

And finally, look closely at how people process data. Understand what they’re doing and respect their workflow, this is why they’re successful -- don’t pressure them to change. For example, 70% of life science researchers are probably using Excel spreadsheets. Don’t disrespect Excel spreadsheets!

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The ATLAS Experiment at the Large Hadron Collider

Mark Neubauer

Department of Physics, University of Illinois at Urbana-Champaign
The pursuit of particle physics is about trying to understand the whole universe. Basically, we’re asking the question, *What is this stuff in the universe, and how is it interacting with each other?* In the standard model, everything in the universe is made of particles—leptons and quarks—and they interact through the exchange of other particles called Higgs-bosons. There are four different component Higgs-Boson particles. Two of them, the Z and W bosons, are positively charged and cause nucleus decay through the transmission of the weak force. The photon causes electromagnetic interactions, and strong interactions are caused by particles called gluons.

These particles are massless, but the particles that actually mediate weak interactions of nuclear activity are actually very massive—in fact, they weigh as much as 90 times the mass of a proton. So the early big puzzle we were trying to solve was to understand why they were so massive. The theory is that the Higgs-Boson is what gives these particles their mass. However, before July 4, 2012, we’d never even seen these particles.

The hypothesis is that throughout the universe particles interact with the Higgs field, and when other massless particles (like the W and Z bosons) traveling at the speed of light interact with the Higgs field, they actually slow down, which gives them mass. The particle that does this is called the Higgs-Boson. That’s what we’ve been looking for with the LHC, which was built primarily to study this particle, although it turns out that there is a lot of other science you can do with the LHC as well.

The LHC is a huge ring, 27 km (17 miles) in circumference that spans parts of France and Switzerland and is where we counter-rotate massive proton bunches (each bunch consists of 100 billion protons) and force them to collide. We put some detectors in various places where these forced collisions take place and study what comes out. If you’re familiar with Einstein’s equation $E=mc^2$, we’re imparting energy to protons and using it to convert it into mass in the form of new particles. And we’re also doing something that perhaps you did as children—we take stuff and smash it together and see what comes out, do it over and over again, except that we are using some very sensitive, very large instrumentation.
The ATLAS experiment involves thousands of barely-visible superconducting magnets that bend the proton beams in a circle using RF cavities to accelerate the protons to make the light visible. A few hundred feet underground there's a detector that monitors protons that are being forced to collide 40 million times/second. The ATLAS Detector is the size of a 6-story building, has about 100 million electronic channels, and observes 40 million collisions/second--all the data produced would fill 100,000 CDs per second!

It’s a great example of big data being used to do big science. Each experiment has 3-4,000 collaborators -- so 10,000 people around the world trying to analyze the data coming out of this thing. That's our big data challenge.

This is what discovery looks like in our field: in this case we measure the energies and angles of two photons and add them together in a particular combination that would create a little bump if there was a new particle that decayed -- we can actually observe a little blip here, which indicates a new formation of decay.
Ideally, we would scoop out the Higgs after we produce it, but it’s too unstable. So here we see another big spike where we don’t expect it, and it happens to be right at the same mass as the other bump, so we see the particle decay in two different ways and that has the mass roughly of a cesium atom all in one simple particle.

The Higgs(-like) boson discovery was based on the analysis of one quadrillion ($10^{15}$) proton collisions and produced 2 million Higgs bosons—that’s a cost of $7000$/Higgs! It’s like looking for a needle in a haystack, however—the vast majority look virtually the same as less interesting processes, and only a few really stand out. We look for very specific signatures and have to do it statistically as an abstraction. So the broader challenge is really about big data.

Annually, the LHC generates 15-25 Pb of data (or 300,000 Blue-Ray discs). We have to simulate the collisions and it turns out that the simulations we derive from refined data sets that we generate in addition to the raw data adds up to this amount. This data is analyzed by 10,000 physicists located all over the world. It’s the distributed nature of this analysis that is one of the big challenges. The LHC Computing Grid was created because we knew we couldn’t have all the data in one place. So we came up with this hierarchical data processing model consisting of 150 computing sites all around the world, 200 PB of disk, and 300,000 cores, connected mostly by 10G networks and a few by 100G networks.
In 2010 I proposed we build a new Tier 2 system here at Illinois, and we actually deployed it in the Illinois campus cluster. Our site is based on 2048 cores and 510/366 TB raw/usable storage and is one of three centers in Midwest Tier-2, along with the University of Chicago and Indiana University. We’re unique in that while some of the other Tier 2 sites pull cycles from shared resources on other campuses, they’re not actually deployed on them.

How the hierarchical data processing system works is that raw data is vaulted at CERN (Tier 0), then distributed to regional Tier 1 sites (Brookhaven in the U.S.), then a number of Tier 2 sites (there are around 10 in the U.S.). Tier 1 sites are where heavy reprocessing of data takes place; simulation and user analysis is done at Tier 2 sites, which are all shared resources. Tier 2 sites are funded by NSF at the level of millions of dollars, and each comprises thousands of CPU cores and several PBs of disk. Tier 3 sites are controlled locally and the data doesn’t have to be shared. We’ve flowed a lot of data between these sites and could easily saturate 10Gb/s links.

A little history: between 2002 and the fall of 2007, we developed a T3 cluster. In October of 2010 we submitted a Tier 2 proposal to USATLAS Computing Management, which was formally accepted in November 2010. At this point we started producing prototype systems, and on October 5, 2011 we had the first successful test of ATLAS production jobs run on the Campus Cluster at Illinois, reading data from our T3gs cluster. On March 1, 2012, our pilot system successfully debuted, using job flocking from the University of Chicago, and in late July 2013 we began upgrading our network to 80Gb (still in progress). Admittedly, our application is rather unique for this cluster—we’re not just a little research group but consist of thousands of researchers all over the world. Our success needs to be cost-effective and depends on campus subsidy and support—power, cooling, infrastructure, staff support—all these things are important and contributed to our being competitive enough to score a Tier 2 site. Our success demonstrates how campus clusters can be leveraged to bring in more funding.

Another important benefit of using the campus cluster is the possibility of opportunistic cycles—other users aren’t necessarily always using all of the cluster all the time, and we can take advantage of that. We also have the opportunity to be involved in the campus research computing ecosystem, which allows us to engage in interdisciplinary interactions, take advantage of others’ expertise, explore new
technologies, and gain visibility for our project. The opportunity to create conversations between multiple users creates the potential for new collaborations. There are also drawbacks, of course. When you do something in a shared environment, you lose direct control over what's going on day to day and have to wait for other people to respond—while we've gotten wonderful support from the campus, there are still things that we could do more quickly and efficiently if we 'd had the chance to tinker for ourselves. Teething pains from deployment of large scale systems are inevitable. And, to quote Spock, "The needs of the many outweigh the needs of the few. Or the one." Sometimes we have downtime delays where we have to wait for other jobs, and they have to wait for us.

Climate System Modeling at Utah

Brian Haymore for Court Strong

University of Utah

The climate research cluster computing community is pretty significant. Two of the models that I work with at the University of Utah are the NCAR Community Climate System Model and WRF. The NCAR CCSM represents about 75,000-100,000 lines of hybrid parallel Fortran 90 code and runs on 100-300 cores at the Utah Center for High Performance Computing, some of which we own outright, some of which are shared resources. WRF regional climate simulations represent another 50,000 lines of parallelized Fortran code for higher-level simulation. These run at a higher resolution on 300-1,000 cores of the Yellowstone supercomputer at Wyoming.

I've been programming nearly my whole life, since I was in high school writing 500 lines of BASIC a night on a Commodore VIC-20. Somewhere along the way I went astray, majored in journalism, and became a TV weatherman for a while. As I was more interested in cogitation than in communications, I found my way back into academia, where I'm trying to make cool things happen on the computers. The three years I spent in the basement writing video games on BASIC don't help me much today—I'm kind of self-taught on Fortran and shell and all that stuff, but I've worked my way up to where my group runs simulations totaling around a million hours per year. Some of that is run on our local resources, and some gets pushed out to the NCAR-Wyoming Supercomputer called Yellowstone, a 74,000-core batch system in Cheyenne. However, we try to run stuff as much as possible locally so we don't have to keep moving big files back and forth.
Above is a visualization of some of the output from the WRF model. On the upper left is a trench, and below it is an overlay of clouds on a topographic map. On the upper right is a visualization of the flow over that complex terrain. These climate models are essentially solving nonlinear partial differential equations on a three-dimensional grid and integrating them four at a time, so they’re quite a piece of software in themselves. Some examples of the kinds of things WRF can simulate are cloud- and continental-scale processes, thunderstorms, downdrafts, rain, hurricanes, forecasts, and fire processes and smoke transport. They can be run locally or at least hemispherically, although usually they’re run at high resolution in a regional configuration. We use the models primarily to simulate precipitations and make long-term predictions, and we also contribute to the model's development—for example, at Utah we've contributed code for fire simulations.
WRF allows you to run different resolutions simultaneously, so you have a coarse outer domain at 36 kilometers inside which you can embed higher resolutions, ultimately stepping your way down to 64 KM while maintaining some kind of computationally efficient scheme. There are a lot of computer science people whose work is devoted specifically to developing the ability to do this kind of programming and enabling communication among these grids, so the outer ones can form the inner ones and vice versa. 

\[
\frac{dT_L}{dt} = -\frac{1}{\rho_w c_w h} F
\]

Cost function
\[
J(h) = \left\{ \frac{1}{n} \sum_{t \in T} \left[ T_L^o(t) - T_L^b(t, h) \right]^2 \right\}^{1/2}
\]

Numerical optimization
\[
\text{arg min}_h J(h); \text{ subject to } h \in [0, \infty]
\]

\[ h = 5.1 \text{ m} \]

Strong et al. (2013), JAMES, in prep.

Because we ourselves are parallel programmers, we do like to get under the hood inside the climate models with which we work. We introduced a model for the Great Salt Lake to simulate this large, shallow water body, and if we don’t know the exact temperature, we’re going to get the weather in its proximity completely wrong. Annually, the Great Salt Lake undergoes a huge temperature swing from 0-23 degrees Celsius during the year, which we can describe in historical simulations, but if we want to know what it will look like in the year 2080, we need to model it. In the graph above, the simulation is red, superimposed against the recorded temperature.

The above graphic shows the kind of workflow that is involved. When we try to run this model off-campus away from our main data stores, we have geographical data (e.g., elevation, land use, soil type...).
(sand, clay, etc.)) that needs to be preprocessed and put onto the specific grid, which is done via an application that creates cdf files, called Geogrid. Then we take meteorological data--some kind of CFSR data, run it via another tool called ungrib, and put it on the model's grid, which creates a set of files are combined by a program called Real to produce the actual work input files. Depending on what you're trying to simulate, the work input files could be hundreds of gigabytes to terabytes in size: they contain the initial conditions for the domains that you're running, the lower boundary conditions to get the model started, and the horizontal boundary conditions, which are spaced temporally so they're all around the model at all levels at all times—that's what mainly contributes to the size. Once we've generated these files we need to get them to the resource where we'll be running the model. It can take about two or three days to port the historical decade simulations over to the NCAR Yellowstone supercomputer, which is why we try to run them locally if we can.

In my experience, the pros of using a condo framework far outweigh the cons. During my 10-12 years as a grad student, postdoc, and visiting scientist before I landed at the University of Utah, I interacted with a lot of colleagues at different universities with different computing setups. Some just put together a makeshift cluster in a closet somewhere and ended up spending a serious fraction of their time—up to 40%—maintaining it. I really didn't want that huge time sink, so during the period when I was interviewing for jobs I looked for a place with good HPC support where I wouldn't have to do it myself. On some level, I might secretly enjoy it, as a programmer myself, but that's not what the University rewards.

The drawback is that I have reduced knowledge about the system--I don't know it nearly as well as I would if I had built it myself. The nine nodes I've been using I purchased with startup funds--I've never actually seen them. I also have reduced control over the system—if the sysadmin decides to update all of the libraries all at once for all of the nodes so that everything is pointing to a soft link which has been updated to the new version, sometimes we find out that we can't compile our code because for some reason it's not backwards-compatible, we can't go back to the old hard link and can't change it. That can be a hassle, but it's a relatively small price to pay for being in a condo framework.

The one thing that is a substantial disadvantage is the idea of retirement date. I understand the issue and have talked to lots of people about it, but, for instance, my car is well past warranty and I'm still driving it. We have this culture where we want to run the equipment into the ground until it melts or falls apart, but then I get an email telling me that a cluster is going to be shut down because it's no longer cost-effective to run. Consequently, someone might pull up to my office with a dolly with eight nodes or something, whereas if I'd actually taken the time to build that thing in the closet next to my office, it would still be there today.

However, even that drawback is substantially outweighed by the benefits, which are really just two: it saves money and it saves time. As new faculty members, we come in and negotiate a startup package with a certain amount of money available to buy nodes, and we can buy more if we’re on a cluster because we’re sharing resources, or maybe even get the University to kick in for the rack, whereas if I build this thing in my closet I have to buy the rack myself. Also, we might license software across these nodes, rather than negotiating individually for software to put on clusters in closets.

And, again, maintaining my own cluster is also a big time sink, which is really the biggest point for me. Instead, someone went out and found a place on campus where they had power and cooling available for this cluster, so we didn't have to negotiate with the owners of our building on campus, and someone else physically assembled the cluster and installed the rack--I'm fortunate enough not to know how
much time that takes. And community knowledge contributes to time savings as well, because if you're in a condo framework, you're sitting on a cluster where your software and hardware is probably similar to that of other users—possibly even identical—so you can ask whether someone else got their code to compile successfully and get a response listing the fourteen flags that you need for it to work, which can save you from having to read 250 pages of compiler documentation. And using a condo framework means I get expert maintenance, too—instead of spending 40% of my time doing maintenance, I can rely on someone else for that support.

So I'm heading into my fifth year at Utah, and I'm up for tenure—and my faculty advisor has told me I have nothing to worry about. And this is because HPC and the condo framework have taken care of so much of that.
Integrating with Campus Infrastructures
Thursday, January 18, 2014

Moderator: Ruth Pordes

Integrating with Campus Infrastructure: Role of the National Network
Tracy Smith
Illinois

Our experience in building a campus research network environment at the University of Illinois has taught us that identifying the purpose of the network we’re building is critical—that an environment optimized for enterprise traffic is not optimized for research traffic, and vice versa, because their needs and requirements are often in conflict. We have adopted the ESI Science DMZ model to address these differences; in the meantime, our network strategy continues to evolve.

A campus research network environment is not one-size-fits-all. It differs in several aspects from an enterprise environment, which is very rigid—that restrictiveness is the reason that many faculty would prefer not to work with central IT. Although we’re required to be rigid by the kind of traffic on the enterprise environment, we recognize that those requirements don’t map to a research environment. A specific example of this is the quasi-religious battle over the security model. The network engineers want to “free the packets,” while the security people want to “protect the packets.” From the perspective of the researcher, that security profile looks a lot different. Once we were actually able to talk about what kinds of security needs and requirements a research environment might have, we realized that the security model might need to differ significantly from that of our enterprise network—for instance, instead of a campus border firewall we might need to implement a passive security perimeter.

Another area that has been a significant opportunity of growth for us is research network management, which differs from enterprise network management in two primary ways. First, I mentioned how rigid our enterprise network is: i.e. we don’t let people in to mess with our network. On the other hand, we want the research environment to be very flexible. On the research network, for example, we expect to have projects that have uptime requirements similar to those of the enterprise network or that require service-level agreements, but conversely, we need the research network to be flexible enough to enable users to do research that requires getting under the hood, such as working with software-defined networking or developing the next networking protocol. Allowing that spectrum of usage is a huge shift for us, and although we’ve often had to measure our progress in baby steps, we are getting there. That is our goal: keeping ourselves relevant and enabling researchers to do the work they need to do.

The second aspect of our research network management model that differs from that of enterprise network management is our collaboration with the National Center for Supercomputing Applications. Historically, NCSA and the campus have had separate networks, and in the beginning, the campus had a wide area network, but because over time we have come to realize the enormous amount of expertise and skill at NCSA, we have worked to develop relationships with them and so leverage that wealth of knowledge, and ultimately partner to build and share management of the campus research network. It has been a great experience—the kinds of knowledge and skills that NCSA engineers have complement our skill sets very nicely, and as a result, it has been a tremendous opportunity for both sides.
The other area that has provided us with an interesting opportunity for growth is funding. Financially speaking, the last several years have been kind of a unique time for the university. On the enterprise side, we have recently adopted a new rate funding model, but our efforts on the research network don’t really fit into it. However, we don’t want to impede research or make it all about cost recovery—I want to build relationships with researchers and have them look forward to discussing their needs with us. Thus, we’ve approached funding the research environment by seeking external grants to cover various aspects of the network, from sources such as the NSF network and the CCNIE program, instead of relying entirely on central funding. We have also received project-specific funding as a result of collaborating with some individual researchers. But we also try to work, if possible, to leverage existing infrastructure. As a result, our Science DMZ uses specific network traffic but applies a physical separation wherever it makes sense. Anything we can do to extend the purpose and shelf life of our enterprise network such that it benefits the research network is centrally funded, so we seek those kinds of opportunities wherever possible to minimize the duplication of efforts and equipment and thus maximize our funding. This approach is continually evolving. Although our funding efforts tend to be creative, our overall plan is to keep it off the researchers’ shoulders so they can focus on their work.

Here’s a current snapshot of the campus research network at Illinois. We’re partnering with NCSA to build our campus advanced research network environment—it is based on a science DMZ model and both NCSA and the campus are connected to it. Our condo campus cluster is an anchor tenant, and we have primary connectivity, which is the “on-ramp” by which local researchers get to wide-area research resources. Right now, that connectivity consists of 100Gb/s via Internet 2, along with multiple 10 Gb/s via our consortium with CIC OmniPop in Chicago, which also has connections to key research servers in that geographic area. That’s what we’ve been doing as part of Central IT—again, it has been a great opportunity for us and has resulted in a great partnership with NCSA.

**Perspectives**

**Guy Almes**  
*EDUCAUSE/Texas A&M University*

At least since the inception of the NSFnet effort in 1986, there has been a close (if sometimes ignored) relationship between high-performance computing and the high-speed wide-area networks that
connect our universities. Initially, this was grounded on the then-challenging task of enabling users from about 200 research universities to access the five NSF supercomputer centers. Over the years, the movement of datasets between the user’s university and the remote supercomputer has been a common source of challenge.

A current, very typical, example is represented by one user community of the Brazos cluster at Texas A&M University. Brazos is, in many respects, a typical campus cluster, with 3,200 cores, Infiniband interconnect, a 200-TByte parallel file system, and a software base including Linux and Torque. Worth noting is the cluster’s 10-Gb/s connection to A&M’s ScienceDMZ, so that the path between the cluster and the Internet2 backbone is a (usually) lightly loaded 10-Gb/s path. One user community is our local high-energy physics group, part of the international CMS collaboration centered on CERN’s Large Hadron Collider. This group’s typical pattern of usage is to identify a CMS dataset of interest, use CMS’s Phedex utility to pull a replica of the dataset from one or several remote CMS sites, execute thousands of several-hour single-core computations on that dataset, store the (smaller) results of those computations, and delete the local replica. It is important to emphasize the value of the ScienceDMZ in ensuring that our well-tuned, but ordinary, use of 10gigE hardware, a parallel file system, Open Science Grid gridftp software, and CMS Phedex software achieves excellent performance in pulling in those dataset replicas.

Given that the datasets vary in size from roughly 3 to 30 TBytes, this performance is essential to project success. The CMS community must be complimented on producing the highly workable Phedex system for transferring dataset replicas among CMS sites and the related storage and catalog systems that support this data-intensive international science collaboration. This discipline-specific data management system, when combined with our very good yet ordinary implementation of the ScienceDMZ idea and the networks such as Internet2, its associated regional networks, ESnet, and international partner networks, make possible the transfer of scientific datasets at rates of several Gb/s sustained over many hours. Taken together, this allows an ordinary campus cluster to be a powerful component of collaborative international data-intensive science.

A newer example is represented by A&M’s Initiative for Digital Humanities, Media, and Culture (IDHMC). In some ways, the pattern is similar. One IDHMC project, for example, is to use optical character recognition (OCR) techniques to process about 45 million images of literature, to produce text versions of hundreds of years of English literature. The total size of the data and or the computational requirement is much smaller than with CMS, but the pattern of moving datasets and computing on them with large numbers of single-core computations is remarkably similar. Also similar is the key importance of data management, including catalogs, careful storing of the data (with multiple replicas), attention to provenance, and support for workflows that access/update the data and aggressively use the computational capacity of Brazos. While our IDHMC colleagues lack the levels of funding and CMS’s tradition over decades of sophisticated computation and data management in support of international collaborative science, they are working effectively to address this issues in their digital humanities context.

Reflecting on these two examples, the importance of data management in support of data-intensive collaborative science/scholarship is key. To an unfortunate degree, such data management is highly discipline-specific and this weakens the ability of campus cluster staff to solve problems for a wide variety of disciplines. But where the discipline can organize a good solution to these data management problems, the campus cluster, with associated parallel file system and networking resources, can
contribute strongly. Of particular importance are the connection of the cluster to the campus’s ScienceDMZ and the careful engineering of that ScienceDMZ to Internet2 and related networks.

To state this in a slightly edgy way, it is relatively easy to provide campus clusters with increasingly powerful compute nodes, but it is more difficult to work with disciplines to support their efforts at data management and then work with the network community to enable the high-value managed data to be quickly moved among collaborating universities.

Key to a vision of campus bridging will be support for such data management in such a way that campus cluster groups can provide local support to national/international (usually) discipline-specific data management schemes. Taking a clue from the Large Hadron Collider community and then applying the basic ideas to other disciplines, our campus clusters can become powerful tools in support of computationally and data-intensive national and international collaborations. This data management focus must then be connected via the ScienceDMZ structure to the increasingly powerful wide-area networks that connect our universities.

Perspectives

Dan Schmiedt  
*Executive Director of Network Services, Clemson*

I've been at Clemson for 18 years. I spent the first fourteen years mostly in the role of network engineer, after which I transitioned into a leadership role. Since then I haven’t been quite so hands-on, and that distance has given me some perspective—what network engineers sometimes call a “bizarre outlook on things.” I've stepped back and asked, “Is this really what we ought to be doing?” Right about the time when I was chief network engineer, I ran into a faculty member on our campus who was collaborating with Stanford on the GENIE project. I've been really fascinated with OpenFlow, which we have since come to call a software-defined network, and I've become an enthusiastic advocate: I'm also the chair of the Internet2 SDN working group, which tries to help shape the way in which SDN will change networking in the future.
Traditionally, the network is considered to be OSI layers 1 through 4, which is handled by network engineering teams. The programmers and systems people are the ones who open up the sockets and send and receive data. The top two layers of abstraction provide a nice bird’s-eye view of things where high-level programs live and we don’t have to think too much about how the hardware works.

However, in the lower layers is a big pile of network protocol amassed over the years to solve various problems. If you’ve ever worked in a networking group, you know that it tends to be kind of chaotic, because you’re responsible for thousands of users who have thousands of users, any one of whom could be causing some issue with some network flow, so you have to be familiar with all those little colored boxes there. That’s life as a network engineer. The network has no layers of abstraction. Network engineers might be classically-trained computer engineers and scientists, English majors, high school graduates—generally, people who are just kind of masters of chaos and have figured out how to run a network. Alex Feltus said earlier that he didn’t know that there was such a thing as a network engineer. We’re a unique breed of person—we kind of do our thing and then fade into the shadows.

What I’m hearing today is that, for any number of reasons, networks are not moving data or doing other things in ways that users, especially as we move into HP 100GB networks. I think we tend to treat the network today as a data “sewer system”: we pour data into it and then get upset when it doesn’t move the data in the way we expect. We might want to think about doing things a little differently.

I don’t have all the answers, but in order to move in a better direction, I think the first thing we need to do is remove that line right there between networking teams and programming and systems teams.

That the network and systems teams of people are two separate groups who come together once in a while—that needs to change. At Clemson, we’re building a Science DMZ as part of our CCMIE project, so we interact regularly both with system people and with researchers like Alex who are actually doing research and getting high bandwidth between their labs and their HPC resources. As a result, we kind of catch up, figure things out, and learn a lot from one another.

Enter the world of software-defined networking. When we say "OpenFlow," we’re talking specifically about an API interface between network hardware (the little blue boxes at the bottom) and a set of network controllers at the bottom. That’s what OpenFlow does: it separates the data plane from the
control plane. Historically in network devices, the data plane and control plane each inside one of those boxes, which makes it hard to do things like network virtualization. When people would talk to me about cloud computing in the past, it would make me, as a network engineer, want to go hide somewhere—I can give you VLANs, I can map things and cross MPLS, but to make a network as truly dynamic as everyone imagines it is...it's not really like that.

Enter OpenFlow. Now, sure, if we want arbitrary packet flow from one place to another, we can do that. However, one thing we need to consider more closely is the interface between that network and upper layer applications. For example, the Internet2 AL2S network uses the OESS system, which can dynamically create Layer 2 circuits across the country. If you can imagine a national 100Gbs network on which it was very easy to create circuits, you could also consider creating circuits in other, more dynamic and more programmatic ways that included things like the kind of file system Guy talked about earlier. We need to think more about this API and what we could do with it.

I mentioned earlier how hard it is, as a network engineer, to interface with research groups. When researchers start talking about cloud computing or some other kind of major networking issue, a network engineer may want to go hide under a desk, but when you describe that problem to a computer scientist or a computer engineer, they see it as a challenge and are thrilled at the prospect of an actual problem on which they can collaborate with you to solve. Before OpenFlow, we hadn’t able to arbitrarily change things about the control point of the network—that ability disappeared as routing protocols and stuff moved from computers onto dedicated network computers, which we now think of routers and switches. Now, with OpenFlow, you can set a grad student loose and say, “Here’s a network problem, here’s an OpenFlow controller and some OpenFlow switches, see what you can do to solve the problem of SMP Windows size not being set correctly.”

An example: the professor I’ve been working with, Casey Wang, was describing to me some network research he wanted to do with GENIE. I kind of shrugged in response, and he said “Well, don’t you think that’s interesting?” And I said, “Well, it probably is, but it’s not the kind of thing we usually run into.” He said, “Well, what kind of problems do you run into?” So I said, “All kinds of stuff, really. Why don’t you come to our technical meetings and just listen in?”

So on the day he and his graduate student, Aaron, attended our meeting, some people at a facility down in Charleston, about 250 miles away, were trying to back up a lot of data onto a server up here on our campus. We had a 10 Gb/s link, but they were only getting 50 Mb/s and saying, “What the heck is wrong with your stupid network?” Of course we said, “There’s nothing wrong with our network!”

The problem was that TCP wasn’t set up properly. Aaron said, “Why can’t the network handle that?” I said, “Well, Aaron, it’s TCP,” and I started to explain it to him, but he said, “Yeah, but what if your network could fake it out, terminate those TCP sessions on each side of the connection, pack up the data, and truck it across to the other side using parallel TCP streams or UDP or something like that?” And I was like, “Yeah, sure!” He said, “I could do that with an OpenFlow switch on each end,” and I said, “OK, do it.”

A week later, he came back and demonstrated it to us. He explained that he was kind of motivated: the ISP connecting his apartment complex off-campus to his advisor’s lab on campus sent packets all the way to DC and back, which resulted in a big latency problem. So he turned on a protocol he’d written and did a file transfer. Previously, he’d been getting around 300kbps or something, but after he turned on an agent that was running on an OpenFlow switch from his apartment to the lab—boom! He started
getting 20 mbps. Yes, it was a hack, and yes, we’ve solved other problems in a similar way, but keep in mind that he did that in a week with a bunch of Python code!

Allowing researchers and students to do the kind of thing that Aaron did is just so important. It’s no longer just about network virtualization -- now networking is a discipline. As someone who has to run a network engineering department, it makes me feel a whole lot better to know that I have a whole team behind me of students and faculty members who are thrilled that not only do we have a very large, high-performance network on campus, but that we’re willing to let them tinker with it in smart ways. I see these guys as our partners.

As the graphic shows, I think this can generate a very important feedback loop. As members of our networking staff, we have people who have been around the block and know networking; students who don’t know really anything about real-world networking but also don’t know what you can’t do; professional networking staff who are familiar with wheel reinvention and who, when you start describing OpenFlow, might say something like, “Didn’t we do a lot of this with ATM in the past?” and help the team stay grounded and realistic; and faculty who understand the research process and who are engaged in teaching and always looking for teachable research problems--if you can give them real problems to solve, that’s even better. So as part of our CCNIE collaboration at Clemson, we have Alex the geneticist in there with Casey the computer engineer, along with our IT networking staff, all working together to try to solve HPC networking problems – they’re all part of an ecosystem to solve problems. My point is that anywhere I can encourage people to think that way, I think we’ll start to see good things happen at other institutions.

Perspectives
Wendy Huntoon
Internet2
One of the things I want to talk about, to which Gus Almes has alluded in his talk, is the convergence of computing, data, and networking. It’s truly important for the computing environment to be integrated seamlessly with the research environment, with the network considered as merely a manageable part of the application workflow. This is something that, from the networking perspective, we don’t really think about --it’s only within the past year that I’ve heard workflow mentioned more than once or twice; however, I think it’s an issue that we’ll be talking about much more in the future.
What's critical is that we are supporting researchers at the start of projects, rather than reacting only after they begin to encounter problems. Currently, the general experience is that we like to think that the network is transparent, even though that's not actually the case, which leads to our reacting to problems rather than proactively anticipating them.

Ideally, we would collect application requirements at the start of a project, which would be a desirable change in practice for both the networking and research communities, from the perspective of both campuses and the national infrastructure. We need to be able to match the infrastructure (including the network) with the application by identifying the holes in the resources that the user needs to use and ensuring that we're actually setting the expectations to match the requirements.

Another important thing is that interaction with researchers should be acronym-free. We sort of joke about that, but if you look how we talk not just about networking but about anything associated with computing resources, we tend to use our favorite acronyms, which are not the acronyms the researcher uses. As a result, they don't understand what we're talking about.

Transparent network access for all resources is also really important, regardless of whether the project is local, regional, national, or international in scope. Illinois is really putting in place an infrastructure to facilitate research projects for researchers, but if we don't do that on a national scale—if other campuses don't have Science DMZs or there are problems with the national network—the ability of researchers to get work done is compromised.

Case studies are a particularly useful tool in this regard. Although most research applications are unique, researchers experience similar problems which are often network-related. Case studies that provide examples of how the network is used can help researchers and campus IT staff identify some of those problems and provide insight about possible ways to address them. For instance, I have talked with researchers who used to ship data storage tapes via FedEx because they had no idea that there was any other way to port data. We need to integrate the campus and national infrastructure to make sure we're clearly articulating what our combined resources make possible, understanding what the researcher wants, and, finally, really trying to meet those expectations.

General Q & A From the Panel

Ruth Pordes: When I think about campus infrastructure, I am thinking about science. At Fermilab, we have an “MZ” that we make as secure as possible, and perhaps we have let that encroach on our research infrastructure, which is naturally architected, so hearing about the Science DMZs at your campuses is very interesting.

Q. (to Guy Almes): As you’ve pointed out, many attempts to realize a unified file system have already been made, and they’ve all failed somewhat. So, do you have any thoughts about what direction this “grand vision” might take?

Guy Almes: I’m not sure about the premise of that particular question—it’s often simply assumed that any effort will fail, and so no one attempts it. However, a positive example would be the experiments Phil Andrews was doing with the Teragrid based on GPFS. There was one demo where the physical limit of the network was 39.6Gb/s, and he was getting an aggregate flow of 27Gbp, with NCSA staff reading a filesystem mounted from SDSC. There are some difficulties—performance is one, as I mentioned, and
it will take some time to first leverage Internet2’s backbone and the corresponding regional infrastructure. Second, there is no question that we need more Science DMZs on campuses. And that would provide the basis for a certain level of in- and throughput. There’s some very interesting work going on in the XSEDE project right now on a wide-area file system built on GPFS that positively supports multiple replicas and caching. There are some negatives, too—as I mentioned earlier, the user ID issue is a hard problem, but not an insurmountable one—but all in all, it’s a very positive step.

Q. We heard this morning from some PIs talking about success stories with their campus clusters, but we’ve also been hearing some disconnect between network engineers and PIs and their students—do you have any success stories you point to? Because from my perspective, the network is upstairs reality, and it doesn’t get faster; it’s so far removed from what I had control over, what I understand, and I’m waiting for it to change.

Guy Almes: A few months ago, when I was talking to one of our CMS guys, who often provided constructive critiques about the problems with the CMS Tier-3 service to our cluster, and I asked him if there was anything positive about his experience. He basically affirmed, absolutely and profoundly, that because of our work, doing high-energy physics at A&M was always pretty constructively critiquing what was not quite right about CMS Tier-3 service providing to our cluster, and I was talking to him one day and said, Was there something positive? And what it came down to was that he absolutely affirmed that, in the collective experience of his group, doing HEP at AM was more productive than at other places. That was very valuable. Many of our research groups see us as enormous enablers of different kinds of science, even if they don’t always come out and say it.

Dan Schmiedt: I’m afraid also that a lot of people think that getting 100 Mb/s transfers is a good thing don’t understand that we really are in a multi-gigabit world, and if you’re not getting that, there’s a problem.

Jim Bottum: I think a lot of people really don’t understand what the network is capable of now. We’ve built up 10-100Gb/s networks, but many people are still living in a 100Mb/s world. We have two problems. First, we haven’t done the things on our campus that would make the network function at top capacity. Even at Clemson, we have a whole pile of Cat3 floating around. Second, we’ve built these friction devices, so that even if you have a 10Gb/s device, if you drop packets, you’re back to 50Mb/s, which is why we’re seeing so many 50 Mb/s numbers—they’re a canonical number for our network and for h, we have even at Clemson a whole pile of Cat 3 floating around. The other thing that’s happened is that we’ve build these friction devices—we may have a 10Gb/s gizmo but you drop packets and you’re back to 50 Mb/s. And that’s why we’re seeing these 50 Mb/s numbers, that’s a canonical number for our network and for the country.

Dan Schmiedt: Using DMZ is a way for my staff to get familiar with operating an SDM network in a semi-friendly environment, at least. I think what I’m hoping will happen is that they begin to ask why we’re not operation the other network in the same way.

Tracy Smith: Historically, networkers like to be behind the scenes—we need to be better about getting out on campus, making the rounds, and letting people know what’s available.

Q: The problem with the network is that there’s a disconnect between the network engineer and the researcher which makes it difficult to translate the knowledge of the network to the user’s experience in
order to figure out out, for example, why they got 50 Mb/s when they should have been getting 10-100Gb/s—there are many examples of problems with WAN performance that have not been resolved.

Wendy Huntoon: I think managing the researchers' expectations is really important. And I think we need to consider not just network performance but overall application performance, which can really improve things. For example, when we worked with some biology researchers at Penn State, they were getting 50Mb/s, but when we looked at the application as well as the network we were able to get sustainable, repeatable performance of 5Gb/s. Scalability is a big issue--working with researchers on performance tuning is useful, but you have to do that on a one-on-one basis, and there are only so many people you can work with. As we upgrade and increase resources, a major issue is figuring out how to scale the infrastructure so that it is easily available to all researchers, and not just the ones with whom we're able to work on an individual basis.

Q: Tracy and Dan both talked about interactions with faculty from the perspective of central IT networking. How do you interact with your campus HPC and research computing teams? They're not working with faculty the way you are. For instance, at Stanford there's networking, and there's us, and technically we're part of the same organization, but we don't have the kind of free flow of information I think we need because we're all busy and can't both make it a priority. How do you make the whole ecosystem work together in terms of networking and your HPC staff?

Tracy Smith: From our perspective, the first step is understanding that that kind of interaction needs to happen—for us, it's one of the areas in which we are making efforts to improve. We need to engage with projects, even just have conversations with researchers. After all, I like to talk about what I'm doing, and everybody else likes to talk about what they're doing, so we try to find opportunities to have those conversations. We don't get it right all the time, so it's an area of focus for us.

Dan Schmiedt: In terms of daily operations in the cluster and network designs at Clemson, part of network engineering is working with HPC engineers, who are hands-on with the switches and network devices that are directly connected to the cluster. They often attend our technical meetings and let us know about hardware and networking issues they are having to which we can apply our experience in operating a large enterprise network. As far as engagement with users goes, one great aspect of the NIE project is that we can work face-to-face with our researcher partners to troubleshoot specific problems they're having. For us, finding projects where we can collaborate with researchers has been been eye-opening in many ways, and it helps us build and strengthen relationships.

Tracy Smith: For us, that involves leveraging relationships with our peers here at NCSA. They bring a different perspective to our conversations.

Guy Almes: One more comment about Science DMZs: another important ingredient is the perfSONAR tools that allow you to measure end-to-end performance. They give us a fascinating way to understand the interrelationships between Science DMZs on different campuses. We've had some complaints about effect of specific data transfer tools between A&M and Vanderbilt on performance and how to improve it. In this case, perfSONAR was working fine at both ends, but the hosts weren't getting good end-to-end performance. Then, suddenly, the performance between hosts improved dramatically, and we were able to consider that problem solved and move on to the next one, but we never figured out what caused the issue in the first place. This isn't a perfect example, but it illustrates two good things about perfSONAR. First, perfSONAR demonstrated very good performance, which proved that the problem wasn't the network itself—it was likely a hardware issue that was resolved when some fix was applied to
the host. Second, perfSONAR kept longitudinal track of the test traffic, which we were able to analyze to identify when, exactly, the problem started to happen.

Miron Livny: One last comment about perfSONAR: perfSONAR and the host are not 100% identical in terms of pathways, so, for instance, perfSONAR could be performing well while the application is not. The Open Science Grid (OSG) is committed to supporting the deployment of perfSONAR in as many places as possible, so anyone who is interested in joining us should let us know.
Moderator: John Towns

Moderator John Towns invited panel members to talk for 10-12 minutes and describe any challenges they have not been able to address satisfactorily, which others could benefit from.

Research computing Services in the Age of Big Data

Erik Deumens
SSERCA

Erik Deumens from the Sunshine State Education & Research Computing Alliance (SSERCA), began his presentation, “Research Computing Services in the Age of Big Data,” defining the alliance as a mixture of state and private universities in the state of Florida (http://sserca.org).

Unifying Research Across the State

The mission of SSERCA is to enable collaboration between researchers in the state of Florida with their colleagues everywhere. In trying to keep SSERCA light, it is a completely virtual organization: all assets are owned by one or more members and all grants are collaborative grants to members. SSERCA performs for and through its members: everyone is moving in the same direction even though not everyone participates through the same efforts. SSERCA also performs data centric research to provide a rich storage infrastructure with close-compute capability at the 6 member facilities: FIU, FSU, UCF, UF, UM, USF, and FAU (pending) with FAMU, UNF affiliates. SSERCA only acts in alignment with members;
for example, there was a SSERCA booth at SC11, SC12 and SC13. There is nothing that SSERCA can do that has a separate agenda from its members.

SSERCA got together through the Florida Lambda Rail (FLR) (http://flrnet.org), where there were discussions of having a robust network but needing to build a cloud-resource infrastructure on top of it, as well as enable collaboration between researchers both inside and outside Florida.

The SSERCA organizational structure has created bylaws, and executive and operational committees that talk to each other on a weekly basis with face-to-face meetings 3 times per year at rotating locations across the state. The operations committee is comprised of the HPC center directors—the power behind SSERCA.

Staff report to the provost or the deans at each location, some to the CIO. It is crucial—whoever you report to in a pure formal resource manner—all three must support of your activity regardless of reporting line.

It is critical to have buy-in from the research community and one-on-one contact is key. One on-going challenge is that here is a large number of faculty members who are very hard to reach, there have to be constant activities to invite people to, hoping word will spread.
At Florida, research computing is under CIO, [http://www.rc.ufl.edu/](http://www.rc.ufl.edu/) with the goal of making researchers at UF more competitive and to be able to provide resources very quickly (in days or weeks instead of months).

Research computing mission at University of Florida:

- Provide high-quality infrastructure for
  - Grant-funded research
  - Scholarly research
  - Interdisciplinary collaborations
- Provide expertise
  - One place to go for research computing help
  - RC provides services, or
  - takes you to the appropriate service provider

Having a virtual organization and collaborating allows us to respond very quickly to researchers who come to us; we can effectively provide a solution or answer that doesn't take 6 months to develop and implement. SSERCA knows the system personnel so that researchers can get going in a matter of days, and the funding has increased because the infrastructure is in place already.

The services provided to the researchers are all virtual, they buy a piece of functional infrastructure with compute cores and GPU capacity; we don't sell nodes, we count them as computer cores.

- Compute core and GPU capacity
  - Buy and use for 5 years, with access to idle cycles
  - Or. buy at $0.02 per hour
- Long term and replicated storage capacity
  - Buy in units of 1 TB for 1 year

The funding agency doesn't necessarily ensure you are in compliance with A21 or all the rules and regulations; knowing that the services are in compliance has helped with clarity.

The Provost subsidizes the staff consultant services, researchers pay $20/hr. The subsidy allows faculty to write in the cost of a graduate student but get a professional programmer for it, which balances affordability with responsible use. If we charged the full cost, then a lot of people couldn't use the services at all.

Researchers benefit over buying by the hour. Buying a node means there is no overhead charged and that they are making a commitment to be working with the program for 5 years. Then researchers have the added advantage that once you are an investor at that level, you use up to 10 times the number of cores purchased if there are resources available. Take an example from last summer: With a $10,000 investment in equipment, would it really be worth it to the grant? If the researchers would have been billed at the cloud rate, the total computing done would have cost $47,000 to the grant. Clearly the grant was well-served by the investment and long-term commitment. This is how we to prove that it was beneficial to the grant, and that the grant was served in the best possible way.

The advantage then is to get access to a secondary type queue; an example of node cost usage for a 5-year purchase being far less than what per-cycle cost would have been for 1 year based on real usage.
Students cannot work independently, because the program doesn’t have the manpower to supervise individual students and answer questions about programming. Students who have a sponsor can easily go to MPI training.

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NCSA/Condo of Condos/MGHPCC/Harvard University

James Cuff

MGHPCC

James Cuff from NCSA/Condo of Condos and MGHPCC/Harvard University who is the Assistant Dean for Research Computing at Harvard reminded us that in the 60s, we had to share machines because it was so expensive. The PC became popular for a reason: because it was mine. Then we started stitching together the cluster, but computers were still not large enough. In 30 years, we have come full circle. What was old is new, what was new is old:

- From centralized to decentralized, collaborative to independent, and back again!
- Bigger, better but further and further away from the scientists’ desktop!

How we will survive as administrators and managers if people don’t feel incentivized? Researchers are not going to join and use resources rather than using a cluster in a closet.

**Challenge 1 #gowestmyson**

Massachusetts Green High Performance Computing Center uses hydroelectric power and serves 5 universities: MIT, Harvard, UMASS, NEU, BU. The center opened in February of 2013 and the first science was in May (ATLAS). There were significant logistics through MIT; going through 1,000 miles latency is an issue.

Now the MGHPCC has a new building with computer rooms, energy vaults, a data center, and room to grow—because no matter how big a boat you build, you’ll always need a bigger boat.

**Challenge 2 #cleanyourroom**

There are no decent tools to help get equipment from an old location to a new location, so we built our own tools to assist: a MySQL shim, tools to see where all our stuff is, and how to track on and off. We also consolidated multiple machines into higher-density ones, but we still have rooms full of stuff—a graveyard—and turning off the old equipment is an operational challenge.

**Challenge 3 #powertothepeople**

For too long the cone of silence has come down once a new building is in place. Let’s be transparent about bills, and power usage. We had a weekly meeting where all 5 institutions discussed operational challenges, where we shared power and electric bills: our share is 65% or 212,578,139 watt hours, which is not comparable to Blue Waters, but it does cost $37,037.71 per month. Now the bill is consolidated, it used to be scattered all over the campuses. The up-side of having it all in one place is that you can voluntarily conserve energy; for example, you can take 30,000 processors off the grid during peak times to see the energy savings. So you can see the consolidation benefit--to delete the old crud.

**Question:** I’m curious about the load check program, if it has great financial incentives: turning off equipment and the mortality rate with power down.

A: Computing is getting a lot more tolerant, but we don’t turn off the storage arrays. We keep machines running and just have the sacrificial lambs. Machines idle more beautifully now, as you saw on Dell’s fresh air example.

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**Perspectives**

**Miron Livny**

**OSG**

*Miron Livny, a Computer Scientist and PI of the Open Science Grid (OSG) has also served as the Technical Director of OSG, is from the University of Wisconsin, and has been leading the Condo project for 30 years. While not an official member of the OSG Council, Livny is a software provider through the Condo project and also is a consumer of cycles, “It takes more energy to keep mice alive than run HPC.”*

In terms of the national and international perspectives of OSG, it is a consortium of 50-60 entities today; a fabric of services of distributed HPC usage delivering 2 million hours and about 1 PB of data movement per day across 100 sites. OSG doesn’t own or maintain any hardware, but they facilitate jobs launched in one location running elsewhere.

OSG is funded jointly by the NSF and DOE with 6 program managers; funding work started in the late 90s. There was a lot of technology coming together, and we had to work to get rid of a lot of wrong job-centric technology that was coming to grid computing. Eventually we moved the whole thing in a more effective way based on the principles of the distributive computing model. OSG is finally in a place where they have the infrastructure that facilitates the Overlay approach to deliver 2 million hours a day, but it has been a long process.

**Challenge 1**

OSG is doing ok on opportunistic process power, but we are still unable to deal with opportunistic storage. The fundamentals of opportunistic storage are not there while we are getting initiatives from above to do big data.

**Challenge 2**

There is no policy or implementation of policy across OSG on how to implement opportunistic cycles.

**Challenge 3**

OSG could and should do much better at Open Science Grid Blueprint Framework.

OSG does have a principle which they are proud of, and it requires real commitment of the organization to maintain. It is all a part of OSG’s success: operating with clear principles, peer to peer, cloud, big data—all these terminologies—how will this happen tomorrow?

**Challenge 4**

We are all facing the acceleration of continuously changing. It is not about the function or how big the data or how fast the machine, it is the acceleration of how fast the change is changing. What is happening around us can change in months.
Challenge 5

What a typical physicist is willing to live with in terms of effort is not what the average biologist can deal with—we don't know how to give scientists the app or “click, download, and run” experience. We don't have the right people. We like to write complex things that require a lot of hand-holding to those who don't know what the shell is.

Are we optimizing the 5% or the 95%? The first thing you cut is travel, it is visible. We are going after the percentage—of what? How many lights are on, which is drawing much more than needed? We should establish a sustainability council. If you're going to measure everything, shut the cash campaign—compute energy is small. It is 25% of the university budget because of desktops. Make sure we focus: the question at the end of the day is do we enable scientific discovery? Energy consumption is part of it, but by saving 2-3%—what is our impact on scientific productivity? Closets at biological labs have things much worse than energy-draining computers.

The Condo of Condos

James Bottom

Condo-of-Condos

Jim Bottom spent the early part of his career at NSF as a management intern then spent 15 years helping Larry Smarr start NCSA. Bottom has spent the last 13 years in the University setting, first at Purdue and now at Clemson where he is the Vice Provost and CIO, and PI of Condo of Condos.

Condo of Condos is not funded yet but is recommended for funding. We saw the benefits of aggregating at the campus level for growth purposes, so Condo of Condos Phase 1 Members are Hawaii, USC, Utah, USC, Wisconsin, Harvard and Clemson.

Condo of Condos Phase I Members

Moving from Big 10 to an EPSCOR state was an eye-opener on challenges: we have far more funding. EPSCOR states are below a certain level of federal funding. A PhD scientist is basically doing system
administration to have the facilities necessary to do research. We are also seeing a national trend, noting that Ed Seidel started a series of reports while at OCI that were good (including Campus Bridging) but didn’t see a lot happening from it. Then one day we learned that some staff was studying the reports, and the idea to see what they could do to bring aggregation across state boundaries: what they couldn’t do nearby due to academic rivalries. From PACI experience that got up to 100 members. They knew the danger of overextending their partners, so they went to NSF about the idea and requested funding to hold a number of workshops. That led to the almost-funded proposal. At the first workshop, they thought it would be about technically integrating between institutions and quickly got to the people side of things which led to Condo of Condos Phase II with the addition of Washington, Stanford, Arizona, Oklahoma, Emory, Ohio and SSERCA.

The Project Vision began to develop as we brought people together for support:
Barr put up the first application. Even though it had a great LINPAK score, on the cluster it wouldn't run. There was no one with expertise to assist. Having gone to Clemson, they knew about the Advanced Cyberinfrastructure Research and Education Facilitators (ACI-REFs). Traditional users will find ways to compute, but there are lots of others out there. The feedback from GIS faculty brought together for discussion was that they were outgrowing their desktops but needed handholding and training to be able to use different types of resources, so the list of project goals developed:

**Project Goals**

- Increase total number of campus ACI users
- Increase diversity of research groups using ACI resources on each campus
- Develop outreach strategies to engage the “long tail” of researchers
- Develop data science practitioners
- Develop a plan for enabling other institutions to join the consortium
- Develop sustainability mechanisms for sustaining project momentum
- Provide technical coordination to allow researchers to focus on science outcomes and not technology

With stimulus money, they researched infrastructure improvement. Clemson has 54 academic departments, 16 were using HPC resources, but now 40 utilize resources and users have increased from 0-600 (including students). NSF is developing plans and sustainability. They couldn't partner with U of Carolina because of competitive differences.

Collaborations can happen in many ways, and there are various threads of connections between individuals: some come together at various times, often serendipitously. Sometimes we struggle to collaborate, so any avenue is good.

**Challenge to date: getting off the ground and funded. But we are close.**

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**General Q & A From the Panel**

Livny shares that many of us feel that we can handle opportunistic computing, but there is great diversity with respect to storage. From the OSG vision perspective, any time you bring two entities together there is a question of sharing and the problem with storage is first cultural. There is a great divide between storage/data and computing people, which is fundamentally flawed. We don’t have a force in our ecosystem that is committed to break this divide. Computing is viewed as scarce but storage is viewed as infinite. People assume that disks are not full, until storage runs out—and then there is panicked cleanup. We have virtual CPUs and move things around but storage isn’t like this. Fundamental change is needed.
James Cuff shares that the number of “sorry” messages he has had to send about CPU failure is small, but that he sends storage failure notes all the time. People’s tolerance for listing a directory and not getting a response is extremely low and work that goes into CPU queues isn’t there for storage queues. No one checks the IO patterns/performance.

We have come full circle in 25 years: you had to ask for storage and wait for it. The UNIX/PC world we’ve created was built around creating trivial environments where you only hurt yourself, but we haven’t done OS research in 20 years. Livney suggests that a main contribution of the grid is to move users back to job control language (JCL).

Deumens questions, is some shift possible? The biological community deals with all the data and thinks in terms of workflows: should we start thinking in terms of workflows? But then we have to come up with file systems that work for this. James Cuff solved this with Hadoop but it doesn’t play well with others. Livney adds that he doesn’t think it was even solved with Hadoop. Workflow is moving in direction of JCL as it does force you to define the resources you want.

Another question was posed about dealing with public vs. private institutions. James Cuff responded that we do sometimes wait a long time for checks, which is why they have a contingency. Sometimes even commercial partners take a while to return checks. Operations meetings for the center are also to keep an eye on the administrative stuff. Deumens adds that Florida is similar and that it is important to know the right people. There is a major value of having the regional organization to help identify the right people. Deumens made sure to add that being able to say that high-level leaders are behind efforts is important.

Livney suggests that we have to keep the communication moving, and that the value and importance of making peer-to-peer links is critical to the future. There are a lot of challenges with working across institutional boundaries. It is only going to work with face-to-face interactions and working across the institutions.

Townes states that technical issues are easy, it is the social engineering of working across institutions and campuses in the future that is our larger issue.
NSF Perspective
Friday, January 17, 2014

Irene Qualters

*Irene Qualters is first and foremost a Program Director and also the Acting Division Director of Advanced Cyberinfrastructure (ACI), which used to be OCI, in NSF.*

Qualters suggests that we think about computational infrastructure holistically, even while boundary lines are blurring between data and computing infrastructures. She is observing that the kinds of discussions surrounding the technical problems on campus being defined as “cultural issues” more than “technical issues”—as being accurate.

In early Earth Cube community discussion among the large data facilities, it was particularly striking that the community met and initially thought they had nothing in common because their data are so different—but they are discovering that they do have very similar problems in many ways. Qualters applauds the leadership demonstrated by the individuals present in meeting to discuss common challenges, and shared approaches. As scientific data from instruments everywhere grow in size, diversity and ubiquity, it is important that the research infrastructure communities evolve strategies that innovate and collaborate with one another. There are challenges and opportunities from an both an innovation and a sustainability perspective as the cyberinfrastructure becomes more and more integral to the conduct of all phases in the discovery process.

In 2013, OCI joined CISE and became the Advanced Computing Infrastructure, (ACI). ACI is inherently multi- and cross disciplinary where the focus is use-inspired, containing ties to directorates. There is a challenge moving into a more focused directorate. ACI, CCF, CNS, IIS are the four subdirectories; ACI and CCF are research CI and the other two are foundational research.

After much community input, the CIF21 strategies remains its guiding document http://www.nsf.gov/publications/pub_summ.jsp?ods_key=nsf12051:
ACI remains pivotal to advancing NSF’s Cyberinfrastructure (CIF21) strategies

CIF21: cyberinfrastructure as an ecological system


There were three major NSF advanced computing infrastructures deployed in 2013 each with very different technologies:

- Blue Waters at Illinois
- Stampede at UT Austin
- NCAR/Wyoming

ACI received over 600 proposals in FY2013 with an award success rate of 29% overall. Going into 2014, appropriation clarification is expected soon. This is a significant improvement over last year’s visibility into availability for award funding.
The impact of mobile devices, social networks and their real-time data component is a factor that is only beginning to be probed from a research CI standpoint.

**Ubiquity in mobile devices, social networks, sensors and instruments have created a complex data-rich environment ripe for new scientific and engineering advances**

This century’s grand challenges often require an expanded and collaborative role for computation and CI throughout the scientific process. Simulation clearly has a heavy involvement in our current computational resources. But as we employ our computational CI to handle not only the increased
volume of observational data but to understand/develop the role of data analytics in discovery and education, the diversity of the computation resources needed will surely increase. This will be accompanied by a more cohesive technical environment to supported integrated workflows.

This century’s grand challenges often require an expanded and collaborative role for computation and CI throughout the scientific process

Smart sensors, data analytics, and simulations have embedded computation into the entire process: theory -> prediction -> experiment -> observation cycle and is reflected in ACI investment portfolio:

This realization is reflected in ACI investment portfolio

Total ACI FY 2013 funding = $210,772,572
In 2014, there will be four upcoming solicitations with an HPC one possibly coming soon:

**Upcoming Solicitations: Webinar on Jan. 27, 2014**

- Data Infrastructure Building Blocks (DIBBs) NSF 14-530 due April 9 – Amy Walton
- Campus Cyberinfrastructure: Infrastructure, Innovation Engineering (CC*IIE) NSF14-521 due March 17 – Kevin Thompson
- Software Infrastructure for Sustained Innovation (SI²) NSF 14-520 - Dan Katz
- Petascale Computing Resource Allocations (PRAC) NSF 14 -518 - Rudi Eigenmann

**Best Practices**

If we think of the cyber infrastructure as an ecosystem, biology teaches us that species diversity is a predictor of resilience: making sure there is diversity in the types, sizes, roles, throughout the ecosystem. But now, new understanding is just emerging, for ecosystems that if one want to successfully adapt and sustain over time—it is equally important to build diverse connections and relationships among the diverse species. Our CI investments have been distinct in diverse forms of computing, data, networking, software. But we have also deliberately supported the building of various fabrics. We have to consider the ecosystem holistically, fostering the development of a portfolio of relationships in concert with a diverse technical portfolio. The diversity in the fabrics supporting various communities will support agility and innovation over time. XSEDE, Condo of Condos, OSG are examples of CI fabrics.

NSF’s computational infrastructure has two key strategies:
- Invest in diverse and innovative national-scale shared resources, outreach, and education complementing campus and other national investments
- Leverage and invest in collaborate flexible “fabrics” dynamically connecting scientific communications with computational resources and services.

We must amplify the strategic importance of deliberately exploring relationships.

**Q&A**

Q: Boundaries (Livny) - what do you plan at the ACI level to take these boundaries and the connection of these boundaries seriously? What can we do to help you address the problem, because it is critical, from
an OSG perspective? The biggest challenge—the concept of sharing compute-cycles and turf, and the budget for computing and data—is a structural problem, not a money problem.

Q: What role is ACI or NSF taking in trying to cross these boundaries between disciplines, and what roles should we play?

A: It is a structural piece but based on experience, there is a very strong cultural barrier. We can push and try to forge relationships but there needs to be discussion about what happens at a community level that happens among the disparate communities. Workshops are an obvious first step. There is appetite within NSF to pursue this but we need help on pace, and we also need your initiative.

Q: Livny finds it difficult to find a channel to communicate examples of collaboration working well.

A: NSF could provide more incentive. The last HPC solicitation combined data CI with computing CI, and we might see more dramatic movement in this vein. It would be useful to have more events where communities come together to talk about what they have that works and how that might bridge to others.
Open Science Grid

Ruth Pordes
OSG

Ruth Pordes is the chair of the Open Science Grid (OSG) Governing Council and Associate Head of the Fermilab Scientific Computing Division, but formerly worked at CERN, and is working toward moving the whole ecosystem forward in a collaborative way by building trust and working together from diverse organizations, policies, and oversight—between the physics community and many other disciplines. Pordes is hoping to provide value to science via the infrastructure.

OSG is a multi-disciplinary partnership to federate multi-level resources to meet needs of research and academic communities. Fermilab is a single-focus lab, so it is natural for Fermilab to work with universities. The project does heavy lifting funded by the DOE and NSF, while the consortium contributes the computer, storage, software, and use. The governing council is a mechanism for building trust, but developing OSG has been a long process.

Core Principle

We should share resources that go unused across multiple scientific communities, “I have spare cycles this month, but I need more later.” This translates into opportunistic access averages around 1.5 million hours per week, which have not yet peaked. This principle can be overlaid and shared on computing used for other things so that the owners don’t give up control of their resources. Common software components allow sharing and also provide evolution to new types of computing that try to protect users from evolutions happening underneath in the fabric. We need expertise to enable sharing and to help new users and communities participate / benefit from OSG. Campus Connect is providing a smooth path from using campus resources to national resources.

Challenging Issues

We need to transition from old to new in people, technologies, and resource types but still keep things running. It takes months to years, not weeks, to transition and moving to the new takes a significant investment. HEP can “gobble up” any computing because they have continuous experience of moving to the new. The main provider of identity certificates at the DOE closed shop which forced a migration to a new provider. We have to ensure transparent use and operation across international boundaries; multicore is a crisis in OSG. We also need to retool codes to not pay through the nose in 5-6 years.

If given $1M, Pordes would support people and the holistic nature of things through training, engagement, help for individuals who can then spread the experience and expertise and help improve the whole ecosystem.

Blue Waters

Bill Kramer
Blue Waters

Dr. William Kramer, Blue Waters Director, NCSA @Scale Program Director, National Center for Supercomputing Applications, University of Illinois shared that Blue Waters is on the Track 1 leadership system from NSF and is novel in a number of different ways.

Several Sub Systems
Blue Waters is the largest Cray subsystem and interconnect in the world: 50% bigger than any other Cray. It is the world’s most intense data storage system with amounts up to 500 petabytes and bandwidth over 1 terabytes/second. Blue Waters has external servers and interfaces at scales that are not common or are unique throughout the world and is also the world’s largest aggregate memory system at 1.6 PB. The mission is to move from evolutionary insight to revolutionary discovery and change. Blue Waters focuses on sustained rather than peak performance:
http://bluewaters.ncsa.illinois.edu/

Community Engagement
The Blue Waters Training allocation is a light-weight proposal process and has a fellowship graduate program. Blue Waters will select a number of PhD students working in HPC to further their research, has training modules for HPC usage, and a virtual school is developing into credit-worthy classes.

How Blue Waters Relates to You
A system like Blue Waters is probably what you’ll have in 5 years. Blue Waters is an XSEDE partner and allows researchers to expand their vision or have co-designs of applications.

Advanced Research Computing: A Canadian Perspective

Chris Loken
SciNet/University of Toronto/Compute Canada

Dr. Chris Loken is Chief Technical Officer of SciNet, an HPC consortium based at the University of Toronto, which is a partner in the national Compute Canada platform. Chris was formerly an astrophysicist and worked in computational fluid dynamics on the academic track but then moved into compute facility management and became the first employee of SciNet in 2008.

Compute Canada (CC) is the national platform for advanced computing in Canada which has evolved by coordinating seven university-based HPC consortia distributed across the country. CC currently operates HPC systems with a total of over 180,000 cores, 500 GPUs and 16 PB of storage. There are a total of 140 technical staff FTEs (employees of the various universities) with 13.5 person-centuries of relevant expertise across the country responsible for all aspects of running and supporting these systems as well as teaching and training users. Systems are open to all university-based researchers who are automatically eligible for “default” accounts that typically average at least 64 core-yrs per year. The majority (~80%) of resources are allocated through an annual Call for Proposals with 270 awards made for 2014. There are currently 1,450 PIs and 4,900 users on CC systems.

After approximately 5 years of lightweight operations, Compute Canada is transitioning to a more robust management and governance structure in response to direction from the funding agency. CC became a not-for-profit corporation in 2012 and is currently developing a new strategic plan as well as
management plan defining the relationship between CC and the four “regions” (West, Ontario, Quebec and Atlantic). Sustained and predictable funding remains a key issue for CC going forward. There are ongoing efforts to improve ease-of-use, and access to, the national platform as well as to better engage with traditionally under-served communities (e.g. social sciences and humanities).

CC faces a number of challenges related to governance as well as funding levels and mechanisms. For example, there is no significant source of funding (outside of health sciences) to build departmental or university level clusters/systems. As a result, CC is essentially the only source of computing resources, support and training beyond the workstation for most Canadian researchers.

Funding for advanced computing in Canada is largely driven by a single national funding agency (CFI - Canada Foundation for Innovation) which has invested $6B in HPC since 1999 but has not awarded funding to CC since 2006 making planning rather challenging. CFI funding needs to be matched by the provinces but, as they have different levels of resources and varying priorities, this has implications for location (and scale) of infrastructure. Individual PIs have recently been strongly encouraged by CFI to use their HPC funding to grow existing CC clusters (condo model) or co-locate their equipment in a CC site.

SciNet, Canada’s largest supercomputer center was formed in 2006 by integrating several existing departmental-level HPC efforts (PSciNet) as well as the research hospitals affiliated with the University of Toronto. A $32M RFP was issued in 2008 to design, build and integrate an energy-efficient datacentre along with two compute clusters and storage that would fit within the (known) 5-yr operating budget. The SciNet datacentre (4,000 sq ft of machine room floor and measured PUE of 1.18 with current 1.5MW of IT load) is off-campus, completely controlled by SciNet and used only for HPC. Key systems include a 31,000 core x86 cluster, 3,300 core Power 6 system and 40,000 cores of BlueGene Q (owned by the Southern Ontario Smart Computing Innovation Platform). A staff of 13 HPC experts is responsible for operating and maintaining the datacentre and systems as well as supporting, teaching and training users.

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**XSEDE**

**John Towns**

*XSEDE*

John Towns, PI and Project Director of Extreme Science and Engineering Discovery Environment (XSEDE) shared the XSEDE tagline, vision, mission, and goals, and the significance of raising awareness of how important this work is to the general public and society in general.
What is XSEDE?

- An ecosystem of advanced digital services accelerating scientific discovery
  - support a growing portfolio of resources and services
    - advanced computing, high-end visualization, data analysis, and other resources and services
  - interoperability with other infrastructures
- A virtual organization providing
  - dynamic distributed infrastructure
  - support services, and technical expertise to enable researchers engineers and scholars
    - addressing the most important and challenging problems facing the nation and world
- A project funded by the National Science Foundation

*Unsolved Challenge*
Billion Dollar Usage

The moderator posed the question, “If you had one billion dollars, how would you spend it in your area?” and Towns limited his analysis to 3 minutes:

**How would you spend $1B (US/CAD) to dramatically improve our national CI?**

**Multiple Efforts! (some of what I would do...)**

- **Co-invest with campuses to develop campus CI:** $200M  
  - 2-3% match from campuses; must integrate with national CI  
  - 2-3 rounds of awards running 3-5 years
- **Establish a national data infrastructure:** $250M  
  - needs to complement the national computing infrastructure  
  - 2-3 rounds of awards running 3-5 years
- **Workforce development:** $40M  
  - expand current and grow new programs to develop CI-savvy researchers: grad student, postdocs, research scientists, faculty, ...  
  - technical staff: systems admins, network engineers, applications support staff, ...  
  - 2-3 rounds of awards running 3-5 years
- **Develop new leadership in our community:** $10M  
  - establish programs to develop leadership  
  - center directors, facility managers, large scale project leads do not have these  
  - 2-3 rounds of awards running 3-5 years
- **Sustain this! $500M**  
  - investment fund to generate ongoing funds for sustaining/expanding these efforts
The growth in this community is limited by leadership: there is not a large pool of folks to draw from.

General Q & A From the Panel

Jim Bottom: economic squeeze is coming and he’s a fan of Massachusetts and Florida getting CEOs to come together. Any discussion of crossing the borders for this? Joining consortium? We are all looking down the future.

Chris: I haven't thought about joining an American consortium but CC is actively developing ties with US entities including participating in this year’s International Summer School in Budapest. 10-15 years ago, Canadian researchers had to find an American collaborator if they needed HPC resources but the national computing situation has improved. From the Canadian context, there is a push to do more with industry such as basic research and there have been some steps toward industry/academic partnerships.

James Cuff: America is a proud nation. There is a national competitiveness on an international platform with top 500 companies. Are we doing enough? Is our national competitiveness sufficient?

John Towns: It is clear that characteristics of students in our universities are changing nationality—more of them are going back to their country after studying. In order for the US research capability to be as competitive as possible, we must collaborate in other countries. This has already been happening organically: rewards and collaborations have rapidly gone international, and we should embrace that or fold. We do need to deal with some policies that don't support this directly, but we have to work in the spirit of finding out how to best support collaborative teams.

Bill Kramer: The influx of international efforts is changing but has always been the case in the US. How many who come here are going to stay and contribute? People who are able to come here compete first to come here, so the challenge is how to keep that experience here beyond just grad school? The competitiveness is good—we are highly competitive. In some ways we are using the wrong metrics to judge that competitiveness. Regarding sustained performance and real problem-solving, we are still the leading nation. If we don't change our approach, we will fall behind and people won't be able to use the productivity we do have. Sustained performance will continue to be the mantra—can we do work on a higher level? NSF recognized that long ago and has that mission philosophy. Everyone wants to be the biggest.

Q: John referred to a need to come up with metrics to measure science, could this group share best practices on how we measure?

John Towns: a list of publications says nothing. How do you take citation indices associated with efforts and get measures that way? Traditionally we throw up system specs, but they don't show what comes out of it. It would be a great conversation: what have you found to be useful metrics? I would love to hear what others have to say about metrics.
Moderator David Richardson welcomed the panel who will discuss the question of how to charge, considering that a large amount of all of our funding comes from federal government. The panel includes Carie Lee Kennedy from Vanderbilt’s Advanced Computing Center for Research and Education (ACCRE), where they were setup by faculty, for faculty—and have remained that way; Jim Bottom from Clemson with the CIO perspective; and John Goodhue, Executive Director of the Massachusetts Green High Performance Computing Center (MGHPCC), sharing how both public and private institutions and state can work together.

**Question for Jim:** as the CIO, to be a major player in research today requires access to lots of computational power, how do you weigh the investor needs with the institutional needs?

Jim: you have to have institutional priorities. Clemson had not had central HPC: everyone was on his or her own. I was brought in specifically to develop it. Over time, the 2008-2009 budget downturns occurred and there were threats of cutting back on HPC. Having a seat at the table representing HPC interest is important. 20-25% of funding is from the University and the overall budget has gone up every year even if the university budget went down. Recently we have had early-out programs for staff and channeled that money into reserves for support and software development groups. The CIO has a fair amount of discretion in their budget and is typically looking for efficiencies, but it is really just a matter with aligning with the university.

**Question for Jim:** did Clemson have a model in place as far as how much of the costs they wanted to recoup from the sponsor world?

Jim: charging scares people away. In an external review of a big project on the west coast, they kept seeing IT activities done by research groups and said that official IT groups cost too much. We had to update the business model, so we brought in Jim Bottom who invented the condo model. We try to make it simple for the researchers, and they have to feel like they are getting a good deal, so the university subsidized the GPUs for the faculty.

**Question for Jim:** how often do you engage the Vice President for Research (VPR), in their view of needs for computational resources?

Jim: the VPR is a supporter of HPC, but he doesn't have a good handle on the needs. We have a faculty committee like the Comp-Pol group at Illinois who help think that through, and it has more of a steering than advisory role.

**Question for John:** with 5 institutional partners putting money into a data center, how do you maintain equity and reasonable allocation of resources?
**Question for John:** with 5 institutional partners putting money into a data center, how do you maintain equity and reasonable allocation of resources?

John: there are 5 different institutional cultures. For example, UMASS is composed of five distinct campuses, and MIT is highly decentralized. Also, research programs at different universities come in different sizes. Harvard started in 1630, and since then we’ve had a long time to practice NOT working together at the institutional level. The MGHPCC represents an interesting shift.

First, we needed commitment from the top. The Board of the partnership originally had the five presidents. Now that the MGHPCC is more established, the Board is composed of VPRs and CIOs.

Second, we kept the business model simple, transparent, fair, and predictable. The MGHPCC is a 501.(c)3 whose members are the five universities, so the bosses are also the principal customers. Each institution pays for what it uses, and pays a proportional share of the cost of carrying capacity for expansion.

Third, we focused on operating principles, not a rule book. The operating agreement relies heavily on cooperation, with few provisions for penalties or sanctions – that has worked very well. There is a high level of engagement and the facility supports many different types of offering.

**Question for John:** there are expectations in the local community to impact the economy, how does that change the outlook on the management side?

John: this is the first time that Massachusetts State Government has invested in a research enterprise that included and involved a combination of public and private universities. The Governor led the way with a belief in the long term economic impact of research, but it was important to deliver tangible near-term benefits as well. By chance, the lowest-cost power source in Massachusetts is a hydroelectric facility located in a community that has been economically distressed for many years. This made it possible to combine a good business choice for the MGHPCC with a development project that had immediate positive impact on the surrounding community. After the facility went into operation, we have been able to exceed expectations with persistent but relatively modest effort – for example, making meeting facilities available to local organizations, volunteer engagement with the school system by people at the various universities, and joint applications for grant funded projects.

**Question for Carie:** you mentioned the center offering flexible HPC resources to a wide audience—how do you leverage the range of computing needs at a comprehensive campus?

Carie: it is actually very simple—it is a small-scale version. There is a huge amount of trust and collaboration between the researchers. If there are special projects and considerations, researchers find a way to make it happen. The goal is to meet everyone’s needs and mostly they are able to do that. One core is the minimum contribution and there are also free guest users who find out what their needs are. Some stay small and some get bigger. Every need is equally important. The largest group has over 400 cores.

**Question for Carie:** what about managing maximum users?
Carie: we have a heavy subsidy with a small requirement from the researcher. As need increases, their contribution increases. Some say, “This is all I have so give me what I can with that.”

**Same question for John: if a person has a fixed amount of grants and needs to upscale, how do you manage?**

John: it depends on the university, how charging is handled, etc. Systems that are more university-wide are better at handling this as it is easier to add incremental capacity to an existing system.

**Question for Carie: you have a hybrid model with both direct procurement and a fee-for-service option—what drives the strategy of choice for researchers?**

Carie: it depends on the size, quantity, and terms of need. Some groups are small enough that it doesn't make sense, because there is a minimal computing need. Sometimes researchers have grant requirements that can't buy capital funds. We meet their needs.

**Question for Carie: if a funding agency isn’t pleased that their equipment is on a rack not owned by them, what do you tell them?**

Carie: we explain the model and have had people from the funding agencies come in, tour the data center, we explain the model, and so far everyone has said ok. There is not a requirement at Vanderbilt that they must use the center. It is ok to use their own cluster.

John: there are two groups to convince—the auditors and people who have to run/sign off on the audit.

**Question: do you gravitate toward the most conservative institution?**

John: When a question comes up, we ask for consensus among experts from all five university compliance groups. Often there is one that has had directly relevant experience during a recent audit.

**Question: with HPC comes a need for large data files and storage—what are the ways you are meeting those needs?**

John: We have been careful to tackle the problems only when we are ready to tackle them. Storage—we are not ready to tackle yet. For the first six months the goal was just figuring out how to stay out of each other’s way and learning about common business interests. Today, vendor management, compliance, and incentives are all part of the conversation, and we are standing up two clusters that are jointly owned and operated by the five MGHPCC universities. From the faculty side, collaborating across university boundaries is easier now that the institutions have equipment in the same place. We have even seen a bit of comparison shopping by teams working together, which has encouraged consistency in the service offerings and cost recovery models. I suspect the next problem we’ll tackle collectively will be identity management, which may simplify access to shared resources.

On a related note, there is a group at BU looking at a new approach to cloud computing. Instead of a monolithic stack, could you build a cloud out of components from multiple vendors—but using the cloud business model? One possible first application might be a service that captures and stores large data sets for common use.
Question for Jim: have you utilized cloud storage at all while satisfying needs?

Jim: make storage available. Faculty members can purchase storage from us in terabyte chunks and get their own file system and mount their own system to move data in and out. It makes it as easy as possible to access their storage within the cluster environment—and their own desktop.

Question for John: how has big data impacted plans going forward?

John: it has affected planning one level down from where we tend to think collectively. After our first 6 months of operation, there were 4-6 PB scattered around data center. However, research groups who are doing things with big data haven't changed the way the center operates, and each of the five institutions accommodate storage needs in its own way. The two multi-university systems that I mentioned earlier are being applied to big-data problems in biology, earth sciences, and other disciplines, but again, they haven't affected the way the data center operates.

Jim: we get ping-ed by people in administration to help them improve business intelligence capabilities. It is a brand new resource and we should be looking for friendly users. It is new to us too, so we understand the reservations. Big data is relative and looking at students, big data is whatever you can't compute or interpret yet.

Question for Carie: what have you done to reduce outreach costs?

Carie: Vanderbilt funding does provide for outreach and training efforts: workshops for new users, intro classes on compiling, nodes, etc. Some may have large classes of 10-14 maximum capacity. If only one person signs up, they still hold the class. Staff will teach various subjects in the workshops, and we try to accommodate and answer online questions and emails. Commonly asked questions are put on the website FAQ to provide access to information. It is an on-going process.

Question for John, do you have a training coordinator on site or embedded in institutions?

John: For the most part, the MGHPCC is serving people who are already well-versed in how to use their systems and applications. All of the MGHPCC institutions have individuals and groups who provide coordinated training and support for their communities.

Question for Jim: in the value-service model, without going beyond contract requirements, are there utilization thresholds that would state that the closet machine is better than the cluster?

Jim: no, the systems stay pretty full, and we seem to keep upgrading enough to stay ahead of the curve. We haven't had complaints of waiting too long in the queue, so it seems to work the way we are running it. People buy on demand and pay roughly 50% of the cost. They have the CI integration group that Barr heads and Condo of Condos came out of that. We have hired an aggressive training and outreach program, and that person has helped paid for himself over and over through non-HPC grants, but very accomplished faculty members are professionalizing the program now. People who don't pay anything get to use the background on demand. We did hear to not do bench-marking before school opens to prevent interfering with classes.

Question for Carie: what if they want to build a cluster?
Carie: there are very few clusters on campus, so it makes it easier for folks to use our services. It is not worth using time to manage it if they don't need it. There are incentives to use the center’s service, but they like that it is optional.

Jim: we don’t force use at Clemson either. Eventually they will see it is a better deal.

John: Research groups at all five universities are generally free to take whatever approach works best for their situation. Options range from building out a dedicated cluster in new computer room space on campus to leveraging an existing system at the MGHPCC. When you offer something that is more convenient and easy to use and more cost effective, people tend to go that route. For example, building out new computer room space involves considerably more effort and lead time than leveraging an existing resource.

**Question regarding cost-competitiveness: is it hard to make this case to researchers because they evaluate the price differently?**

John: There are a several issues that can distort perceived cost. One is that infrastructure costs such as power and cooling are usually built into the overhead rate, and are sometimes perceived as “free” as a result. Another is the “Best Buy syndrome”, where people compare two very different kinds of service – for example, the cost per terabyte for a USB disk drive compared to a high performance, RAID-protected, fully backed up disk array. These distortions will always be a challenge, but are happening less often.

Jim: have your CFO desegregate the power bill and send it to the department head!

Dave: even when collecting a full overhead, you still lose $0.10 to $0.20 on the dollar.

Jim: if your institutional goals align, financially incentivized them to work with central IT. There is a trend toward efficiencies, and you can motivate them in other ways.

John: It is important to align incentives in a way that encourages people to choose solutions that make the most efficient use of power and other resources.

**Question for Carie: how do you maintain the competitive edge in terms of timely replacement of inefficient models?**

Carie: we used to be on a 3-year but are now on 5-year replacement model. Some jobs can run on older hardware, others need the newest hardware. The range of hardware fits the various jobs.

**Question for John: what do you do when you get to build in replacement costs?**

Note – my response below is to a different question. You may want to delete it or move it elsewhere.

John: With respect to measuring and managing overall costs, the MGHPCC has been the first opportunity in many cases to do systematic measurement of all of the costs associated with providing and supporting a computing service. It is therefore difficult to do backward-looking comparisons. For example, it is not easy to isolate the cost of a computer room that is embedded in an on-campus classroom building. Looking forward, we will be doing benchmarking against alternatives such as
Amazon or commercial data centers. The goal is to keep our costs below those benchmarks. Another important consideration is that we live in a business where the game changes every 18 months to 2 years and are dealing with institutions with planning horizons as long as 50 years. That means we need to think beyond the quarter-by-quarter concerns that can constrain commercial services.

Dave: most of our business models are predicated on a longer depreciation allowance because they haven't been updated. The minute you plug the machine in, it's like driving a car off the lot. Someone else will come along. It is difficult to ascertain how to view that—how to get people to view it along those lines.

**Question for John or Jim: how do you convince the people to invest in your process vs. find a better value in the marketplace?**

John: it is not either or, but the decision process is straightforward —if the commercial marketplace can provide something that is better, faster, and cheaper, then the faculty will migrate there. If you try to prevent them, you're wasting your time and money. Anyone who is operating a service that is not thinking that way is doomed.

Jim: if the commercial marketplace can help someone and serve their needs, most of our information is anecdotal. There are hidden costs. Our upgrade model is twice a year, so it seems to be staying ahead of the curve.

John: commercial services do upgrades too, and have to accommodate those costs in their pricing model.

James Cuff: It’s important to think clearly about the content of the service as well as the price. For example, the hands-on help that many university HPC services provide is rarely available with commercial services

**Question: how do you become the leader, socialize it, and develop the skill set to make everyone aware?**

John: The first thing you need is to be efficient at what you do. It is also unnecessary to know everything or be everything in order to lead. Better to learn about, encourage, and publicize what others are doing,

Virginia Tech, has come out before and challenged the administrator dealing with technology refresh, and why we haven't gotten different business models. We know the investments needed to keep the building maintained, but this has to be a priority not just security.

Dave: we paid for that at the time with our own money and asked to charge the DOE and give it away to everyone else—which you can’t do. The business model should never drive the science, but it has to be factored into the 5th not the 9th inning.

John Towns: regarding the business model driving the science, first it is a question about compliance. We have found a wide range across campuses with regard to their tolerance for risk, appropriate funds, and compliance. For many institutions, this is a new way of dealing—with a single source of funds. In some case the agency is matched by institutional funds. With NSF money, NHS, and institutional funds, there is a wide range of aversion to risk as to the allow ability of the business models. It makes doing
things and getting it done a challenge depending on the risk of aversion. If the campus is going to have to deal with an audit, they are driving to a zero risk. As a result, there is push-back on the ability for faculty to do research because they can't spend the money.

**Question for Carie: so how do we deal with that locally?**

Carie: regarding compliance at the university level, you have to find a balance between research and compliance and meeting both needs at the same time. For example, different types of services with different pricing to match needs. You can meet their needs with justification, so that if audited you are prepared for it.

**Question: how do we build a model that is reasonable and can be administered?**

Institutions are risk adverse, and you have to find the right people. If you have heard that other institutions have gone through an NSF audit, it makes you feel better because we operate under same rules.

**Follow-up question from John Towns: traditionally, a researcher buys a cluster and works through their local purchasing people. But now the Condo-style arrangements bring in the operator of the condo research and are making purchases even though they own the funds; if there is an issue of inappropriate use of funds, who is responsible? They've come to us. It is not our reward, but they've still come to us—where should the responsibility really lie?**

John: we have to recognize that condos are different and becoming more pervasive, so we are turning. We saw a similar transition with campus networks in the 90s, which were first deployed within departments and research groups, but eventually became a campus-wide service. We have to get to a place where computing cycles become that kind of resource. Both funding agencies and offices of sponsored programs are learning as condos condo-style arrangements evolve.

James Cuff: In my area at Harvard, we are already at a point where dollars for clusters are invested in condos as the first option. We are investing for sustainable delivery of computing resources in the same way that we invest to ensure that the lights always go on when someone turns on the switch.

**Question: is the shared services model the new model?**

John: The principal argument for shared services across multiple institutions is that scale, cost and utilization matter. Savings of 5% really do matter, and scale helps with that. Offering a service that is jointly operated by multiple institutions is not for everyone, but it can yield significant rewards. Whether it will work depends on both technical and human factors. For example, it is important that the user community be geographically close enough to ensure low network latency and affordable bandwidth to a centrally located facility. Equally important, especially at the outset, is good chemistry among the leaders of the participating institutions. The MGHPC would not have happened if the presidents of the five universities had not been able to get along, or if the VPs of Research and CIOs had not been willing to work together to follow through.

Dave: the PI role is the responsible party on fiduciary responsibility. Others are in loop trying to ensure consistency but ultimately the PI is responsible.
John Towns: it is a service they are purchasing and the service provider doesn’t get tied up on whether it was legal or not. We want to help facilitate but we know nothing about their award and its condition. We want to help but can’t be held responsible. You can’t put all of this back on the service provider, separate from the PI.