

Annual Report for Period:09/2007 - 08/2008**Submitted on:** 07/18/2008**Principal Investigator:** Livny, Miron .**Award ID:** 0621704**Organization:** U of Wisconsin Madison**Submitted By:**

Avery, Paul - Co-Principal Investigator

Title:

Sustaining and Extending the Open Science Grid: Science Innovation on a PetaScale Nationwide Facility

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Contribution to Project:

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Worked for more than 160 Hours: Yes

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Research Experience for Undergraduates

Organizational Partners

Boston University

Brookhaven National Laboratory

California Institute of Technology

Cornell University

Fermi National Accelerator Laboratory

Columbia University

Indiana University

Information Sciences Institute

Lawrence Berkeley National Laboratory

Purdue University

University of North Carolina

Stanford Linear Accelerator Center

University of California San Diego

University of Chicago

University of Florida

University of Illinois at Urbana-Champaign

University of Wisconsin-Madison

University of Wisconsin-Milwaukee

DOSAR

Other Collaborators or Contacts

The OSG relies on external project collaborations to develop the software to be included in the OSG Virtual Data Toolkit and deployed on the

shared common distributed infrastructure.

The external projects OSG has worked with over the past year are:

- Community Driven Improvement of Globus Software (CDIGS),
- SciDAC-2 Center for Enabling Distributed Petascale Science (CEDPS),
- the Condor Project,
- the dCache Collaboration,
- the Data Intensive Science University Network (DISUN),
- the Energy Sciences Network (ESnet),
- Internet2,
- LIGO Physics at the Information Frontier,
- Fermilab Gratia Accounting,
- the Storage Resource Management collaboration at LBNL,
- the U.S. Large Hadron Collider experiment Software and Computing Projects.

Activities and Findings

Research and Education Activities: (See PDF version submitted by PI at the end of the report)

OSG provides an infrastructure that supports a broad scope of scientific research activities, including the major physics collaborations, nanoscience, biological sciences, applied mathematics, engineering, computer science and, through the engagement program, other non-physics research disciplines. The distributed facility is quite heavily used, as described in the attached document showing usage charts.

OSG continued to provide a laboratory for research activities that deploy and extend advanced distributed computing technologies in the following areas:

- * Integration of the new LIGO Data Grid security infrastructure, based on Kerberos identity and Shibboleth/Grouper authorization, with the existing PKI authorization infrastructure, across the LIGO Data Grid (LDG) and OSG.
- * Support of inter-grid gateways which transport information, accounting, service availability information between OSG and European Grids supporting the LHC Experiments (EGEE/WLCG).
- * Research on the operation of a scalable heterogeneous cyber-infrastructure in order to improve its effectiveness and throughput. As part of this research we have developed a comprehensive 'availability' probe and reporting infrastructure to allow site and grid administrators to quantitatively measure and assess the robustness and availability of the resources and services.
- * Scalability and robustness enhancements to Condor technologies. For example, extensions to Condor to support Pilot job submissions are being developed, significantly increasing the job throughput possible on each Grid site.
- * Deployment and scaling in the production use of 'pilot-job' workload management system ũ ATLAS PANDA and CMS Glidein. These developments were crucial to the experiments meeting their analysis job throughput targets.
- * Scalability and robustness enhancements to Globus grid technologies. For example, comprehensive testing of the Globus Web-Service Gram which has resulted in significant coding changes to meet the scaling needs of OSG applications
- * Development of an at-scale test stand that provides hardening and regression testing for the many SRM V2.2 compliant releases of the dCache storage software required by the WLCG MOU.
- * Integration of BOINC-based applications (LIGO's Einstein@home) submitted through grid interfaces.
- * Further development of a hierarchy of matchmaking services, ReSS or Resource Selection Services, that collect information from more than 60 OSG sites and provide a VO based matchmaking service that can be tailored to particular application needs.
- * Investigations and testing of policy and scheduling algorithms to support 'opportunistic' use and backfill of resources that are not otherwise being used by their owners, using information services such as GLUE, matchmaking and workflow engines including Pegasus and Swift.

* Comprehensive job accounting across 60 OSG sites, publishing summaries for each VO and Site, and providing a per-job information finding utility for security forensic investigations.

The key components of OSG's education program are:

* Organization and participation in more than 6 grid schools and workshops, including invited workshops at the PASI meeting in Costa Rica and the first US eHealthGrid conference, and co-sponsorship of the International Grid Summer School in Hungary.

* Active participation in more than 5 'Campus Infrastructure Days (CI Days) events. CI Days is an outreach activity in collaboration with Educause, Internet2, TeraGrid and the MSI institutions. Each event brings together local faculty, educators and IT personnel to learn about their combined needs and to facilitate local planning and activities to meet the cyber-infrastructure needs of the communities.

* Invited participation in the TeraGrid Supercomputing 07 education workshop, participation in the HPC University sponsored by TeraGrid, and funding contributions from TeraGrid to OSG grid workshops.

* Support for student research projects from the University of Chicago, looking into usability issues.

Findings: (See PDF version submitted by PI at the end of the report)

* Scientists and researchers can successfully use a heterogeneous computing infrastructure with job throughputs of more than 15,000 CPU days per day, dynamically shared by up to ten different research groups, and with job-related data placement needs of the order of Terabytes.

* Federating the local identity/authorization attributes with the OSG authz infrastructure is possible. We know there are multiple local identity/authorization implementations and it is useful to have an exemplar of how to integrate with at least one.

* The effort and testing required for inter-grid bridges involves significant costs, both in the initial stages and in continuous testing and upgrading. We have not yet adequately automated the validation and regression tests.

* Availability and reliability testing and interpretation are very valuable, but not yet complete. It is a good way to stimulate responsible site administration.

* The scalability and robustness of the infrastructure is slowly improving, but has not yet reached the scales needed by the LHC when it reaches stable operations. The goals for the commissioning phase in FY09 have been met but, especially for data movement and storage, not met over the needed sustained period of months (to years).

* The job 'pull' architecture does indeed give better performance and management than the 'push' architecture.

* Automated site selection capabilities are in their infancy û especially when faced with the plethora of errors and faults that are encountered on a loosely coupled set of independent computing and storage resources used by a heterogeneous mix of applications with greatly varying I/O, CPU and data requirements.

* Analysis of accounting and monitoring information is a key need which requires dedicated and experienced effort.

* Transitioning students from the classroom to be users continues to be a challenge, especially given the limited effort OSG can dedicate to this activity.

* Many communities are facing the same challenges as OSG in educating new entrants to get over the threshold of understanding and benefiting from distributed computing.

Findings enabled by the Distributed Infrastructure:
Science Deliverables

Physical Sciences:

LIGO: LIGO has advanced its capabilities to deliver large workflows for the binary inspiral searches. These workflows, consisting of tens of thousands of individual jobs, are necessary to analyze LIGO dataset in the search for binary inspirals of compact stellar objects such as neutron stars and black holes. Working closely with the developers of the Pegasus Workflow Planner, LIGO scientist, post-docs and technical staff have

also been able to develop common abstract workflow generation tools which can be used to submit to either the LIGO Data Grid or the Open Science Grid. This effort continues to identified further technological advances needed in the areas of data storage and data management which will allow even greater opportunities for scientific deliverables associated with the binary inspiral analysis in the coming year.

In addition, LIGO identified the Einstein@Home application late last year as a good candidate application to migrate onto the Open Science Grid based on experiences with migration of Einstein@Home onto the German DGrid. This was a particularly appealing project as the Einstein@Home Project had prior experience with vetting scientific results from computational resources not under the management of the project. A scientific 'credit' based accounting system is provided by the Einstein@Home Project which allows accounting of meaningful scientific results collected from computational resources around the world. Working with the principal developers of the Einstein@Home application on the DGrid, and the OSG, LIGO was able to identify changes to the codes which would allow the same infrastructure to be used on both the DGrid and on the Open Science Grid. Credits began to accumulate from Einstein@Home jobs running on the Open Science Grid in January 2008. By June of 2008, Grid Computing Resources on the DGrid and the Open Science Grid were the largest single contributor of credits (scientific results) for this important periodic source analysis with approximately 15% of the credits from grid resources being delivered by the OSG. Currently, a primary limitation to the number of Einstein@Home jobs running on the OSG has been the cumulative number of OSG sites supporting the Globus WS-Gram interface. LIGO has worked with several enthusiastic OSG site administrators to increase this count, while at the same time worked with OSG Executive Team to identify a path for more standardization of WS-Gram on the OSG as a whole. In addition, LIGO has been working with the developers of Einstein@Home to understand the development and compatibility issues which would allow more general grid interfaces to be used, opening up a new class of sites available to contribute to the scientific credits in the coming year.

LHC: OSG has delivered the necessary throughput and reliability to meet the needs of the US ATLAS and CMS experiments for their data challenges and simulation production in late 2006, early 2007. Interoperability with and contributions to the WorldWide LHC Computing Grid have been a success. Data distribution at rates of more than 1.2 GBytes/sec from the CERN 'Tier-0' to the Brookhaven and Fermilab Tier-1s and fourteen University Tier-2s was achieved.

CMS: US-CMS relies on Open Science Grid for critical computing infrastructure, operations, and security services. These contributions have allowed US-CMS to focus experiment resources on being prepared for analysis and data processing, by saving effort in areas provided by OSG. OSG provides a common set of computing infrastructure on top of which CMS, with development effort from the US, has been able to build a reliable processing and analysis framework that runs on the Tier-1 facility at Fermilab, the project supported Tier-2 university computing centers, and opportunistic Tier-3 centers at universities. There are currently 13 unfunded Tier-3 centers registered with the CMS datagrid in the US, which have begun to provide additional simulation and analysis resources to the US community. In addition to common interfaces, OSG has provided the packaging, configuration, and support of the storage services. Since the beginning of OSG the operations of storage at the Tier-2 centers have improved steadily in reliability and performance. OSG is playing a crucial role here for CMS in that it operates a clearinghouse and point of contact between the sites that deploy and operate this technology and the developers. In addition, OSG fills in gaps left open by the developers in areas of integration, testing, and tools to ease operations. The stability of the computing infrastructure has not only benefitted CMS. CMS' use of resources has been very much cyclical so far, thus allowing for significant use of the resources by other scientific communities. OSG is an important partner in Education and Outreach, and in maximizing the impact of the investment in computing resources for CMS and other scientific communities.

In addition to computing infrastructure OSG plays an important role in US-CMS operations and security. OSG has been crucial to ensure US interests are addressed in the WLCG. The US is a large fraction of the collaboration both in terms of participants and capacity, but a small fraction of the sites that make-up WLCG. OSG is able to provide a common infrastructure for operations including support tickets, accounting, availability monitoring, interoperability and documentation. As CMS goes from development into stable operations, the need for sustainable security models has become more important. The common security infrastructure and personnel provided by OSG is a significant service to the experiment.

ATLAS: US ATLAS depends crucially on the OSG infrastructure. All our facilities have the OSG software stack as the base upon which we install the ATLAS software system.

Over the past 3 years ATLAS developed in the US the PanDA distributed production and analysis system based on just-in-time (pilot based) workflow management, now in use ATLAS-wide, and since fall 2006 the PanDA effort has been a part of the OSG's workload management effort as well. Both ATLAS and OSG have benefited from this activity. The OSG WMS effort has been the principal driver for improving the security of the PanDA system, in particular its pilot job system, bringing it into compliance with security policies within the OSG and WLCG. OSG WMS effort has also deepened the integration of PanDA with the Condor job management system, which lies at the foundation of PanDA's pilot submission infrastructure. For the OSG, PanDA has been deployed and offered as a tool and service for general OSG use. In the last year a team of biologists used PanDA and OSG facilities for the protein folding simulation studies (using the CHARMM simulation code) underpinning a research paper that has been submitted for publication. Their use of PanDA continues, and the PanDA/OSG team is also

soliciting new OSG user communities. In the coming year we plan to increase the scope of PanDA's offerings to the OSG community, drawing on its proven capabilities serving all ATLAS distributed production worldwide. Enhancements will include mechanisms by which VOs and the OSG itself can monitor and control resource usage; record, track and address failure modes at the application and facility levels; and gather and publish VO/site specific attributes that guide workload brokerage for VO applications. Reciprocally the OSG WMS effort will continue to be the principal source for PanDA security enhancements, further integration with middleware and particularly Condor, and scalability/stress testing of current components and new middleware integration.

(US) ATLAS has sought to minimize grid middleware dependencies in general for well known reasons. Where we still have middleware dependencies, we often still have problems. The OSG has been helpful in mitigating or minimizing the problems. Examples:

- * GRAM dependency in CondorG submission of pilots. Not sufficiently scalable to support analysis in Panda. OSG program includes a 'pilot factory' effort to work around this by doing site-local pilot submission without every pilot seeing the gatekeeper and GRAM.
- * glexec. This has been validated and deployed for production by FNAL/CMS. It will be added to the OSG software stack so we can pick it up easily for integration ourselves via the OSG stack.
- * OSG-standard site configuration. Provides a 'known' environment on OSG WNs for more homogeneity in execution environment. This lessens the application-level work of establishing homogeneity.
- * Tools for resource discovery. The tools we have are provided by OSG, and while they need improvement, we'd be in much worse shape without them; it would be very difficult to gather the information on resource availability, health, and access rights that is required to run a distributed system on all the resources available.

Another area in OSG US ATLAS is taking advantage of its storage management. US ATLAS Tier-2 sites running dCache are greatly benefiting from the support provided by the OSG Storage Group in terms of seamless code integration and help with operational issues. At BNL (ATLAS and STAR), and at some US ATLAS Tier-2 sites we have Xrootd deployed. The integration and support effort that has started as part of the Storage Group's program is much appreciated. Also, though OSG may not have much impact on SRM 2.2 development and deployment timeline, and quality, we are benefiting from having OSG help to integrate this mandatory software component with the rest of the middleware stack.

We also greatly benefit from the new OSG-wide accounting services, which are now part of OSG releases, as well as the information services that is providing OSG site information to the application layer.

We benefit and rely on the VDT and OSG packaging, installation, and configuration processes that lead to a well-documented and easily deployable OSG software stack, and the OSG integration and validation processes that precede incorporation of new services into the VDT.

The RSV infrastructure is used to probe the status of compute and storage element resources and provide a local web display of this current and historical status that is proving useful to US ATLAS site administrators. In addition, the results of these probes are collected centrally by the GOC and forwarded to the WLCG Site Availability Monitoring system to provide a top-level system view of site performance that can be reviewed by top-level US ATLAS, WLCG and OSG management to assess reliability.

US ATLAS relies on the OSG Gratia accounting infrastructure to collect usage statistics (normalized CPU-hours) consumed on a VO-basis at each of its computing facilities. These also are summarized monthly and reported by WLCG for review of compliance with MOU agreements between the WLCG and the US ATLAS Research Program.

There are other components of the operational infrastructure that are becoming routinely used by US ATLAS and ATLAS Operations teams - namely the trouble ticketing system (which distributes tickets received by the OSG from within the OSG and the EGEE service to the US ATLAS RT tracking system) and the OSG OIM system which is now becoming used to communicate downtimes of US ATLAS resources on the OSG to WLCG and International ATLAS.

US ATLAS benefits from the VDT packaging efforts to include middleware components from gLite that ATLAS has elected to use but were not part of the OSG environment. These include the LCG-Utils package, needed by ATLAS, and client libraries and API bindings for the LFC file catalog service which US ATLAS will migrate to this year.

We also benefit from and rely on the infrastructure maintenance aspects of the OSG such as the GOC and others that keep the virtual US ATLAS computing facility and the OSG facility as a whole operational. We have PanDA running on ALL OSG sites (not just ATLAS) and are poised to take advantage of opportunistic resources on the OSG to do further Monte Carlo simulation and distributed analysis for ATLAS.

D0 at Tevatron: During the extremely successful reprocessing of over 500 million data events in 2007 on OSG, D0 and OSG co-developed the infrastructure necessary to efficiently handle both the D0 reconstruction algorithm and large data transfers at a number of OSG sites. Since this infrastructure was in place and D0 developed a working relationship with OSG, it was natural to continue to exploit the OSG resources in a number of different areas.

Monte Carlo events are now routinely run on a number of OSG sites. Nearly 4 million of the 12 million Monte Carlo events generated each week are on OSG sites. The D0 experiment relies heavily on Monte Carlo for studying systematics, efficiencies, etc. and very few publications would be possible without large Monte Carlo samples. Having OSG provide over 30% of the Monte Carlo events is a tremendous resource and allows D0 to publish results much faster.

In addition to Monte Carlo generation, D0 also uses the OSG infrastructure for its primary processing of data. Previously all D0 data was processed on a private farm. However, only one person understood the farm well and it was becoming obsolete. D0 decided to run its primary processing on OSG which provides for a larger core group of experts, allows D0 to share its resources with other experiments and if necessary use other's resources in times of need. Currently the primary processing of data is run only on D0 resources (not opportunistically). This is possible since D0 currently has the necessary computing power to process the incoming data in a timely manner. However, in the future as D0 nears the end of its run, it is foreseen that D0 will need to begin to use opportunistic computing for its processing of data. Since papers will continue to be published after D0 stops collecting data, having the ability to use OSG is critical for continued success in publishing papers in the long term.

CDF at Tevatron: The GRID and OSG are critical components of CDF's overall computing strategy and are essential for the experiment to continue to produce high quality physics results in a timely fashion with ever increasing data sets. Since 2005, CDF has moved nearly 100% of its Monte Carlo production to GRID sites around the world. With these sites, CDF typically produces in excess of 500 Million simulated events/year. These simulations of physics processes are crucial to properly estimating our systematic uncertainties. These Monte Carlo data sets also provide simulated signal samples for which physicists can tune their analysis selection criteria. CDF does not use the GRID to reconstruct its 'raw' data. The reconstruction software is so efficient that local resources can keep up with the data being collected.

CDF publishes over 40 refereed journal publications/year and typically ~250 conference presentations each year on the wide variety of physics of physics where it tests the standard model from every available angle. This kind of success would not be possible without the GRID computing resources and the OSG tool kit with which to access it. The limiting factor in our producing results is people, not computing.

Nuclear physics: The STAR experiment has continued to use the OSG data movement capabilities between LBNL, BNL and new sites on the OSG at Wayne State, Sao Paulo in Brazil, and in tests at the University of Illinois at Chicago. STAR is converting its simulation production to run on OSG, has worked with the Troubleshooting team to solve problems in efficiency, and through solving problems of robustness and configuration with the Fermilab FermiGrid site has moved its simulation into production on the OSG infrastructure.

Astrophysics: The Sloan Digital Sky survey has continued to use the OSG infrastructure for analysis as needed. The Dark Energy Survey simulation activities are ramping up. Both experiments have been able to achieve their deliverables this part year û issues of availability and robustness are being addressed.

Multi-Disciplinary Sciences: The Engagement team has worked directly with researchers in the areas of: biochemistry (Xu), molecular replacement (PRAGMA), molecular simulation (Schultz), genetics (Wilhelmsen), information retrieval (Blake), economics (clemson, need name), mathematical finance (Buttimer), computer science (Feng), industrial engineering (Kurz), and weather modeling (Etherton). The computational biology team led by Jinbo Xu of the Toyota Technological Institute at Chicago now uses the OSG for production simulations (see below). The following non-physics VOs are registered with OSG and are at various stages of contributing to and making use of the distributed facility: CompBioGrid: Virtual Cell biology group from the University of Connecticut; GADU genome analysis database update from Argonne National Laboratory; GLOW multi-disciplinary science from the University of Wisconsin; GRASE: multi-disciplinary science from the University of Buffalo; GROW geographical information systems from University of Iowa; Nanohub nanotechnology (see Engagement report below), SBGrid, structural biology at Harvard University.

Computer Science Research: A collaboration between OSG extensions program, the Condor project, US ATLAS and US CMS is using the OSG to test new workload and job management scenarios which provide 'just-in-time' scheduling across the OSG sites using 'glide-in' methods to schedule a pilot job locally at a site which then requests user jobs for execution as and when resources are available. This includes use of the 'GLexec' component, which the pilot jobs use to provide the site with the identity of the end user of a scheduled executable.

Findings of the Distributed Infrastructure: The OSG Facility

OSG Facility: The facility has provided operational, security, troubleshooting, software, integration, and engagement capabilities and support. In the second year of the project, the facility has added focus to the following areas: 1) improvement to storage management services, both middleware software in the VDT and deployed services on the fabric include new releases of dCache and SRM; 2) improvement to the process for non-disruptive upgrades of middleware components; 3) increasing interoperability with WLCG; and 4) testing and scalability improvements.

The usage of the facility continues to grow; the usage varies depending on the needs of the stakeholders and during stable normal operations is providing over 300,000 CPU wallclock hours a day with peaks occasionally exceeding 400,000 CPU wallclock hours a day with approximately 25-35% of this being opportunistic resource sharing. The success rate is variable and hard to measure and depends as much on the user end-to-end success and failure measurements as on those at the level of the infrastructure; currently the infrastructure reports success rates over 90%.

Middleware: The OSG Software stack has gone through evolutionary but significant changes that have resulted in new functionality for OSG users, as well as improvements in stability and quality of information. These changes were embodied in two major software releases, OSG 0.8 (December 2007) and OSG 1.0 (June 2008). These upgrades have greatly improved the quality of information available to users and management in three ways. First, in OSG 0.8 we introduced Resource and Service Validation (RSV) software, which allows sites to test various aspects of their functionality and know where problems are. The quality of this testing was improved in OSG 1.0, and the results are shared with the WLCG's GridView for reporting site availability. Second, we have updated the Gratia accounting software, which reports on the usage of sites (both jobs and storage). This information is used both within OSG and to report to WLCG, and new versions of Gratia have significantly improved the quality of the accounting information. Third, the Generic Information Provider (GIP) was significantly improved in OSG 1.0, and provides real-time information about sites to enable decisions about where jobs might be run, both by the OSG Resource Selection Service (ReSS) and the WLCG Workload Management System. The OSG Software stack has improved supports for WLCG users by providing new needed software. This includes data access tools on compute nodes (such as lcg-utils, which was added in OSG 1.0 and improved versions of SRM client tools), and improved versions of dCache for storage management.

The OSG software stack requires regular maintenance and improvements and we have added support for several new platforms (RedHat Enterprise Linux 5, Debian 4, Mac OS X) that our stakeholders need, while dropping support for older platforms that are no longer used (such as Fedora Core 4). We have also resolved or fixed dozens of software defects and the software packages have been upgraded to ensure users have a stable environment. For example, the OSG 1.0 release had about 25 software components updated to new versions (compared to OSG 0.8), each of which required integration and testing effort. Some software was added or changed in order to improve OSG's infrastructure. For example, we added a mechanism to allow sites to easily update the Certificate Authority list, which allows them to be able to authenticate new users. In the past, slow updates have prevented valid users from accessing sites. We also changed our software to depend on the operating system's version of OpenSSL instead of a specific version shipped with Globus and thus enabled greater security by putting the responsibility for updating this critical piece of security software into the hands of operating system vendors who are well positioned for doing this in a timely and secure fashion.

The OSG software has two major ongoing initiatives. First, we are improving the support for WLCG client data management software, a critical item for WLCG users. We are also considering revising the mechanism by which we package software, to allow us to more easily distribute and update software to our users.

Operations: OSG Operations provides a central point for operational support. The Grid Operation Center (GOC) performs real time monitoring of OSG resources, supports users, developers and system administrators, maintains critical information services, provides incident response, and acts as a communication hub. Goals of the OSG Operations group are the preservation and strengthening the autonomy of OSG resources, building operational relationships with peering grids, providing reliable grid infrastructure services, ensuring timely action and tracking of operational issues, and responding quickly and accurately to security incidents. In year2, the GOC was able to ensure the continued operation of the OSG facility, provide robust monitoring, registration and documentation services to the community, and improve the services for publishing information to the user organizations and sites.

The GOC has recently completed implementation of the OSG Information Management (OIM) database which provides the definitive source for listing OSG entities at the person, resource, support agency, or virtual organization level; this system was upgraded to include administrative and scheduled maintenance information for each resource to enable RSV/SAM reporting to the WLCG. Work continues on validating the provisioned information and adding functionality. Another major deliverable was the Resource and Service Validation (RSV) system upgrade which has added storage monitoring, reporting to WLCG, and several improvements for administrator maintenance. The RSV system enables WLCG reporting of availability statistics of ATLAS and CMS Tier 2 resources. These systems are operational, but the final step in this process, planned for July 2008, is accuracy validation and approval of this data by ATLAS and CMS to complete the reporting to the WLCG Management Board.

The GOC is actively planning for the LCH turn on. We anticipate that this will place additional strains on the current systems and policies based on an increased user base and load. Thus the GOC is defining and clarifying policy for ticket response, expectations for participant interactions, and acceptable timescales for tickets opened at the GOC.

Integration and Site Coordination: The mission of OSG integration is to improve the quality of grid software releases deployed on the OSG and enable greater success by the sites in achieving effective production.

In the last year, the Integration effort delivered high quality software packages to our stakeholder resulting in smooth implementation of the OSG 0.8.0 and OSG 1.0 releases; several process innovations were key to these results. During the release transition of OSG 0.6 to 0.8, and from OSG 0.8 to OSG 1.0, several iterations of the Validation Test Bed (VTB) were made using a 3-site test bed which permitted quick testing of pre-release VDT updates, functional tests, and install and configuration scripts. The ITB was deployed on 12 sites providing compute elements and four sites providing storage elements (dCache and BestMan packages implementing SRM v1.1 and v2.2 protocols); 36 validation processes were defined across these compute and storage resources in readiness for the production release. Pre-deployment validation of applications from 12 VOs were coordinated with the OSG Users group. Other accomplishments include both dCache and SRM-Bestman storage element testing on the ITB; delivery of a new site configuration tool; delivery of a facility-wide logfile collection infrastructure for troubleshooting; a program of client/server tests for WS-Gram with functional and scalability measurements for typical site configurations.

The OSG Release Documentation was significantly upgraded; this collection of wiki-based documents capture processes that enable install, configure, validation methods used throughout the integration and deployment processes. These documents were updated and received review input from all corners of the OSG community (33 members participated for the OSG 1.0 release) resulting in a higher quality output.

The community of resource providers comprising the OSG Facility is diverse in terms of the scale of computing resources in operation, research mission, organizational affiliation, and technical expertise, leading to a wide range of operational performance. A Sites Coordination activity was launched in July 2007 to provide a forum and organization structure to establish common metrics for good site performance, to share technical expertise and best practices for grid and fabric services as relevant, and to address feedback from the OSG Users Group. Two face-to-face meetings have been held, and the group meets by phone monthly.

Troubleshooting: The troubleshooting team continues to be effective in developing solutions to high-impact end-to-end problems encountered by the users and VOs. The Troubleshooting team works with OSG VO stakeholders and other Facility teams on quickly resolving each identified troubleshooting problem arising in both production and testing environments. Another major contribution was to help OSG sites make transitions from Release 0.6.0 to Release 0.8.0. In addition, a Troubleshooting FAQ was established to help OSG users and VOs quickly resolve their typical problems.

Engagement: A major priority of Open Science Grid is helping new user communities benefit from the infrastructure we are putting in place by working closely with these communities over periods of several months. The Engagement activity brings the power of the OSG infrastructure to scientists and educators beyond high energy physics and uses the experiences gained from working with new communities to drive requirements for the natural evolution of OSG. To meet these goals, engagement helps in: providing an understanding of how to use the distributed infrastructure; adapting applications to run effectively on OSG sites; engaging the deployment of community owned distributed infrastructures; working with the OSG Facility to ensure the needs of the new community are met; providing common tools and services in support of the engagement communities; and working directly with and in support of the new end users with the goal to have them transition to be full contributing members of the OSG.

During this program year, the Engagement team has successfully brought three lead researchers and their teams into full production use of the Open Science Grid (Xu, Blake, Wilhelmsen). These users represent, respectively, the science domains of Biochemistry, Information and Library Science, and Genetics. A Research Highlight has been published for one of these groups, and there is a commitment from the other two for Fall of 2008; and OSG was cited by the winner of the SC07 Storage Challenge as a result of Engagement efforts. There are roughly ten emerging users we are engaged with at various stages that we are working to convert into production users.

Additional activities of the Engagement team during the reporting period include: hosting the 2007 OSG annual meeting; convening a computational Biology workshop at the 2007 OSG annual meeting; representing OSG at CI-Days events; participating in the Campus Champions program in partnership with TeraGrid and CI-Days; contributing the match making technology used to assist new users as an open source project on SourceForge; assisting PRAGMA with OSG usage; investigating OSG/EGEE interoperability via the WISDOM application.

In April 2008, the Engagement team was awarded a grant from the NSF CI-TEAM proposal to continue these efforts for an additional three years. Current initiatives include scaling up our efforts to more effectively manage the Engagement process, working more closely with the OSG EOT and Users group efforts, communicating our activities to the broader OSG community, actively recruiting a more diverse set of OSG users, and helping new users implement systems that leverage OSG.

Campus Grids: The Campus Grids team's goal is to include most US universities in the national infrastructures. By helping universities understand the value of campus grids and resource sharing through the OSG national framework, this initiative aims at democratizing cyberinfrastructures by providing all resources to users and doing so in a collaborative manner.

In the last year this team has enabled several campuses to start the process of joining the OSG. Following the NYSGrid CI Days in December 2007, Rochester Institute of Technology (RIT) has deployed a condor based campus grid of several thousand nodes. The SBgrid project (<http://www.sbgrid.org>) from Harvard has also become very active in OSG and deployed two new resources; a team of OSG experts from Clemson, RENCi and Wisconsin engaged with Harvard to help finish the configuration of these two sites. Clemson and RENCi staff went to Duke University and helped bring up a new ATLAS Tier-3 site. The New Jersey Higher Education Network (<http://www.njedge.net/>) contacted us after they concluded that OSG had the framework to help them build their regional cyberinfrastructure; a plan has been setup to enable their users on OSG and add a new resource before the end of summer 2008.

Security: During the last program year this team undertook a multi-faceted approach that successfully met the primary goal of maintaining operational security of OSG. The Security Test & Evaluation (ST&E) controls, which were defined in the OSG Security Plan, have been implemented and completed; subsequently, we reviewed our controls against the NIST guidelines and referred to applicable NIST guidelines. We responded to 4 security incidents (average of 1.3 days until a security advisory released to sites) and addressed 9 software vulnerabilities (the responses were completed in 8 days at maximum and fixes by VDT team were developed in 17 days on average). None of the vulnerabilities and incidents so far caused a disruption of OSG operations. As part of our ST&E, we revised and improved our Incident Response Procedure based on our findings from the incidents/vulnerabilities and we generated a roadmap plan for OSG's security needs.

We have continued our active participation into the Joint Security Policy Group (JSPG) mandated by the WLCG. In addition to the policies prepared by JSPG, we worked on the Privacy Policy, OSG Registration and Termination Policy, and VO-specific policies. And, we informed our VOs about the policies that they should be preparing for their own use and prepared policy templates for helping them.

We identified the key infrastructural needs to maintain operational security and generated a requirements document, jointly with EGEE, for tools needed for security management. DOEGrids workflow for issuing user certificates has been updated based on user inputs. As a follow up action to a recently discovered security vulnerability, we have asked the International Grid Trust Federation (IGTF) to form an incident response team and we participate in this team on a voluntary basis.

Findings of the Distributed Infrastructure: Extending Science Applications

In addition to operating a facility, the OSG includes a program of work that extends the support of Science Applications both in terms of the complexity as well as the scale of the applications that can be effectively run on the infrastructure. We solicit input from the scientific user community both as it concerns operational experience with the deployed infrastructure, as well as extensions to the functionality of that infrastructure. We identify limitations, and address those with our stakeholders in the science community. In the last year of work, the high level focus has been threefold: 1) improve the usability and scalability, as well as our understanding thereof; 2) establish and operate a workload management system for OSG operated VOs; and 3) establish the capability to use storage in an opportunistic fashion at sites on OSG.

Scalability, Reliability, and Usability: As the scale of the hardware that is accessible via the OSG increases, we need to continuously guarantee that the performance of the middleware is adequate to meet the demands. There were three major goals in this area for the last year and they were met via a close collaboration between developers, user communities, and OSG.

* At the job submission client level, the goal is 10,000 jobs running simultaneously and 100,000 jobs run per day from a single client installation, and achieving in excess of 95% success rate while doing so. The job submission client goals were met in collaboration with CMS and DISUN, using glideinWMS. This was done in a controlled environment, submitting jobs only to a subset of well managed sites. In the future, we will focus on making this level of successful operations possible for a larger set of applications, and across a larger set of sites in a less controlled environment.

* At the storage scheduling level, the present goal is to have 1Hz file handling rates. For Gbyte file sizes this would translate into close to 10Gbps data transfer capacity. The SRM scalability was achieved in collaboration with the dCache developers, and demonstrated with transfers between SRM v2.2 test stands operated by OSG and DISUN.

* At the functionality level, the present goal is to roll out the capability of opportunistic space use. The roll-out of opportunistic storage was exercised on the OSG ITB preceding OSG v1.0. This still needs to be adopted more widely on the OSG production infrastructure to be useful and that is planned for year 3.

In addition, we are working on WS-GRAM scalability and reliability in collaboration with LIGO, DISUN, CDIGS/Globus, and OSG.

In the area of usability, an 'operations toolkit' for dCache was started. The intent was to provide a 'clearing house' of operations tools that have been developed at experienced dCache installations, and derive from that experience a set of tools for all dCache installations supported by OSG. We expect this to significantly decrease the cost of operations, and lower the threshold of entry. Site administrators from both the US and Europe have uploaded tools, and a first release was derived from that. This release has been downloaded by a number of sites, and is in regular use across the US, as well as some European sites.

Finally, work has started on putting together a set of procedures that would allow us to automate scalability and robustness tests of a Compute Element. The intent is to be able to quickly 'certify' the performance characteristics of new middleware, a new site, or deployment on new hardware. Once we have such procedures, we can then offer this as a service to our resource providers so that they can assess the performance of their deployed or soon to be deployed infrastructure.

Workload Management System: The primary goal of the OSG Workload Management System (WMS) effort is to build, integrate, test and support operation of a flexible set of software tools and services for efficient and secure distribution of workload among OSG sites. There are currently two suites of software utilized for that purpose within OSG: Panda and glideinWMS, both drawing heavily on Condor software.

In the area of WMS development and support, the Panda WMS system continued as a supported WMS service for OSG with reports of good results from the user community. In addition to being the main computing platform of ATLAS, it was used by the CHARMM biology team. A working prototype was created of the Panda Pilot Factory, a utility designed to enhance scalability of the pilot job framework utilized in Panda. And several updated versions of glideinWMS were released to address issues related to Condor version compatibility, ease of installation and monitoring.

In the area of Security enhancements, the Panda Pilot job software has been updated with the capability to change the effective user ID from the identity of the Pilot Job submitter to one of the end user, based on glxexec privileged executable. Successful testing has been performed on properly configured OSG sites. In addition, similar functionality was built into the glideinWMS system and tested. The OSG Privilege group (Fermilab) in conjunction with DOEGrids and BNL, have identified a need for an automated system to manage the request and renewal of host grid certificates. In order to serve this need, a package (Certify) has been developed, that uses the DOEGrids Grid Administrator interface to programmatically handle certificate transactions, and has the ability to track grid cert status across all site hosts.

This program of work is important for the science community and OSG for several reasons. First, having a reliable WMS is a crucial requirement for a science project involving large scale distributed computing which processes vast amounts of data. A few of the OSG key stakeholders, in particular LHC experiments ATLAS and CMS, fall squarely in that category, and the Workload Management Systems developed and maintained by OSG serve as a key enabling factor for these communities. Second, drawing new entrants to OSG will provide benefit of access to opportunistic resources to organizations that otherwise wouldn't be able to achieve their research goals. One example of such a research groups is the CHARMM team of biologists, who, thanks to simulations run on the Panda system, have successfully produced results to be used in an upcoming publication. As more improvements are made to the system, Panda will be in a position to serve a wider spectrum of science disciplines. And finally, recent security enhancements will ensure compliance with OSG security policies and guarantee alignment of OSG WMS software with policies of member sites of ATLAS and CMS collaborations, thus allowing for a wider deployment and use of their software.

Storage Extensions: The Storage Extensions area contributes to the enhancement of software used in Storage Elements on the Open Science Grid. This includes additional features needed by users and sites, as well as improvements to the robustness and ease-of-use of middleware components. During this last year we focused on robustness and access.

Robustness is an important aspect of the grid Facility, both in terms of computational throughput and attraction of new communities to the OSG. Robustness includes the features of software quality, ease-of-use (both in installation and operation), interoperability, and monitoring. We improved robustness by: 1) negotiating interoperability conventions for Glue Schema 1.3 Storage entries; 2) creating Gratia probes for dCache Storage Elements; 3) collecting tools from OSG sites and providing the OSG Storage Operations Toolkit. In addition, we contributed Storage Element inputs to the XACML Interoperability plan.

Access to the grid by VOs is necessary for its utilization. Here the issues are not only literal authorization in terms of a site's policy, but availability of the knowledge needed to make use of OSG capabilities. Our work with Role Based Access Control and Space Reservation supported enabling technologies in this area, and direct work with sites and VOs is leading to increased use of Storage Elements in OSG, in ways that lead to greater scientific production. In area of Access, we: 1) supported testing of Space Reservation with the Fermigrid, BNL, UChicago, UCSD and LBNL sites; 2) supported testing of opportunistic storage with the ATLAS, CDF, CIGI, SBGrid, and SDSS VOs; 3)

worked with ATLAS on Bestman /xrootd and Bestman RBAC/GUMS support; 4) wrote and supported role-based authorization in dCache and Bestman; and 5) updated Generic Information Provider scripts for Glue Schema 1.3.

Users Group: A strong underlying objective within OSG is to engage, facilitate, enable, support, and sustain Science communities to produce Science using the OSG. The Users Group serves as liaison between the Science communities (VOs) and the rest of OSG including Middleware, Operations, Storage, Security, Engagement, Troubleshooting, and Sites coordination. Thus the OSG Users Group collaborates to address requirements, feedback, issues and roadmaps of our Science community. Some of the major work items in the last year were:

- * The Science communities were canvassed for inputs and their requirements were compiled for OSG Release 1.0, with 14 VOs outlining needs and expectations.

- * The VO Science application validation of sites on Integration Testbed (ITB) was completed for OSG 0.6 and OSG 0.8, and most recently, for OSG 1.0. In partnership with OSG Integration Group, a rigorous OSG process has been designed and is regularly executed with each software release to assure high quality. Each participating Science stakeholder exercises a stake in vetting, suggesting changes, and signaling an official approval toward readiness of an official OSG release. In the recent ITB validation, 12 Science stakeholders (i.e., VOs) participated, 7 VOs ran real Science applications, 6 VOs participated in storage validation, of which, 4 VOs conducted introductory validation of opportunistic storage. In terms of process execution, this was a coalition of 36+ experts, 20+ from VO communities. After rigorous validation and feedback, official 'green flags' toward OSG 1.0 were given by ATLAS, CDF, CIGI, CMS, DOSAR, Dzero, Engage VO, Fermilab VO, LIGO, nanoHUB, SBBGrid, and SDSS/DES.

- * VO usage feedback and direct dialog was completed in 2007, with more than 20 VOs participating. The annual OSG Users meeting was organized at BNL in June of 2008, with emphasis on VO security. In addition, weekly teleconferences are conducted on a regular basis.

The OSG Users group continues to provide strong interfaces between the Science communities and all facets of the OSG to assure that the needs of the science communities are understood and translated into work activities in OSG to address the needs of the stakeholders.

Training and Development:

Training and outreach to campus organizations, and the development of the next generation of scientist, together with targeted engagement activities, is a core part of the OSG program. The OSG Education and Training program brings domain scientists and computer scientists together to provide a rich training ground for the engagement of students, faculty and researchers in learning the OSG infrastructure, applying it to their discipline, and contributing to its development.

From August 2007 through July 2008 the OSG has sponsored and conducted numerous training workshops for students and faculty and participated in additional invited workshops. This has enabled grid computing training and education for over 130 students; of which about 30% were from under-represented groups and about 20% women.

Four major OSG sponsored 'Grid School' training events (3 full days each) were conducted in the past 12 months: 1) Great Plains Grid School, August 2007, University of Nebraska at Lincoln; 2) Florida International University Grid School, January 2008; 3) Tuskegee University Grid School, Feb 2008; and 4) Georgetown Grid School, April 2008. To further OSG outreach goals, the FIU and Tuskegee Grid Schools brought leading grid experts and scientific colleagues to two important minority serving institutions, while the Nebraska Grid School was hosted at an NSF EPSCoR state university. Following each of these workshops, feedback is gathered, tabulated and studied, and follow-on research and engagement assistance opportunities are provided with access to the hands-on curricula and to OSG EOT staff. In addition to these major training events, OSG staff conducted several smaller training and outreach workshops:

- * Two workshops in the education track of the Supercomputing 2007 conference, Reno, NV Nov 2007;

- * Tutorial at the OSG All Hands Meeting March 6, 2008 at UNC/RENCI.

- * 1-day Grid workshop for the NSF-sponsored Pan-American Advanced Studies Institute (PASI): Cyberinfrastructure for International, Collaborative, Biodiversity and Ecological Informatics, Costa Rica, June 2008

- * Invited EOT talk at Minority Serving Institutions' Research Partnership (MSIRP) Conference, May 13, New Orleans

- * Half-day Grid workshop at the HealthGrid 2008 conference, June 2008, Chicago

- * 1-day CI-days Grid Workshop, May 2008, Clemson University

The content of the training material has been enhanced over the past year to include a full module for OSG Grid site administrators, and the end-user training content was updated to include training on SRM/dCache and Bestman. Work continues to enhance the on-line delivery of user training, but many users and students nationwide have already made use of this self-paced module, both for Grid introduction and as a refresher after taking an in-person Grid School.

The OSG Education team coordinated the selection of students who participated at ISSGC 08, and arranged sponsorship for US-based students to attend this workshop. In addition, OSG staff provides direct contributions to the International Grid School by attending, presenting, lab exercise development, and student engagement.

OSG staff will conduct a grid training school in South Africa July 25-28 2008 (just after the filing of this report) at The University of Witwatersrand, Johannesburg, South Africa. Over forty attendees from South African universities and other African nations are registered. This training event will use Grid facilities that have been deployed over the past year as part of the OSG international outreach program, and will involve South African students that attended the Great Plains grid school in 2007 followed by Grid Administration training at the UChicago CI. And OSG and the UChicago Computation Institute hosted a visit by 3 faculty members from the evolving nation grid of Colombia, and 2 Columbian students followed on to attend the Georgetown Grid School and one student attended the Florida International Grid School.

OSG collaborates with Educause, Internet2 and TeraGrid to sponsor day-long workshops local to university campus-wide CyberInfrastructure (CI) Days. These workshops bring expertise to the campuses to foster research and teaching faculty development, IT facility planning, and CIO awareness and dialog. Ongoing dialog and coordination between the EOT programs of TeraGrid and the Supercomputing conference education programs take place frequently during the year.

Outreach Activities:

U.S. Outreach

- * Workshop at the High Performance and Distributed Computing (HPDC 2008): <http://indico.cern.ch/conferenceDisplay.py?confId=27789>
- * Joint EGEE and OSG Workshop on VO Management in Production Grids.
- * The fourth annual Cybersecurity Summit for NSF Large Research Facilities will be held May 7th, 2008 at the Sheraton Crystal City in Arlington, Virginia.
<http://roadrunner.ltnet.net/drupal/?q=node/15>
<http://www.educause.edu/About+EDUCAUSE/MemberCommittees/CommitteeMembers/959?CODE=CYB08>
- * Contributions to the DOE Grass Roots Cyber Security R&D Town Hall Meetings and mathematics and security workshop.
- * Contributions to the Building Effective Virtual Organizations (BEVO) workshop in January 2008.
- * Contributions to the NRC report, 'Integrated Computational Materials Engineering.'
- * International Research Networking Collaborations workshop
- * Participation in and presentations for the Campus Infrastructure Days, a collaboration with Internet2, Educause, TeraGrid and other projects.
<http://cidays.org/Presentations>
- o Clemson University CI Days, May 19-21, 2008
- o New Mexico CI Days; March 10-11, 2008
- o Elizabeth City CI Days, January 4, 2008
- o NYSGrid CI Days Workshop - December 2007

International Outreach

- * Co-editorship of the highly successful International Science Grid This Week newsletter, www.isgtw.org which is becoming a recognized communication vehicle for publishing of science and technologies of grids.

- * Training at Cyberinfrastructure for International Collaborative Biodiversity and Ecological Informatics Pan-American Advanced Studies Institute, <http://ciara.fiu.edu/eco/>
- * International Workshop on Digital Divide, Mexico City, October 2007, <http://fismat.uia.mx/HEP/ICFADDW2007/>
- * Contributions to High Throughput Computing Week November 2007, e-Science Institute, Edinburgh <http://www.nesc.ac.uk/esi/events/831/>
- * Presentations at the online International Winter School on Grid Computing <http://www.iceage-eu.org/iwsgc08/index.cfm>
- * Distributed science workshop, Peru, December 2007

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Web/Internet Site

URL(s):

www.opensciencegrid.org

www.isgtw.org

Description:

OSG web site for general, publication, and technical information about the project.

OSG sponsored weekly eNewsletter

Other Specific Products

Product Type:**Teaching aids****Product Description:**

OSG has developed web based training materials for Grid Schools. These have been reused by other organizations doing training in the field: in particular schools in South America in Columbia, Argentina and Brazil.

Sharing Information:

Shared through being available through the web and personal contacts of Grid school educators and students.

Product Type:**Technical Know-How****Product Description:**

OSG is developing an experienced and expert workforce in the operational, management and technical aspects of high throughput production quality distributed infrastructures. This experience includes the use, diagnosis, security and support of distributed computing technologies including Condor, Globus, X509 based security infrastructure, data movement and storage, and other technologies included in the Virtual Data Toolkit.

Sharing Information:

Through engagement and outreach with new site and users of the OSG.

Contributions**Contributions within Discipline:**

The OSG has delivered to the science of the physics collaborations who are the major stakeholders and helped to refine and advance the capabilities of distributed computing technologies.

Contributions to Other Disciplines:

In the nine months since the start of the OSG project engagement activities have succeeded in:

- * Protein Modeling and Design: Adaptation and production running opportunistically using more than a hundred thousand CPUhours of the Rosetta application from the Kuhlman Laboratory in North Carolina across more than thirteen OSG sites.
- * Weather Modeling: Production runs of the Weather Research and Forecast (WRF) application using more than one hundred and fifty thousand CPUhours on the NERSC OSG site at Lawrence Berkeley National Laboratory.
- * Nanotechnology Simulations: Improvement of the performance of the nanoWire application from the nanoHub project on sites on the OSG and TeraGrid, such that stable running of batches of five hundred jobs across more than five sites is routine.
- * Molecular Dynamics Simulations: Production running using more than twenty thousand CPU hours of the CHARMM molecular dynamic simulation to the problem of water penetration in staphylococcal nuclease using opportunistically available resources across more than ten OSG sites.
- * Information and Library Science: OSG resources were used to implement a method for retrieving, analyzing and finding relationships in published research texts from multiple disciplines. A total of 162,000 documents from a variety of scientific fields were analyzed. This work, amounting to 15,000 hours, was completed in about 28 hours using the grid resources of the OSG.
- * Developing working relationships with additional research groups to fill the pipeline of potential new users. These upcoming production runs include WRF modeling from UC Davis, and two senior researchers in molecular and biochemistry.
- * Progress in Campus Grids at Wisconsin and Fermilab, and engagement with the University of California at Davis researchers and campus IT support staff towards a university-based cyberinfrastructure. Triggered exploration of new methodologies for identifying, assessing and resolving security vulnerabilities in multi layered, multi vendor distributed software stacks.

Contributions to Human Resource Development:

See Training and Development section under Activities and Findings

Contributions to Resources for Research and Education:

The OSG infrastructure currently provides access to the following resources. It must be remembered that OSG does not own any resources. They are all contributed by the members of the OSG Consortium, and are used both locally and by the owning Virtual Organization. Only a percentage that varies between 10 and 30% are in general available for use by the OSG.

processing resources on production infrastructure: 84
 # Grid interfaced data storage resources on prod. infrastructure: 15
 # Campus Infrastructures interfaced to the OSG: 4
 # National Grids interoperating with the OSG: 2
 # processing resources on the Integration infrastructure: 20
 # Grid interfaced storage resources on integration infrastructure: 2
 # Cores accessible to the OSG infrastructure: ~44,000
 Tape storage accessible to the OSG infrastructure: ~10 Petabytes
 Disk storage accessible to the OSG infrastructure: 3 Petabytes
 CPU Wall Clock usage of the OSG infrastructure: Average of 13,000 CPU days/ day

The OSG Virtual Data Toolkit

The OSG Virtual Data Toolkit (VDT) provides the underlying packaging and distribution of the OSG software stack. VDT continues to be the packaging and distribution vehicle for Condor, Globus, myproxy, and common components of the OSG and EGEE software. VDT packaged components are also used by EGEE, the LIGO Data Grid, the Australian Partnership for Advanced Computing and the UK national grid, and the underlying middleware versions are shared between OSG and TeraGrid.

In the first nine months of the OSG project the VDT has been further extended to include: OSG accounting probes, collectors and a central repository for accounting information, contributed by Fermilab; The EGEE CEMon information manager which converts information from the MDS2 LDIF format to Condor ClassAds; Virtual Organization (VO) management registration software developed for the World Wide LHC Computing Grid (WLCG) and used by most physics collaborations; An additional implementation of storage software, interfaced through the Storage Resource Management (SRM) interface. The dCache software, provided by a collaboration between the DESY laboratory in Hamburg, and Fermilab, is also in use by the WLCG and High Energy Physics experiments in the US. VDT releases are tested on the OSG Integration Grid before being put in production. VDT is an effective vehicle for the rapid managed dissemination of security patches to the component middleware. Patches and updates are provided to the installation administrators for security and bug fixes.

Contributions Beyond Science and Engineering:

None

Special Requirements

Special reporting requirements:

OSG has put in place activities that meet the terms of the Cooperative Agreement and Management Plan:

- * The Joint Oversight Team met to hear about OSG progress in February 2008 in Washington DC. OSG is following up on the feedback.
- * The Science Advisory Group (SAG) met June 12, 2007. The presentations are posted as OSG Event-68. The OSG Executive Board has addressed feedback from the Advisory Group. Another meeting of the SAG is planned for Fall 2008.

Two intermediate progress reports were submitted to NSF in February and June of 2007. They are available as OSG documents 570 and 632. Document 672 (OSG Highlights) was presented to DOE in July 2007. A DOE annual report was submitted February 2008.

Change in Objectives or Scope: None

Animal, Human Subjects, Biohazards: None

Categories for which nothing is reported:



OSG Mid-Year Metrics

OSG-769

July 16, 2008

Revision 4

1. Document Overview

The Metrics Defined for Year 2 (OSG document #740) were divided into three parts – “Open” metrics which represent how well we are engaging the community, “Science” metrics representing how well we serve the science stakeholders, and “Grid” metrics which emphasize quantitative measurements of the entire Open Science Grid.

This report provides a mid-year view of achieving the goals defined for US LHC and LIGO. There are 4 science goals for the LHC VOs, CMS and ATLAS, and 2 science goals for LIGO.

To quote from the Metrics Definition Document: *“We have deliberately tied our milestones and metrics to those of the WLCG and LHC experiments, as part of our contributions to the World Wide LHC Grid Computing Collaboration. This means that we have used the metrics from the WLCG Combined Computing Readiness Challenge (CCRC’08), the ATLAS Full Dress Rehearsal (FDR-2) and the CMS Computing and Software Analysis (CSA08). For LIGO the metrics are tied to the goals of the planned program of work and the output from the quarterly meetings between LIGO and OSG management.”*

2. Summary of Results

The following table gives a summary of the results of achieving the goals defined for US LHC:

Metric	CMS Result	ATLAS Result
50% of sites meet WLCG MoU Operational targets	6/7 sites for CPU 6/7 sites for disk ¹	5/5 sites for CPU 1/5 sites for disk ¹
50% of sites deploy SRMv2.2 by February 2008	7/7 sites	5/5 sites
50% of sites meet WLCG MoU reliability targets	DELAYED –OSG reporting to WLCG will start in July 2008 ²	DELAYED – OSG reporting to WLCG will start in July 2008 ²

¹ This is as of June 2008, which was before some site’s 2008 disk purchasing.

OSG meets VO needs for CCRC'08	6/7 goals achieved	3/4 goals achieved
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These metrics are discussed in full in Section 3.1.

The following table achievements for the LIGO goals.

Metric	LIGO
Usage of OSG storage for LIGO	DELAYED
Production running	ACHIEVED

These are discussed in Section 3.3.

3. Year 2 Metrics

3.1. *WLCG Collaboration Metrics*

3.1.1. **Metric 1: WLCG MoU operation targets for CCRC'08**

Goal:

1. More than 50% of CMS Tier-2 sites reporting at least pledged capacity. CPU: ACHIEVED (6/7 sites). Storage: ACHIEVED (6/7 sites)
2. More than 50% of ATLAS Tier-2 sites reporting at least pledged capacity. CPU: ACHIEVED (5/5 sites). Storage: MISSED (1/5 sites)

Explanation:

The WLCG Combined Computing Readiness Challenge in 2008 defined as its goal the WLCG MOU targets for Tier-2 capacity.

Measurement:

The WLCG MoU operational targets deal with the size of each Tier-2 site with respect to the CPU capacity, online disk, and network capacity. We take the numbers as reported during June 2008, shortly after the second phase of CCRC'08. The targets written in the MoU apply to LHC turn-on; accordingly, some sites have planned for large expansions between the end of CCRC'08 and beginning of LHC collisions. These expansions are not reflected here.

For CMS, the targets are given in the megatable (The WLCG Collaboration 2007). The targets for the fiscal year 2008 and the capacity during July 2008 are given here:

² The capability to measure reliability was not mature enough at the time of this report. CMS VO specific results shown at end of report.

Site	2008 CPU Goal (KSI2K)	June 2008 CPU (KSI2K)
T2_US_Caltech	1000	1000
T2_US_Florida	1000	998
T2_US_MIT	1000	1000
T2_US_Nebraska	1000	710
T2_US_Purdue	1000	1000
T2_US_UCSD	1000	1000
T2_US_Wisconsin	1000	1000
Totals	7000	6708

The June values were taken from (Bloom 2008). Note that the original source indicates the entire cluster size; the numbers here reflect the portions controlled by CMS. Over 50% of the CMS sites have achieved their MoU targets for CPU. For online disk space, the megatable (The WLCG Collaboration 2007) again provides targets and (Bloom 2008) provides the June 2008 values:

Site	Target disk (TB)	June 2008 disk (TB)
T2_US_Caltech	200	200
T2_US_Florida	200	136
T2_US_MIT	200	200
T2_US_Nebraska	200	200
T2_US_Purdue	200	200
T2_US_UCSD	200	200
T2_US_Wisconsin	200	200
Totals	1400	1336

For disk, 6 out of 7 sites have met the 2008 targets. Again, these numbers represent the amount controlled by CMS.

Finally, the megatable specifies that all sites should have 10Gbps connections to FNAL; 100% of the sites have reached this goal. For the specific rate goals from the different worldwide CMS Tier-1, see the information provided section 3.2.2; the WAN goals were achieved for 6 out of the 7 Tier-1 sites.

For ATLAS, site targets for CPU and disk space ending FY08Q3 are summarized (Gardner 2008). The CPU targets are given below.

Site	June 2008 (KSI2K)	2007 Goal (KSI2K)	2008 Goal (KSI2K)
US-NET2	1031	394	665

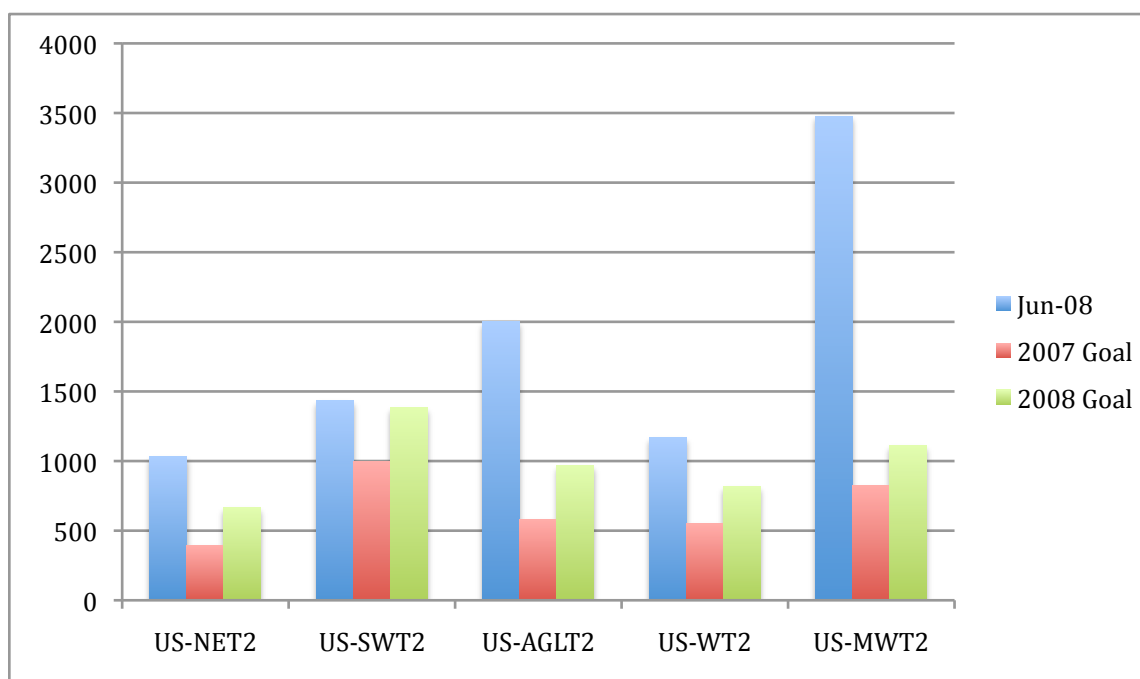
US-SWT2	1437	998	1386
US-AGLT2	2000	581	965
US-WT2	1171	550	820
US-MWT2	3478	826	1112
Totals	9117	3349	4948

All 5 ATLAS sites have met the CPU targets as of June 2008.

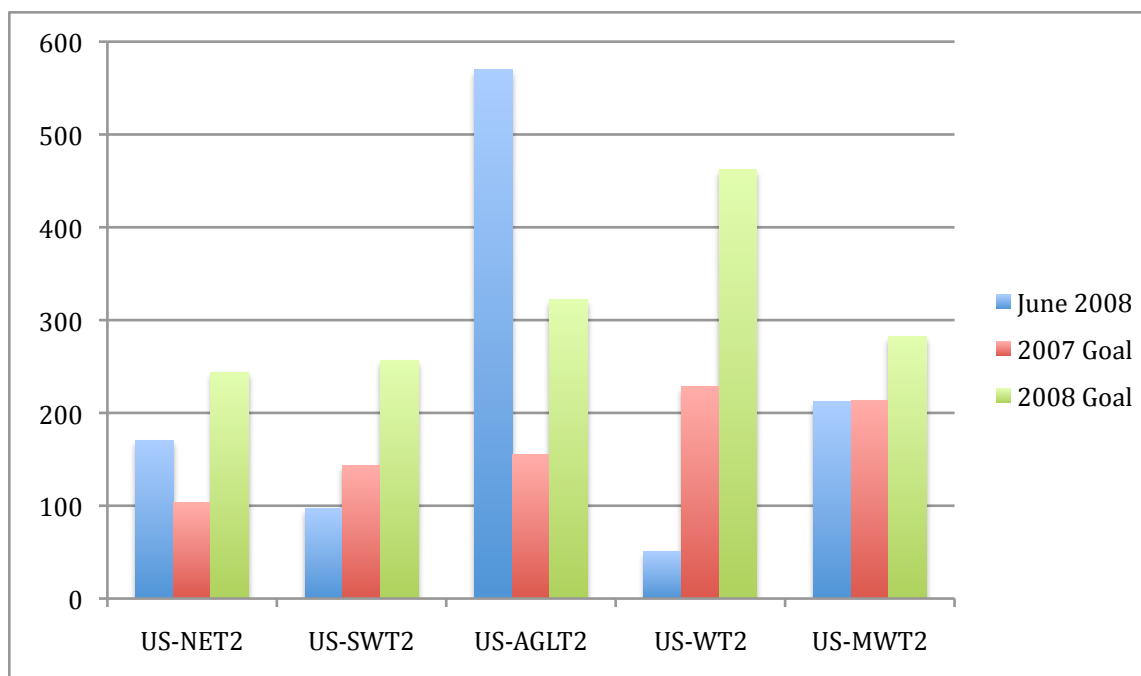
The disk space targets are given below.

Site	June 2008 (TB)	2007 Goal (TB)	2008 Goal (TB)
US-NET2	170	103	244
US-SWT2	97	143	256
US-AGLT2	570	155	322
US-WT2	51	228	462
US-MWT2	212	213	282
Totals	1100	842	1566

Graphically, the deployed CPU versus WLCG pledge is shown below.



All US ATLAS sites have exceed their CPU pledge for 2008. For disk-storage, the situation is shown here:



As of June 2008, one of the five ATLAS sites has achieved the 2008 disk goal. The remaining sites have a large disk procurement milestone of September 15, 2008.

3.1.2. Metric 2: US LHC Tier-2s with SRM V2.2 capable storage service

Goal:

1. More than 50% of US CMS Tier-2s sites have a SRM V2.2 capable storage services in February 2008. ACHIEVED (6/7 sites)
2. More than 50% of US ATLAS Tier-2s sites have a SRM V2.2 capable storage services in February 2008. ACHIEVED (5/5 sites)

Explanation:

Availability of SRM V2.2 capable storage services was a deliverable of the contributing Grid infrastructures and sites to the start of the CCRC'08 in February 2008.

Measurement:

The deployment of SRM v2.2 storage service on US CMS Tier-2 sites was recorded in (Bagliesi and Bloom 2008). 6 out of 7 sites were upgraded to SRM v2.2 prior to February 2008; the last site was upgraded on February 13, 2008. As of May 2008, SRMv1 endpoints are no longer needed by the experiment, completing the rollout of SRM v2.2 for USCMS Tier-2 sites (Bonacorsi, Decommissioning SRMv1 endpoints at Tier-2's for CMS 2008).

For ATLAS sites, the list of used endpoints is kept in CVS (ATLAS DDM 2008). As of May 2008, the Tier-1 and all Tier-2 sites have SRM v2.2 capable end-points, including endpoints located at the following facilities:

- US-BNL, US-NET2, US-SWT2, US-MWT2, US-WT2, US-AGLT2
- There are additional ATLAS endpoints that are not subject to the WLCG MOU which have no immediate plans to upgrade their storage elements.

3.1.3. Metric 3: WLCG MOU Critical Service availability

Goal:

More than 50% of US LHC Tier-2s sites meet the WLCG MOU Critical Service availability goals in September 2008

Explanation:

The WLCG MoU states the reliability of a Tier-2 site should be 95%, where reliability is the site's availability divided by the scheduled availability³. CMS has further clarified "scheduled availability" for a Tier-2 to only include "working hours"⁴

Measurement:

The mechanism for measuring the availability – RSV – was developed in Q1 2008, and delivered to the sites in Q2 2008. Although preliminary measurements are available in May and June, it was agreed that July would be the first month where the experiments would certify the results at the WLCG level. This allows for sites to develop experience with the RSV tool and an understanding of how the availability algorithms work [as the WLCG algorithm is fairly intricate (Sonvane, et al. 2008)].

As of the beginning of July, we have all ATLAS and CMS Tier-2 sites reporting availability numbers.

Availability numbers will be available from OSG availability reports or the GridView development server (GridView 2008).

³ The original documents call this "availability", but the accepted terminology now refers to this as "reliability"

⁴ Working hours are defined to be 8:00-17:00, Monday through Friday, excluding holidays.

3.2. US ATLAS and US CMS Related Metrics

3.2.1. Metric 4: OSG Infrastructure meets US ATLAS metrics for CCRC'08

Goals:

1. Distribute 200 Mbytes/sec data for one week from CERN to the Tier-1 and Tier-2 sites. The BNL share of CCRC08 data was 81TB to tape, 252TB to disk. The BNL share of FDR-2 data was 100TB on disk. ACHIEVED.
2. Run 10,000 simultaneous jobs across ATLAS facility (Including OSG, EGEE, and NorduGrid). ACHIEVED.
3. Re-process M5 data at BNL every day. DELAYED – reprocessing delayed to post-CCRC08
4. SRM V2.2 compliant storage service at Tier-1 and all Tier-2s. ACHIEVED
5. 30M events produced for FDR-2 in parallel with full data flow from DAQ system through to Tier-2s, with ongoing data processing and analysis (Bos 2008). NO DATA YET PROVIDED

Three of the four goals with known statuses were achieved.

Explanation:

ATLAS defined metrics for the WLCG Combined Computing Readiness Challenge in 2008. OSG contributed to meeting these.

Measurement:

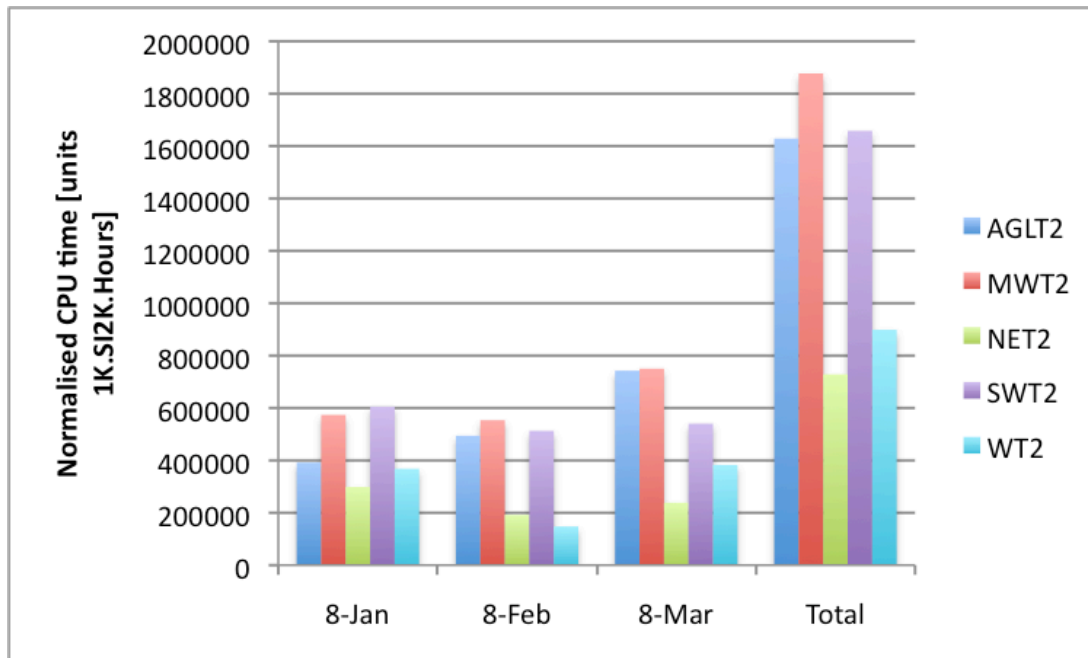
The ATLAS metrics for CCRC'08 were given in (Bos 2008) prior to CCRC'08 and in (Campana 2008) post-CCRC'08. The goals are grouped into two sections – computing and transfer goals.

Computing Goals

We have the following computing goals for US ATLAS sites:

- Simulate 30 million events
- Tier-1 site (BNL) reprocesses M5 data every day – DELAYED. In (Campana 2008), it is noted that, while reprocessing did occur, it was not attempted at challenge rates. This will be an area of focus post-CCRC08.
- 100TB of data resides on BNL disk – ACHIEVED

During the first three months of 2008, the contributed CPU time to WLCG from the five US ATLAS Tier-2 facilities is shown below. In total, more than 6.5 million CPU hours were delivered during this time period in support of FDR-1 simulation, reconstruction and analysis.



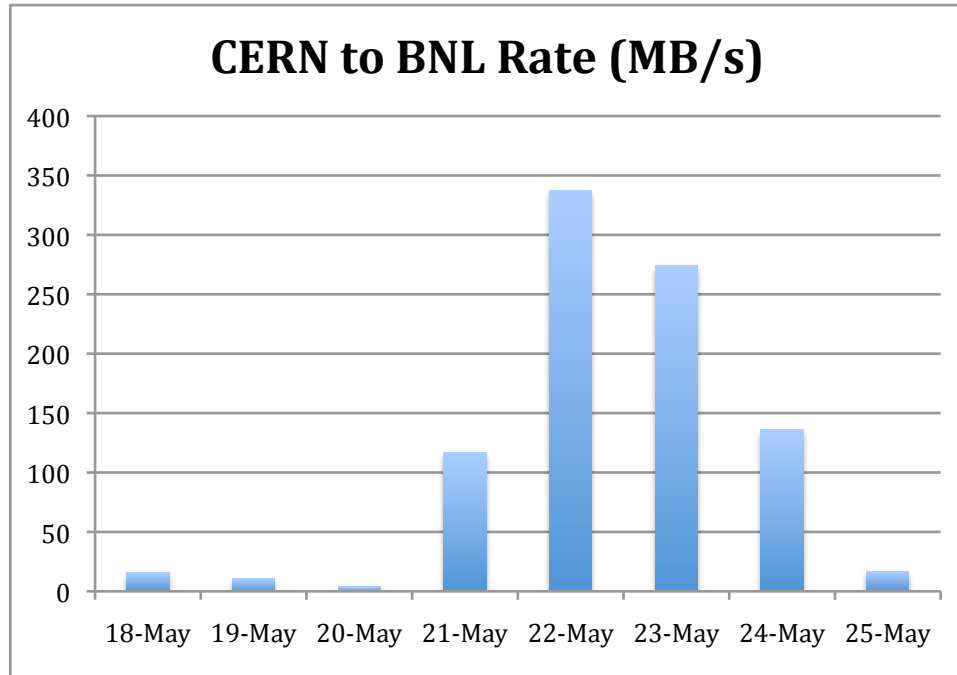
Panda-based analysis queues supporting distributed analysis (via the Pathena program) previously at the Tier-1 have now been configured for each of the Tier-2 facilities. These queues were exercised for FDR-1 (Shibata 2008).

Transfer Goals

As with CMS, the ATLAS transfer goals for CCRC'08 were more thorough; while some are given in (Bos 2008), they are broken into weekly goals in (Campana 2008). A review of the goals' status is given in (Klimentov 2008).

- **Week 1: Tier-0 to Tier-1 Transfers**
 - Sites hold complete replica of 90% of dataset. ACHIEVED.
 - Dataset replication completed within 48hrs. ACHIEVED.
- **Week 2: Tier-1 to Tier-1 Transfers**
 - Every channel should finish 90% of datasets. BNL ACHIEVED for 9/10 channels.
- **Week 3: Simulated Tier-0 data exports**
 - BNL sustains peak rate for 24 hrs: The peak rate was 337MB/s, achieved on May 22.
 - BNL sustains nominal rate for 3 days: MISSED (only achieved nominal rate for 2 days). The average rate is defined to be 287MB/s in (The WLCG Collaboration 2007) and 298MB/s in (Campana 2008). The Week

3 Tier-0 to Tier-1 transfer rates are graphed below.



- **Week 4: Full system exercise.** Emulate 14 hours of data taking plus MC production
 - Tier-0 to Tier-1: import 90% of subscribed datasets. ACHIEVED
 - Tier-1 to Tier-2: Complete copy of AOD to Tier-2. ACHIEVED
 - Tier-1 to Tier-1 (functional): import 90% of subscribed datasets. ACHIEVED
 - Tier-1 to Tier-1 (throughput): BNL receives all AOD/ESD. ACHIEVED

During this time 210 FDR datasets were distributed from the Tier-1 to each Tier-2 using the DDM infrastructure and SRM endpoints. The endpoints were space-token managed storage locations. The table below summarizes the results of the data distribution exercise.

Site	Files assigned	Files copied successfully	Datasets Assigned	Datasets Successful
US-NET2	1925	1925	210	210
US-AGLT2	1925	1922	209	210
US-SWT2	1925	1925	210	210
US-WT2	1925	1925	210	210
US-MWT2	1925	1925	210	210
Totals	9625	9622	1049	1050

3.2.2. Metric 5: OSG Infrastructure meets US CMS metrics for CCRC'08

Goals:

1. Demonstrate [CMS data transfer goals](#) of 100% of 2008 Tier-1 to Tier-2 WLCG Rate Goals. MISSED (only 6 of 7 links passed). The last link did not pass due to problems at a foreign T1.
2. Three out of five tested Tier-2 “regions” should meet their 2008 WLCG rate goals of 126 Mbytes/second from FNAL. ACHIEVED.
3. Demonstrate data distribution at 100% of 2008 Tier-0 Rates. ACHIEVED
4. Demonstrate data distribution at 100% of 2008 Tier-1 Rates. ACHIEVED
5. Demonstrate the replication of a sizeable dataset within 4 days from one Tier-1 to others. ACHIEVED
6. [Analysis Goals](#): Phase 1: Centrally submitted analysis at 2008 data taking rates. Phase 2: Chaotic submission from Tier-2 sites. Phase 3: Tier-2 Latency measurement. ACHIEVED
7. Produce 120M events worldwide. ACHIEVED (US Tier-2 portion: 20%)

Six of the seven goals were achieved.

Explanation:

CCRC'08 tested the entire computing infrastructure for worldwide CMS. It also can be used as a measurement for how well OSG sites and infrastructure were meeting USCMS needs. The wide ranging goals for CCRC'08 means that there are many areas in computing with goals; CMS CCRC'08 goals can be broken into three areas:

- Analysis Goals: The analysis exercise was highly successful, with about 50k jobs submitted during the first week and 100k jobs submitted during the second week. CMS has not yet released results from the third week of analysis activities.
- Production Goals
- Transfer Goals: The transfer goals were an elaborate test of all the different types of production links, including Tier-0 to Tier-1, Tier-1 to Tier-1, and Tier-1 to Tier-2. Four out of five goals were achieved; the remaining goal involved target rates for 7 Tier-1 sites, of which 6 were realized.

Below, we give a detailed analysis of the accomplishments in all three areas.

Measurements:

Analysis Goals.

The analysis portion of CCRC'08 is split into three phases:

Phase 1: Central submissions

CMS computing experts centrally submit jobs to many sites. There were two rounds of submissions; all 7 Tier-2 sites participated. There were 9.3k jobs in Round 1 and 40k jobs in Round 2; the success rates were 99.6% and 86%, respectively (Wuerthwein 2008).

Phase 2: Chaotic Submissions

The CMS computing personnel (plus any physicists) submitted jobs from their Tier-2 sites to any other Tier-2 site. This phase ran from May 19 through May 25. The number of jobs run at each site is given in a table below.

Site	Number of Jobs	Success Rate
T2_US_Caltech	10045	100%
T2_US_Florida	18955	87%
T2_US_MIT	4241	100%
T2_US_Nebraska	21567	80%
T2_US_Purdue	8080	99.9%
T2_US_UCSD	25323	99.9%
T2_US_Wisconsin	21696	96%
Totals	109907	92%

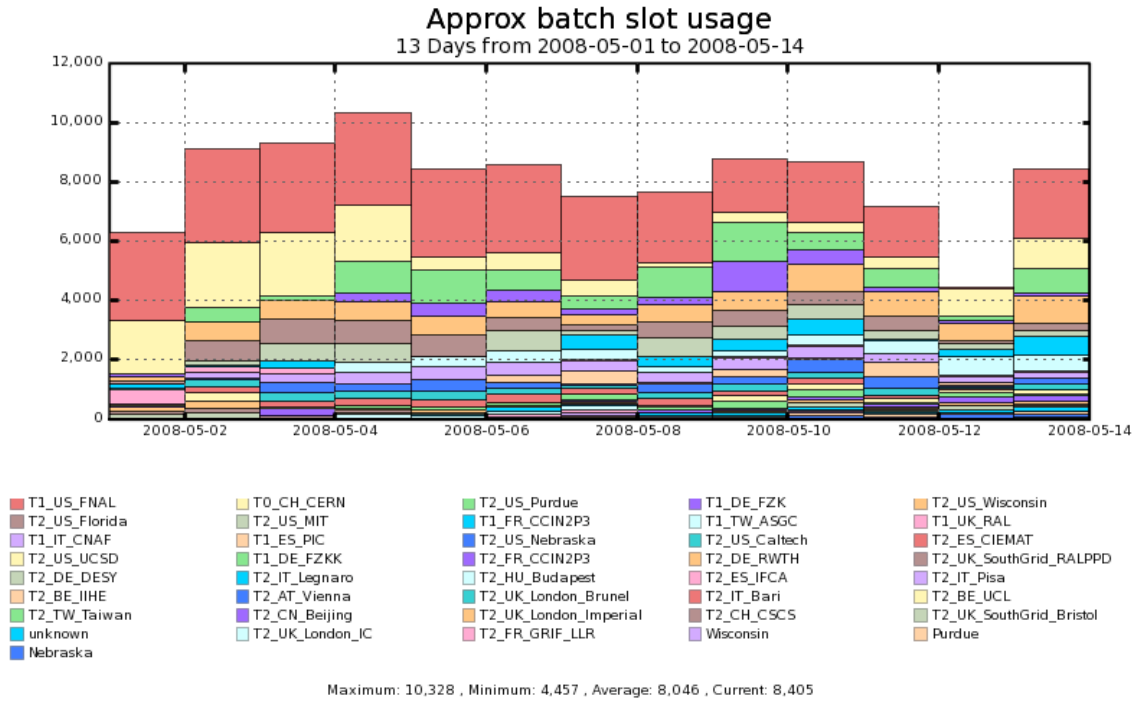
Source (ARDA Dashboard 2008).

Phase 3: Latency Measurement

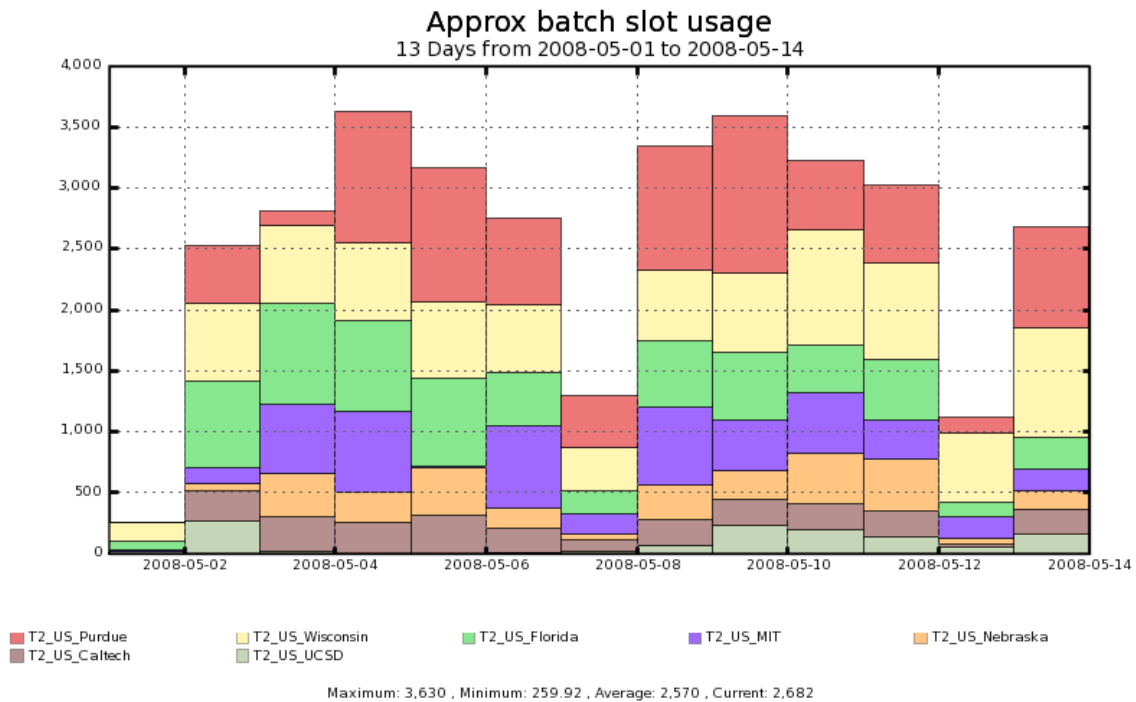
The third phase involved sites selecting a dataset not locally available, measuring the time it took to transfer it, and run an analysis over the entire dataset. Participation from sites in this exercise was very limited because it did not fit into the 1 month schedule of CCRC08, and was done largely the week after CCRC08. CMS finds that transfer of ~1TB dataset completes within 2-4 hours, with the latency being dominated by edge effects. This time can increase substantially when the source is a site that is experiencing storage problems.

Production Goals

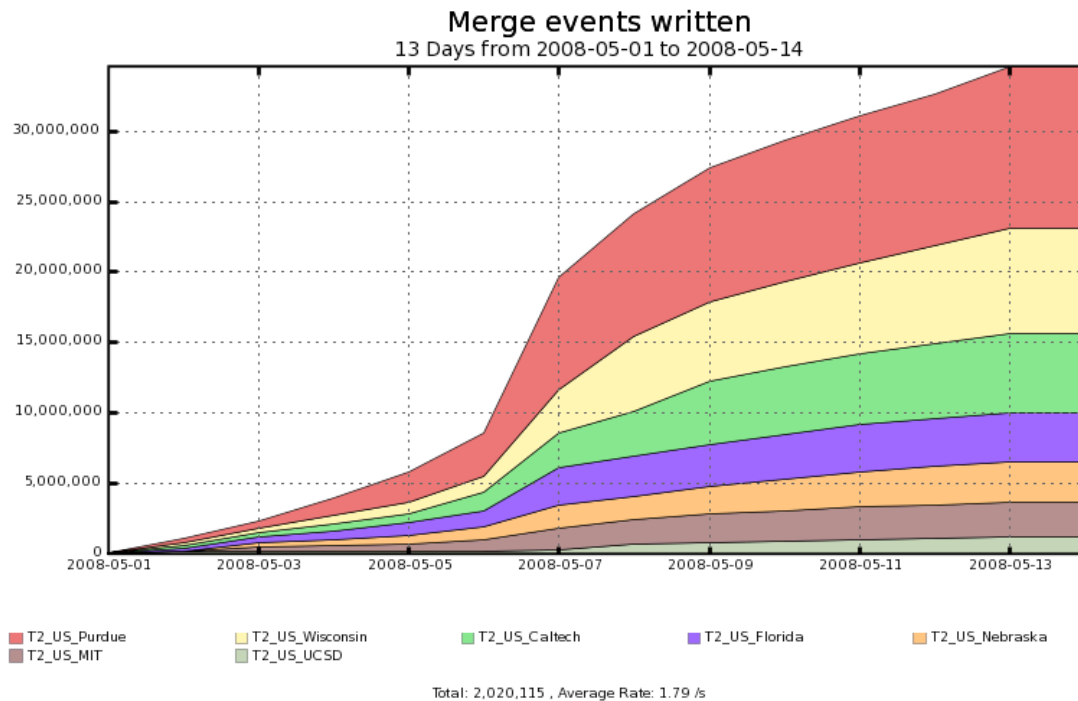
There was a major round of production to provide events for the CCRC'08 exercise in CMS. The physics groups requested 120M events, and over 150M were produced (Gutsche, et al. 2008). The entire production run was started on May 1 and finished by May 13. There was, on average, 8000 batch slots occupied worldwide, as shown on the plot below:



Filtering on the US Tier-2 sites, there were on average 2500 batch slots used.



Finally, we show a graph of the number of events written throughout the exercise; US Tier-2 sites contributed 30M events, or about 20% of the total.



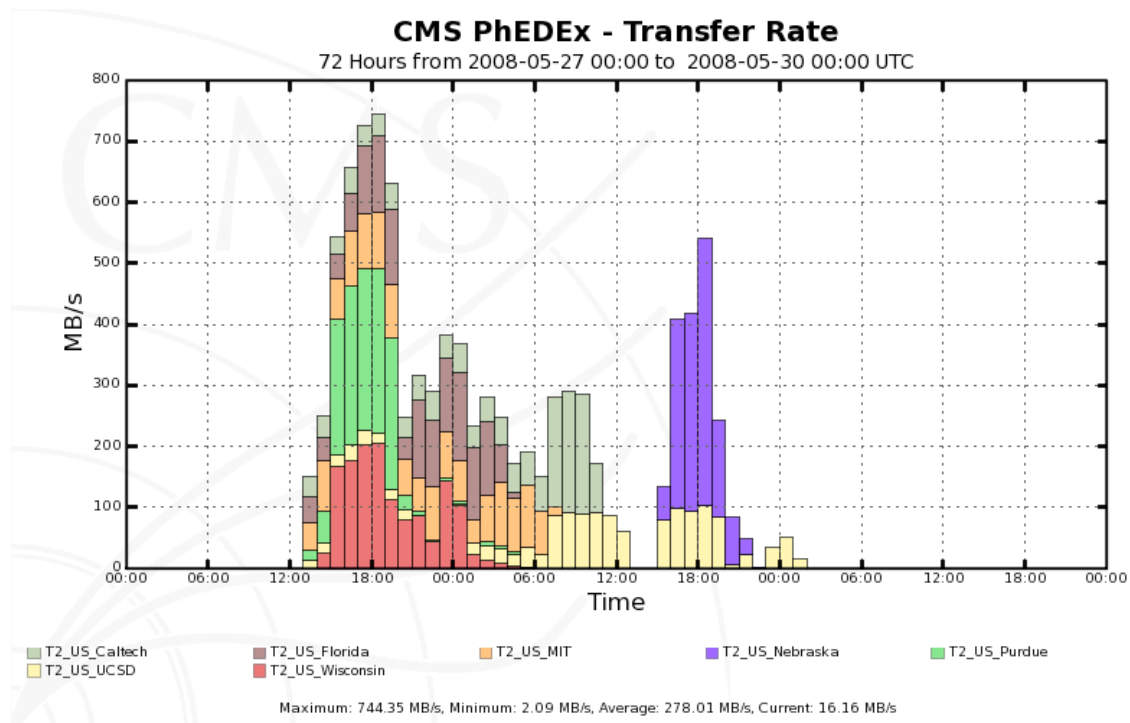
During the exercise, T1_US_FNAL reprocessed over 100M events and provided skimming for approximately 1M events.

Transfer goals

CMS had an elaborate set of transfer goals for CCRC'08, laid out in (Teodoro and Magini 2008). We first examine the Tier-2 transfer goals, then the Tier-1 goals for FNAL. Overall, the entire process was highly successful – all the goals were achieved with the exception of one entry in the transfer table.

Tier-2 Goals:

- **Ability to measure transfer latency.** CCRC'08 was the first time that statistics were available for block latency measurement (Tuura 2008). **ACHIEVED.** [These statistics are available here](#). While the actual block latencies are high, being able to measure them will allow problems to be diagnosed and solved.
- **Demonstrate 100% of 2008 Tier-1 to Tier-2 WLCG Rate Goals.** 6/7 **ACHIEVED.** Each Tier-1 has a stated goal for transfers to the US region. Seven Tier-1s were tested (transfers from Tier-1 CERN were de-scoped), and all except ASGC met the minimum rate as stated in (Bonacorsi, Klem, et al. n.d.). With the exception of ASGC, the US region led in the average transfer rate for non-regional transfers.
 - In fact, FNAL to US Tier-2 had the largest average and peak transfer rates; the peak transfers are shown in the graph below.
 - The table below references the total number of files transferred during this 48 hour time period.



This table shows Tier-2 statistics from the 2 day period, May 27 12:00 through May 29 12:00.

Site	Number of files Transferred	Number of TB Transferred
T2_US_Caltech	1998	4.7
T2_US_Florida	2079	5.0
T2_US_MIT	1998	4.8
T2_US_Nebraska	6808	10.3
T2_US_Purdue	2278	5.6
T2_US_UCSD	2634	5.8
T2_US_Wisconsin	2220	5.5
Totals	20015	41.7

Tier-1 Goals

- **Regional Participation.** Three out of five tested Tier-2 “regions” should meet their 2008 WLCG rate goals from FNAL, including the US region. **ACHIEVED.** This metric was achieved; 8 regions were tested and all passed.
- **Demonstrate 100% of 2008 Tier-0 Rates.** **ACHIEVED.** Pass the WLCG nominal rate for 3 days a week for two weeks of May. This was accomplished during the weeks of May 11 and May 18 (Bockelman 2008)

- **Latency. ACHIEVED.** Demonstrate the replication of a sizeable dataset within 4 days to other Tier-1s; target is replicating the dataset to 6 Tier-1s (Bauerdick and Bonacorsci 2008).

3.3. *LIGO Related Metrics*

Goals:

1. Demonstrate use of OSG grid accessible storage for LIGO application
2. Effective throughput of Einstein@Home on OSG accessible resources.

Measurements:

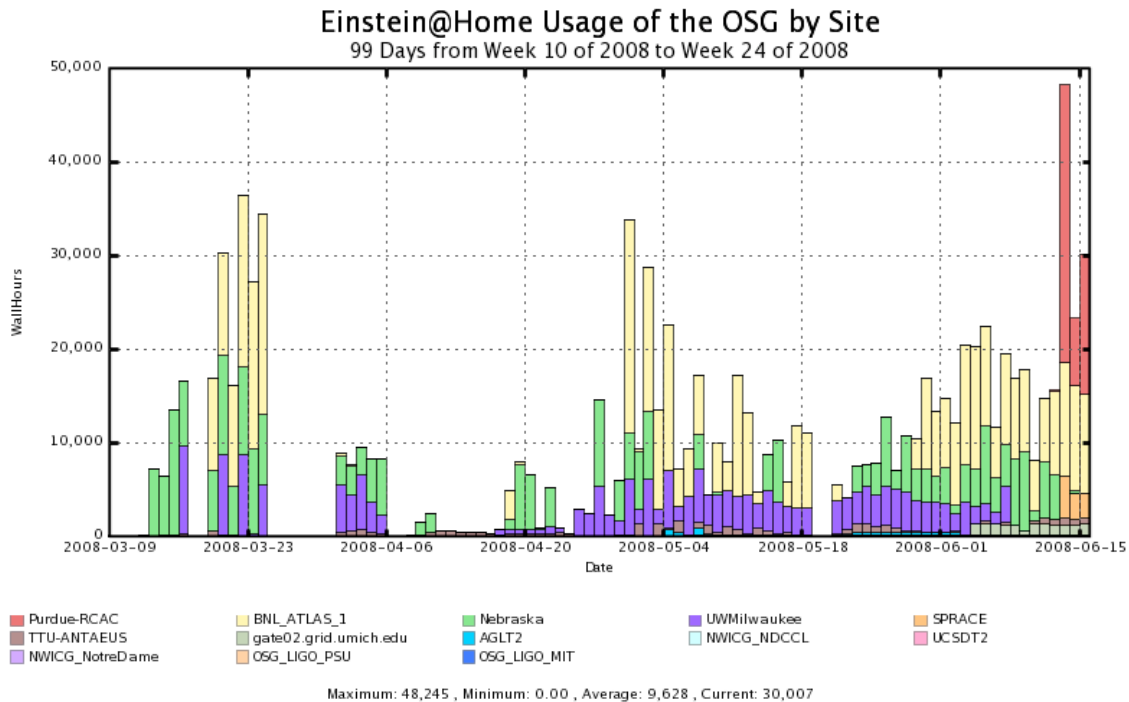
The measurement of Goal 1 for this metric has been delayed until the final report.

The LIGO Einstein@Home application presents two unique difficulties:

1. The grid-enabled version of this application was developed on D-Grid, a German Grid.
2. The application uses the Web Services version of GRAM; this version of GRAM was previously widely utilized on the OSG

The first is an interoperability problem, while the second is a deployment problem. The first was tackled successfully in February 2008 as the D-Grid participants were able to quickly adopt the grid application to the OSG. The second has been slower; sites are starting to adopt the WS-GRAM interfaces as LIGO asks for it, but have not been enabling this on their own.

The outcome has been a success – LIGO regularly utilizes over opportunistic 1000 CPUs a day and peaks up to about 2000 CPUs a day. This translates to up to 50,000 wall hours a day, as the next graph shows:



LIGO has run on 13 different OSG sites with varying levels of success. This graph is taken from a VO-specific instance of Gratia, the OSG's accounting tool (Gratia Project 2008).

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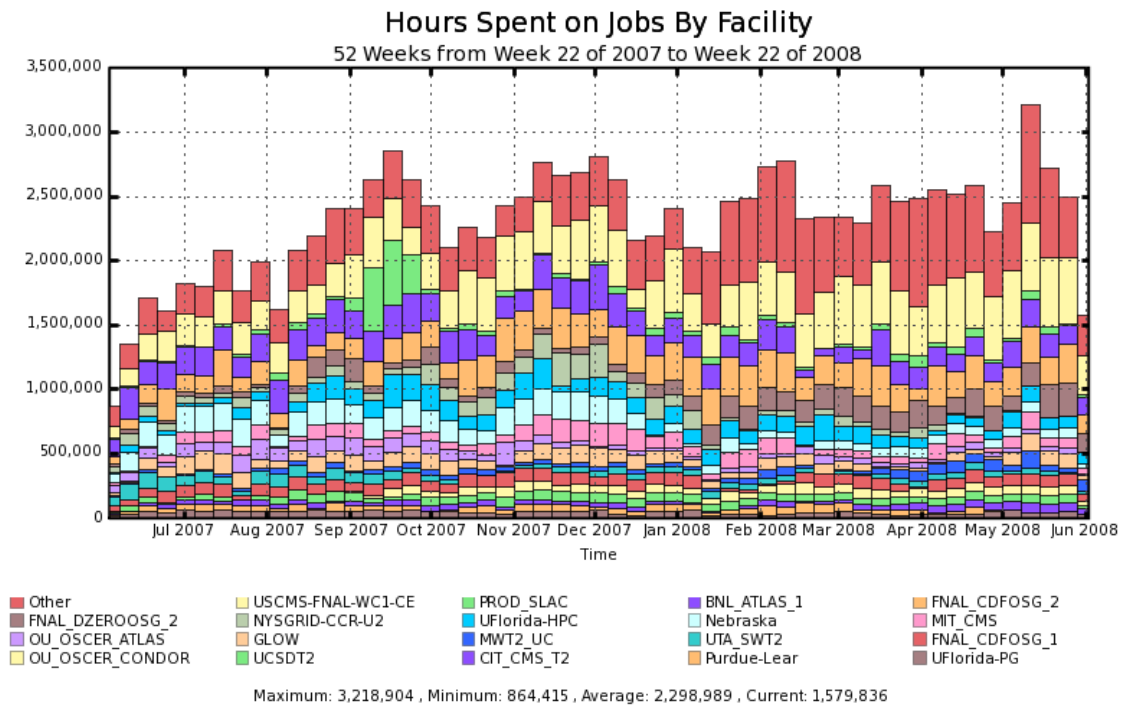
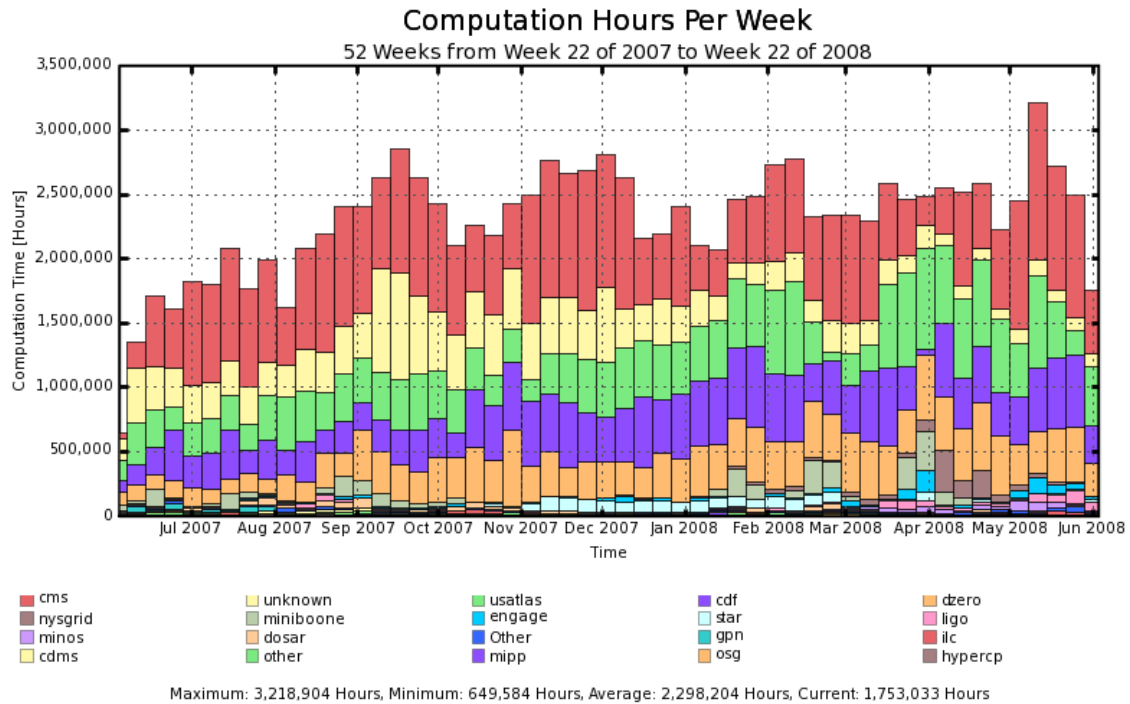
5. Additional Info

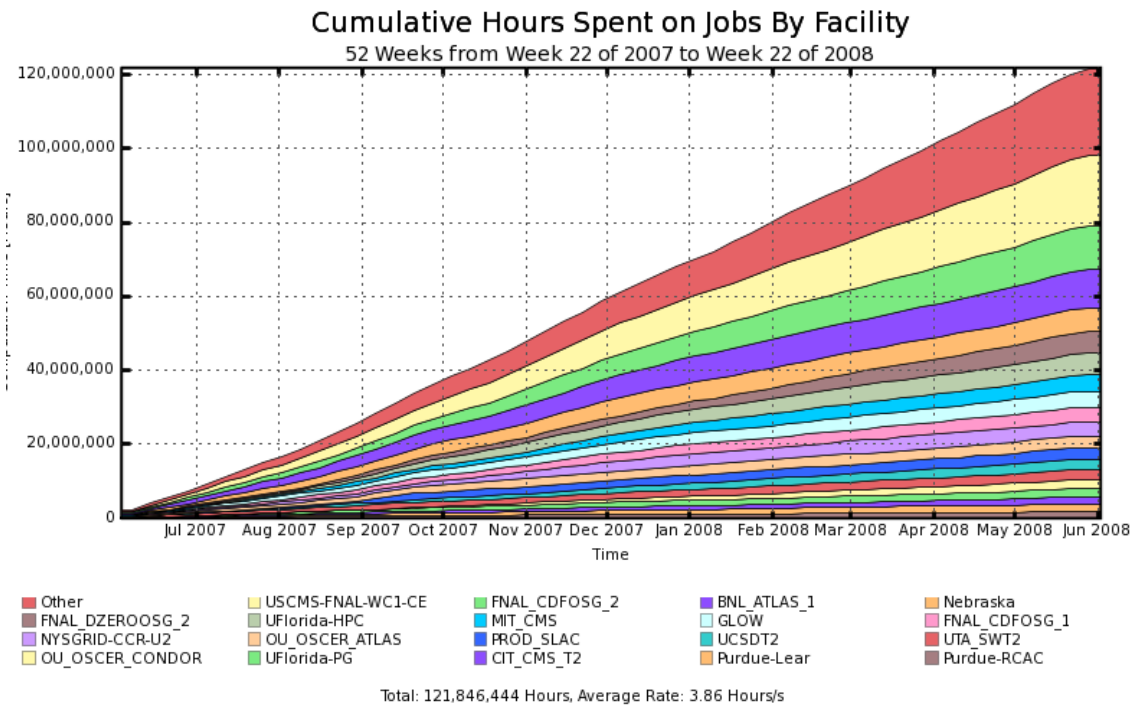
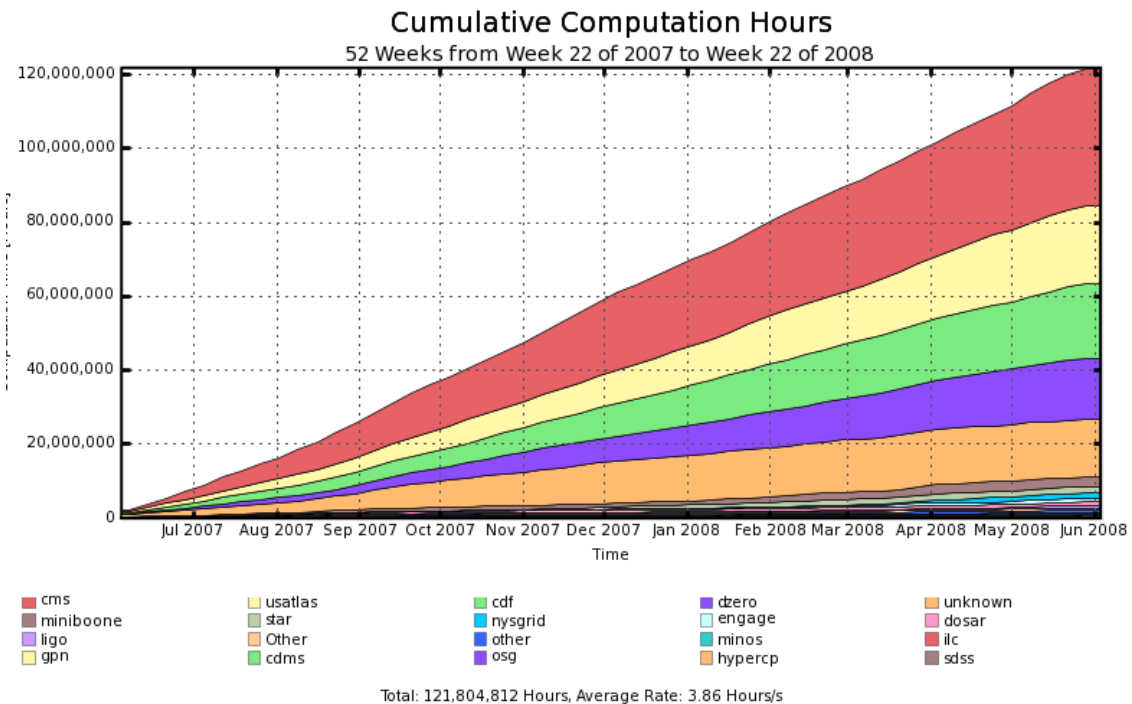


Site Availability Measured by CMS VO tests

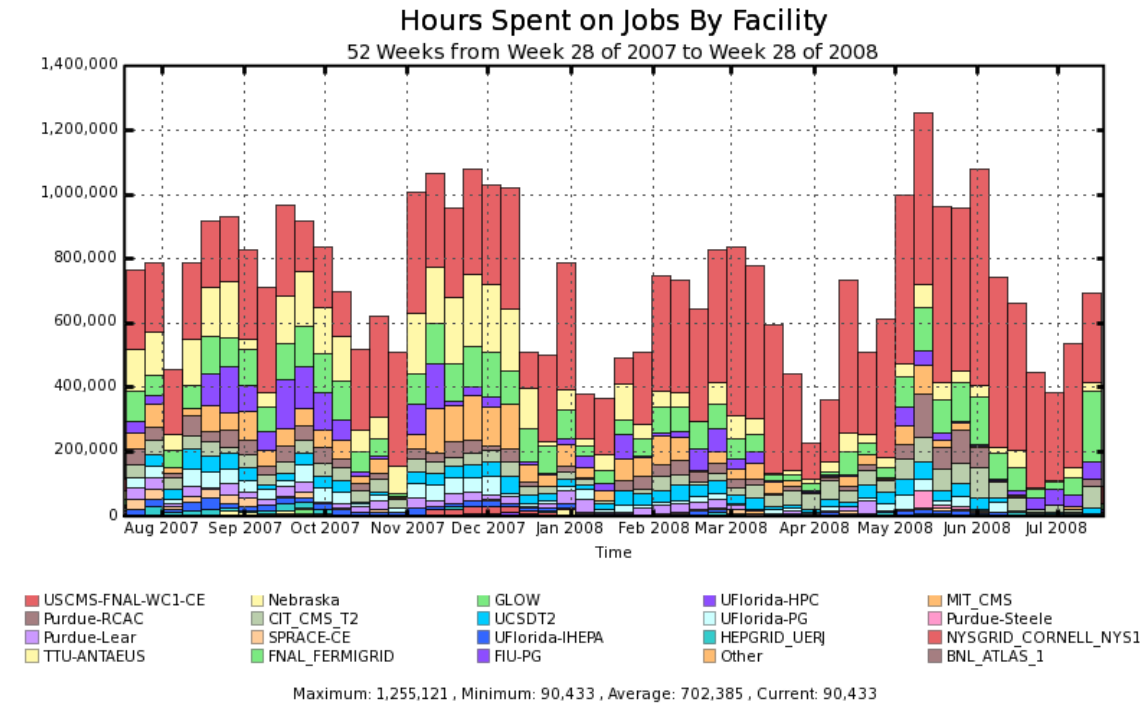
Production on Open Science Grid

1. Open Science Grid Facility Summary



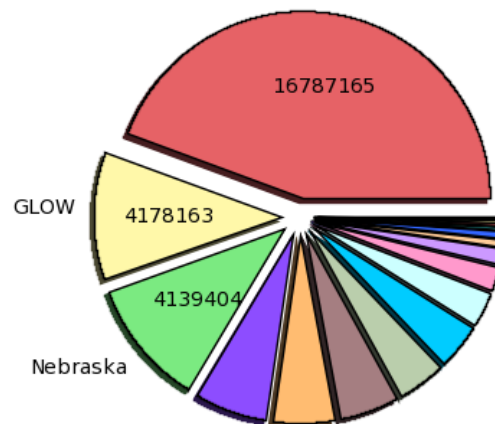


2. CMS on Open Science Grid



Wall Hours by Facility (Sum: 37816304 Hours)

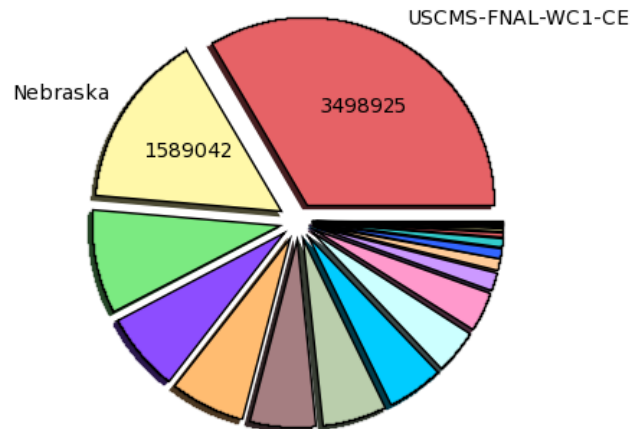
52 Weeks from Week 28 of 2007 to Week 28 of 2008
USCMS-FNAL-WC1-CE



USCMS-FNAL-WC1-CE (16787165)	GLOW (4178163)	Nebraska (4139405)	MIT_CMS (2373212)
UFlorida-HPC (2006299)	CIT_CMS_T2 (1928926)	Purdue-RCAC (1557461)	UCSDT2 (1487756)
UFlorida-PG (1126960)	Purdue-Lear (799720)	UFlorida-IHEPA (513119)	SPRACE-CE (281869)
HEPGRID_UERJ (233719)	NYSGRID_CORNELL_NYS1 (127123)	TTU-ANTAEUS (103369)	Purdue-Steele (79792)
FIU-PG (34222)	Other (32472)	FNAL_FERMIGRID (15222)	BNL_ATLAS_1 (10330)

Job Count by Facility (Sum: 10452058)

52 Weeks from Week 28 of 2007 to Week 28 of 2008

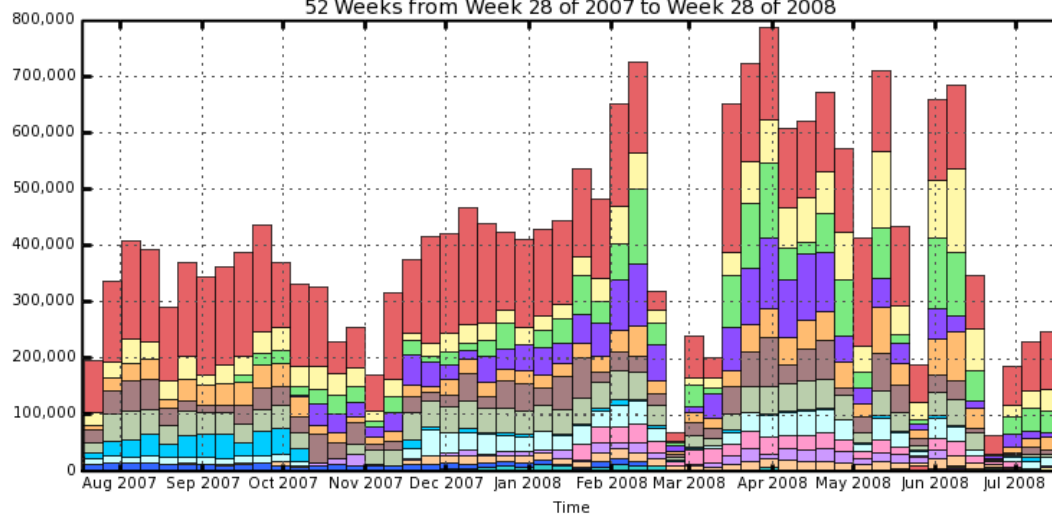


USCMS-FNAL-WC1-CE (3498925)	Nebraska (1589042)	GLOW (939775)	Purdue-RCAC (709030)
UCSDT2 (681208)	UFlorida-HPC (594264)	CIT_CMS_T2 (583721)	MIT_CMS (510182)
UFlorida-PG (408623)	UFlorida-IHEPA (355983)	Purdue-Lear (171685)	SPRACE-CE (106405)
HEPGRID_UERJ (86331)	TTU-ANTAEUS (80713)	Purdue-Steele (51639)	Other (31646)
OSG_INSTALL_TEST_2 (21540)	NYSGRID_CORNELL_NYS1 (11506)	UCR-HEP (10401)	NYSGRID-CCR-U2 (9438)

3. ATLAS on Open Science Grid

Hours Spent on Jobs By Facility

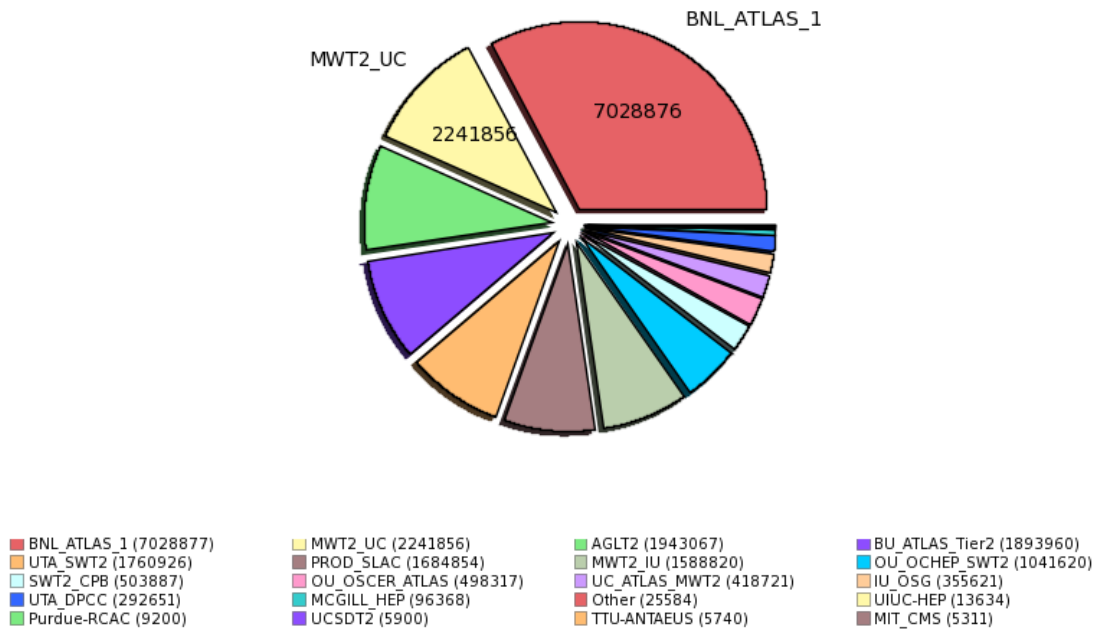
52 Weeks from Week 28 of 2007 to Week 28 of 2008



Maximum: 789,362 , Minimum: 4,153 , Average: 397,012 , Current: 4,153

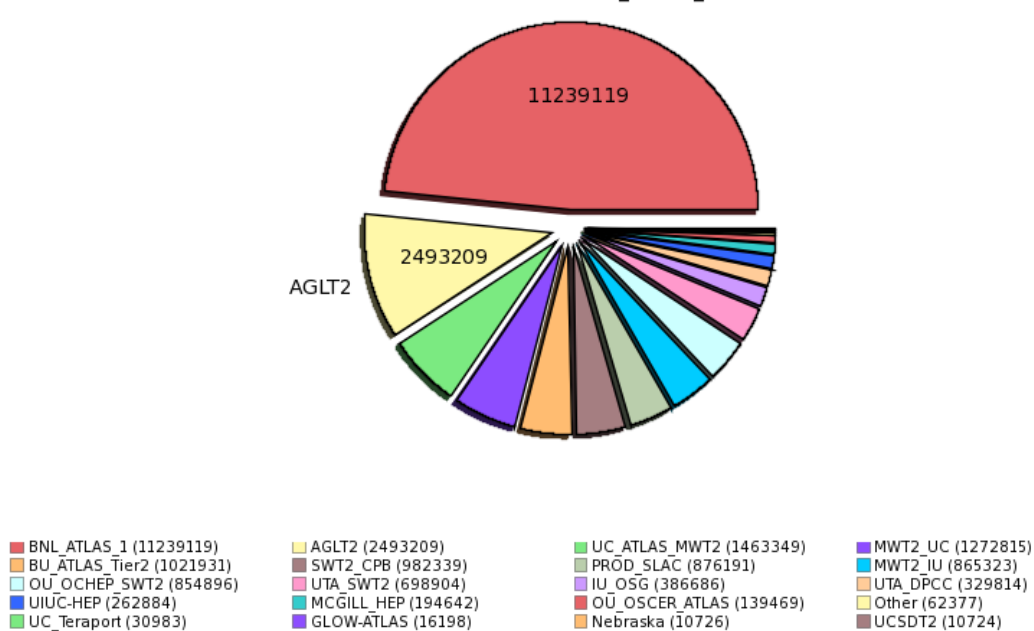
Wall Hours by Facility (Sum: 21414913 Hours)

52 Weeks from Week 28 of 2007 to Week 28 of 2008

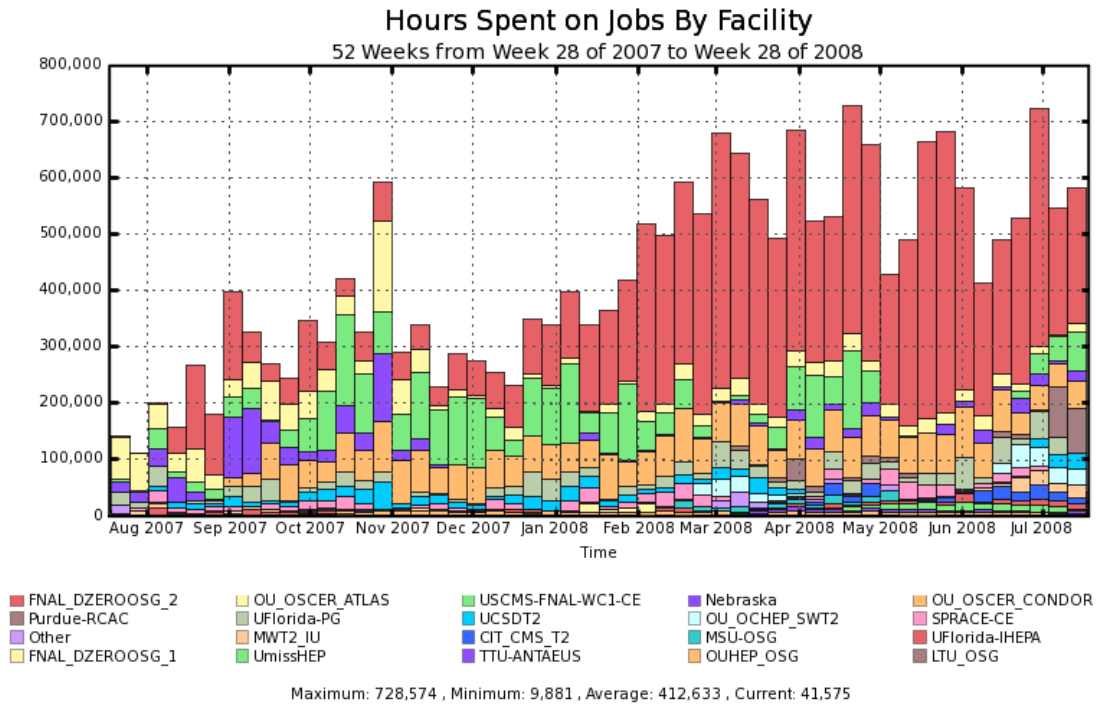


Job Count by Facility (Sum: 23212579)

52 Weeks from Week 28 of 2007 to Week 28 of 2008

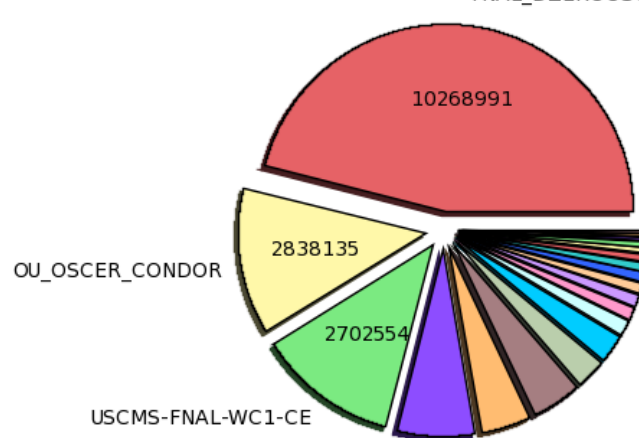


4. D0 on Open Science Grid



Wall Hours by Facility (Sum: 22272385 Hours)

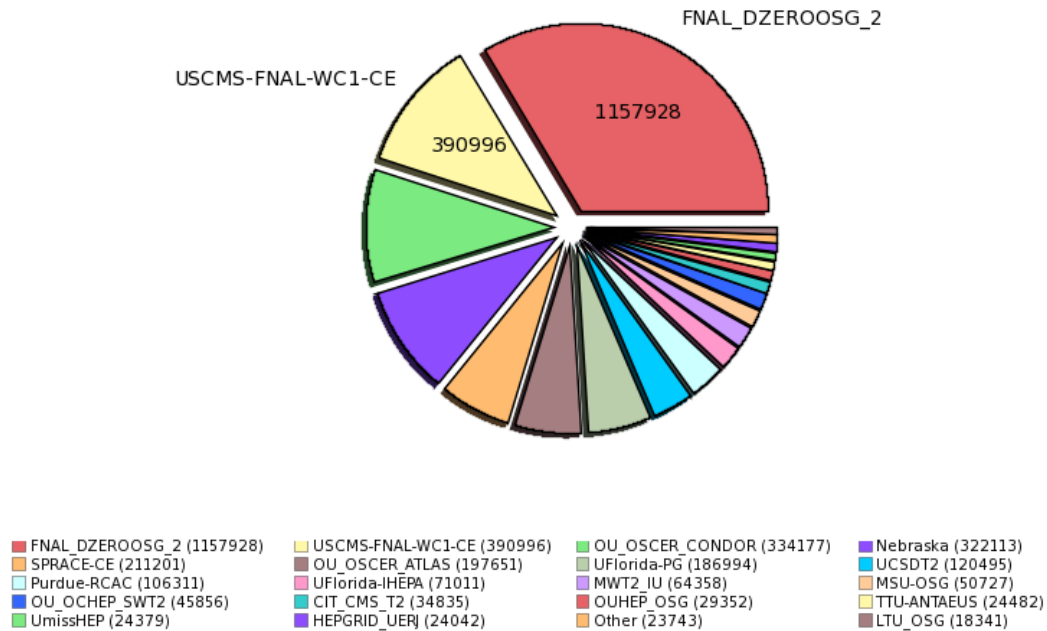
52 Weeks from Week 28 of 2007 to Week 28 of 2008



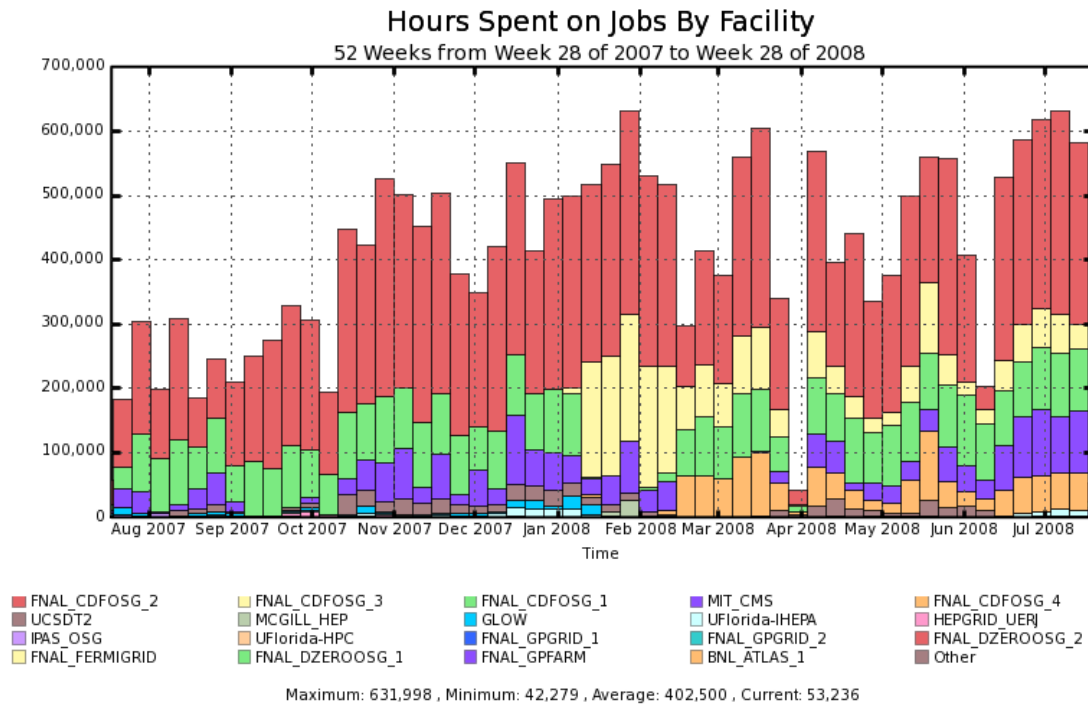
FNAL_DZEROOSG_2 (10268992)	OU_OSCER_CONDOR (2838135)	USCMS-FNAL-WC1-CE (2702555)	OU_OSCER_ATLAS (1506692)
Nebraska (970329)	UFlorida-PG (966445)	UCSDT2 (574001)	SPRACE-CE (540703)
Purdue-RCAC (292604)	OU_OCHEP_SWT2 (263366)	OUHEP_OSG (229392)	UFlorida-IHEPA (203965)
CIT_CMS_T2 (194870)	MWT2_IU (172443)	UmissHEP (133936)	Other (123331)
MSU-OSG (108773)	TTU-ANTAEUS (71180)	LTU_OSG (63208)	FNAL_DZEROOSG_1 (47467)

Job Count by Facility (Sum: 3438992)

52 Weeks from Week 28 of 2007 to Week 28 of 2008

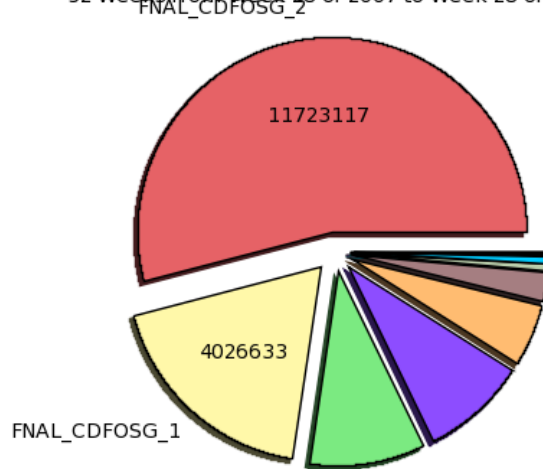


5. CDF on Open Science Grid



Wall Hours by Facility (Sum: 21679939 Hours)

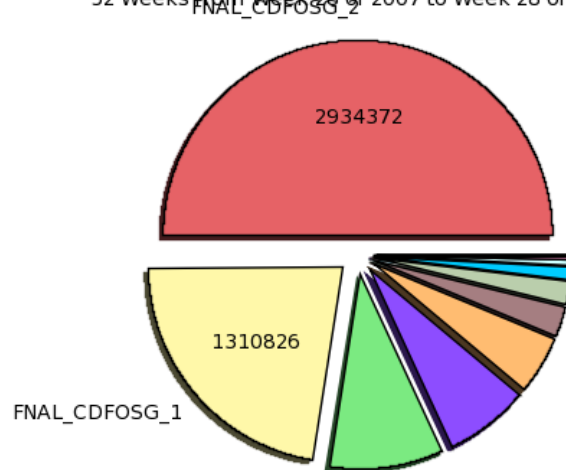
52 Weeks from Week 28 of 2007 to Week 28 of 2008



FNAL_CDFOSG_2 (11723118)	FNAL_CDFOSG_1 (4026633)	FNAL_CDFOSG_3 (2083152)	MIT_CMS (1904565)
FNAL_CDFOSG_4 (1107800)	UCSDT2 (514085)	GLOW (129001)	UFlorida-IHEPA (127249)
MCGILL_HEP (31117)	HEPGRID_UERJ (23360)	IPAS_OSG (9443)	UFlorida-HPC (372)
FNAL_GPGRID_1 (22)	FNAL_GPGRID_2 (22)		

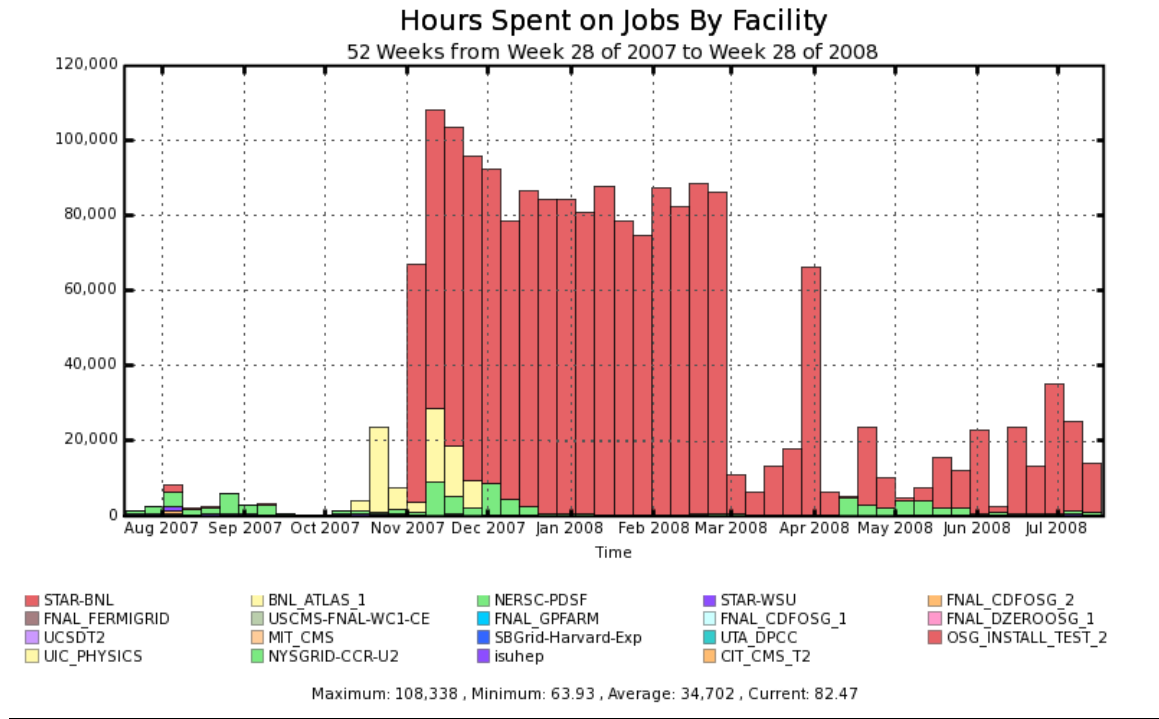
Job Count by Facility (Sum: 5859487)

52 Weeks from Week 28 of 2007 to Week 28 of 2008

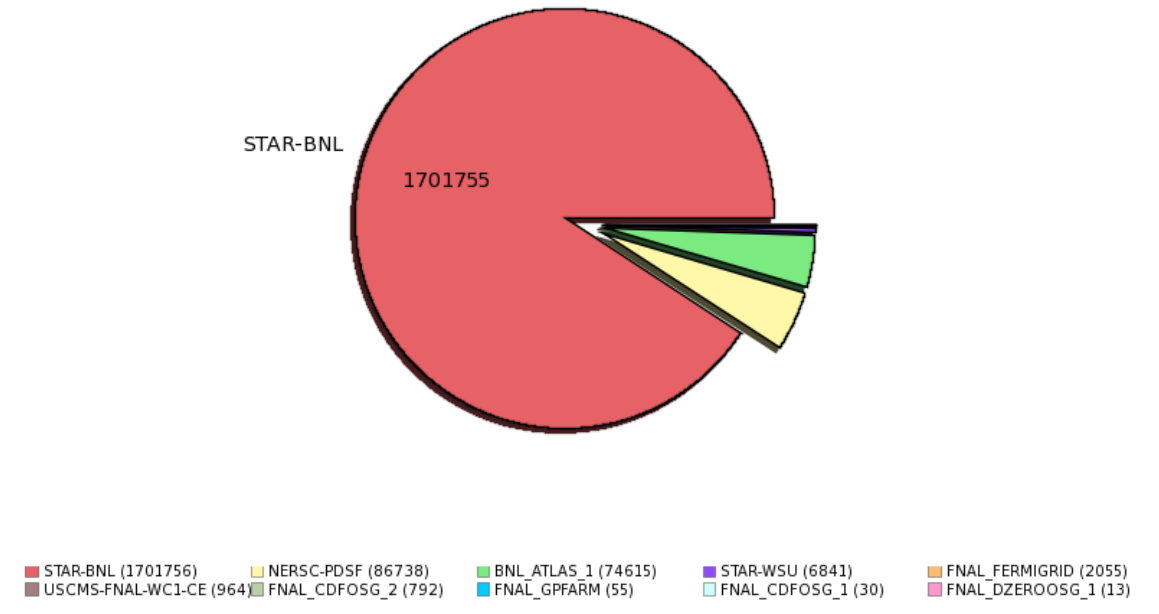


FNAL_CDFOSG_2 (2934372)	FNAL_CDFOSG_1 (1310826)	FNAL_CDFOSG_3 (555832)	MIT_CMS (412183)	FNAL_CDFOSG_4 (278304)
UCSDT2 (143630)	UFlorida-IHEPA (113528)	GLOW (62078)	HEPGRID_UERJ (27736)	MCGILL_HEP (15294)
IPAS_OSG (5566)	FNAL_GPGRID_1 (33)	UFlorida-HPC (31)	FNAL_GPGRID_2 (30)	FNAL_DZEROOSG_1 (11)
FNAL_DZEROOSG_2 (9)	TTU-ANTAEUS (8)	FNAL_FERMIGRID (7)	FNAL_GPFARM (5)	Other (4)

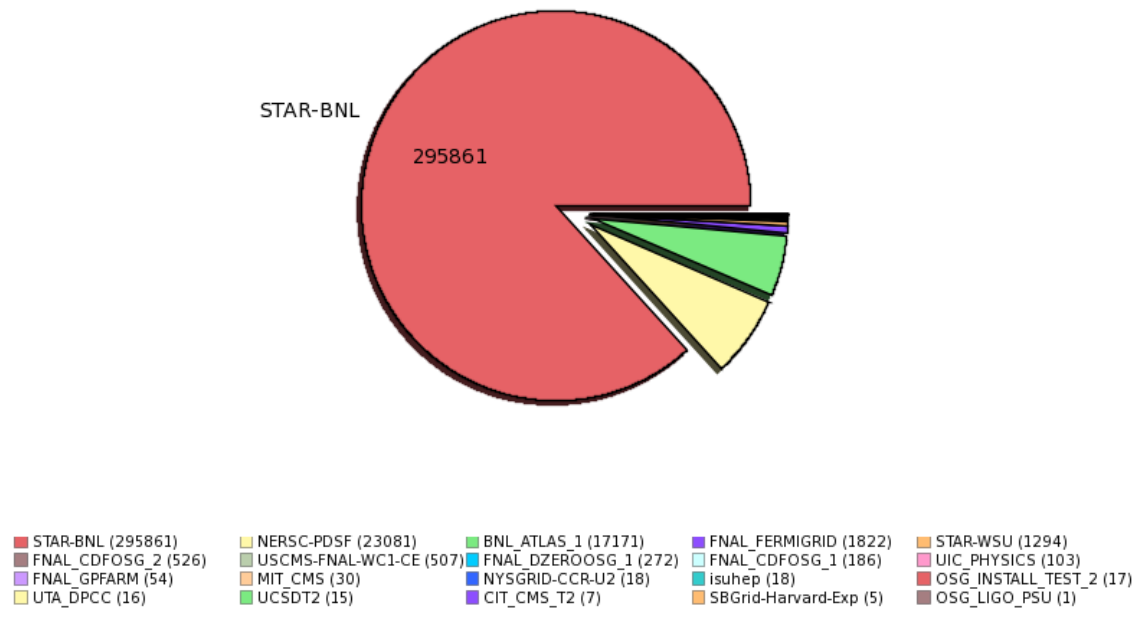
6. STAR on Open Science Grid



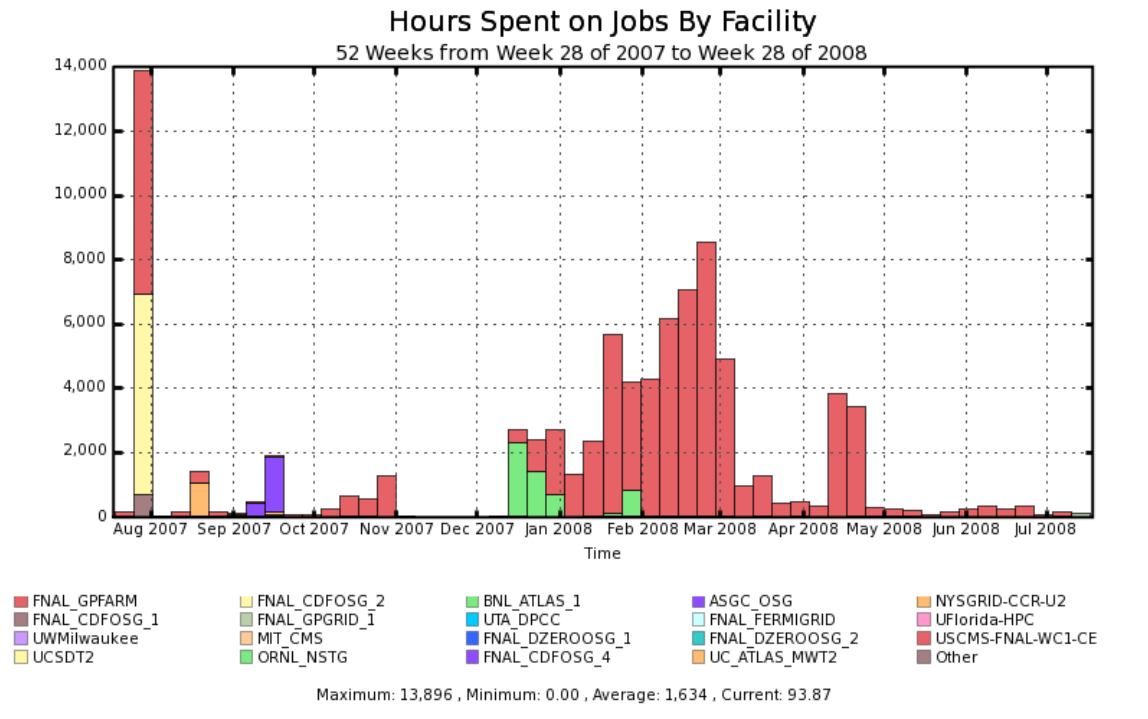
Wall Hours by Facility (Sum: 1873857 Hours)
52 Weeks from Week 28 of 2007 to Week 28 of 2008



Job Count by Facility (Sum: 341004)
52 Weeks from Week 28 of 2007 to Week 28 of 2008

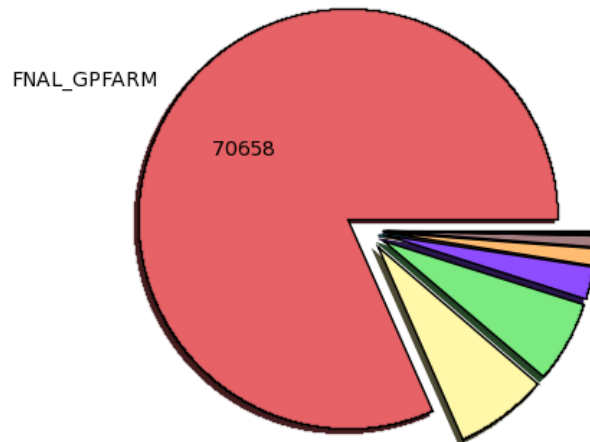


7. SDSS on Open Science Grid



Wall Hours by Facility (Sum: 86616 Hours)

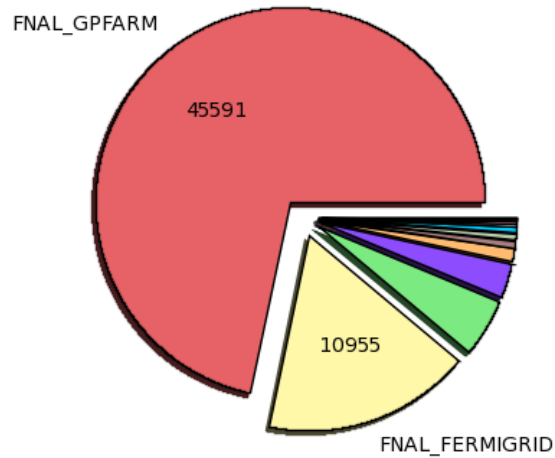
52 Weeks from Week 28 of 2007 to Week 28 of 2008



FNAL_GPFARM (70658) FNAL_CDFOSG_2 (6240) BNL_ATLAS_1 (5457) ASGC_OSG (2132) NYSGRID-CCR-U2 (1131)
 FNAL_CDFOSG_1 (711) FNAL_FERMIGRID (106) FNAL_GPGRID_1 (97) UTA_DPCC (84)

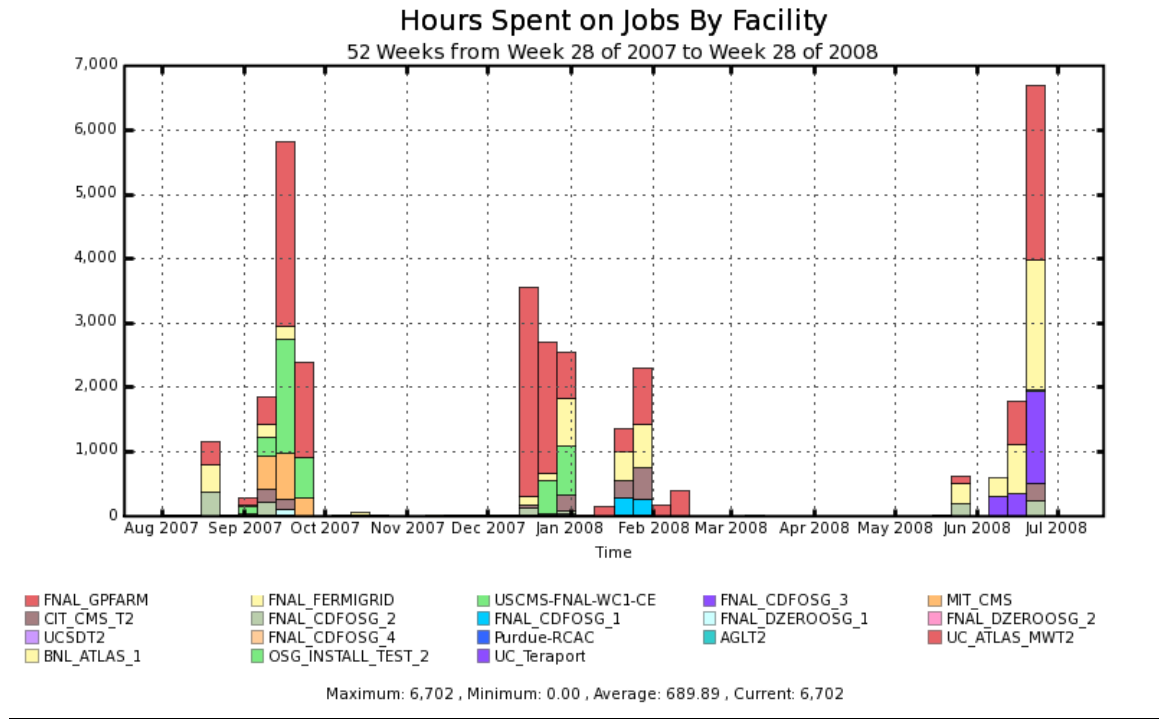
Job Count by Facility (Sum: 63553)

52 Weeks from Week 28 of 2007 to Week 28 of 2008

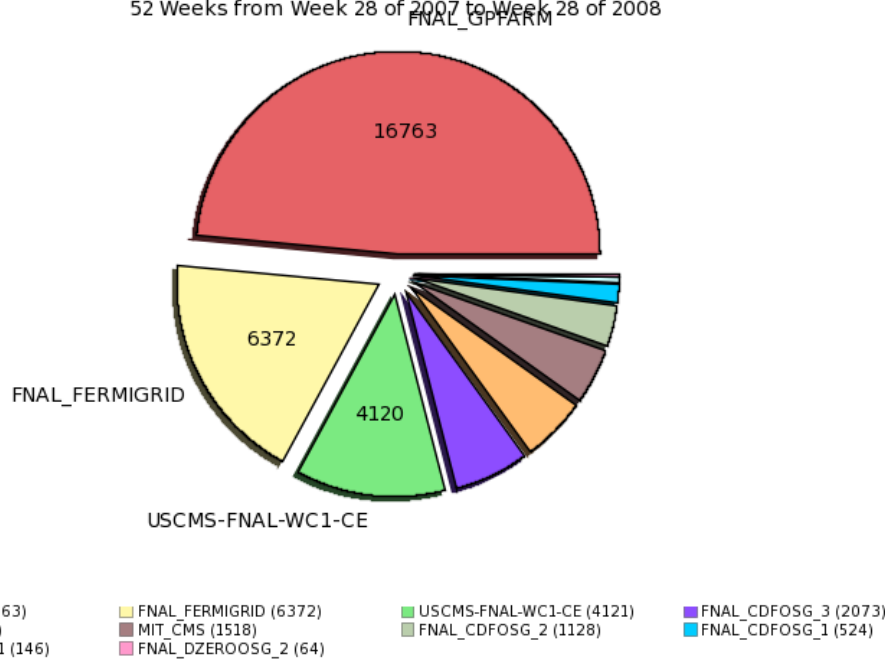


FNAL_GPFARM (45591) FNAL_FERMIGRID (10955) FNAL_CDFOSG_2 (3079) BNL_ATLAS_1 (1785) ASGC_OSG (675)
 FNAL_CDFOSG_1 (368) FNAL_DZEROOSG_2 (340) NYSGRID-CCR-U2 (303) FNAL_GPGRID_1 (179) FNAL_DZEROOSG_1 (101)
 ORNL_NSTG (32) USCMS-FNAL-WCI-CE (32) UWMilwaukee (25) UFlorida-HPC (18) Other (14)
 UTA_DPCC (14) MIT_CMS (13) UCSDT2 (12) OSG_INSTALL_TEST_2 (8) UC_ATLAS_MWT2 (8)

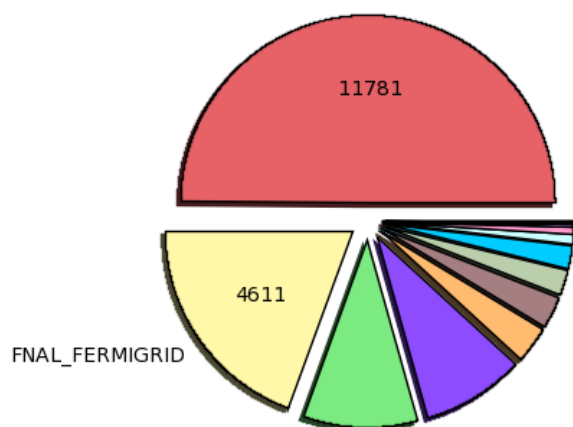
8. DES on Open Science Grid



Wall Hours by Facility (Sum: 34488 Hours)
52 Weeks from Week 28 of 2007 to Week 28 of 2008



Job Count by Facility (Sum: 23595)
52 Weeks from Week 28 of 2007 to Week 28 of 2008

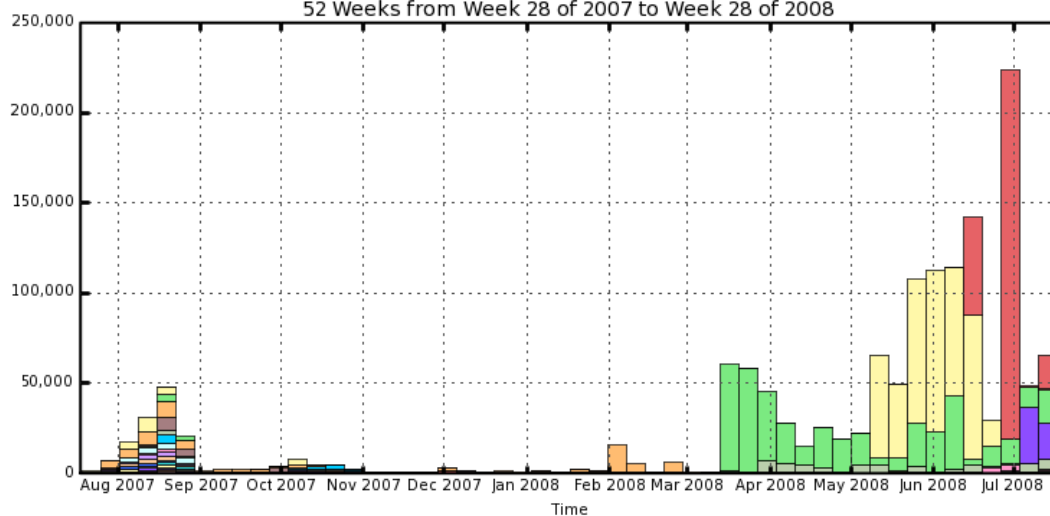


FNAL_GPFARM (11781)	FNAL_FERMIGRID (4611)	CIT_CMS_T2 (2332)	USCMS-FNAL-WC1-CE (2080)
FNAL_DZEROOSG_1 (743)	FNAL_CDFOSG_2 (655)	FNAL_CDFOSG_1 (508)	MIT_CMS (456)
FNAL_CDFOSG_3 (193)	FNAL_DZEROOSG_2 (142)	UCSDT2 (33)	UC_ATLAS_MWT2 (16)
AGLT2 (12)	UC_Teraport (8)	OSG_INSTALL_TEST_2 (8)	FNAL_CDFOSG_4 (7)
Purdue-RCAC (6)	BNL_ATLAS_1 (3)	FNAL_GPGRID_1 (1)	

9. LIGO on Open Science Grid

Hours Spent on Jobs By Facility

52 Weeks from Week 28 of 2007 to Week 28 of 2008

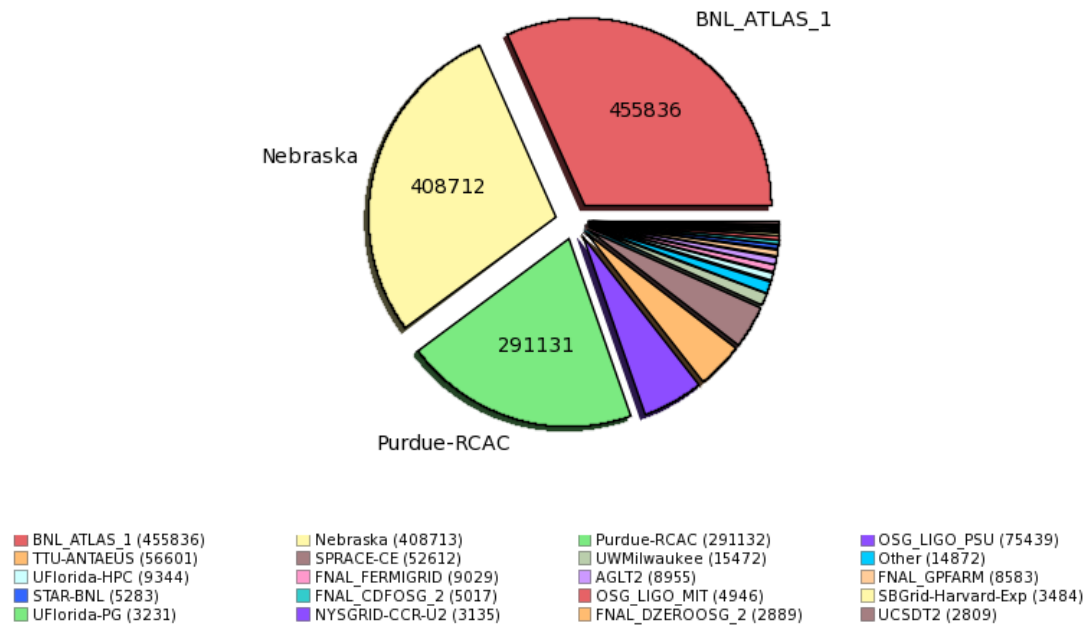


Purdue-RCAC	BNL_ATLAS_1	Nebraska	SPRACE-CE	OSG_LIGO_PSU
UWMilwaukee	TTU-ANTAEUS	UFlorida-HPC	Other	AGLT2
FNAL_GPFARM	FNAL_FERMIGRID	STAR-BNL	NYSGRID-CCR-U2	OSG_LIGO_MIT
FNAL_CDFOSG_2	SBGrid-Harvard-Exp	UCSDT2	UFlorida-PG	FNAL_DZEROOSG_2

Maximum: 224,327 , Minimum: 9.88 , Average: 26,618 , Current: 13,271

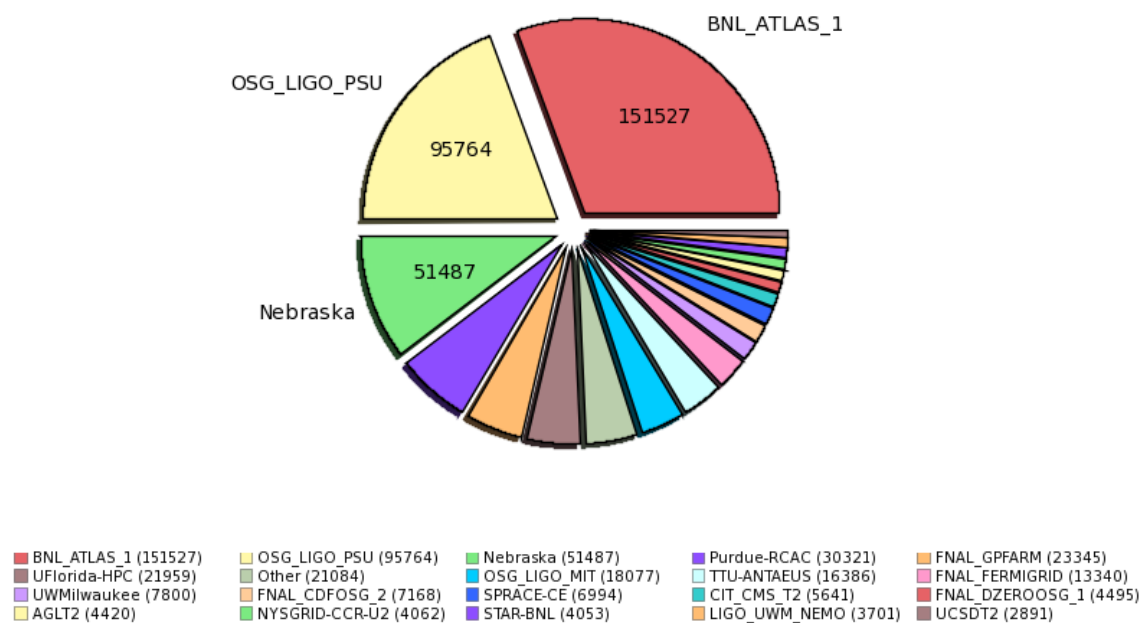
Wall Hours by Facility (Sum: 1437380 Hours)

52 Weeks from Week 28 of 2007 to Week 28 of 2008

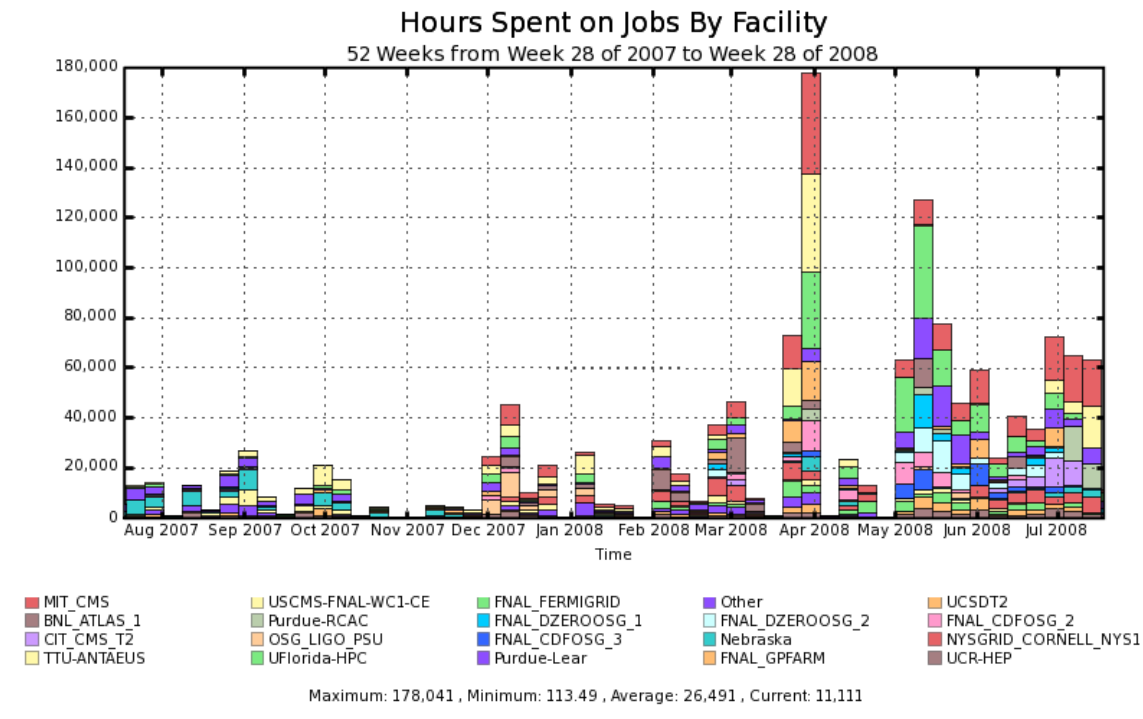


Job Count by Facility (Sum: 494515)

52 Weeks from Week 28 of 2007 to Week 28 of 2008

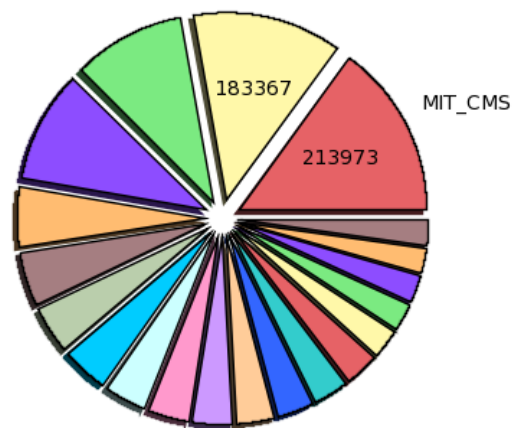


10. Engage on Open Science Grid



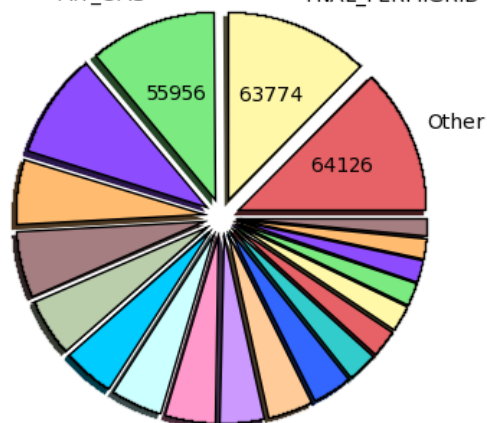
Wall Hours by Facility (Sum: 1424942 Hours)

52 Weeks from Week 28 of 2007 to Week 28 of 2008



MIT_CMS (213973)	FNAL_FERMIGRID (183368)	Other (139287)	USCMS-FNAL-WC1-CE (137587)
NYSGRID_CORNELL_NYS1 (73234)	BNL_ATLAS_1 (66628)	UCSDT2 (57930)	Nebraska (57696)
FNAL_DZEROOSG_2 (52408)	FNAL_CDFOSG_2 (50848)	FNAL_GPFARM (48716)	Purdue-Lear (46443)
UCR-HEP (44711)	UFlorida-HPC (43297)	TTU-ANTAEUS (42099)	Purdue-RCAC (36236)
FNAL_CDFOSG_3 (34376)	CIT_CMS_T2 (33177)	OSG_LIGO_PSU (31547)	FNAL_DZEROOSG_1 (31381)

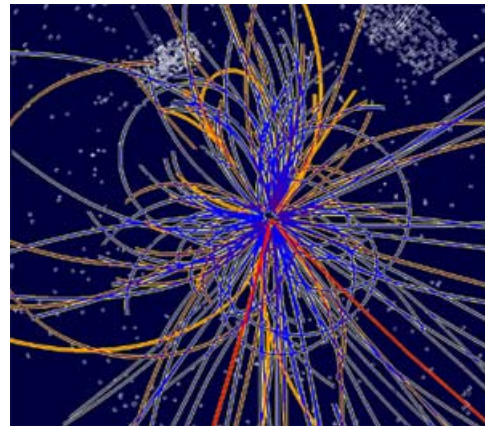
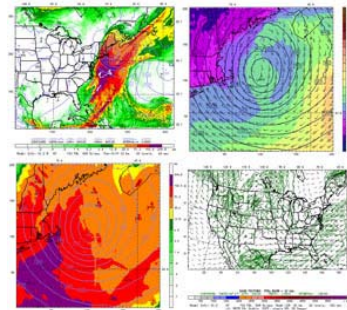
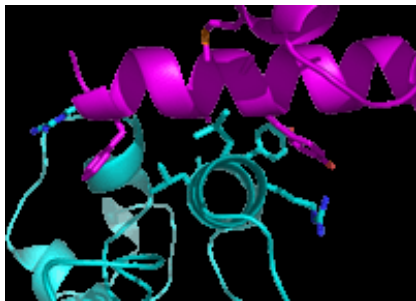
Job Count by Facility (Sum: 509194) 52 Weeks from Week 28 of 2007 to Week 28 of 2008



Other (64126)	FNAL_FERMIGRID (63774)	MIT_CMS (55956)	USCMS-FNAL-WC1-CE (46310)
UCSDT2 (28868)	TTU-ANTAEUS (28795)	NYSGRID_CORNELL_NYS1 (25092)	BNL_ATLAS_1 (22804)
Nebraska (22593)	FNAL_GPFARM (21906)	UCR-HEP (19602)	FNAL_CDFOSG_2 (19391)
Purdue-Lear (17261)	UFlorida-HPC (13278)	FNAL_DZEROOSG_2 (12077)	Purdue-RCAC (11358)
FNAL_CDFOSG_3 (9896)	CIT_CMS_T2 (9317)	GLOW (8821)	OSG_LIGO_PSU (7969)

Open Science Grid Research Highlights July 2007 – June 2008

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Computing the unseen: The search for dark matter	8
Open Science Grid crunches through CMS simulations.....	10
Grids work like a CHARMM for molecular dynamics	12
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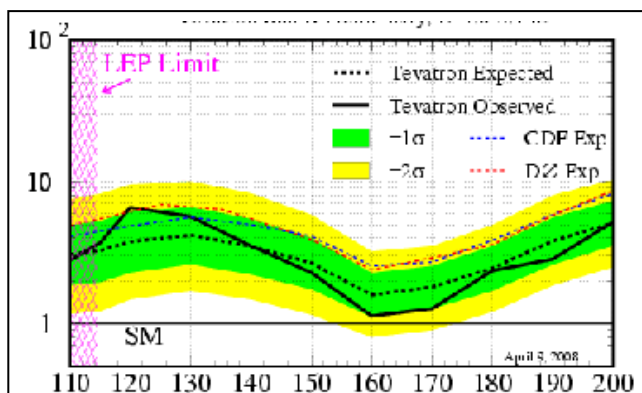
Friendly but fierce competition for the Higgs

The two Tevatron experiments at Fermilab, CDF and DZero, have nearly ruled out the hoped-for mass value for the Higgs boson—the particle regarded by some as one of the last big mysteries of the universe. Its discovery could help explain dark matter, dark energy and why particles have mass.

Against a tradition of friendly rivalry, the Higgs search provides sufficient motivation for these competitors to combine their analyses. Teams from each experiment run simulations on the Open Science Grid and compare their models to actual data. The process of combining results is a significant analysis in itself. The scientists must account for the unique uncertainties in each component of their different detectors.

“You don’t want one group to say they’ve discovered the Higgs and, using the same data, the other group to say it’s background,” says CDF physicist Tom Junk. “That would be embarrassing.”

Sharing hard-earned data requires trust.



This diagram plots the limit (at 95% confidence level) of Higgs production (y-axis) for different possible Higgs masses (x-axis). Each mark along the y-axis is a multiple of the Standard Model rate of Higgs production, and this rate is shown as a straight line at “1.” The more data Fermilab scientists collect, the closer their observed limits will get to the Standard Model rate.

Notice that the “observed” line comes vertically closest to 1, the Standard Model rate, at 160 on the x-axis. Fermilab physicists have amassed nearly enough data to make a statement about whether the Higgs exists at the mass value 160 GeV/c².

Image courtesy of the Tevatron New Phenomena & Higgs Working Group on behalf of CDF and D0.

“We spend almost the entire year dug down in our trenches, staring across at each other,” says DZero’s Wade Fisher. “Now we’re giving them our data, saying, ‘Here, open up the hood and poke around the engine a bit’.”

Through their combined efforts, the joint CDF/D0 collaboration has amassed enough data to state with 90% certainty—and likely 95% by year’s end—that the Higgs does not have a mass of 160 GeV/c².

That may seem a funny way to state a result, but it gets to the heart of the matter. The Large Hadron Collider, CERN’s massive new accelerator, will be seven times more powerful than the Tevatron. Its Higgs “sweet spot,” however, sits at 160 GeV/c². If the Higgs isn’t there, the CERN experiments will have to work harder to find it.



Members of the Higgs combination team clockwise from top left: Gregorio Bernardi (DZero); Tom Junk (CDF), Mark Kruse (CDF), Matt Herndon (CDF); Nils Krumnack (CDF); Wade Fisher (DZero); Wei-Ming Yao (CDF).

Image courtesy of the D0 and CDF collaborations.

Meanwhile, the Tevatron physicists will continue to accumulate and process data.

“Two years ago, we didn’t appear to have much chance of finding the Higgs,” said CDF’s Mark Kruse. “The use of Open Science Grid resources has

enabled us to run more simulated samples, and larger ones, which in turn has enabled us to exploit the data in increasingly sophisticated ways. I think people are starting to believe we have a realistic shot at the Higgs.”

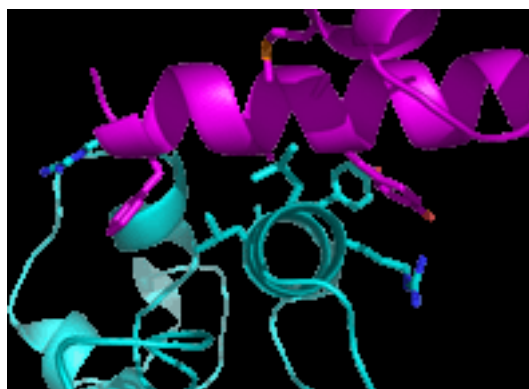
*Jennifer Lauren Lee, Fermilab
June 2008*

Matchmaking for Science

The Renaissance Computing Institute connects researchers with computing resources on the Open Science Grid

Computing enables much scientific research today, but finding the right high-end computing resources is often a challenge.

Brian Kuhlman, a biochemistry and biophysics professor at the University of North Carolina at Chapel Hill and head of the Kuhlman Laboratory in the UNC School of Medicine, needs thousands of compute hours each year to create modules of different protein configurations and determine their abilities to combine with one another. It's work that could lead to new treatments, and eventually cures, for serious diseases such as diabetes, Alzheimer's, HIV/AIDS and many cancers. And it requires computing power well beyond that of his own small research lab.



A De Novo designed protein-protein interface created with the Rosetta application developed at the University of Washington.

Image courtesy Brian Kuhlman, UNC Chapel Hill.

Catherine Blake, an assistant professor in UNC's School of Information and Library Science, works with RENCI through the Faculty Fellows program to develop a method for retrieving, analyzing and finding relationships in published research texts from multiple disciplines. The work could help researchers find research results in other fields that relates to their own fields of study and lead to more productive research practices and more cross-disciplinary sharing and collaboration.

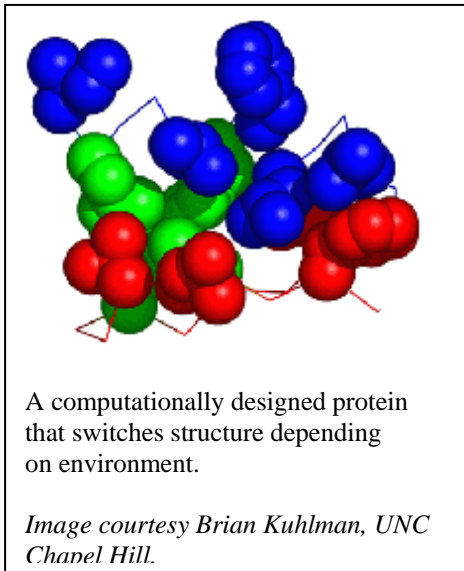


Catherine Blake

The project, called "Claim Jumping through Scientific Literature" required a staggering amount of computing time in its first phase. With help from RENCI, Blake's team analyzed 162,000 documents from a variety of scientific fields using a process called *dependency parsing*, which analyzes the grammatical structure of sentences to find meaningful relationships among words in different documents and from different fields. Generating these results on a high-end desktop computer would have required about 15,000 hours—about seven and a half years of 40-hour work weeks, said Blake.

Both Kuhlman and Blake looked to RENCI not only for the technical expertise of its staff and on-site resources, but also for its connections to a nationwide network of expertise and resources in computing and technology. Through

RENCI, they found the Open Science Grid, a consortium of universities, national laboratories, scientific collaborations and software developers dedicated to meeting the ever-growing computing and data management requirements of scientific researchers. Supported by the U.S. Department of Energy Office of Science and the National Science Foundation, OSG provides access to its members' independently owned and managed resources through a common grid infrastructure that uses high-performance networks to connect computing systems scattered across the country. As the leader of engagement activities for OSG, RENCI works with researchers to introduce them to the OSG and its resources and help them develop the skills needed to use the OSG national cyberinfrastructure.



After being introduced to the OSG through RENCI, Kuhlman's team was soon running large-scale jobs on the OSG with Rosetta, molecular modeling software used to study protein design, protein folding, and protein-protein interactions. Kuhlman's team used more than 150,000 CPU hours on the OSG in 2007—work that would have taken years on computers in the Kuhlman Lab.

For Blake and her research team, more than seven years of work was completed in about 28 hours using the grid resources of the OSG.

“We had the monumental task of parsing 162,000 documents with several thousand sentences each,” she said. “It was an ideal project for the grid

because the job is already carved up into small pieces that can use computer resources anywhere.”

“Having RENCI here at Carolina helped us access the OSG,” added Kuhlman. “That has been a huge time saver, but even more important, it has made it possible for us to examine questions that would otherwise be unanswerable,” said Kuhlman.

*Karen Green, Renaissance Computing Institute
March 2008*

Stormy weather: Grid computing powers fine-scale climate modeling

During spring, summer and early fall, sea breezes can combine with mountainous terrain to trigger heavy precipitation and stormy conditions.

This phenomenon, known as *convective precipitation*, is inherently difficult to predict and requires fine-scale atmospheric modeling.

Thanks to guidance from the Renaissance Computing Institute and access to computing power from the Open Science Grid, a team from the University of North Carolina, Charlotte, is now increasing the accuracy of these storm predictions.

Multiple models increase accuracy

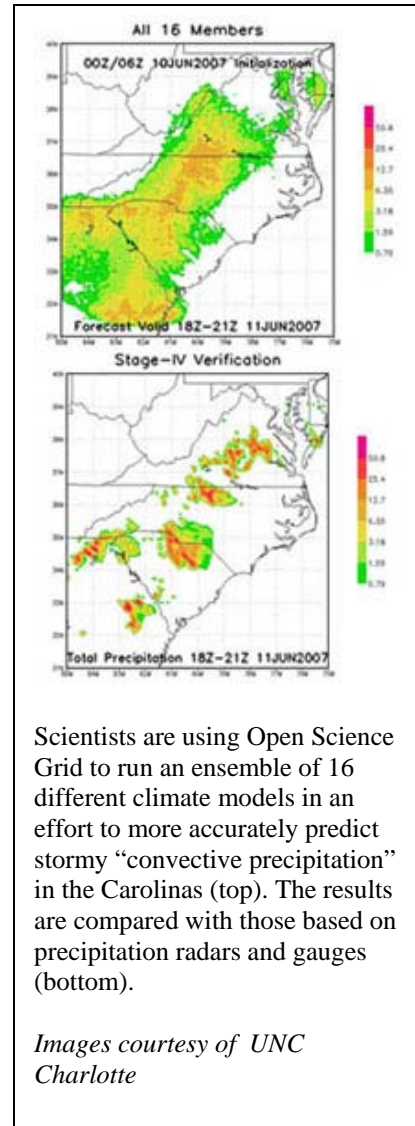
Brian Etherton and his colleagues in the Department of Meteorology at UNC Charlotte are using the Weather Research and Forecasting (WRF) system—a next-generation mesoscale numerical weather prediction system—to model volumes of space over the Carolinas at a fine resolution of around four kilometers.

In modeling these spaces, many quantities, such as wind and temperature, can be assumed to be constant throughout a particular volume. Others, like rain drops and the reflection of sunlight off clouds, vary within it. Different physics packages can be used within WRF to represent different physical phenomena and conditions.

Assembling ensembles for forecasting

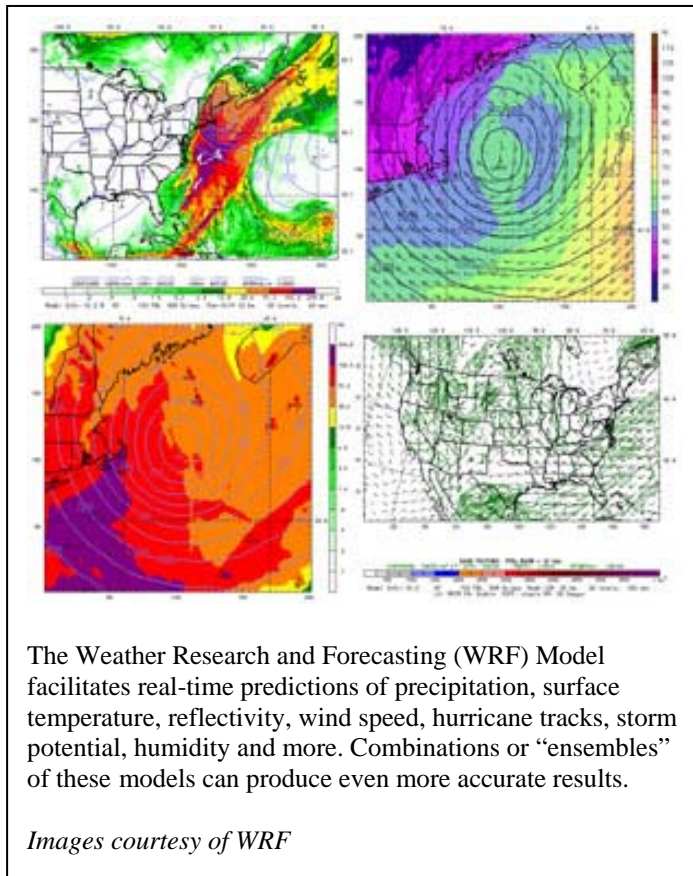
Etherton's team analyzes individual WRF model runs as well as “ensembles” of multiple runs, comparing generated results to real-world observations and varying parameter values for each run. The accuracy of results produced by ensembles is established as unbeatable compared to individual models alone.

The ensembles run thus far consist of 16 forecasts per day, differentiated by start time and a variety of physical parameterizations such as air/surface exchanges of heat and moisture.



Scientists are using Open Science Grid to run an ensemble of 16 different climate models in an effort to more accurately predict stormy “convective precipitation” in the Carolinas (top). The results are compared with those based on precipitation radars and gauges (bottom).

Images courtesy of UNC Charlotte



And the result? Probabilistic forecasts determined using the 16-member ensemble are far more accurate than those based on any one model run.

Introducing cumulus clouds

Etherton’s team is now using additional OSG resources to study the effect of another parameter: the impact of cumulus clouds transporting heat and moisture.

“These cumulus schemes were originally designed for use on larger grids of around 30 kilometers,” says Etherton, referring to volumes of space. “Their validity for such small grid sizes [4km] has always been in question. By running the

ensemble both with and without a cumulus scheme, we can quantify the benefits or drawbacks of using a convective scheme at a four kilometer resolution.”

Etherton and his team continue to make groundbreaking progress in understanding the impact of convective schemes. Their work will not only improve the forecasting of sudden stormy conditions, but will also influence longer-term climate modeling, both areas of increasing importance.

*Leesa Brieger, Renaissance Computing Institute,
and Anne Heavey, Open Science Grid
February 2008*

Computing the unseen: The search for dark matter

Think you've seen it all? Think again.

Everything we can see and detect makes up only four percent of the universe, according to Michael Weinberger, a physicist at Texas A&M University and member of the Collider Detector at Fermilab collaboration.

Weinberger and his CDF colleagues are conducting a search that could shed light on the universe's "dark matter"—material that doesn't emit or reflect radiation but is predicted by astrophysical observations to outnumber visible matter by nearly six-to-one—and they are using grid technology to expedite their hunt.

The elusive B_s decay

The key to the search is the ability to measure the rate at which B_s particles, known for their quirky ability to change rapidly between matter and antimatter, decay to form two muons. According to the Standard Model, a well-established theory that describes elementary particles and their interactions, this decay is extremely rare.

"It is comparable to you being picked randomly from the entire population of the U.S.," Weinberger explains.

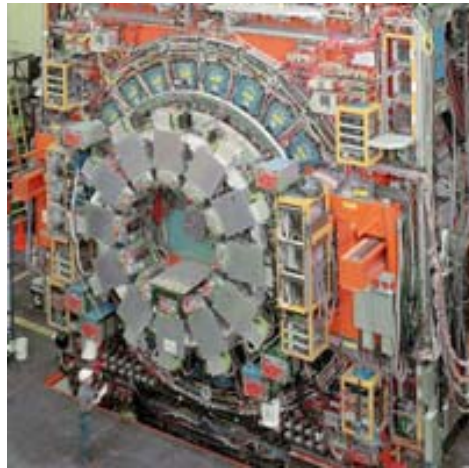
At such a low rate, researchers cannot expect to identify this decay among the trillions of proton-antiproton collisions produced by Fermilab's world-class accelerator, the Tevatron.

An invisible solution

However, alternate models such as "supersymmetry" predict that this decay is up to 1000 times more common. An observation of the rare B_s decay could provide evidence for this theory, in which each known elementary particle has a heavier superpartner.

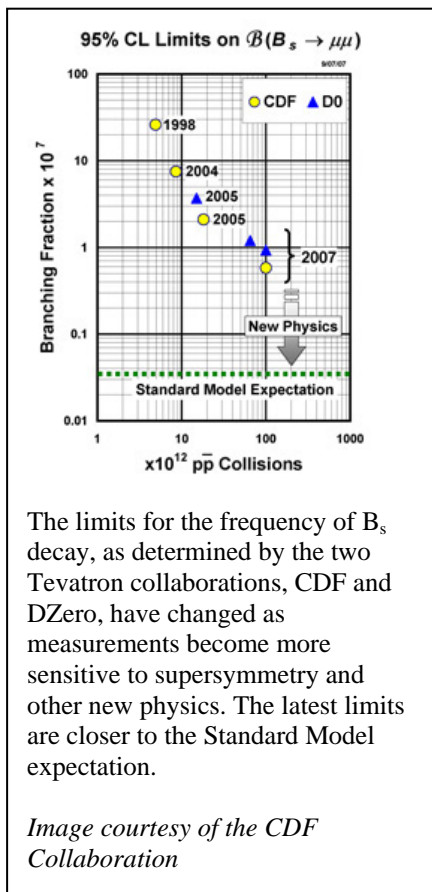
"One reason we like supersymmetry is that we haven't seen any of the particles," says Weinberger.

This makes the lightest uncharged superparticle, which would be stable if it exists, a good candidate for the dark matter scattered throughout the universe.



Researchers are using the Collider Detector at Fermilab detector to help in the search for dark matter, hoping to observe a B_s particle decay, which could provide evidence of supersymmetry and dark matter.

Image courtesy Fermilab



Grid technology enables push to new limits

To distinguish the decay from more abundant, look-alike processes, researchers employ sophisticated statistical tools developed using simulations of the particles as they travel through the CDF detector. Producing these simulations requires enormous computing power and the collaboration relies on the Open Science Grid and EGEE for the task.

“CDF is dependent upon grid technology,” says CDF co-spokesperson Rob Roser. Donatella Lucchesi, University of Padova professor and one of the collaboration’s computing coordinators, estimates that 20 percent of all CDF’s computing currently uses grid resources. She expects that to double by the end of 2008.

The researchers have not observed the rare B_s decay, but they have set the world’s best limit on how often it can occur—no more than approximately ten times the Standard Model rate. This result narrows the search for dark matter and is significantly more

precise than previous measurements. Much of the improvement is attributable to a larger data set and refined techniques for identifying and distinguishing particles, but credit is also due to the speed gained from unprecedented computing capacity.

“We have been able to produce many of the competitive results in high-energy physics because we can exploit grid resources,” Lucchesi notes.

Apparently, that’s true even when the computers have to work in the dark.

*Susan Burke, Fermilab
February 2008*

Open Science Grid crunches through CMS simulations

In the lead-up to the launch of the Large Hadron Collider (LHC) and the four massive physics projects that depend on it, scientists around the world have been giving their data processing muscle a serious workout, with superb results.

As part of the Compact Muon Solenoid experiment, Open Science Grid scientists are crunching through Monte Carlo simulations of what might happen when protons collide inside the CMS detector. Millions of proton collisions must be simulated to gather a meaningful result.

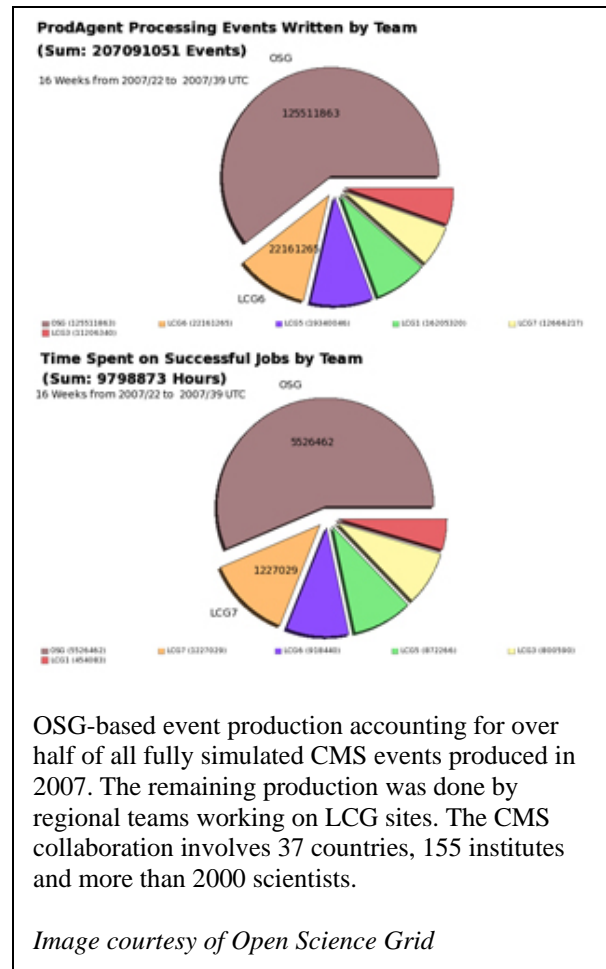
The use of OSG resources to simulate these events continues to be a spectacular success, with OSG-based event production accounting for over half of all fully simulated CMS events produced in 2007.

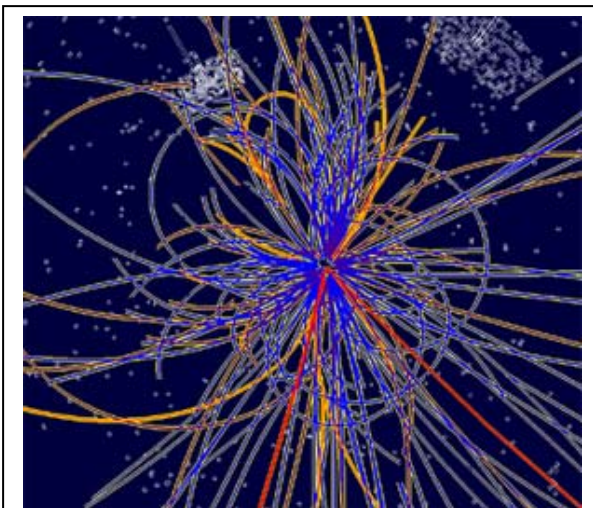
Simplicity and specificity

One key to success has been the combined use of the CMS ProdAgent workload management tool and JobRouter, coupled with the familiar Condor-G mechanism, for dispatching jobs to OSG sites. The CMS LHC Computing Grid (LCG) Production Teams used ProdAgent to drive jobs into the EGEE middleware and resource brokers and also produced a large sample of simulated events at a number of LCG sites.

Dave Evans from Fermilab and Alessandra Fanfani from INFN led the development of the ProdAgent software.

“ProdAgent allows CMS to run production across a diverse set of globally distributed systems, from grids like OSG and LCG to single farms such as the Tier-0 facility at CERN,” says Evans. “The software consists of components—developed by collaborators from all across the CMS experiment—that communicate with each other using a message passing system. This design allows us to break down a very complex workflow into a set of atomic components that work together to form an efficient, coherent system.”





The Compact Muon Solenoid experiment measures the characteristic paths traveled by particles created when protons and heavy ions collide at unprecedented energies.

Image courtesy of CERN

Black hole defense

The JobRouter Condor component, developed by Dan Bradley at Wisconsin University, is used in the OSG ProdAgent instance to dynamically route jobs to various computer farms at OSG sites.

“The JobRouter performed very well in balancing the workload under changing conditions,” says Bradley. “The software also managed to mitigate site-level ‘black holes’: sites that suddenly start rapidly failing most or all jobs.”

For individual worker-node black holes, a simple approach was used to limit the rate of failures on the node in order to prevent rapid consumption of all jobs waiting in the queue at the site in question.

The approach relied heavily on the dCache storage systems at the involved OSG sites, which were used to store the input/output data files required or produced by the jobs running locally. This significantly reduced the load on each site’s grid gatekeeper, by limiting data flow to control and debugging information only.

Summary

From June 2007 through September 2007, OSG produced about 126 million of 207 million fully simulated events and integrated consumption of about 5.5 million CPU hours. This feat was achieved—thanks to excellent software support from CMS, prompt attention by the OSG site administrators and useful monitoring tools developed by Brian Bockelman at Nebraska—using a single production server. The server comprised four CPUs with 4GB of memory and was able to handle up to 30,000 jobs in the Condor queue and to manage up to 4000 jobs running in parallel (limited due to maximum number of CPUs available) across ten OSG sites: eight in the U.S. and two in Brazil.

This work was supported in part by the CMS project and a Data Intensive Science University Network grant from the National Science Foundation.

*Ajit Mohapatra, University of Wisconsin and OSG
December 2007*

Grids work like a CHARMM for molecular dynamics

In 1963, Richard Feynman said that “everything that living things do can be understood in terms of the jiggling and wiggling of atoms.”¹

Molecular dynamics aims to better understand these jiggles and wiggles, using numerical methods to simulate the ways in which atoms and molecules move.

One tool facilitating this work is CHARMM—or Chemistry at HARvard Macromolecular Mechanics—a software application developed at Harvard University for modeling the structure and behavior of molecular systems.

CHARMM has multiple applications, but for Ana Damjanovic of the National Institutes of Health and Johns Hopkins University in Baltimore, Maryland, U.S., molecular dynamics simulations are the name of the game.

CHARMMing simulations

Damjanovic is using CHARMM to help her learn more about the interactions between proteins and water, an understanding of which can ultimately aid the design of medicinal drugs.

“I’m running many different simulations to determine how much water exists inside proteins and whether these water molecules can influence the proteins,” Damjanovic says.

“Water in protein interiors can play important functional roles—such as in enzymatic catalysis or charge transfer reactions—and when a protein moves, it can shift the position of these water molecules.”

“One of the bottlenecks in simulating how proteins function is that many functionally important motions occur on timescales of microseconds and longer, but molecular dynamics simulations can only sample real-time in nanoseconds,” Damjanovic says. “Sometimes even the processes that occur on nanosecond timescales, such as water penetration in some proteins, are not sampled properly with only a few simulations. To get better statistics, one needs to run many, many different simulations.”



X-ray crystallography at room temperature reveals only one water molecule (shown as a red sphere) near the protein residue of interest (shown in the box). The protein is a variant of staphylococcal nuclease.

Image courtesy of Johns Hopkins University

¹ Feynman, Richard (1963). “Lectures on Physics” 1: 3-6.

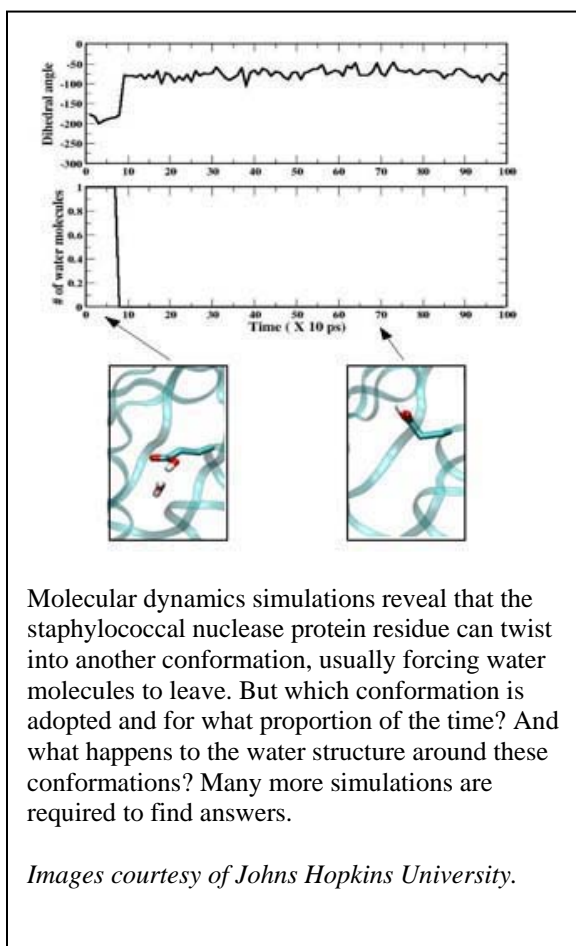
This is where it pays to have access to grid computing, which provides the large number of processors necessary to obtain meaningful sampling.

Using your CHARMM on grids

Tim Miller of the National Institutes of Health is working with Damjanovic to optimize the CHARMM application for running on the Open Science Grid.

“We have developed workflow management software for submitting and babysitting the jobs,” Miller explains. “Since molecular dynamics jobs usually take days to complete, and Open Science Grid sites are optimized for shorter jobs, each long job is split into many, many little jobs.”

The workflow uses customized PanDA software, developed at Brookhaven National Laboratory for the US ATLAS high energy physics experiment, to submit jobs to compatible Open Science Grid sites.



“Now our workflow software can keep track of the rather large number of jobs—what’s submitted and what’s left to be done—and it can then automatically submit the work that’s to be done,” Miller says. “If a job fails, this is detected and the job is then resubmitted. There are multiple threads running as well, and they can branch out and run two different types of analysis on the same structure.”

Damjanovic says her access to Open Science Grid with the newly developed workflow software has worked like a charm.

“All I had to do is initially submit my simulations,” she says. “A month later, I had statistical analysis of lots and lots of simulation. No pain, and no babysitting.”

*Jen Nahn
October 2007*

Keeping up with Moore's Law

Better, faster, and ever tinier—nanotechnology is set to shrink cell phones, computers, hair dryers, you name it. Silicon nanowire transistors, promising devices for tiny future integrated circuits, may become a driving force.

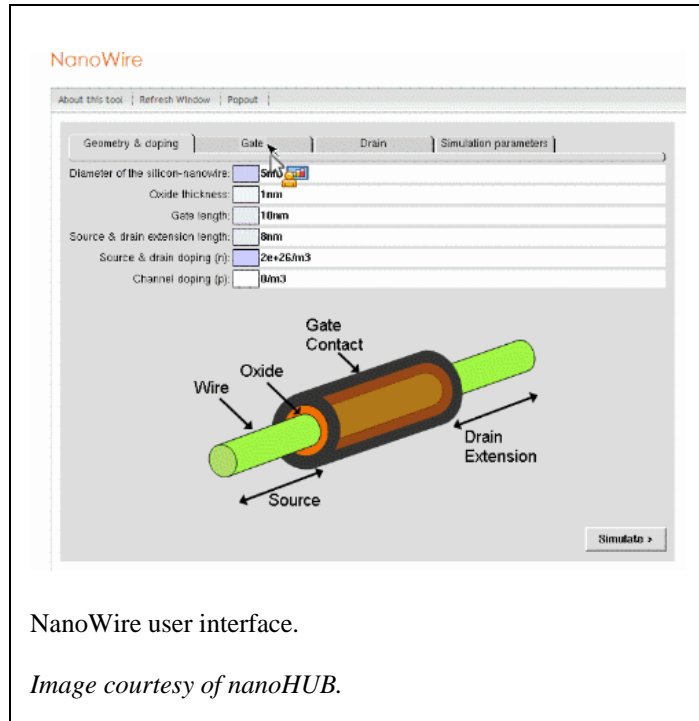
But before you can put a supercomputer in your pocket, researchers need to understand how material properties vary on an atomic length scale, and how to exploit those properties. Computer modeling serves as

virtual microscope to peer into these materials as well as a testing ground to find the best new circuit design. NanoHUB is a portal to “nano-modeling” tools, among them

NanoWire, that can run on grids.

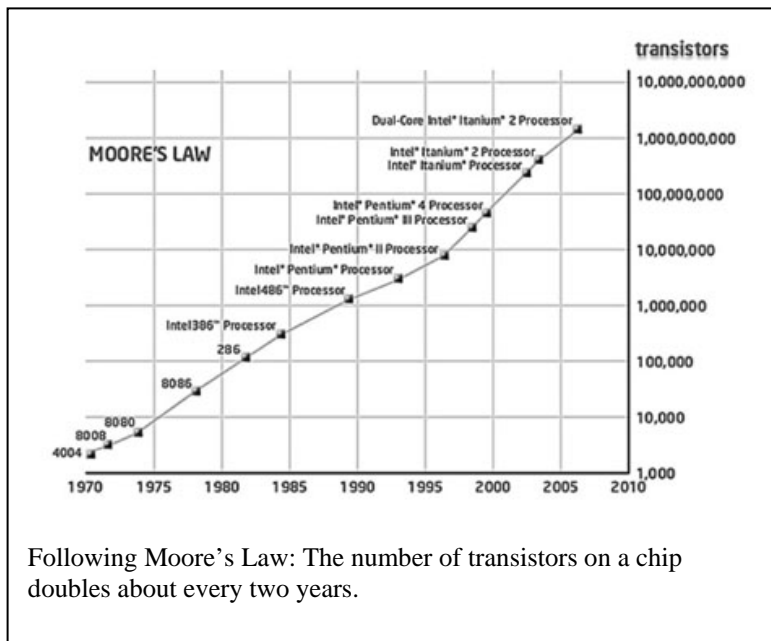
Researchers set up a NanoWire simulation through a graphical interface that allows input of device parameters and ranges of voltages to test. A simple click on “Simulate” transparently sends a set of parallel processes off to Open Science Grid, TeraGrid and/or the local cluster at Purdue. The computers send back complex and enticing electrostatic potentials and quantum

eigenstates. NanoWire makes the results easy to interpret, and the researchers are on their way to optimizing transistor designs.



NanoWire user interface.

Image courtesy of nanoHUB.



Following Moore's Law: The number of transistors on a chip doubles about every two years.

Saumitra Mehrotra and K.P. Roenker of the University of Cincinnati have run simulations on the OSG to study the effects of varying transistor variables such as body thickness, gate length and gate dielectric thickness on nanowire transistor voltages.

“We ran over 500 3-D simulations under varying conditions and gained an insight into how superior the silicon nanowire MOSFET device is relative to traditional MOSFET transistors,” Mehrotra said. “And an understanding of its limitations.”

They were able to optimize a nanowire device design for both high performance and low operating power applications, thus advancing a future technology expected to help continue the transistor scaling and extend Moore’s Law.

Anne Heavey
September 2007