XSEDE

eXtreme Science and Engineering Discovery Environment

2012 Q3: July 1, 2012, through September 30, 2012

<u>XSEDE Senior Management Team</u>

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XSEDE QUARTERLY REPORT

Contents

1 Overview

The Extreme Science and Engineering Discovery Environment (XSEDE) is the most advanced, powerful, and robust collection of integrated digital resources and services in the world. It is an integrated cyberinfrastructure ecosystem with singular interfaces for allocations, support, and other key services that researchers can use to interactively share computing resources, data, and expertise.

1.1 Project Context

Scientists, engineers, social scientists, and humanities experts around the world—many of them at colleges and universities—use advanced digital resources and services every day. Computational technologies and resources such as supercomputers, visualization systems, storage systems and collections of data, software, and networks are critical to the success of those researchers, who use them to advance our understanding of our world, and to make our lives healthier, safer, and better. XSEDE integrates these resources and services, makes them easier to use, and helps more people use them. XSEDE currently supports 13 supercomputers and high-end visualization and data analysis resources across the country.

Digital services, meanwhile, provide users with seamless integration to NSF's high-performance computing and data resources. XSEDE's integrated, comprehensive suite of advanced digital services is developing and implementing tools, methods, and policies to federate with other high-end facilities and with campus-based resources, serving as the foundation for a national cyberinfrastructure ecosystem. Common authentication and trust mechanisms, global namespace and filesystems, remote job submission and monitoring, and file transfer services are examples of XSEDE's advanced digital services. XSEDE's distributed systems architecture allows open development for future digital services and enhancements.

XSEDE also provides the expertise to ensure that researchers can effectively use the supercomputers and tools. Those include:

- Extended Collaborative Support that includes teaming with individual research groups or with research communities to extend their capabilities.
- An advanced hardware and software architecture rooted in user requirements and hardened by systems engineering that allows for individualized user experiences, consistent and enduring software interfaces, improved data management, and ways for campus resources to be transparently integrated into the overall XSEDE infrastructure.
- The XSEDE User Portal, a web interface that allows users to monitor and access XSEDE resources, manage jobs on those resources, report issues, and analyze and visualize results.
- Coordinated allocations of NSF's high-end resources and digital services.
- A powerful and extensible network, in which each XSEDE service provider is connected to a Chicago-based hub at 10 gigabits per second and has a second 10 gigabit-per-second connection to another national research and education network.
- Specialized community-provided services that serve a particular function and allow for rapid innovation and experimentation.
- Advanced cybersecurity to ensure that XSEDE resources and services provide confidentiality, integrity and availability of information
- Training, Education, and Outreach efforts that expand the scope and scale of activities to foster greater community participation in XSEDE-based projects through curriculum development, live and web-based training offerings, outreach at professional society meetings, and engagement of under-represented faculty and students.
- Advanced support for novel and innovative projects.

- A fellowship program that brings Campus Champions working closely with Extended Collaborative Support Service staff on user identified challenges for up to a year.
- The Technology Insertion Service, which allows researchers to recommend technologies for inclusion in the XSEDE infrastructure and enables the XSEDE team to evaluate those technologies and incorporate them where appropriate.

1.1.1 Communities Served

The national, and global, user community that relies on XSEDE for HPC resources has grown tremendously. XSEDE continued to see increased HPC resource user numbers in Q3 2012, with 863 new users added in the quarter. The number of open individual accounts reached 6,964, and the number of non-gateway individuals charging jobs was 2,148. An additional 1,624 users submitted jobs via science gateways—that is, over 40% of XSEDE users submitting jobs worked through gateways; this is a new high in the number of XSEDE users submitting jobs via gateways. Counting current individual accounts and gateway users together, the XSEDE community numbered 8,588 users.

Further details can be found Appendix E.

1.1.2 XSEDE's Integrated, Distributed Environment

XSEDE is taking on the difficult but necessary task of documenting a clearly specified architectural design for its distributed systems architecture. Given the nature of the end game of the proposal competition that ultimately resulted in the XSEDE award, the project has had to substantially redesign the architecture originally proposed in order to incorporate innovative and important elements of the previously competing proposal. While this has been difficult and has led to some confusion, the project is making progress in this area and will begin to produce design documents that specify the architecture in detail during the coming months.

1.1.3 Project Governance

The XSEDE project has established an organizational structure and governance that promotes efficient and effective project performance. As this is a distributed project involving 17 partner institutions and with many other stakeholders including NSF, and thousands of users, it was necessary to establish a governance model that balances efficiency and inclusiveness. The XSEDE governance model has strong central management to provide rapid response to issues and opportunities, delegation and decentralization of decision-making authority, openness to genuine stakeholder participation, and improved professional project management practices including formal risk management and change control.

The XSEDE governance model is geared towards inclusion of, and responsiveness to, users, service providers, and the NSF scientific community. The various stakeholders have input through three distinct advisory bodies, which have direct access to the XSEDE Project Director and the XSEDE senior management team through regularly scheduled meetings. In order to remain well informed of the requirements of the user community, XSEDE leadership receives advice and counsel from the User Advisory Committee, the XD Service Providers Forum, the XSEDE Advisory Board, and the TEOS Advisory Committee. These advisory committees are intimately involved with XSEDE management in guiding the project towards optimal operations, service, and support for users.

The XSEDE project is managed by a senior management team consisting of the PI/Project Director as chair, the co-PIs and key leaders of major areas of the XSEDE project, the Chair of the User Advisory Committee, and the Chair of the XD Service Providers Forum. This team is constituted from those responsible for the day-to-day operation of the project and is the highest-level management body in the organization. In order to be responsive to both the user community and the set of Service Providers with whom we will collaborate, the chairs of the User Advisory Committee and the XD Service Providers Forum are members of this team.

1.2 Project Highlights

The first quarter of Program Year 2 (PY2) has seen the project transition from a startup mode in PY1 to a project delivering value on a regular basis. This is clearly evidenced by the regular reporting of science and engineering success XSEDE has supported and enabled. In Section 2 of this report you will note a few of them we have highlighted this quarter ranging from molecular bioscience, to environmental science to planetary physics results that are very high-impact science or engineering research.

XSEDE continues its high level of support of researchers with our Extended Collaborative Support Services staff engaged in over 90 active projects during this past quarter covering a variety a areas. The requests for such support continue to be very strong via the allocation request process. Of particular note, at XSEDE12, ECSS management met with over 50 ECSS staffers as an opportunity for this very large distributed team to connect with one another and discuss critical topics such as streamlining work plans and coordination of efforts.

Through these engagements we continue to support important science and engineering advances; we provide highlights on 6 additional successes supported by XSEDE across a variety of domains in Section 2 of this report.

After an extensive program development period, the first fellows have finally been selected for the Campus Champion Fellows program. As described in the press release, our four initial fellows include Dirk Colbry from Michigan State University, Naseer Idrisi from the University of the Virgin Islands, Liwen Shih from the University of Houston-Clear Lake and Jack Smith from Marshall University.

XSEDE's Allocations team continues to coordinate peer-review of XSEDE's over-requested computing resources, and began discussing storage allocations for implementation. Requests totaling 1.1B SUs (SUs locally defined to each resource) were reviewed at the September 2012 Reviewer recommendations totaled 390M SUs with 379M SUs available. The September XRAC is historically the one that sees the most requests and several research teams were asked to shift their requests to the December XRAC next year and will do so to assist in leveling out the demands across the four XRAC events annually.

More than a dozen training events took place, including a number of large summer courses with hundreds of attendees while demand for both beginner and advanced training continues to grow.

In this quarter the XSEDE Operations team's efforts led to the completion of several milestones such as the production of the first security risk, threat, and vulnerability report; the addition of duplicate account notification and correction packets to AMIE; the implementation of state tracking mechanisms for proposal submissions and account requests; the deployment of the initial configuration instance of the new XSEDE ticket system; and the installation of the root of the namespace and secure token server for the GFFS Beta deployment.

Overall, we achieved over 99.8% uptime for all but one of the production central services (that one being "only" having a 98.7% uptime) while fielding over 2,400 tickets of which over 35% were closed within 2 business days. The User Engagements team has completed its evaluation and recommendation of a new ticket system. Approved in Q2CY2012, the new system will further improve user issue analysis, and thus drive improvements to all of the other user services activities (web documentation, XUP, training, allocations, etc.) as well as XSEDE resources.

In addition work began to support variable length awards in the Partnerships Online Proposal System (POPS), to prepare for the next increment to the XSEDE software environment, and to evaluate one-time password (OTP) solutions for federation.

As has historically been the case during the summer, a significant amount of outreach was conducted focused on faculty professional development through a series of summer workshops. However, we have also continued our efforts working with institutions on the creation of formal programs, co-sponsored student workshops, contributed to the XSEDE conference, worked to create computational modeling exercises for inclusion in the pre-service curriculum for science and math teachers, and initiated work on a repository for shared, computational science training and education materials.

Though we have been as diligent as possible, we are being faced with some “good problems” in our outreach efforts—the Campus Champions and the XSEDE Scholars Program are solid and rapidly growing beyond the resources initially allocated to support them. At the same time, it has become clear that other Outreach services, notably Student Engagement and the Campus Champions Fellowships (a joint project with ECSS) are in need of reevaluation to achieve their desired impact.

The TEOS community requirements activities have continued to move forward with updates and responses to the Community Needs Survey summary. The TEOS Advisory Committee (AC) generated a brief set of recommendations for the TEOS Level 3 managers. TEOS managers also received recommendations from the NSF review in June. The Community Requirements Manager synthesized the major points of these recommendations for a TEOS management team meeting at XSEDE 12.

A significant amount of effort in PY1 was expended on establishing many processes and practices to support the efficient and effective execution of the project. The Use Cases have very much emerged as an effective vehicle for XSEDE to gather needs that are articulated in a manner that the Architecture and Design team can work with effectively. Our first use of this practice with Campus Bridging is now leading toward a finalized Level 3 decomposition of the XSEDE Architecture in this area. With help from the Systems and Software Engineering (S&SE) team who is adopting ownership of the process, we are beginning to develop a clear practice that is shepherded and coordinated across project teams. Likewise, SD&I has now conducted its second semi-annual planning activity, identifying many tasks they need to accomplish. With guidance from the UREP (managed by S&SE) they were able to develop a clear schedule of activities informed by that prioritization process.

With our Sciforma project management software in place, we have fully populated all projects we had planned to track with this tool into the system. Next quarter we will be able to begin to reap the benefits of the effort.

During this first quarter of PY2 we have also functionally merged the activities of the Technology Insertion Service into the regular operation and conduct of the XSEDE project. Though awarded one year earlier than the primary XSEDE award, it was always intended to be an integrated activity with the rest of the XSEDE project. Though we will continue to formally submit reports for the formally independent award from NSF, the management of the activity is now been fully merged as it had always been intended.

2 Science and Engineering Highlights

2.1 Atomic, Molecular and Optical Physics: Dissociative Recombination of Electrons with Molecular Ions and Rotationally Inelastic Collisions of Rotating Molecules and Atoms (A. Peet Hickman, Lehigh University)

Physicist A. Peet Hickman of Lehigh University and colleagues used Abe at the National Center for Supercomputing Applications and Blacklight at the Pittsburgh Supercomputing Center in quantum-mechanical studies. In findings reported in *Chemical Physics Letters* (March 2012), they investigated dissociative recombination (DR), the process by which electrons combine with molecular ions to form an excited molecule that breaks up into neutral fragments. DR is important in many low-density plasmas because it affects charge balance, transforming two oppositely charged particles into two neutral particles. Hickman's calculations (using GAMESS, primarily with Abe) addressed the DR reaction involving $N2H^+$, important for understanding nitrogen chemistry in the interstellar medium. Their study provided theoretical confirmation that it is unlikely that low-energy DR can rupture the strong N2 bond. In a more recent project, Hickman and colleagues investigated the collision between rotating molecules and other atoms, which is very relevant for experiments at Lehigh University of rotating NaK (sodium-potassium) colliding with other atoms (such as He, Ar, or K). The researchers used Blacklight (to run code that Hickman wrote) for extensive electronic-structure calculations of a potential-energy surface, including dependence on the NaK bond length. Their theoretical results are in good agreement with some of the main features of the experimental results (see figure), and provide several predictions that can be tested in future experimental work, among them that the vibrational level has a great effect on the rate for rotational transitions. Experimental work is underway to test this prediction. Further calculations have shown that orientation of the molecules tends to be preserved in collisions with He, even when the rotational energy changes significantly, and that this effect is also very sensitive to the vibrational level. The calculations involved solving several hundred coupled differential equations, and Blacklight (which achieved 87 percent memory utilization on 96 cores) was particularly suitable, says Hickman, because of its large memory per processor.

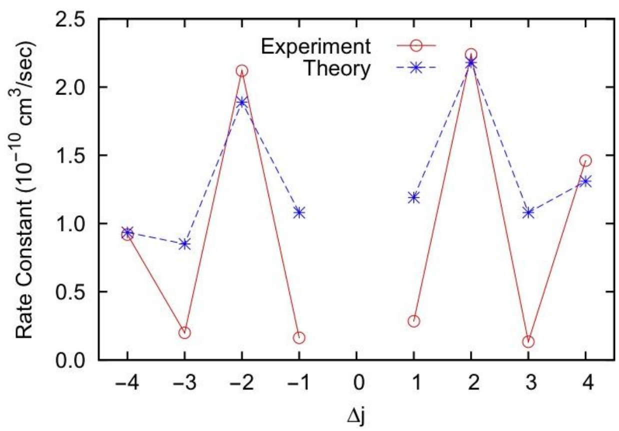

Figure 2.1. Comparison of experimental and theoretical rate constants for rotationally inelastic scattering of He + NaK at T = 600 K. These preliminary theoretical calculations were carried out for vibrational level (v) = 15. In agreement with experiment, rates for inelastic transitions with an even change in rotational quantum number (ΔJ) were found to be larger than those with odd ΔJ.

2.2 Biophysics: Protein Folding using REMD (Justin MacCallum, SUNY at Stony Brook)

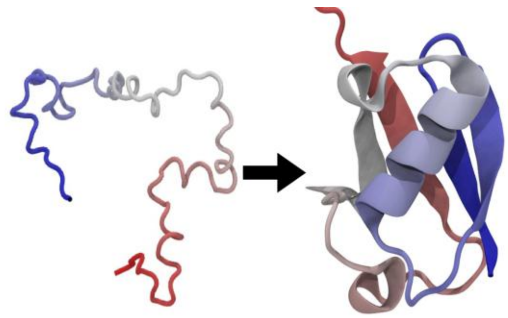

Figure 2.2. Starting from an extended chain (left) and using sparse data from solid-state NMR experiments the protein is simulated to create a model of the protein's structure (right).

Proteins are nothing without their shape. In fact, that three-dimensional shape, called the protein structure, is the determiner of a protein's function. That's why there is an important need to know what the native structures of proteins are, so scientists can better understand how they work, explains Justin MacCallum, a junior fellow at the Laufer Center for Physical and Quantitative Biology at Stony Brook University. His team of researchers — including post-doc Alberto Perez and led by Laufer Center Director, Ken Dill — used NCSA's Forge and its GPU/CPU architecture in their quest to develop computational techniques for determining protein structure. Because of the shared resources through XSEDE, MacCallum was able to transfer his work to the Keeneland supercomputer at the Georgia Institute of Technology upon the retirement of NCSA's Forge. Understanding the mechanisms of proteins helps advance fundamental biology knowledge and also can lead to practical applications, such as improved drug designs and designs of novel enzymes. Proteins are made up of chains of amino acids held together by peptide bonds. The chains then fold, turning into their structure. There is much to learn about folding and the structures, and MacCallum is developing theoretical techniques that can be combined with experimental techniques other than crystallography to get protein structures. He is using a hybrid approach that combines detailed molecular dynamics simulations with distant restraints derived from bioinformatics, evolution, and experiments. The restraints serve to restrict the size of the conformational space to be searched and make the computation tractable on current computer hardware. In some cases, they've been able to get reasonable structures from surprisingly little data. For example, one protein with which they were working had some sparse data available from solid-state nuclear magnetic resonance (NMR) experiments. That protein folds on a millisecond timescale. By inputting the NMR data into the tool, the protein folded on a 50-nanosecond timescale. Trying to get something from almost nothing is what makes the CASP (Critical Assessment of protein Structure Prediction) competition so interesting. For the first time, 2012's CASP organizers provided hypothetical data to competitors to see if extra information improved the outcomes. MacCallum says that was a good way to test their tool, and they were pleased with the one result they know to date.

2.3 Climate Science: Mid-Century Warming in the Los Angeles Region (Alex Hall, University of California, Los Angeles)

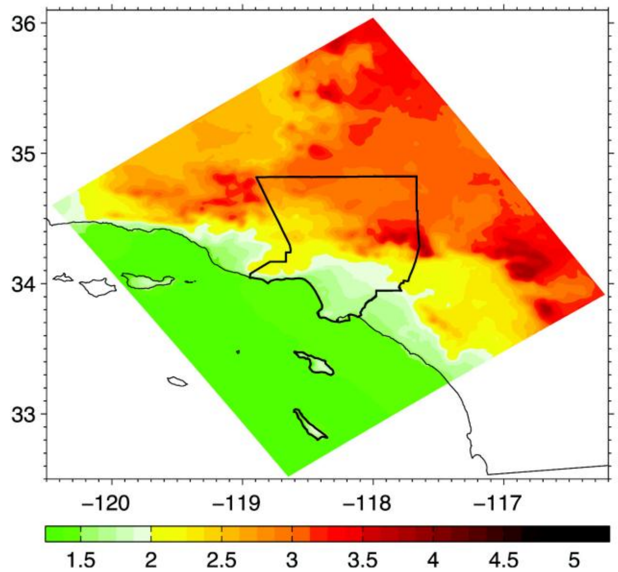

Figure 2.3. This graphic, gridded in degrees of latitude/longitude, shows change in warming (difference between 1981-2000 baseline and 2041-2060) in the greater Los Angeles metropolitan region as an annual mean surface air temperature in °F (increasing from green to red).

Through a ground-breaking initiative in regional planning, a coalition of municipalities, academic institutions, and businesses in the Los Angeles region are working to develop a Climate Action Plan that accounts for the local effects of global climate change. To lay a credible foundation for this work, Alex Hall, a professor in the Department of Atmospheric and Oceanic Sciences at the University of California, Los Angeles (UCLA), is leading an effort in computational modeling. In June 2012 he and his colleagues released a study, “Mid-Century Warming in the Los Angeles Region,” that is the first published study assessing effects of global climate change at the scale of a metropolitan region. For computational resources, Hall relied on XSEDE — in particular, Blacklight at the Pittsburgh Supercomputing Center (PSC) and, initially, Ember at the National Center for Supercomputing Applications — along with the National Energy Research Scientific Computing Center (in Berkeley, Calif.) and UCLA in-house computing. Because global climate model (GCM) results lack the detail needed to give a clear picture at regional scale, Hall and colleagues did extensive calculations to downscale GCM results to the local features of the Los Angeles area. To reliably capture information at fine enough detail on which to base planning, Hall and colleagues applied an innovative two-stage approach that drew on the archived results of 19 GCMs. The study predicts that, for the years 2041 to 2060, temperatures in the greater Los Angeles area will be higher — compared to the last 20 years of the 20th century — by an average of 4-5° F. The number of extremely hot days — temperature above 95° F — will triple in the downtown area, says the study, and quadruple in the valleys and at high elevations. The 2041-2060 model presented two scenarios for LA conditions at mid-century — “business-as-usual” with greenhouse gas emissions continuing, and a scenario with reduced emissions. The model shows that, even if the world succeeds beyond expectations in drastically cutting back greenhouse emissions, the greater LA area will still warm to about 70 percent of the business-as-usual scenario.

2.4 Environmental Biology/Behavioral Genomics: Using Next-Generation Sequencing to Identify Genetic Differences in the Social Lives of Mammals (Eileen Lacey and Matthew MacManes, University of California, Berkeley)

In the foothills of the Santa Cruz Mountains, two closely related species of mice share a habitat and a genetic lineage, but have very different social lives. The California mouse (Peromyscus californicus) is characterized by a lifetime of monogamy; the deer mouse (Peromyscus maniculatus) is sexually promiscuous. Researchers from the University of California, Berkeley examined the differences between these two species of mice on a microscopic and molecular level. They discovered that the lifestyles of the two mice had a direct impact on the bacterial communities that reside within the female reproductive tract of the species. These differences correlate with enhanced diversifying selection on genes related to immunity against bacterial diseases. The results were published in the May 2012 edition of *PLoS One*. Post-doctoral researcher Matthew MacManes performed a genetic analysis on the variety of DNA present in each species, revealing hundreds of different types of bacteria. He found that the promiscuous deer mouse had twice the bacterial diversity as the monogamous California mouse. Since many bacteria cause sexually transmitted infections (like chlamydia or gonorrhea), he used the diversity of bacteria as a proxy for risk of disease. The researchers next studied how the bacterial diversity in the promiscuous mice might translate into changes to the genes involved in immune function. MacManes hypothesized that selective pressures caused by generations of bacterial warfare had fortified the genomes of the promiscuous deer mouse against the array of bacteria it hosts. Based on a comparison of the two species' genotypes, he confirmed that the promiscuous mice had much more

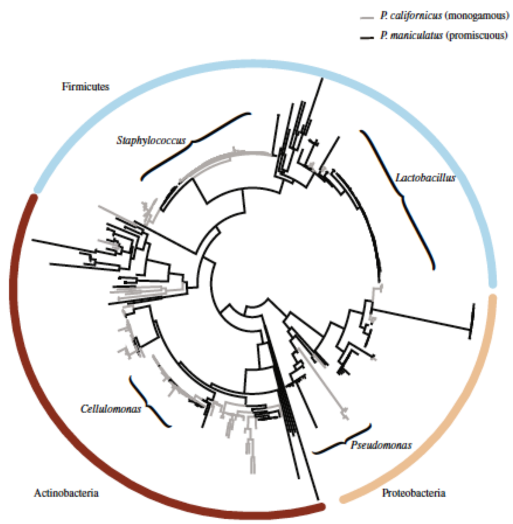

Figure 2.4.1. Phylogeny of the 16S rRNA sequences used in this study. Gray branches correspond to the bacterial sequences recovered from the monogamous P. californicus, while the black branches related to the promiscuous P. maniculatus. Phylotypes recovered in both host species were relegated to the host in which they were more common.

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Figure 2.4.2. The colonial tuco-tuco (Ctenomys sociabilis) in its native Patagonian environment (volcanic ash). The tuco-tuco is a species of subterranean rodent, related to the common guinea pig, of interest in behavioral genomics because it exhibits within one species extremes between social and solitary living conditions.

diversity in the genes related to their immune system. The results match findings in humans and other species with differential mating habits. They show that differences in social behavior can lead to changes in the selection pressures and gene-level evolutionary changes in a species. To analyze datasets too big for their university laboratory clusters, the researchers used NSF supercomputers allocated through the Extreme Science and Engineering Discovery Environment (XSEDE), including Ranger at TACC. The alignment and analysis that MacManes accomplished on Ranger in a few weeks would have taken years with his local resources, allowing him to rapidly find insights about the relationship between genes and behavior. For related genomics work, MacManes used Blacklight at the Pittsburgh Supercomputing Center (PSC), and received consulting support from Phil Blood at PSC. In the study, MacManes looked at differences in gene expression related to the transition from social to solitary living in the colonial tuco-tuco, a species of burrowing rodent. Presenting a unique case for studying social behavior, some tucos live in groups while others leave their burrow system to live in solitary conditions. MacManes used messenger RNA extracted from the hippocampus (a brain region implicated by prior research in social behavior) of captive tucos housed as two control groups — in social and solitary conditions. The extracted tissue was sequenced and yielded 56 billion base-pairs of raw data. XSEDE consultant Phil Blood of PSC installed pre-compiled modules of about 20 programs typically used in genomics assembly and analysis, which, says MacManes, were extremely helpful in identifying a number of genes that are differentially expressed according to tuco social behavior. Using 640 gigabytes of RAM (80 cores) on Blacklight, the assembly required 14 days of computing, with subsequent analysis extending for months. MacManes identified a number of genes that are differentially expressed according to tuco social behavior, and the researchers have a manuscript reporting their findings in preparation.

2.5 Molecular Biosciences: Simulations of Protein Folding and Aggregation (Joan-Emma Shea, University of California-Santa Barbara)

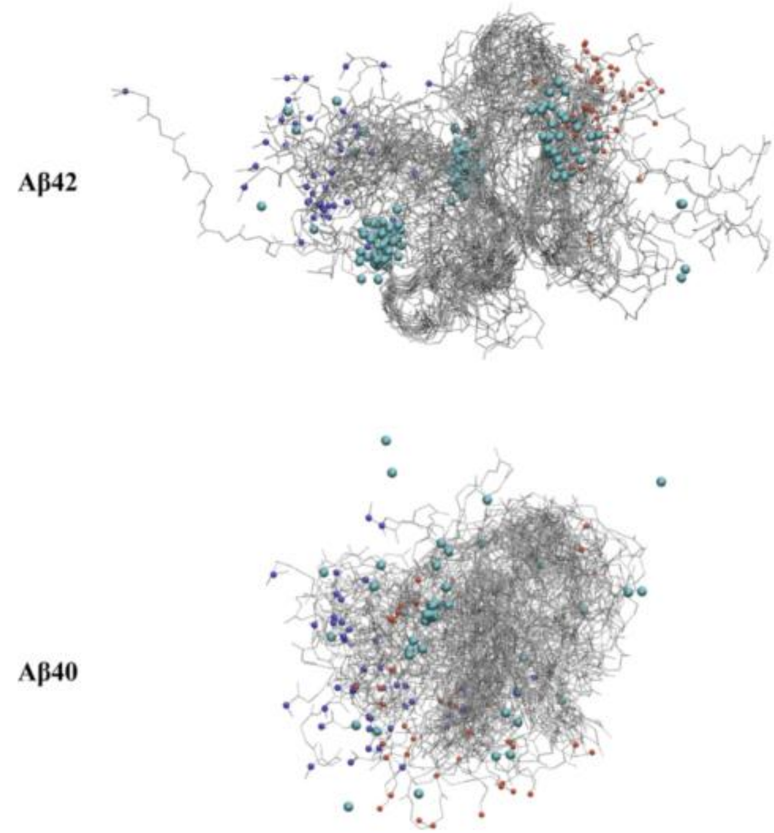
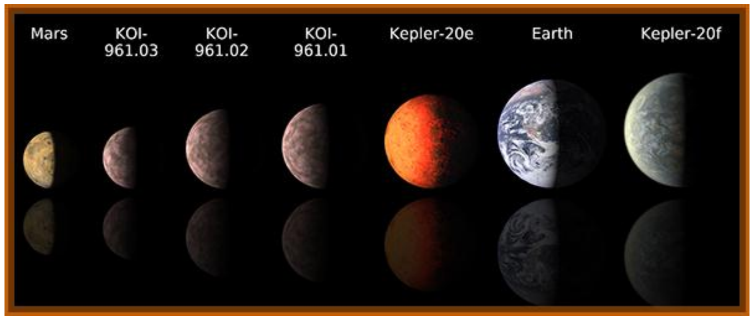


Figure 2.5. Binding of Aβ(39−42) to Aβ42 and to Aβ40. The positively charged N-termini and negatively charged C-termini are indicated by small blue and red balls, respectively. The C-terminal fragments are noted by the larger cyan balls.

Alzheimer’s disease is one of the most dreaded and debilitating illnesses. Currently, the disease afflicts 6.5 million Americans and the Alzheimer’s Association projects it to increase to between 11 and 16 million by 2050. Long knotty fibrils, formed from misfolded protein fragments, are almost always found in the brains of diseased patients. These accumulations, known as amyloid plaques, were presumed to be the cause of the disease. However, new findings support a hypothesis that the amyloid plaques are a by-product of the disease rather than the toxic agent. This paradigm shift changes the research focus to smaller, intermediate molecules that form and dissipate quickly, and are difficult to perceive in brain tissue. In 2007, Shea and Michael Bowers, professor of chemistry and biochemistry at UCSB received a grant from the National Institutes of Health to investigate small peptide-based inhibitors that would prevent these oligomers from forming. To understand the structure, formation and behavior of amyloid accumulations in the brain. the Shea group at University of California-Santa Barbara relies upon computer simulations. Since 2007, Shea has run thousands of simulations of amyloid peptides using the Ranger supercomputer at the Texas Advanced Computing Center (TACC). The simulations helped to identify the important structures that are adopted by these peptides at a resolution that exceeds what can be examined experimentally. In a recent paper in *Biophysical Journal*, Shea and postdoctoral researcher Luca Larini studied the conformations adopted by small oligomers of peptide amyloids encountered within the cell. They found that hairpin-shaped forms of the peptide initiated the aggregation of oligomers that ultimately led to the formation of a fibril. The supercomputer simulations have not only helped uncover the role of oligomers in the onset of Alzheimer's, but they are aiding in research that is trying to stop oligomer formation altogether. A paper in the November 2011 edition of *Biochemistry* described how a class of small molecules known as c-terminal inhibitors stopped the formation of oligomers, possibly halting disease progression. Since 2009, the project has used more than 13 million hours of compute time on TACC's Ranger and Lonestar supercomputers. The simulations are helping researchers identify where the inhibitors bind and are leading to new ideas about how inhibition can be improved.

2.6 Planetary Science: Search for new life (Travis Metcalfe, Space Science Institute)



The National Aeronautics and Space Administration's (NASA) Kepler spacecraft is currently on the hunt for Earth-like planets (exoplanets) throughout the Milky Way and is surveying a multitude of stars to determine how many might support orbiting exoplanets. For a planetary body to be labeled "Earth-like," its orbit must reside within the habitable, or Goldilocks (not too hot, not too cold) zone of the host star, a distance suitable for water and possibly life to exist; and it must be no more than 25 percent larger than the radius of the Earth. Kepler recently grabbed headlines with the discovery of Kepler 22b, the first planet discovered by the spacecraft that resides in the Goldilocks zone, but it failed the size test. The only method for judging a planet's size is to compare it to the star it's orbiting. And to know the planet you first have to know the star, a task being taken up by a team led by Travis Metcalfe of the Space Science Institute in Boulder, Colorado. Metcalfe was on the team that catalogued both Kepler 22b and its host star. To process the mountains of data being produced by Kepler's far-flung observations, Metcalfe used Kraken, an XSEDE-allocated resource managed by the University of Tennessee's National Institute for Computational Sciences (NICS). Metcalfe's team is measuring the properties of the stars being orbited by potential exoplanets — properties such as radius, mass, age, and bulk composition, or the proportions of individual gases throughout the star. Through an XSEDE Science Gateway, Metcalfe also is using his Asteroseismic Modeling Portal (AMP) featuring an easy-to-use interface coupled with a low-level artificial intelligence algorithm that allows users to quickly attain much-needed stellar data. For example, the data gathered by Kepler can be easily plugged into the AMP interface and the observed star modeled, thus giving researchers precious clues as to a star's true identity, which is especially important because quantifying a star's age using traditional, observational methods presents unique difficulties. Science Gateways provide easy-to-use, leading-edge tools to researchers across the scientific spectrum. The data from the Gateway gives astronomers a better idea of the qualities of any orbiting planets, a valuable tool to better understand the wider universe. Previously, said Metcalfe, his team could observe and model 12 stars in a decade, compared to hundreds every few months with the one-two punch of Kepler and Kraken. It's only in the last year that the team has been applying the AMP gateway to exoplanet host stars. And Kepler keeps the work coming, sending data for hundreds of stars every month. "We're analyzing five, 10 stars at a time," says Metcalfe, adding that his team is trying to keep up: "Kepler is specifically built for this purpose. We've never had this much data before." Metcalfe's team has been utilizing Kraken for three years now, and could not keep pace without it. So far, the team has classified approximately 100 stars, including several with planets (including Kepler 22b), said Metcalfe, and the team hopes to do 100 more this year alone. "Little jobs like ours aren't given high priority by default," said Metcalfe. "It's been outstanding to have people (at NICS) help push us through with minimal impact on the big users … The staff at NICS has been really helpful."

3 XSEDE Project Office 1.1

3.1 Overview

With only some exception, progress has been quite good in the Project Office this past quarter—though many were quite busy supporting the XSEDE12 meeting in July. The one exception has been with respect to the Industry Relations program noted below.

The Use Cases have become an effective vehicle for XSEDE to gather needs that are articulated in a manner that the Architecture and Design team can work with effectively. We have begun to develop use cases in a variety of areas as the design results of our first use of this practice with Campus Bridging is now leading toward a finalized Level 3 decomposition of the XSEDE Architecture in this area. Training on use case development has been very helpful but will require ongoing effort since we are regularly encountering stakeholders unfamiliar with the process and we go on.

Our Systems and Software Engineering (S&SE) effort has really begun to gel this quarter. With the emergence of the use of Use Case to identify researcher and stakeholder needs, S&SE staff have stepped up to help manage this process and in particular to work on engaging additional stakeholders for input. Complementing this, the User Requirements Evaluation and Prioritization (UREP) working group has met to help provide prioritization to the many tasks on the list to be done by SD&I.

Processes we have put in place are beginning to show benefits for the project. SD&I has now conducted its second semi-annual planning activity, identifying many tasks they need to accomplish. With guidance from the UREP as noted above, they were able to develop a clear schedule of activities informed by that prioritization process.

With our Sciforma project management software in place, we have fully populated all projects we had planned to track with this tool into the system. Next quarter we will be able to begin to reap the benefits of the effort.

3.2 Project Management and Reporting 1.1.1

Project Management Software Tool

A test environment has been created for testing changes to the Sciforma PM software tool. The Sciforma PM software tool underwent additional customization to make it more usable for identifying the best available resources for a task as well providing additional reports. The enhancements are currently undergoing acceptance testing. Production implementation of these updates is expected in Q4. Sciforma has distributed version 5.0 which has a new token model. Tokens are used to give access to functionality for each user of the system. The new model will free up over 40 tokens which will allow us to accommodate some of the additional user of the system due to organization changes etc. without having to purchase additional tokens. Version 5.0 will be implemented in production along with the previously mentioned enhancements. All existing ECSS projects have been created in Sciforma as have the reporting schedules and the overall XSEDE Schedule.

Reporting

The combined Annual and Q2 2012 Report was completed.

Quarterly Meeting

The fifth XSEDE Quarterly meeting was planned and held September 11/12 in Champaign, IL.

3.3 Systems and Software Engineering 1.1.2

During the quarter ending 9/30/12, the Systems and Software Engineering Team (S&SE) has accomplished the following:

Gathering New User needs and Capabilities

Early in the project we expected that users would be willing and eager to send in requests for new capabilities. As it turns out, this was a somewhat naïve perspective – users are simply more used to "making do" and coping rather than asking for new things. Until we can reeducate users about this process, we will need other ways to gather information about what users need and want to guide XSEDE development activities. With this in mind S&SE has becomes involved with the user facing project areas of XSEDE (ECSS, the NIP group in particular, User Engagement, Campus Champions, etc,), joining in their regular conferences calls and email discussions to tease out new user needs and capabilities. We are also reviewing reports of meetings, "Birds of a Feather" sessions, surveys, and other user outreach events for similar information. The information collected is of a widely disparate nature – some simple requests, some that are much more difficult and have architectural significance. We've begun discussion about how best to get these capabilities and needs into the XSEDE "pipe" for processing by the appropriate XSEDE group and will hope to formalize this process within the coming quarter.

Requirements Analysis

Working with the Use Cases and associated documents developed by the Architecture and Design (A&D) group for Campus Bridging, S&SE has gone through these Use Cases and pulled out addition requirements to be added to the baseline System Requirements Specification. We will continue this activity for new use cases that come out of A&D.

User Requirements Evaluation and Prioritization

The User Requirements Evaluation and Prioritization (UREP) working group reviewed and ranked work that was proposed by the XSEDE Software development and Integration Team. Results of this review will guide the activity and work carried out by the SD&I group during the next 2 quarters. This was the first such review of SD&I proposed work by the UREP, and we learned much from the process. We are hoping to make this a regular, biannual, event. Additionally, two new members were added to the UREP during this quarter, Jeff Pummill and Mark Miller. Both are also members of the User Advisory Committee and bring a unique, and much needed, user perspective to the UREP.

Establishing an XSEDE Component Registry

S&SE and members of the XSEDE Architecture and Design (A&D), Software Development and Integration (SD&I) and Operations (OPS) groups began work to develop a registry of XSEDE components. The goal of this effort is to provide XSEDE management with a mechanism to easily track key components throughout XSEDE processes, from the architectural stage, through development and integration, and on to production operation. This will enable us to provide better tracking and reporting about the status of new capabilities that we have added to help XSEDE evolve and grow in response to changing user needs.

XSEDE Digital Object Repository

XDOR, the XSEDE Digital Object Repository, will be used to preserve all the key documents and digital objects for the XSEDE project via the University of Illinois IDEALS digital repository for research and scholarship. During this quarter we developed documentation and procedures for using XDOR. We also recruited another member for the XDOR committee, Jim Ferguson from NICS, to help with reviewing and processing documents and to help decide on an appropriate document numbering and organizational structure for XDOR.

3.4 Architecture and Design 1.1.3

During Program Year 1 (PY1) the A&D team worked to establish a process for collecting, documenting and reviewing use cases with quality attribute scenarios and associated XSEDE architectural level 3 decomposition responses. Our first architectural area, Campus Bridging, was the focus. This was very much an important team and process building exercise however, we learned that process was too slow to meet the needs of the other XSEDE software engineering teams (SD&I, SYS-OPS, Security and S&SE). We had to come up with a more “fine-grained” approach that would allow us to focus on a single use case at a time, rather than a complete set, so that we could continually provide new actionable use-cases for SD&I and SYS-OPS to put through their processes and ultimately into production. To accomplish this the A&D team focused on engaging all XSEDE Architecture Area leads in the development of use cases and corresponding quality attribute scenarios in the first quarter of PY2. This strategy is particularly important in that Felix Bachmann’s XSEDE effort will be ramping down in PY2 and ending by PY3. This allows us to make optimal use of Felix’s time by allowing all the area leads to engage with him immediately, rather than one area at a time. Another benefit to engaging all area leads now is that if there are unforeseeable delays in the development of use cases for our planned focus area, as we saw with Science Gateways, the A&D can move ahead to use cases from other areas that are ready.

Architectural Area Leads Identified

The following people were identified as having in depth knowledge and understand of how researchers want to make use of XSEDE resources for each particular area.

- Campus Bridging
    - Rick Knepper
    - Craig Stewart
- Science Gateways
    - Nancy Wilkins-Diehr
    - Suresh Marru
- Computing
    - High Performance Computing
        - Mark Fahey
        - Sergiu Sanielevici
    - High Throughput Computing
        - Mike Wilde
    - Scientific Workflows
        - Ravi Madduri
        - Marlon Pierce
- BIG Data
    - Data Analytics
        - Nick Nystrom
        - Shawn Strande
    - Data Movement, Storage, Backup & Archival
        - Christopher Jordan
        - Kurt Seiffert
    - Visualization
        - Kelly Gaither
        - Sean Ahern
        - David Bock
- Connecting Instrumentation
    - Rick McMullen

    - Jim Shank
    - Lothar Bauerdick
- Collaboration
    - Scott Lathrop
    - Jeff Pummill

Use Case Development Training

All area leads have been invited to participate in our weekly A&D Team call. We've been using this time to discuss new use cases as they are being developed while all other area leads can listen, ask questions, and start thinking and working on the use cases for their areas. Participation on these calls has been excellent and we have seen early use case development from Science Gateways, High Performance Computing and Data Analytics. All other area leads have been asked to prepare at least one use case by October 25th, 2012.

Susan Mehringer from CAC has been developing a Virtual Workshop, web-based training module, based on materials from Felix Bachmann's tutorial XSEDE'12 tutorial in Chicago. We plan to have this available for all members of the community in Q2.

Area leads have also been invited to listen in on the A&D reviews of the use cases to prepare them for their reviews in the future. These reviews include the stakeholder review, where the area leads are asked to confirm that the architectural response to their use cases is appropriate and the active review with the SD&I, SYS-OPPS, Security, and S&SE teams.

Development of a Use Case Registry

David Lifka (A&D), JP Navarro (SD&I), Victor Hazlewood (SYS-OPS), and Janet Brown (S&SE) have started development of a "Use Case Registry" system. Use cases describe, "what a user wants to do with XSEDE" and how they expect it to perform and behave. This registry system will allow our team members and XSEDE management to track any use case throughout the software engineering cycle. Once a use case is created by an area lead or anyone with a high priority requirement and it has been reviewed and accepted by A&D, it will enter the system and be tracked through the various documentation, development, testing and review procedures of A&D, SD&I, SYS-OPS, Security and S&SE. This will ultimately provide important metrics as to what new services are made available to the XSEDE user community over a specified period of time.

Q1 Activities

- XSEDE Architecture Level 3 Decomposition – *Final reviews before being ready to be public facing*
- Campus Bridging
    - *L3 documentation completed for all 5 initial use case*
    - *2 of 5 use cases reviewed and approved by SD&I, SYS-OPS, S&SE & Security*
    - *L3 documentation to be released with appropriate information stating whether a use case has been approved by SD&I, SYS-OPS, S&SE & Security*
- Science Gateways
    - *3 of 5 initial use cases and quality attribute scenarios completed*
    - *Remaining 2 of 5 use cases completed and ready for review*

Q2 Planned Activities

- XSEDE Architecture Level 3 Decomposition - *public facing before the end of October*
- Campus Bridging

- *All 5 of the initial use cases reviewed and approved by SD&I, SYS-OPS, S&SE & Security*
- *Level 3 documentation to be released with appropriate information stating whether a use case has been approved by SD&I, SYS-OPS, S&SE & Security before the end of October*

- Science Gateways
  - *All 5 initial use cases and quality attribute scenarios completed*
  - *A&D Internal and stakeholder reviews completed*
  - *Review of initial use cases started by SD&I, SYS-OPS, S&SE & Security*
  - *Level 3 documentation completed for all 5 initial use cases*

- Other Architectural Areas
  - *1 or 2 initial use cases submitted for each area to be reviewed and discussed on weekly A&D team calls and accepted as a use case submission*
  - *Level 3 decompositions for individual use cases from any area will be prioritized and completed based on their availability*

- Use Case Registry System
  - *Planning and initial development for use case registry system continues*
  - *Details of procedural steps from each of the software engineering teams will be documented and reviewed*
  - *Initial tracking system will be developed*
  - *All use cases submitted, previously and new, will be entered into the system*

3.5 External Relations 1.1.4

3.5.1 Accomplishments

The External Relations team was focused on the XSEDE12 conference for much of the first month of the quarter, contributing to daily communications updates, signage at the hotel — including a daily schedule posted outside each room being used for that day, and photography and reporting for key events during the conference. Successful media coverage included placement of nine conference-related stories from four XSEDE ER writers and extensive blog posts from deputy director of EGI, with whom ER enjoys a collaborative relationship.

The announcement of the PRACE-XSEDE open call for Expressions of Interest in joint projects also was released during XSEDE12 and was published by more than one media.

Follow-up for XSEDE12 included: creating itemized list of communications-related expenses, mailing out all award certificates for recipients unable to receive them in person at conference, creation of certificates of appreciation for conference sponsors, and posting links to presentations, and award/recipient information on conference website.

ER promoted the following events via XSEDE website, Facebook, Twitter, User News, and through email lists directly to all XSEDE staff and the media: NCSA's Alan Craig as new XSEDE DHS, Eclipse Parallel Tools Platform user call, XSEDE User Engagement monthly calls, NSF's Research Data Alliance planning meeting, OpenACC GPU Workshop, NSF award for Science Gateways Institute planning, NSF-XSEDE Cloud Use Survey, and NCSA's Petascale Day.

ER regularly contributes copyediting and/or distribution of XSEDE documents, writings, and announcements, which include the following for this quarter: ISGTW story with Jim Kinter focus, I-CHASS announcement of Kevin Franklin's appointment to XAB, XSEDE13 SIGAPP in-cooperation request, first cohort of Campus Champions Fellows, Campus Champions Support position job posting, revised Science Gateways and What is XSEDE? flyers, and Steve Gordon's paper, "Advancing Computational Science Education through XSEDE."

The team continues to contribute to monthly newsletters with internal and external focus, Inside XSEDE and What's New in XSEDE, respectively, which are widely disseminated.

Greeted visitors, answered questions, and represented XSEDE in the Governor's Tent during opening day at the Illinois State Fair.

Participate on bi-weekly basis in planning for XSEDE13, on Key Leads and Logistics & Local Arrangements committees, and regarding communications needs. Contributions this quarter include: draft of tax-exempt letter, preparation of documents necessary for in-cooperation status and publishing of proceedings in ACM Digital Library, design and production of print and online banner, revisions to sponsor letter, design and production of conference website.

Several communications staff joined the ER team this quarter, including: Liz Murray, NCSA; Greg Kline, Purdue; Ruth Pordes, OSG; Ken Chiacchia and Shandra Williams, PSC; and Ceci Jones Schrock, Indiana. Science writer Caitlin Rockett left NICS and the ER team in July.

A priority project for ER this quarter was production of the annual highlights book, with distribution scheduled for mid-November at SC12. Work this quarter included: ranking and selection of story ideas with input from XSEDE senior leadership, issued RFPs for design and printing and selected vendors, approved design concept, created drafts, addressed senior leadership requests, and provided final copyedited stories.

Planning for the XSEDE exhibit at SC12 in Salt Lake City included: developing cost comparisons for booth, creating booth design and securing final approval, coordinating all paperwork associated with booth, selection and ordering of items for booth – notepads, pens and stickers, creating signup Doodle for staffing the booth.

Created online registration and connected to payment system for quarterly meeting.

Collaborated with TEOS staff to produce discipline-specific handout for use at discipline conferences and first draft of general TEOS informational flyer. Also participated in discussion of how and where to house educational materials TEOS wants to share with the public, including materials generated by TEOS-based events.

Followed up on recent events and produced certificates for 60+ participants in EU-U.S. HPC summer school, and posted Extreme Scaling Workshop presentations on the event website.

Finalized Program Year 2 communications plans and timeline.

Continued efforts include: participating in document repository discussions, including selecting IDEALS as the repository and discussing file naming conventions; regularly maintain updates to XSEDE website, including replacing rotating graphics on homepage; for each quarter -- create registration form for meeting participants and contribute science highlights and ER team accomplishments to quarterly report; strategic communications plan still in progress.

3.5.2 Media Hits

XSEDE saw its most successful quarter thus far, with more than 60 news items published on XSEDE-related topics, as tracked during the quarter. An Excel file containing specific media hits has been submitted for inclusion in the Appendix.

3.5.3 Challenges

NCSA is still working on filling an open XSEDE ER position.

3.6 Industry Relations 1.1.5

As discussed in our PY2 Program Plan, this area made no progress in PY1 with intent to initiate activity in PY2. The first step in that process was to work with the XAB to schedule a further discussion of the notional plans and programs and develop the ideas further. This is to be followed by the development of a clear plan for the remainder of PY2 and to project forward future activities. This has been hampered by difficulty in scheduling the interaction with the XAB. Though the plan was to have this program area documented and more fully developed by the end of the first quarter of PY2, we did not complete this as yet. The interaction with the XAB is scheduled for October 12, 2012. We will be working to draft a program description by the middle of November.

3.7 Software Development and Integration 1.1.6

In February of 2012 the Software Development and Integration (SD&I) team conducted its first *semi-annual* planning activity that identified over 100 software development and integration activities. With Operations input we prioritized 16 of those activities and started working on them during the 4th quarter of project year 1 (April – June 2012). During this past quarter SD&I made significant progress on these 16 activities by conducting joint design reviews with Operations, developing and preparing the software for XSEDE integration, conducting software testing, and handing off deliverables to Operations, most notably:

- We delivered an Execution Management Services (EMS) based on UNICORE 6 with GridFTP stage-in/out support for production deployment by Operations.
- We delivered a new increment of the Globus Online Data Transfer Services for production deployment by Operations and which addresses all the security issues identified by Operations during PY1 3Q. Most notably: the integration of OAuth limited proxies to reduce the impact of stolen credentials, improved integration and documentation in the User Portal, and several internal security design and operational improvements.
- We prepared an enhanced GridFTP service for production deployment by Operations that addresses known defects and replaces software inherited from TeraGrid with an upgrade that has undergone the more rigorous XSEDE software engineering and testing process.
- We prepared a new integrated increment of Genesis II GFFS and EMS UNICORE 6 for beta deployment and use by the Campus Bridging effort. This increment provided requested documentation improvements and several other important improvements.

In summary, during this quarter 1 of 16 projects was canceled, 10 of 16 were complete, and 5 of 16 are still in progress.

In preparation for a new round (increment 3) of development activities, in September we launched our second *semi-annual* planning activity to identify software projects to be worked on during the 2nd and 3rd quarters of project year 2 (October 2012 thru March 2013). This planning activity was significantly different to previous planning activities in that for the first time we used the Systems & Software Engineering (S&SE) coordinated User Requirements Evaluation and Prioritization (UREP) team as described in the XSEDE Systems Engineering Management Plan (XSEMP). The UREP, which includes both XSEDE senior management and user representatives, was able to prioritize SD&I proposed activities based on user needs and other strategic factors. The UREP will ensure that future SD&I development efforts align with the needs of users, other program areas, and strategic initiatives.

Other systems engineering improvements in this quarter include the first ever active design review of Campus Bridging Use Cases intended to validate that SD&I is able to turn Architecture

& Design produced Use Cases and Level 3 architecture decomposition documents into specific development and integration. We also launched an effort to re-design and streamline our activity management workspace. With a queue of over 100 proposed projects, a dozen active projects, over a dozen activity development and testing leads, and over 30 staff members, it is essential that we have an organized activity planning and execution workspace that is both easy for our staff to use, helps us apply engineering best practices to our activities, and provides the information external stakeholders like senior management, project managers, and the system's engineering office need.

4 XSEDE Operations 1.2

4.1 Overview

The Operations group consists of ~30 FTEs and is responsible for implementing, delivering, maintaining, and evolving an integrated cyberinfrastructure capability of unprecedented scale that incorporates a wide range of digital capabilities to support the national scientific and engineering research effort. The Operations group follows the XSEDE project management methodologies detailed in the Project Execution Plan by allocating and coordinating staff in accordance with the XSEDE work breakdown structure (WBS), scheduling tasks in the XSEDE project schedule, and identifying and reviewing risk on an ongoing basis. Operations staff is subdivided into six teams based on the WBS:

1.2.1 Cybersecurity
1.2.2 Data Services
1.2.3 XSEDEnet (Networking)
1.2.4 Software Testing and Deployment
1.2.5 Accounting and Accounts Management
1.2.6 Systems Operational Support

In this quarter Operations' teams efforts led to the completion of several milestones such as the production of the first security risk, threat, and vulnerability report; the addition of duplicate account notification and correction packets to AMIE; the implementation of state tracking mechanisms for proposal submissions and account requests; the deployment of the initial configuration instance of the new XSEDE ticket system; and the installation of the root of the namespace and secure token server for the GFFS Beta deployment.

In addition work began to support variable length awards in the Partnerships Online Proposal System (POPS), to prepare for the next increment to the XSEDE software environment, and to evaluate one-time password (OTP) solutions for federation. All project schedule items for Operations WBS 1.2 were updated for the baseline project schedule and are reflected in Appendix B. The Operations group completed all tasks scheduled for this quarter. All risk items for the group's activities were reviewed and are listed in Appendix C. No risks were triggered during this quarter.

4.2 Cybersecurity 1.2.1

The Security Operations team's focus is the availability, integrity, and security of XSEDE related information, data, and services. No vulnerabilities were identified within this quarter that required XSEDE-wide notification, and there were no known compromised user accounts and no security issues with XSEDE resources. Key advances in the 1st quarter of project year 2 include: 1) Completion of the Risk, Threat, and Vulnerability Assessment; 2) Commitment from InCommon to move forward on TAGPMA membership and accreditation for their host certificate service; 3) Plans for establishment of an XSEDE CA; and 4) GX-Map upgrades. What follows is a complete list of activity updates during this quarter which are more fully documented on the Cybersecurity page of the XSEDE staff wiki:

XSEDE Certificate Service - lead Randy Butler (NCSA):
At the end of the fourth quarter we had begun to detail options for an XSEDE-wide automated host CA service with the goal to put it into service by the end of the calendar year. Our plans changed after discussions with InCommon management led to their interest in pursuing TAGPMA accreditation for their host CA service. InCommon is moving forward with this and we have agreed to utilize this host CA service, once accredited for XSEDE's needs and thus no

longer have a need to establish our own host CA service. Until the InCommon CA is available XSEDE will be relying on CAs already available and accredited at XSEDE SPs.

September TAGPMA meeting – Lead Jim Marsteller (PSC):
These meetings occur twice per year and they function as a coordination and oversight of the international collection of certificate authorities. Members of the Cybersecurity group represent XSEDE at these meetings to ensure that we follow TAGPMA's lead and voice our opinions, concerns and ideas to aid in the federation of X.509 certificates. At that TAGPMA meeting, Derek Simmel (PSC), the TAGPMA Chair, led the discussion over two time sensitive issues: addressing the cryptographic weaknesses of SHA-1 and the accessibility to CAs over IPv6. Almost all TAGPMA APs are able to generate/sign using SHA-2 now, or will be able to before December 31, 2012. About half of the TAGPMA APs support availability of their CA resources via IPv6. Others have no plans to provide availability via IPV6 - some due to limitations of their network service at their organizations. Two new members were inducted at the last meeting: CIDETYS of Panama and redCLARA <http://www.redclara.net>. XSEDE SPs attending the meeting included PSC, NCSA, and OSG along with representation for XSEDE.

InCommon Membership – lead Randy Butler (NCSA):
University of Illinois has now paid the InCommon Membership fees and is working on the execution of the membership agreement.

XSEDE OTP Service Coordination - lead Victor Hazlewood (NICS):
Matt Ezell who was leading this activity has left employment at NICS and the activity has been handed off to Victor Hazlewood temporarily. We are in the early phase of evaluating potential solutions for a federated OTP service and evaluating RSA and Duo authentication technologies.

XSEDE Federation Risk Assessment - Lead Adam Slagell (NCSA):
An XSEDE risk, threat, and vulnerability analysis has now been completed and a draft report has been produced. The effort highlighted a number of medium and low risks, and helped to establish priorities for a risk mitigation plan.

SD&I and A&D Collaboration:
Members of the Cybersecurity Operations team (Butler, Fest, Marsteller, Slagell) were heavily involved in the SD&I discussions about the security of Configuration Items. These included SD&I activities SDIACT-097 (Basic EMS Unicore), SDIACT-050 (Oauth for Globus Online), SDIACT-101 (EMS and GFFS) and SDIACT-015 (modify Genesis II/GFFS to use SAML). Additional discussions about the XSEDE security architecture have occurred between the Architecture and Design (A&D) team and Cybersecurity Operations in regard to use cases currently being developed in A&D.

4.3 Data Services 1.2.2

Data Services activities for this quarter included maintaining the existing operational infrastructure, such as GridFTP servers and archive resources, improving documentation for data resources in XSEDE, and preparing for upcoming software deployments and accounting changes.

Data Services staff have worked this quarter on investigating GridFTP logging capabilities and log analysis. Additional logging capabilities have been identified and requested via SD&I activity 31 (SDIACT-031) and are currently under development for potential deployment across XSEDE.

The XSEDE-Wide File System (XWFS) process has now proceeded past the technology evaluation phase and into a phase of cost analysis for configuration options and coordination with SD&I and A&D to introduce XWFS into the XSEDE design and deployment process.

Several SD&I components affecting Data Services are in preparation for deployment, including updates to GridFTP, Globus Online, and the Global Federated File System. Staff participated in testing and operational readiness reviews for all such components. In addition, Data Services consulted on accounting for storage allocations and on use cases for Architecture and Design.

The Albedo wide-area file system, a resource developed under the TeraGrid project, has been officially retired after over 3 years of operation. Data Services has been responsible for the maintenance of this resource and assisted user services staff in identifying and migrating user data to appropriate resources.

4.4 XSEDEnet 1.2.3

The Networking team's primary focus is monitoring, maintaining, and improving XSEDEnet. Discussions were held with network service vendors Internet2 and NLR this quarter to determine if they could meet the need for future XSEDE Service Provider connectivity. Network contracts with NLR were up for renewal in August 2012 (first quarter PY2) and NLR has agreed to extend the current contracts on a month-by-month basis while discussions are ongoing.

Work has continued with collecting and analyzing perfSONAR information to help understand XSEDEnet capability and use. All XSEDE perfSONAR hosts were updated with a Web100 kernel.

Figure 47, Appendix E shows traffic utilization of the Chicago-Denver link for 3Q2012. Figure 48, Appendix E shows link utilization as a percentage. Traffic offered load into XSEDEnet links for 3Q2012 is shown in Figure 49, Appendix E.

The following table summarizes network outages for the quarter by site.

Site	Available	Down	Uptime	Downtime	Times Down
FutureGrid	99.56%	0.03%	91 days 23:20:14	0:39:46	4
IU	99.70%	0.03%	91 days 23:18:34	0:41:26	4
NCSA	99.81%	0.04%	91 days 23:5:16	0:54:44	6
CHIC	100.00%	0.00%	92 days 0:0:0	0:00:00	0
DENV	100.00%	0.00%	92 days 0:0:0	0:00:00	0
PURDUE	99.72%	0.03%	91 days 23:18:33	0:41:27	4
SDSC	96.48%	0.07%	91 days 22:31:30	1:28:30	14
UCAR	98.81%	0.04%	91 days 23:13:15	0:46:45	5
PSC	99.65%	0.04%	91 days 23:6:54	0:53:06	5
TACC	99.78%	0.08%	91 days 22:19:55	1:40:05	9
NICS	99.66%	0.05%	91 days 22:58:30	1:01:30	10

4.5 Software Testing and Deployment 1.2.4

Operations Software Testing and Deployment (ST&D) identifies resources for software testing, conducts acceptance testing and operational readiness reviews of software, and aids the deployment of software at service providers. In this quarter the ST&D group added the campus bridging coordinator and service provider coordinator to the group to support campus bridging and service providers and completed the acceptance test report for Global Federated File System (GFFS), which uses the data access components of Genesis II. The actual testing for this configuration item (CI) was completed in the previous quarter. The GFFS CI was accepted for a limited beta deployment at a small number of SP sites, followed by a pilot project for user usage at six campus-bridging sites.

This beta deployment for GFFS was a major area of effort in the ST&D group this quarter. A Genesis II container service comprising the root of the GFFS namespace and a Kerberos-backed security token service was deployed at NCSA. Requirements for the six campus-bridging pilot projects were also collected. The addition of SP and campus-bridging coordinators to the ST&D group at the beginning of the quarter greatly helped these efforts.

In the previous quarter, the Software Development and Integration (SD&I) group began a number of new software projects based on primarily on feedback from ST&D. The ST&D group developed operational readiness review (ORR) documents and acceptance test plans for several of the expected CIs, in particular Basic EMS (SDIACT-97) and Globus Online (SDIACT-50 and SDIACT-100). The ORRs for these CIs are expected to be conducted early in the next quarter.

	PY1 Q1	PY1 Q2	PY1 Q3	PY1 Q4	PY2 Q1
CI Readiness Reviews Completed	0	0	2	1	0
CI Acceptance Tests Performed	0	0	2	1	0
CIs Accepted for Beta	0	0	0	1	1
CIs Accepted for Production	0	0	0	0	0

4.6 Accounting and Account Management 1.2.5

The Accounting and Account Management (A&AM) group maintains and improves the interfaces, databases, and data transfer mechanisms for XSEDE-wide accounting of resource allocation and usage. There were several advances made by the A&AM group during the first quarter of PY2:

Due to the fact users can now create their own XSEDE User Portal accounts, there is an increased possibility of duplicate user accounts within the XSEDE Central Database (XDCDB), and within the account management databases at the various SPs. To address this issue, three new packets for the Account Management Information Exchange (AMIE) system were developed. The first packet, *notify_person_duplicate*, allows an SP to notify the XDCDB of the detection of a duplicate account. The second packet, *request_person_merge*, is sent by the XDCDB to the relevant sites to inform them of which account is the “kept account”. The third packet, *notify_person_ids*, allows SPs to manage account ids and usernames as mapped in the XDCDB.

Work was completed on the new “xdusage” command, which is a complete re-write of the TeraGrid-era “tgusage”, command, which became unsupported at the end of TeraGrid. This command is currently undergoing software testing and will be released to the sites in the second quarter of this program year.

Mechanisms were implemented for tracking the state of proposal submissions and account requests as they move through the process of being approved. The A&AM group is coordinating with the User Information and Interfaces (UII) group to develop interfaces within the XUP to display this data.

The Keeneland Initial Delivery System (KIDS), a new allocable XSEDE resource, was configured in POPS and the XDCDB and work continued to integrate FutureGrid into XSEDE as a Level 1 SP.

Work was begun in POPS to support variable length awards. Currently, all awards are one year in length. Allowing for variable length awards will provide better support for training and educational awards, as well as for untraditional award types, e.g. software testing on FutureGrid resources. This work will be completed in the second quarter of PY2.

4.7 Systems Operational Support 1.2.6

The Systems Operational Support (SysOps) group is responsible for operating the XSEDE Operation Center and providing system administration for the ever-evolving set of XSEDE centralized services. Significant progress was made in the following WBS tasks in Q1 of PY2: 1.2.6.10, 1.2.6.12, and 1.2.6.13. Tasks worth noting include deploying the first operational phase of the new XSEDE ticket system, continued work on setting up the backup XSEDE Operations Center, and installation/deployment of the root of the namespace and secure token server for the Genesis II Beta deployment. Even though there were several planned and unplanned outages during Q1 of PY2 the SysOps team maintained high overall uptime, which ensured data integrity and availability. By leveraging failover resources, where appropriate, user-facing downtime was greatly minimized. As such, no central service experienced any less than 98.71% uptime for Q1 of PY2.

4.7.1 XSEDE Operations Center

During Q1 of PY2 the XSEDE Operations Center (XOC) fielded 2,421 tickets and closed 2,028 tickets. Among these 2,175 were submitted via email to help@xsede.org, 18 were submitted via the XSEDE User Portal, and 228 were submitted via phone to the XOC. There were 880 tickets closed within 2 business days, which equates to 36% for the reporting period. There were a total of 2,021 tickets responded to within 24 hours, which equates to 83% for the reporting period. Table 16, Appendix E shows the ticket breakdown (opened/closed) for each major resolution center. Figure 16 in Appendix E shows tickets broken into the 7 distinct problem categories with significant representation.

4.7.2 Central Services

There were several outages both planned and unplanned that affected various central services during Q1 of PY2. Many of these outages were the result of individual servers or sites experiencing unexpected technical difficulties or routine maintenance. Outages varied between site-specific power events, networking interruptions, system failures, planned activities, and user initiated interruptions.

The following table describes each service that experienced an outage, the corresponding downtime/uptime, the nature of the outage (e.g. Planned or Unplanned), and the total number of hours down:

Service	Percentage of Uptime (Number of downtime hours)	Planned Outage(s)	Unplanned Outage(s)	Total Outage(s)
Inca	**98.71%**	26 hours	2.5 hours	**28.5 hours**
Karnak	**99.98%**		.5 hours	**.5 hours**
Majordomo	**99.92%**	1.8 hours		**1.8 hours**
Sciforma	**99.84%**	3.5 hours		**3.5 hours**
Speedpage	**99.95%**	1 hour		**1 hour**
User Portal	**99.98%**		.5 hours	**.5 hours**

XDCDB	**99.97%**		.75 hours	**.75 hours**
XDCDB Backup	**98.91%**		24 hours	**24 hours**

4.7.3 INCA

At the time of this report, the Inca deployment was executing 1011 tests for XSEDE software and services. Of these, 120 of these tests were running for six central XSEDE services: Inca, Information Services, Karnak, MyProxy, User Portal, and XDCDB. The table below shows the definition of an outage for each service and the uptime percentages as detected by Inca. All services fall within acceptable limits of their high availability service definition.

NOTE: Uptime numbers shown below will vary from the above uptime numbers. The numbers represented below show all of the outages that INCA detected during the reporting period. Any outages or race conditions within the INCA system could prevent INCA from detecting further outages. For official uptime numbers, the data in the 'Central Services' section should be used.

Service	Definition of outage	Uptime (Details of outages)
Inca	Inca status pages are unavailable or not able to fetch data from the database (i.e., test details page fails to load). Tests every 5 mins.	**98.7%** (One scheduled outage for database upgrade for 26 hours, one unplanned outage for 2.5 hours)
Information Services	Information Web pages are unavailable. Tests every 15 mins.	**100%** (No outages detected)
Karnak	Karnak front page fails to load. Tests every 30 mins.	**99.98%** (One outage for < 30 minutes of downtime)
MyProxy	MyProxy server does not respond to credential query check. Tests every hour.	**100%** (No outages detected)
User Portal	Portal front home page fails to load correctly. Tests every 30 mins.	**99.98%** (One outage for a total of 30 minutes of downtime)
XDCDB	Connection to database refused or slow (using check_postgres.pl script). Tests every 5 mins.	**99.96%** (One outage for a total of 50 minutes of downtime)

4.7.4 Syslog Monitoring Project

The Cornell Center for Advanced Computing (CAC) has partnered with XSEDE sites in order to provide a novel approach to systems administration and monitoring. CAC gave a presentation at the XSEDE conference in July to the Systems Operations group. This demonstration showed how CAC could assist with tools, applications, and systems knowledge for log analysis and monitoring of other sites. The CAC team is ready for more partner sites to participate in further testing and evaluation of predictive log analysis and near real-time reactive monitoring.

4.7.5 Globus

During the reporting period, there were 57 million files transferred to and 45 million files transferred from XSEDE endpoints using Globus Online (GO). In total GO facilitated transfers of 311 TBs to and 325 TBs from XSEDE endpoints. In total, there are 218 distinct GO XSEDE users. Diving deeper we know that of the total files transferred 25 million were transferred from Globus Connect (GC) to an XSEDE endpoint and 9 million files were transferred from an XSEDE endpoint to GC. In total 37 TBs of data were transferred from GC to an XSEDE endpoint while 34 TBs were transferred from an XSEDE endpoint to GC. Of the previously mentioned distinct XSEDE GO users, 138 of them are distinct GC users. This data does not include stats from automated performance testing.

In total, there were 34 tickets opened for the GO team. The tickets can be lumped into the following categories: user education, endpoint operational issue, bug fix, feature request, and user action required notification. The table below shows the number of tickets that fit within each distinct category.

Category	Number of Tickets	Explanation and Details
User Education	10	Information provided to resolve the problem.
Endpoint Operational Issue	9	Problems using a specific endpoint.
Bug Fix	12	A problem occurred that warrants a change/fix to the GO software/system.
Feature Request	1	GO lacking in some way and an improvement/new feature is identified.
User Action Required Notification	2	Unsolicited email sent to user(s) for a problem that they should be aware of.

5 User Services 1.3

5.1 Overview

User Services activities continued to grow and improve in the first quarter of the second project year, leveraging experiences and feedback gained during PY1. Training continued its high rate of offerings, and began preparations for upcoming training for new systems (Keeneland, Stampede) for certification programs. Documentation efforts continued to expand and refine technical information. The XUP portal added new features including publication gathering/tracking capabilities and improvements in allocations monitoring. User Engagement completed the analysis and reporting of information from the first annual XSEDE User Survey, and continued to make progress on the implementation of the new ticket system. Allocations received a record number of requests for cycles (1.1B SUs), and made progress on the implementation of storage allocations in 2013. Overall, the user services efforts continue to operate smoothly, while incrementally improving in scope and quality. Significant new capabilities will be completed in the next quarter, including storage allocations and also Keeneland and Stampede training and documentation.

5.2 Training 1.3.1

The XSEDE training efforts continued apace in this quarter. More than a dozen training events took place, including a number of large summer courses with hundreds of attendees. Demand for both beginner and advanced training continues to grow.

Planning for training certificates is well under way, with core course requirements being defined, and train-the-trainers materials under development. Much emphasis is being placed on developing content for new systems as well. A multi-site course on using accelerators for Keeneland will be offered early in the coming quarter, with Stampede training beginning later in the quarter. A strong tutorial presence at SC12 is also expected. Conversations are under way to coordinate training activities with the Blue Waters effort as well, as that system should also come online shortly and share many training needs with XSEDE.

Overall, in both delivery and in course development, XSEDE remains on track to deliver on the milestones for this year.

5.3 User Information & Interfaces 1.3.2

Both the XSEDE web site and XSEDE User Portal (XUP) released new features and met deliverables for this quarter. The XSEDE web site continued to expand and organize the online content by updating storage information and adding end dates for XSEDE resources based on feedback from the User Advisory Committee to help users decide what resources they want to apply for in the future. The UII team also created updated user guides for Keeneland and Globus Online.

This quarter also included new features in the XSEDE user portal including a new publication-gathering feature. This enables users to select a project and specify a list of publications associated with the project; staff can also enter in staff publications. In less than a month since the release there were over 120 publications entered by staff and users. The portal also released a dynamic feedback feature that displays a feedback tab on each page of XUP, enabling users to easily submit feedback from any page on the portal without having to navigate to a different page. The team also refreshed the welcome page to include the user’s avatar and recognize campus champions with their logo and a link to the campus champion’s area. In addition, the team expanded the allocation usage drill down graphs for users and PIs. They can now view jobs and SU usage for an allocation or individual users and drill down by month, week, or day. This data can be downloaded to CSV format for further processing. For a better user experience the portal team also added a *forgot username* feature to help users automatically retrieve their username without having to go through the helpdesk. Complementary activities for staff include migration of the XSEDE user and allocation queries to a new secure site that allows only staff to access these queries using their portal username and password and a staff publication listing feature on the staff site.

The Knowledgebase (KB) team expanded and improved the KB articles by adding 62 new KB items and updated existing articles to insure accuracy for a total of 538 documents for over 85,000 document retrievals.

Within the reporting period there were over 42K file transfers accounting for over 3.6TB of data transferred via the portal file transfer service. The overall usage of both the web site and user portal continue to increase with over 2.3 million hits on the web site and over 1.5 million on the user portal. Furthermore, over four thousand XSEDE users logged in to the user portal and out of 2,253 users running jobs on XSEDE almost 70% of them were logging in to the user portal.

5.4 User Engagement 1.3.3

XSEDE User Engagement is organized as two working teams: Feedback and Consulting. The Feedback team focuses on proactive support, while the Consulting team focuses on reactive support.

5.4.1 Feedback

The Feedback team completed all required feedback activities and required reporting for the quarter, except for the quarterly focus group (which was completed during the first week of PY2Q2 due to scheduling conflicts). The team also completed the PY1 XSEDE Annual User Survey and associated reporting. A review of feedback activities over the first year of the project was conducted, and the resulting lessons are being applied to improve planned feedback activities for the second year of the project.

The Feedback team conducted a BoF entitled "XSEDE – Review and Directions after One Year" at the XSEDE 12 conference. The BoF examined developments within XSEDE during the first year of the project and solicited associated feedback. Preliminary results from the PY1 XSEDE User Survey were used to motivate discussion about potential improvements to XSEDE, and associated feedback was collected, as well. A report documenting the event is posted on the XSEDE Staff Wiki for reference.

The Feedback team completed data mining on the tickets submitted to help@xsede.org during the previous quarter. As in previous quarters, the majority of tickets were related to routine operational issues. Aside from routine operational issues, the most common issues across XSEDE were related to data transfer, GPU computing, storage facilities, and specific software packages (such as Gaussian, AMBER, Gromacs, LAMMPS, and VASP). None of the issues and trends observed this quarter are considered significantly problematic. A report documenting the results of the quarterly data mining activities is posted on the XSEDE Staff Wiki for reference.

The 2012 XSEDE Annual User Survey was designed to gather information about user satisfaction with XSEDE services and to determine if XSEDE users are better provisioned with cyberinfrastructure services than researchers who are not users of XSEDE. On May 1, 2012, the survey was sent to 5,000 current XSEDE users and to 5,000 NSF principal or co-principal investigators funded between 2007 and 2011 who were not current XSEDE users. The final report is based on data from 734 respondents that completed at least 50% of the survey before it closed on June 11, 2012. The survey results indicate a high overall level of satisfaction with XSEDE services. Results concerning the provisioning of XSEDE researchers with cyberinfrastructure services are less conclusive but appear positive. The final report is posted on the XSEDE Staff Wiki for reference.

5.4.2 Consulting

The Consulting team conducted all required consulting activities for the quarter and made solid progress towards the milestones associated with the deployment and release of the new XSEDE ticket system and the associated consulting policies and procedures. A development instance of the new system is in place, and work is underway to configure and customize the system. Production deployment of the new system is expected to occur in PY2Q3. Finally, a cost-risk-benefits analysis for the proposed XSEDE CRM is underway, and the associated report is expected to be submitted to the XSEDE Senior Management Team next quarter.

5.5 Allocations 1.3.4

This objective encompasses the allocations process, both for Startup, Education and Campus Champion allocations as well as the merit-review XRAC Research request process, the POPS system for request handling and management, mechanisms by which allocation PIs manage allocations through transfers, extensions and so on, and interfaces by which allocation PIs manage the users who are authorized to use their allocations. Operationally, this objective includes the XRAC review process, the Startup allocations review and decision process, and the maintenance and operations of the POPS system.

The table below shows the overall allocations management activity handled by POPS and the allocations staff for the reporting period. Note that for Transfers, the table shows only the positive side of the transaction to show the total transfer level; there is a corresponding negative amount, adjusted for resource exchange rates.

Table 1: POPS Requests and Award

	Research				Startup				Education				Campus Champions			
	# Req	SUs Req	# Awd	SUs Awd	# Req	SUs Req	# Awd	SUs Awd	# Req	SUs Req	# Awd	SUs Awd	# Req	SUs Req	# Awd	SUs Awd
New	63	217,740,159	50	100,040,537	158	23,248,424	129	16,550,113	19	1,441,013	18	1,344,002	12	9,464,030	11	8,426,003
Prog. Report	1	1,000,000	1	700,000	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Renewal	94	585,485,478	86	279,574,869	18	2,489,527	13	1,379,003	1	50,001	1	50,002	9	7,953,114	9	6,125,013
Advance	30	34,657,356	24	13,596,905	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Justification	4	22,394,000	2	368,000	0	0	0	0	0	0	0	0	0	0	0	0
Supplemental	29	53,223,328	19	42,515,809	22	2,227,024	19	1,492,012	0	0	0	0	5	410,010	4	245,001
Transfer	87	35,232,555	76	19,141,240	38	2,534,179	34	1,504,928	5	106,566	4	42,500	1	2,600,000	5	190,000
Extension	67	n/a	60	n/a	53	n/a	51	n/a	1	n/a	1	n/a	1	n/a	1	n/a

The September quarterly allocations meeting, XRAC, was planned and held in Champaign-Urbana, IL. The next two XRAC meetings have been scheduled for Orlando FL. in December 2012 and Las Vegas, NV. in March 2013.

Requests totaling 1.1B SUs (SUs locally defined to the respective resources) were requested at the September 2012 XRAC meeting. However, as history has shown, the September meeting is always the largest requested XRAC meeting. The allocations team worked with the SPs and found eight large research groups that were offered the opportunity to move to the December 2012 XRAC in hopes of balancing meetings; these eight groups accepted. Supplements were provided to the groups on the compute resources they had requested so they could continue their research while their awards are on hold until January 2013. Reviewer recommendations totaled 390M SUs with 379M SUs available. Only a few moves were needed to bring recommended awards in line with the individual resource available limits. However, the XSEDE Allocations staff and XSEDE site representatives are faced with a difficult situation of continued requests for supplements, transfers, and startups but no significant pool of SUs to satisfy the user community requests!

The XSEDE Allocations staff received 440 tickets within the reporting period. Most, if not all, were addressed and a high rate of user satisfaction achieved.

Lastly, XSEDE Allocations staff along with the XSEDE Operations/A&AM, led by Steve Quinn, are working on improving reporting of not only PI awards to their respective program officer but also to the entire XSEDE community via quarterly award announcements in conjunction with the XSEDE ER team.

6 ECSS – Projects 1.4

6.1 Overview

The Extended Collaborative Support Service (ECSS) pairs members of the XSEDE user community with expert ECSS staff members for an extended period to work together to solve challenging science and engineering problems through the application of cyberinfrastructure. In depth staff support, lasting weeks to up to a year in length can be requested at any time through the XSEDE allocations process. Expertise is available in a wide range of areas, from performance analysis and petascale optimization to the development of community gateways and work and data flow systems. ECSS staff members also participate in reviewing adaptive proposals associated with XRAC meetings.

We divided ECSS efforts in two, one designated as Projects, headed by Ralph Roskies; the other, designated as Communities, headed by Nancy Wilkins-Diehr. These groups have very close interactions, with common Project Management support. All told, ECSS consists of 37 FTEs, spread over ~80 people at about a dozen sites.

At XSEDE12, ECSS management met with over 50 ECSS staffers. We discussed streamlining work plans, stressing that they can be modified, and they need not try to encompass all contingencies up front. We reiterated that we can drop projects whose PIs or contact people are not responsive to repeated attempts to engage them. We also issued a template for final reports which should make it easier to fill those out. We stressed the value of including testimonials from projects that are being helped.

ECSS-Projects consist of ESRT (Extended Support for Research Teams) and NIP (Novel and Innovative Projects).

In Q3, ECSS-Projects has also begun to contribute to the A&D effort. Mark Fahey and Sergiu Sanielevici are developing the use cases and attribute scenarios for High Performance Computing, and Nick Nystrom (PSC, ECSS NIP) develops the use cases and attribute scenarios for Data Analytics with Shawn Strande (SDSC). They have drafted early versions of the use cases and expect to complete this work during Q4.

We grappled with the user survey finding that seemed to indicate that only 28% of users were aware of ECSS. We will be working ER and the Campus Champions to raise awareness of ECSS.

We discovered that we were not getting data from allocations on time extensions. Sometimes we think a project is winding down, but it has received an extension or a supplement. We will be coordinating more closely with Allocations on this.

Detailed metrics are contained in the individual reports below.

ECSS¹s Project Managers (Karla Gendler and Natalie Henriques) have continued their tasks of maintaining spreadsheets for project requests, active projects, project assignments and staffing. They review and track work plans, entering staff allocations on each project and quarterly objectives into the spreadsheets. They manage and attend ECSS meetings and XSEDE PM meetings, posting notes and action items to the ECSS wiki once the meeting has concluded. They provide ECSS information to the XSEDE PM office and relay information from the PM team to ECSS. They also maintain the ECSS wiki and mailing lists. They coordinated the gathering of information for this quarterly report and have published all of the information to the wiki. They have entered all the projects in Sciforma, the project management software, and continue to work on transferring the remaining information from their spreadsheets to the software. Testing and customization continues on the software as the PM team is working to make it usable by ECSS managers and staff.

6.2 Extended Support for Research Teams 1.4.1

An ESRT project is a collaborative effort between an XSEDE user group and one or more ECSS staff members, whose goal is to enhance the research group's capability to transform knowledge using XD resources and related technologies. Typical ESRT projects have a duration of several months up to one year and include the optimization and scaling of application codes to use 100,000 nodes or more per job; aggregating petabyte databases from distributed heterogeneous sources and mining them interactively; or helping to discover and adapt the best work and dataflow solution for simulation projects that generate ~100 TB of persistent data per 24-hour run. The first year of the XSEDE ESRT program is also managing projects transitioned from the TeraGrid ASTA program, and all of the ASTA projects will be completed by the end of June 2012.

A request for ESRT support is made by the principal investigator (PI) of a research team via the XSEDE resource allocation process. If the request is recommended by the reviewers and suitable to be an ESRT project, and if staff resources are available, a statement of work for up to one year will be developed by in collaboration by the PI, the ESRT team leader, and the ESRT manager and project manager. The work plan will include staff assignments from the pool of available advanced support experts who have the necessary skills. The ESRT team leader, working with the ECSS project manager, will be responsible for project tracking and reporting and for requesting additional resources or assistance from XSEDE management as needed.

Metrics that quantify ESRT requests this quarter and total active projects are provided in Table 2 and Table 3.

Table 2 ESRT project metrics for this quarter

Metric	XRAC	Startups/Edu
Number of requests	7	9
Number of projects initiated	7	9
Number of work plans completed	1	4

Table 3 ESRT project breakdown

Metric	XRAC	Startup/Edu
Number of active projects	26	19

As of Oct 2012, there are 13.2 FTEs assigned to ESRT from NCSA, NICS, PSC, SDSC, and TACC.

Table 4 summarizes the number of requests, unjustified/rejected requests, work plans completed (and as such projects in progress), and work plans still in process.

Table 4 ESRT project metrics since XSEDE began.

	Requests	Not justified	Work plans completed	In process
Jun-Aug startups (2011)	12	8	4	0
Aug XRAC	10	2	8	0
Sep-Dec startups	12	9	3	0

Dec XRAC	11	6	5	0
Jan-Mar startups (2012)	11	4	7	0
Mar XRAC	13	6	7	0
Apr-June startups	12	9	3	0
June XRAC	11	4	4	3
July-Sep startups	9	1	4	4
Sep XRAC	7	-	1	6
Totals	**108**	**49**	**46**	**13**

For the first 15 months, there has been one main challenge with managing the ESRT program - the management of projects and people. ESRT has a large distributed staff and many different projects with different start/end dates. The project management staff is excellent and has helped tremendously, but we eagerly await the project management software to replace email and spreadsheets.

The following sections highlight a few projects that provide examples of the kind of work that is being done in the ESRT program.

6.2.1 Cyberinvestigations of Compressible Turbulence (Donzis, Texas A&M U.)

ECSS Project Team: Vince Betro (UTK)

The goals of this ECSS project are to (1) create an MPI/OpenMP hybrid code version with optimized performance that beats non-hybrid performance by 1.5 times with the same resources and (2) determine and implement via smarter reads/writes a more scalable file format within the code.

The file format being used currently is a well-known binary format (HDF5), which means that it is quite portable. Moreover, there are two implementations of I/O: one that uses a large file and does collective reads and writes and one that uses small files gathering information to the root process. HDF5 is well-suited to both implementations, so there is no reason to change the file format. Rather, the focus became on speeding up the I/O. The reason for this is that large node counts are needed to properly decompose the domain when dealing with high Reynolds number, viscous flows and therefore the I/O time needs to be as minimal as possible.

Under the original MPI_IO implementation for a weak scaling problem where the mesh gets finer but the work per core stays constant: a job with 8K cores runs in 159,755,913 seconds; a job with 16K cores runs in 466,281,565 seconds (which is a 3x SLOWDOWN); and a job with 32K cores runs out of memory. The method where the root process collects all the data and writes is actually much faster than the MPI_IO implementation, but clearly has limitations because of memory. And there is no technical reason the MPI_IO method should be slower. It was determined, that the MPI_IO implementation with collective communication, resulted in all processes reading/writing simultaneously and that was placing an excessive amount of work on the OSTs for very large processor counts.

In order to combat this slowdown, an attempt was made to see if simple file striping would correct the issue, but after trying stripe counts of 2, 4, 8, 16, 32, and all OSTs with no noticeable gain in performance, both this and a growth in the MPICH_UNEX_EVENT_BUFFER environment variable were scrapped as simple solutions. Ultimately, by adding collective buffering and by using the following MPI_IO environment variables in combination with file striping the performance was increased such that 1) 32,000 and 64,000 core jobs can now run successfully with MPI_IO and faster than with the original multi-file implementation and 2) as one grows the core count (fixed work per core), the wall time now grows slowly. Also, use of subarray data types was retained thus allowing memory use per core to scale better than with a root process having to control all I/O. See Table 1 and Figure 1 for complete details.

Table 1: MPI_IO environment variables used

MPICH_MPIIO_HINTS (to all files read and written)	
Romio_cb_write	Enable
Romio_ds_write	Disable (deprecated call)
Romio_cb_read	Enable
Romio_ds_read	Disable (deprecated call)
MPICH_MPIIO_HINTS_DISPLAY	1 (DEBUG ONLY)
MPICH_MPIIO_XSTATS	1 (DEBUG ONLY)
MPICH_MPIIO_CB_ALIGN	1 (aligns with lustre striping/boundaries)
MPICH_PTL_MATCH_OFF	1 (disables registration of recv requests w/portals) (to overcome PtlMEMDPost() failed: PTL_NO_SPACE)
Lfs setstripe outdata –c -1	Set from head directory

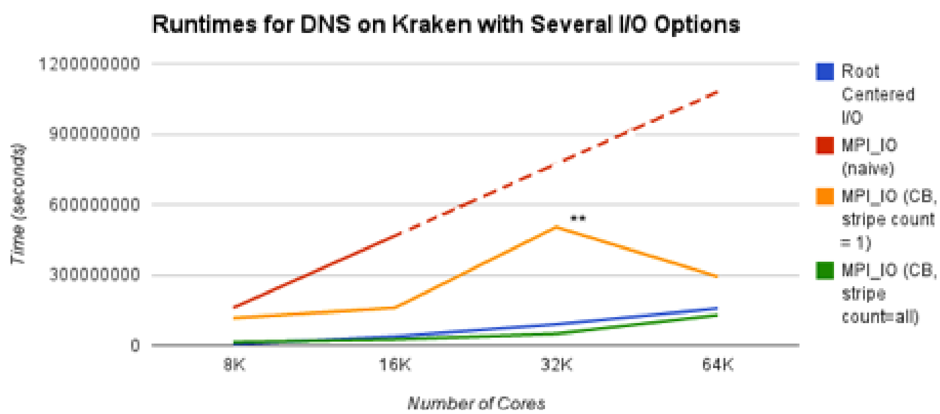


Figure 1: Runtimes for a DNS weak-scaling (fixed amount of work per core) problem on Kraken with several I/O options. The collectively buffered I/O with large stripe count is now the fastest I/O implementation. Note that the 32K and 64K runtimes (MPI_IO naive) with non-collectively buffered I/O are projections.

6.2.2 *Statistical Approaches to Integration of Mass Spectral and Genomic Data of Yeast Histone Modifications (Ma, U. Illinois Urbana)*

ECSS Project Team: Darren Adams (NCSA)

Although this was anticipated to be a fairly short collaboration, it has grown beyond the initial expectations. The project's goal is to improve performance of the "histone" code, and in particular, data storage and possible parallelization of linear algebra routines.

The following progress has been made:

- A new HDF5 data format has been developed and implemented
- OpenMP parallelization improvements

* Parallelization of the main algorithm using OpenMP
* Demonstrated scaling on first part of main loop from ~400 seconds down to <100 seconds
* Scaling to less than 30 seconds should be achievable running on more than 64 cores

- And the following software engineering improvements:
  * Implemented Cmake build and test system
  * Improved handling of numerical precision
  * Established regression tests

Building on this, the next steps are: (1) improve vectorization of second part of main loop, (2) determine scaling on Blacklight, and finally (3) allow team to complete their evaluation of the method using the rest of their allocation running jobs with 256 processes on Blacklight. It is expected that the main iteration update will complete in approximately 1 minute, which would bring their turnaround time down to less than 1 day. With better vectorization of the second loop, the team should be able to run on Blacklight with anywhere from 64 to 256 (maybe more) processes. These runs will allow them to further evaluate their algorithm and publish results.

There are further opportunities to investigate parallelization approaches for their code including hybrid MPI/OPenMP and GPU optimization of sections of the code. It looks quite promising to radically improve performance using these techniques resulting in an extremely successful collaboration.

6.2.3 Computational Models of Volcanic Jets (Ogden, UCSD)

Active ECSS Project Team: Amit Chourasia (SDSC)

The actively remaining part of this ECSS project is to create visualizations of data to communicate results and process studied by volcanic simulations. In particular, the goal is the visualization of simulation data to show ash, rock, and steam distribution in 3D. The PI is interested in identifying and showing rock deformation as well. Advanced visualization abilities will provide better communication of the complex processes studied here to both the scientific and general community. Visualization of volcanic eruptions presents the challenge of illustrating the large deformation undergone by the surrounding rock while still including the volcanic flow field parameters that are of interest to the volcano research community.

The PI had previously used Tecplot for visualization of this project. The ECSS project team has been able to use VisIt, an open source software for visualization, after some modifications and fixes to the software for this work. The bugs and limitations that were identified during this process were passed to the VisIt developer community who were prompt and helpful. The PI provided a new set of data from nine simulations and the work is ongoing for visualizing this new dataset.

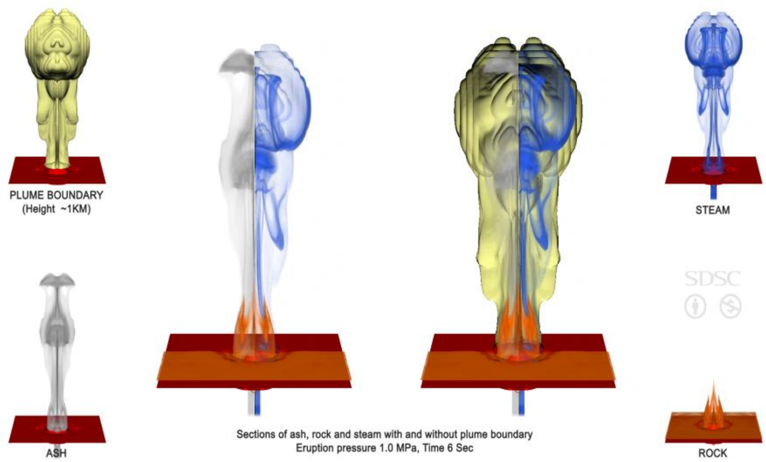


Figure 2: Sections of ash, rock, and steam with and without plume boundary.

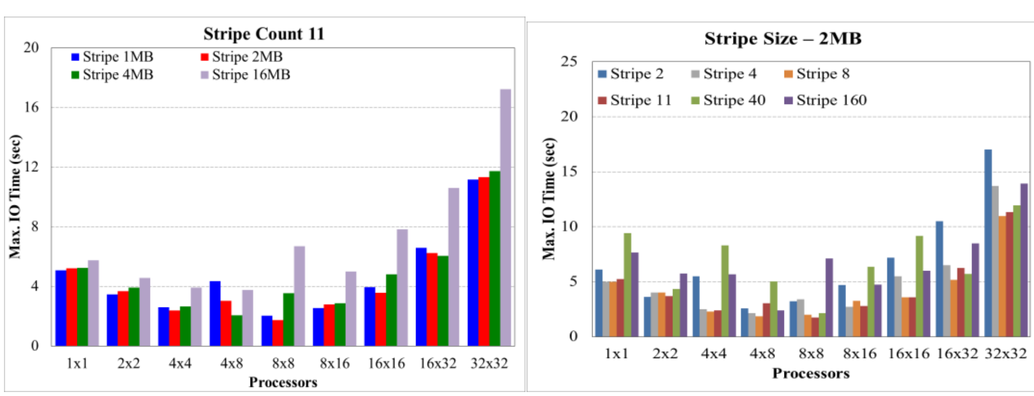
Additional images and movies available at http://visservices.sdsc.edu/projects/volcano/, with the latest movie at http://visservices.sdsc.edu/projects/volcano/movies/volcano_eruption.mov.

6.2.4 Extreme Event Impacts on Air Quality with a Changing Global Climate (Fu, UTK)

ECSS Consultant: Kwai Wong (NICS)

This project aims to develop a renovated tool and technique to examine the extreme event impacts on air quality induced by the changing global climate in present and the future from regional to global scale. With more and more extreme events observed, an improvement in model performance is required to be capable of forecasting the air quality in a shorter time. As the current I/O module embedded in the Community Multiscale Air Quality (CMAQ) Modeling System accounts for 15-20% of the total simulation time, it will save a significant time in dealing with the data input and output when performing a long-term simulation. Additionally, there is an MPI bottleneck that limits scalability in CMAQ. The current best performance occurs when CMAQ runs with 64 MPI processes, and increasing or decreasing the number of processes will reduce the model performance. Future simulations regarding extreme event impacts on air quality would benefit from improving performance of the code.

A series of experiments on a fixed sized problem in setting different stripe counts and stripe sizes were performed for optimum I/O settings (**Error! Reference source not found.**). Preliminary tests on managing I/O have been performed by two different methods: parallel-NetCDF and regular NetCDF. With the stripe count set to 11 and the stripe size set to 2 MB, an Eastern US domain-size data of one time step (approximately 1.59 GB) takes two to three times more I/O time for regular NetCDF than that for parallel-NetCDF (Figure 4). In addition, utilizing 64 processors in parallel-NetCDF tests gives the best I/O performance (the smallest maximum I/O



time); either decreasing or increasing the processors results in reduced performance.

Figure 3: Examples of I/O performance for a fixed problem size in terms of fixed stripe count (left) and fixed stripe size (right)

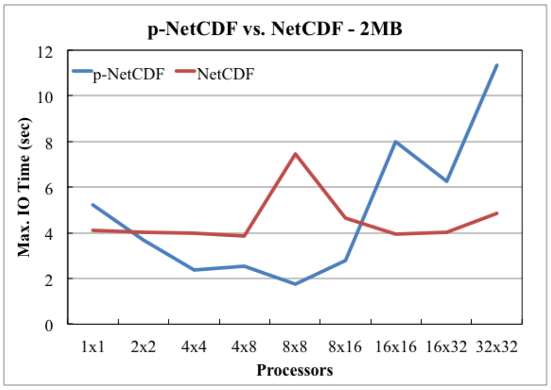


Figure 4: I/O performance for a strong-scaling problem (fixed size) using parallel-NetCDF (blue) and NetCDF (red).

6.3 Novel and Innovative Projects 1.4.2

The mission of the Novel and Innovative Projects (NIP) team is to provide proactive efforts to develop and sustain XSEDE projects by non-traditional (to HPC/CI) users. Activities range from initial contact to the conception and execution of successful projects, including those that receive extended collaborative support. The scope of NIP includes disciplines whose practitioners have rarely availed themselves of HPC/CI resources in the past. It also includes demographic diversity, such as researchers and educators based at MSIs and EPSCoR institutions, and SBIR recipients. Bringing these communities to XSEDE leads to the consideration of applications and programming modes that have not been the focus of HPC in the past, such as those necessary for data analytics and informatics, and of innovative technologies such as streaming from instruments, mobile clients, and the integration and mining of distributed, heterogeneous databases. The implementation of campus bridging processes and technologies will be particularly important for these communities.

Biweekly teleconferences and the use of the project wiki and email list have been successful in catalyzing communications among team members, who benefit from each other's contacts and expertise and share best practices.

Since the beginning of the program (July 2011), the NIP team (5.64 FTEs on September 30, 2012) has initiated and executed 21 outreach events; engaged 42 groups of potential XSEDE users; and mentored 65 XSEDE user groups. Team members are currently involved in the technical execution of 10 ECS projects and were involved in 3 ECS projects that were completed on September 30. They are leading the planning of 3 possible future ECS projects recommended by reviewers.

An important activity has been our effort to organize the workshop "Extending High Performance Computing Beyond its Traditional User Communities" at the 8th IEEE International Conference on eScience in Chicago, see http://www.psc.edu/index.php/escience-2012-workshop . Working with an international program committee assembled by leveraging our NIP efforts over the past year, we were able to attract 10 excellent paper submissions of which 9 will be published in the IEEE proceedings of the conference. 6 of these papers relate to work performed on XSEDE systems with NIP support. We assembled a program featuring the presentation of 8 of these papers as invited talks, in the areas of Digital Humanities, Genomics, Public Health, and Cloud Computing. We also invited a talk about Computational Economics and one about the National Center for Genome Analysis Support (http://ncgas.org/). But most importantly, we built in discussion sessions to encourage interactions among all presenters and participants, generating cross-fertilization and a set of requirements and use cases that NIP can bring to the XSEDE Systems Engineering process. The outcome of this October 8 workshop will be discussed in the next quarterly report.

We have built a close connection between NIP and the XSEDE systems engineering, user engagement, and technology investigation services. Systems engineering staff now attend each of our biweekly NIP teleconferences and take note of the feedback our team members pick up from the potential and current users they contact and mentor. We have launched specific efforts to develop use cases for data-centric and GIS related applications. We have also launched an effort to identify tools and technologies that are of cross-cutting relevance to NIP efforts, such as Python, R, MySQL, neo4j, and Matlab. We are assembling reading lists and materials and are thinking about organizing internal training events for current NIP and other ECSS staff to increase their expertise in these technologies, but we are also considering whether we need to request the flexible contract hiring of one or more experts in the application of these technologies.

One of the first four ECSS Campus Champion Fellows, Dirk Colbry of Michigan State University, has joined the team working on the NIP-supported ECS project *"Interactive Large Scale Media Analytics"* (PI Virginia Kuhn, USC). Dirk is helping to install the multimedia content management software system *Medici* (*medici.ncsa.illinois.edu)* on Gordon; he also developed an annotated bibliography of video analytics software. Next, he will research and test color video analytic software to see what would be helpful, and then integrate the resulting software into *Medici*. The NIP team has also referred *Medici* for evaluation by the XSEDE Technology Investigation Service, for possible deployment as an XSEDE-wide capability.

An example of a successful project helped by NIP is that led by Mao Ye, assistant professor of finance at the University of Illinois. As reported in the October 4 edition of *XSEDE News*, *https://www.xsede.org/high-speed-trading-study*, this team studies NASDAQ market data to investigate practices such as odd-lot trades (of fewer than 100 shares) and increasing the speed of computerized trading from microseconds to nanoseconds. Working with the NIP team since the inception of our program in July 2011, Ye's group has been using PSC Blacklight and SDSC Gordon. Their investigation of odd-lot trading has led the Financial Industry Regulatory Authority (FINRA) to consider including odd lots in reports of trade-and-quote (TAQ) data, which may reduce the current lack of transparency which can skew perceptions of the market. Ye et al.'s investigation of high-frequency trading (HFT) calculated the ratio of orders cancelled to orders executed, finding evidence of a manipulative practice called "quote stuffing," in which HFT traders place an order only to cancel it within 0.001 seconds or less, with the aim of generating congestion. (See Figure 5 below.) This analysis provides justification for regulatory changes, such as a speed limit on orders or a fee for order cancellation. Testimony at a September hearing before the U.S. Senate Subcommittee on Securities, Insurance and Investment cited this study by Ye et al., referring to it as "ground-breaking".

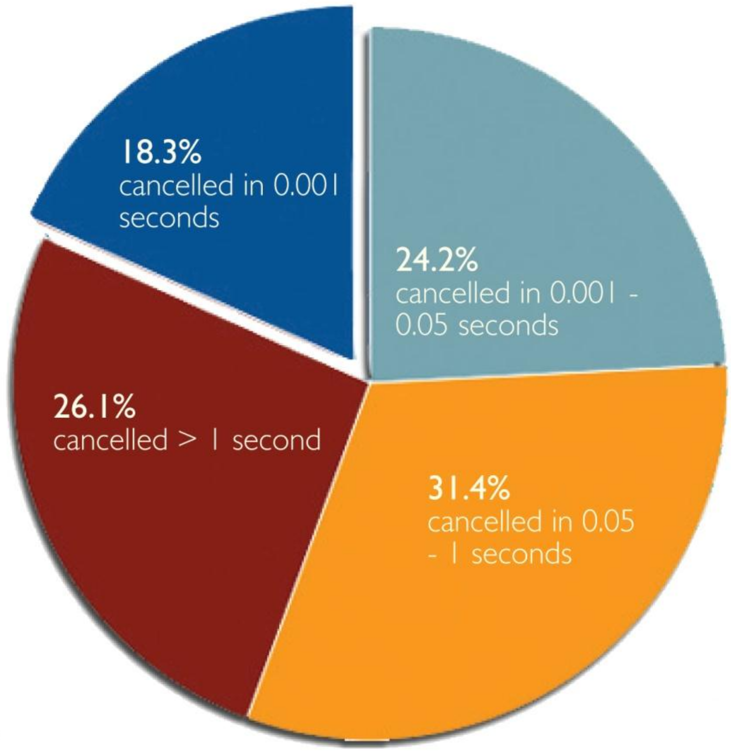


Figure 5: On August 30, 2011, about three million orders were submitted to the NASDAQ exchange to trade the stock SPDR S&P 500 Trust. This image shows that 18.3 percent of the orders were canceled within one millisecond, and 42.5 percent of orders had a lifespan of less than 50 milliseconds, less time than it takes to transfer a signal between New York and California. More than 40 percent of orders, in other words, disappeared before a trader in California could react.

7 Extended Collaborative Support Service – Communities 1.5

7.1 Overview

Requests continue to come in through the XSEDE allocations process for Extended Support for Community Codes (ESCC) and Extend Support for Science Gateways (ESSGW). 29 ESCC projects and 17 ESSGW projects are currently in progress. Work in both of these areas is also internally initiated by XSEDE. In ESCC, these include projects to optimize commonly used community codes. This work is reviewed and approved by the newly formed XSEDE User Advisory Committee. In ESSGW, internally initiated work includes development of science gateway use cases for the XSEDE architecture team.

ECSS staff contributed significantly to the success of the XSEDE12 program, filling key roles in the organizing committee including chair of the technical program and chairs of several of the technical tracks. Staff gave tutorials, presented posters, reviewed submissions, served as judges in the best paper and poster competitions and more.

The ECSS Symposium continues each month and is open to the public to highlight work going on in ECSS projects and allow ECSS staff to learn from one another. The speakers this reporting period were:

- Coupling Climate and Hydrological Models: Interoperability Through Web Services. Presenter: Kathy Saint (SGI), PI: Cecelia DeLuca (UCAR), ECSS staff: Haihang You (NICS)
- DNS of Spatially Developing Turbulent Boundary Layers. Presenters: David Bock, Darren Adams (NCSA), PI: Antonio Ferrante (U Washington)
- Efficient Implementation of Novel MD Simulation Methods in Optimized MD Codes. Presenters: Lonnie Crosby (NICS), Phil Blood (PSC), PI: Greg Voth (U Chicago)

The symposium audience includes the user community, Campus Champions and staff. There was no symposium in July due to the XSEDE12 conference.

After an extensive program development period, the first fellows have finally been selected for the Campus Champion Fellows program. As described in the press release, our four initial fellows include Dirk Colbry from Michigan State University, Naseer Idrisi from the University of the Virgin Islands, Liwen Shih from the University of Houston-Clear Lake and Jack Smith from Marshall University.

Dirk, a research specialist at the Institute for Cyber-Enabled Research at Michigan State University, **is paired with Ritu Arora**, a research associate in high-performance computing at the Texas Advanced Computing Center (TACC) at the University of Texas at Austin. Colbry brings many years of high-end computing expertise to the program and hopes to learn more about large-scale data analysis. Colbry and Arora are supporting PI Virginia Kuhn's Interactive Large-Scale Video Analytics project. Kuhn is associate director of the Institute for Multimedia Literacy and assistant professor in the School of Cinematic Arts at the University of Southern California (USC). The project focuses on indexing, tagging, and searching vast media archives in real time, applying a hybrid process of machine analytics and crowd-sourcing tagging. SDSC's data-intensive Gordon supercomputer will be used as a resource for this project.

Idrisi, an assistant professor at the University of the Virgin Islands' Center for Marine and Environmental Studies, **is paired with Kwai Wong**, a computational scientist with the National Institute for Computational Sciences (NICS) at Oak Ridge National Laboratory. They are supporting principal investigators John Bryant Drake and Joshua Fu at the University of Tennessee

Knoxville, both of whom are doing climate simulation. Working with Wong, Idrisi will expand his knowledge in parallel programming while contributing a domain viewpoint to the projects.

Shih, professor and computer engineering chair at the University of Houston-Clear Lake, **is paired with Yifeng Cui**, a research scientist at SDSC. Their project focuses on Cui's work on physics-based seismic research in collaboration with SDSC and the Southern California Earthquake Center (SCEC). Thomas Jordan at USC is the SCEC principal investigator. Phil Maechling is SCEC's information technology architect and also a member of the XSEDE Advisory Board.

Smith, a research staff member with Marshall University and cyberinfrastructure coordinator at the West Virginia Higher Education Policy Commission, **is paired with Yaakoub El Khamra**, a research engineering/scientist associate with TACC. Smith has extensive experience in many programming areas, as well as chemistry and material science, and would like to use knowledge gained in the Fellows program to grow research programs in new areas. They are working on the projects of PI Ronald Levy (Rutgers) and PI Thomas Bishop (Louisiana Tech). Both involve the use of SAGA software to manage large numbers of loosely coupled bioinformatics calculations.

Accepted Fellows, with the support of their home institution, make a 400-hour time commitment and are paid a stipend to allow them to focus time and attention on these collaborations. The program also includes funding for two visits, each ranging from one to two weeks, to an ECSS site to enhance the collaboration. Funding is provided to attend and present at a Fellows symposium at the annual XSEDE conference.

7.2 Extended Support for Community Codes 1.5.1

Extended Support for Community Codes (ESCC) efforts are aimed at deploying, hardening, and optimizing software systems necessary for extensive research communities to create new knowledge using XD resources and related technologies. ESCC projects are focused on helping users with community codes and tools on XSEDE systems.

Over the past quarter, three new ESCC projects were requested, one was related to a supplemental request and the other two were associated with startup allocations. Also, there was another request for assistance with the Trinity code on Blacklight. This request will be folded into the Genomics Community Capabilities project. There were no XRAC requests for ESCC.

The supplemental request for the iPlant Collaborative project seeks help in using the SAGA/BigJob infrastructure to integrate InterProScan into the XSEDE environment. This will build upon two previous projects that succeeded in integrating the SAGA/BigJob framework into the XSEDE environment on Kraken, Lonestar, and Ranger.

One startup request sought to test a new implementation of ADIO in MVAPICH 2 at the scale of 1024 tasks or more on Lonestar. Since this could greatly impact the file system if the user was not careful, a project was created and a consultant assigned to coordinate test runs and provide performance feedback.

The other startup request was for assistance in using two ION nodes on Gordon to measure the performance of a large scale distributed sort algorithm using distributed flash storage rather than spinning disk. However, after contact, the PI's determined they would not need ECSS support and could be accommodated by the ticketing system.

Below is a summary of the progress of an ECSS project to provide an example of the type of support being provided.

AMBER Force Field Consortium to Develop the Second Generation of General AMBER Force Field (PI Junmei Wang, UT-Southwestern)

ECSS Team: Xiao Zhu (TACC)

A key focus of this project is to develop general reliable and widely applicable force fields for proteins, nucleic acids and drug-like molecules. The successful development of high quality molecular mechanical force fields facilitates the understanding of the molecular mechanisms of biological events and the functions of biomolecules. The knowledge gained will enable the design of new biomolecules. Moreover, a high quality scoring function for conducting molecular docking can be developed using the high quality mechanical force fields.

Objective:

The objective of this project is to develop fast charge methods that resembles the HF/6-31G* RESP and MP2/aug-cc-pvTZ RESP charges for the second generation of general AMBER force field (GAFF2). Specifically, the focus will be on two schemes: (1) following the scheme of AM1-BCC (semi-empirical with bond charge correction) and doing least square fitting to get charge correction directly; (2) parameterizing the electronegativity-like parameters with the Gasteiger charge scheme using genetic algorithm (GA) optimization

A set of programs and scripts have been developed to derive the BCC parameters. All programs and scripts have been validated to derive fast charges resembling the MP2/aug-cc-pVTZ RESP charges using a relative small set of 120 molecules. The group set out to calculate the MP2/aug-cc-pVTZ RESP charges for training set molecules containing 6000 molecules, which represent different compound classes and functional groups. So far calculations have been finished for about 4000 molecules. Completion of the first scheme will be dependent upon the availability of reference data. At this point, 60% of the reference data has been calculated, and the optimization phase will not start until this data is complete.

A genetic algorithm (GA) program was implemented to optimize the electronegativity-like parameters so that the point charges calculated by the Gasteiger scheme reproduce the MP2/aug-cc-pVTZ electrostatic potentials (ESP) from Gaussian. Validation of the code has been performed using a small set of 300 molecules. 60% of this calculation has been completed. The team will focus on improving the high-throughput performance to efficiently include 6000 reference molecules in the training set as in the first approach.

7.3 Extended Science Gateways Support 1.5.2

The Extended Support for Science Gateways (ESSGW) is tasked to provide assistance to researchers wishing to access XSEDE resources through web portals and science gateways. The group assists both new and advanced groups and has experience in the use of web technologies, grid software, fault tolerance, complex workflows, and security and accounting aspects of the program.

The progress on ECSGW projects is listed further in this section. This quarter, the ECSS Science Gateways group has worked significantly with the other groups in XSEDE. The accomplishments include:

- Leading gateway community engagement
- Working with the Architecture and Design team to finalize five gateway use cases. This exercise resulted from an extensive survey of gateway architecture and how it interacts with XSEDE architecture. The effort was coordinated through contributed use cases from many teleconferences.
- Initiated a gateway documentation exercise which will describe the various layers of gateway architectures. This is being developed through technology knowledge sharing sessions and will result in the release a gateway cookbook by XSEDE 13.
- Participated in XSEDE 12 Panel discussing Security for Science Gateways and Campus Bridging.

Architecture & Design Use Case effort:

The gateways developers within the ECSS Science Gateways group have expended significant effort assessing current and future needs of gateways currently in production. This exercise has resulted in a survey of gateway architecture as it relates to XSEDE integration. The team has worked through the requirements gathering phase in coordination with the XSEDE Architecture team. This quarter concluded the initial phase of this exercise and extracted the common XSEDE requirements into comprehensive use cases for gateway security, execution management, data movement, large file uploads and information services.

Open Science Grid:

ECSS Science Gateways group personnel Yan Liu and Shaowen Wang are interacting with users requesting OSG access. The initial users include support requests from University of Delaware and the Northeastern University. The ESSGW team provides direct user support with backend support from OSG staff. The University of Delaware team has successfully ported their code on OSG and started production runs using OSG resources. They became the first user group (PI: Qaisar Shafi) to use both XSEDE and OSG resources for their research through the XSEDE science gateway user support. The 'sampleapp' package developed for this specific support was made generic as an EOT resource to train future XSEDE users with OSG allocation. Next quarter will continue the support and in collaboration with OSG team will work on publishing a major revision of the OSG wiki page on XSEDE user portal.

XSEDE 12 Gateway Tutorials:

At XSEDE 12 Conference, members of the ECSGW spearheaded two gateway tutorials:

- "Hands-on Tutorial for Building Science Gateway Applications on Cyberinfrastructure" Yan Liu (NCSA), Nancy Wilkins-Diehr (SDSC), Suresh Marru(IU), Marlon Pierce(IU), Ramider Singh(IU).
- "Developing Science Gateways using Apache Airavata API" with Suresh Marru(IU), Marlon Pierce(IU), Lahiru Gunathilake(IU), Sudhakar Pamidighantam (NCSA), Ye Fan (NCSA) and Matt McKenzie (NICS).

Through these tutorial audiences were presented with hands-on, practical insights into gateway building. The tutorials also provided insights into aspects of open community software development practices to not just use open software but to learn how to contribute, get recognized and also have a say in future directions.

The morning tutorial focused on providing insights into introducing XSEDE capabilities: account access, data resources, HPC clusters and job management services, software environment, and information services. The tutorial provided exercises for programmatically developing XSEDE-enabled application using the SimpleGrid Application Programming Interface (API). The tutorial demonstrated developing web application using Web 2.0 technologies (JavaScript, AJAX, and Ext JS) to enable community-wide shared access to deploy iGoogle-like Web app gadget using Apache Rave.

The afternoon tutorial taught lessons on executing compute jobs and workflows on XSEDE resources through grid interfaces; wrapping command line applications and turning them into Web accessible programmable interfaces; and learning about open community development process to contribute to existing software with proper contribution governance models. The tutorial was based on Apache Airavata, a software toolkit to build science gateways. Using Airavata the participants composes, executed monitoring applications and workflows on XSEDE Ranger Cluster.

7.3.1 ESSGW projects

7.3.1.1 Dark Energy Survey Simulation Working Group:

The ECSS supported development of python scripts that prepare the TACC Ranger environment for DESSIM community account jobs, and developed workflows using Apache Airavata for the full set of N-body job functions (initial condition preparation and multiple submissions of the N-body code itself). Each simulation models roughly 10 billion mass elements, a size that was state-of-the-art just a few years ago. The initial project was renewed to include support for data management of the N-body runs and to extend the workflow's capabilities.

The support accomplishments this quarter include:

- Running simulations effectively on XSEDE resources
- Workflows running from a configured working directory and storing all job related data in same directory for better data provenance and archiving
- Workflows running multiple simulations in parallel on one or more XSEDE resources
- Workflows understanding and recovering from middleware failures
- Optimization of job working directories, addition of special configurations to job RSL to capture job information for data provenance and archiving
- Working with the group to enable SDSC Trestles to run the workflow. Code porting and Gram5 testing on Trestles are still in progress.
- Working with TACC to debug job cancellation issues

7.3.1.2 Cyber-enabled investigations of turbulence studies of mixing and dispersion:

In the past quarter, the ESSGW support looked into available data management options at XSEDE sites (iRODS, Albedo, GFFS) and came up with several potential designs to address the user's request. After further discussion with XSEDE staff, the support team focused two solutions: 1) portal or downloadable client that interacts with GFFS that interacts with the archives and 2) portal that interacts with iRODS that interacts with the archives.

Based on the effort involved, the team feels the first approach is more promising. The next step is to try it on a GFFS testbed (GFFS is not yet a production resources) to better understand the system.

7.3.1.3 *VLAB**:***

The VLAB project provides petascale computations in mineral physics with the Quantum ESPRESSO codes. The ESSGW support is helping the VLAB project team to build workflow infrastructure to perform first principles calculations of unprecedented magnitude and scope in mineral physics. The project is focusing on optimizing the execution of the Quantum ESPRESSO software for materials simulations in XSEDE systems. This quarter, the gateway support focused on working with the VLab gateway developer in porting Quantum ESPRESSO to the XSEDE Ranger Cluster, enabling job submission through Apache Airavata gateway building framework.

7.3.1.4 Galaxy Deployment for the Scripps Research Institute (TSRI):

The project focused on assisting the researchers at TSRI to manage, map, and analyze the terabytes of data generated from gene sequencing experiments. The project plans to sequence multiple complete human methylomes which have reduced complexity using specialized mapping software required such as Bismark , BS_Seeker. These software programs map the raw reads to four separate human reference genomes using GALAXY and BOWTIE. This quarter the gateway was running smoothly with occasional maintenance requests.

This ESSGW project is in the process of being aligned with the "The Galaxy Bioinformatics Platform on XSEDE", an ECSSGW project that will enable the public Galaxy site at PSU to submit jobs to XSEDE resources.

7.3.1.5 CyberGIS:

CyberGIS Gateway was successfully used and demonstrated at the First International Conference on Space, Time, and CyberGIS (CyberGIS'12), which drew around 100 attendees from multiple science domains (http://www.cigi.illinois.edu/cybergis12/index.php). A hands-on tutorial on how to do CyberGIS-based problem-solving on XSEDE by coupling cyberinfrastructure, GIS, and spatial analysis was well-received by about 70 scientists and students on August 6. In September, CyberGIS Gateway was awarded 5.58M service units (SUs) from the XSEDE allocation committee to further enhance and extend CyberGIS research for the year of 2012-2013.

The ESSGW team also engaged two social science domains in the use of CyberGIS: culturomics and political science. In culturomics, the heat map analytical service has been deployed on Trestles and Ranger to service community use through the GISolve Open Service API. In political science, the redistricting research code has been investigated for parallelization. For high-performance spatial analysis and modeling, we continued to develop scalable algorithms for large- and multi-scale parallel agent-based models (ABM) using XSEDE.

The following research publications have been produced:

Ye, S. Covino, T. P., Sivapalan, M., Basu, N. B., Li, H., and Wang, S., "Dissolved Nutrient Retention Dynamics in River Networks: A Modeling Investigation of Transient Flows and Scale Effects." Water Resources Research, in press.

Next quarter the ESSGW personal will continue to work with researchers in political science in developing a scalable algorithm for large-scale redistricting problem-solving based on our parallel genetic algorithm library which can scale to 16,384 processors on Ranger. We will enhance the heat map analytical service to leverage the shared-memory architecture on Blacklight for large-scale analysis. As we add several new XSEDE clusters in our 2012-2013 allocation, we will port all current CyberGIS applications to and test, profile, and deploy on those resources.

7.3.1.6 Galaxy Bioinformatics Platform on XSEDE

This quarter, the progress of this project has been slow but some incremental efforts have been made.

The project is exploring various data management options. Globus online allows users using the galaxy instance to move their data/files from one XSEDE site to another, or from their laptop or desktop. So far the tasks to verify user XSEDE account is completed. GFFS is a similar capability and includes ability to submit a job to the XSEDE compute resources. Work is ongoing to assess its feasibility. PSC-designed data transfer testing from the TeraGrid program ("speedpage") and gridftp monitoring has been added to Galaxy portal. The Data Supercell for syncing reference data has been ongoing.

This ESSGW project is being re-aligned in co-ordination with the PI to make mid-course corrections and work towards a concrete goal.

7.3.1.7 Social Science Gateway

This quarter the ESSGW support has started with an example SAS script that calls out to R for statistical analysis, modified it to call out to Swift, which submits R jobs to the local SSG compute resource and to Blacklight@PSC. Swift manages data staging in and out of the compute resources. Over the next quarter, the project plans to move forward more quickly on the workplan milestones.

7.3.1.8 Coupling climate and hydrological models interoperability through web services

A climate to hydrological coupling strategy has been developed utilizing the two community standards, ESMF and OpenMI. The Earth System Modeling Framework (ESMF) is widely used within the HPC Earth System Model community and OpenMI is a common standard within the hydrological community. Currently, the team has a working system in which a climate model running on a local LINUX cluster is coupled (one way) to a hydrological model running on a local personal computer utilizing Web services. These systems are not publicly accessible and the results at present are not reproducible by others. Data transfer is done via an external netCDF file but streaming will be implemented in the short term.

The team seeks to move this prototype to an XSEDE environment in order to complete the development of a viable one-way coupling strategy and to pave the way towards the investigation of two-way coupling paradigms. ESSGW staff participate in a weekly meeting, work with project members to solving problems including account issues, Web server issues, and reservation setup for development and demos. Results were presented at the August 21, 2012 ECSS symposium.

Co-author a journal paper "Jonathan L. Goodall, Kathleen D. Saint, Mehmet B. Ercan, Laura J. Briley, Sylvia Murphy, Haihang You, Cecelia DeLuca, and Richard B. Rood. Coupling Climate and Hydrological Models: Interoperability through Web Services. Submitted to Journal of Environmental Modeling & Software, 2012.".

7.3.1.9 UltraScan Science Gateway

The ESSGW project focused on enabling the gateway to use Trestles to run the jobs. The support assisted in working with SDSC staff and project staff to explore different options to fix the issues.

The ESSGW staff also assisted with grid middleware challenges on PI's gateway cluster where job status was not getting updated because of Gram SGE service went down.

Key accomplishments include:

- Enabling job submissions to Trestles from the Ultrascan portal for the community
- Understanding grid failures and providing solutions and workarounds to solve the problems
- Improving error messages for the users to understand failures work with them to develop alternative solutions

7.4 Extended EOT Support 1.5.3

Over this quarter, ESTEO continues to contribute to many tutorials, mentoring opportunities, meetings, as well as presented numerous talks and presentations at scientific and high performance computing conferences. In many cases, ESTEO staff initiated the contributions, developing and delivering the content at a number of venues especially including XSEDE12, and delivered content accepted for XSEDE12 as well as worked on preparations for SC12.

A large amount of ESTEO work for the period culminated in not only delivering content for the XSEDE12 conference (tutorials and papers), but organizing the conference as well. Phil Blood (technical program chair) and Amit Majumdar (deputy chair) coordinated the technical program for the conference, and Jay Alameda (chair) and Suresh Marru (deputy chair) coordinated the software track in the technical program. Additionally, XSEDE ESTEO staff presented posters amd hosted BoFs at the conference, in addition to reviewing submissions and assisting in the best paper competition. Of special note are the numerous tutorials presented at XSEDE12, including:

- Accelerator programming: OpenACC and intermediate CUDA
- Introduction to XSEDE
- Introduction to Visualization
- Toward Improved Performance Solutions (TIPS) on XSEDE Systems
- Hands-on Tutorial for Building Science Gateway Applications on Cyberinfrastructure
- Developing Science Gateways using Apache Airavata API
- Introduction to Unix/Linux
- A New and Improved Eclipse Parallel Tools Platform: Advancing the Development of Scientific Applications

During the period, staff continued to provide outreach and training activities even as they prepare new material for large events later in the year. Staff participated in summer institute programs at TACC and at SDSC; additionally, many publications were submitted or accepted for publication in domain journals by members of the ESTEO group.

A number of staff, including Amit Majumdar, Bilel Hadri, Marcela Madrid, and Ross Walker mentored students this quarter. This also included mentoring activities at tutorials, as needed.

We also continue to review web tutorials and provide new content.

The full list of training courses for the period is available online at https://www.xsede.org/web/xup/course-calendar.

8 Education and Outreach WBS 1.6

8.1 Overview

The TEOS team has continued to make good strides in achieving the TEOS goals and objectives. And the team is improving its resources and services through the findings from the external evaluation team.

The TEOS team is continuing to strive to improve communications both internally and externally. Internally, the TEOS team now includes representatives from all TEOS partners in bi-weekly coordination calls. Externally, the TEOS team is planning to launch a TEOS Symposium, similar to what ECSS has been providing, in the spring of 2013. Also, the TEOS team is developing a set of TEOS services documents to better articulate the resources and services provided by TEOS to the external community. This information will be disseminated via the XSEDE web site, through flyers at conferences and meetings, and through presentations about XSEDE.

The first annual XSEDE12 Conference was held July 16-20 in Chicago, bringing together more than 600 people to help celebrate the launch of XSEDE and to engage the community in becoming more deeply involved in utilizing XSEDE's resources and services.

8.2 Education WBS 1.6.1

Over the past quarter, the education program has focused primarily on faculty professional development through a series of summer workshops. However, we have also continued our efforts working with institutions on the creation of formal programs, co-sponsored student workshops, contributed to the XSEDE conference, worked to create computational modeling exercises for inclusion in the pre-service curriculum for science and math teachers, and initiated work on a repository for shared, computational science training and education materials. Each of these activities is discussed in detail.

8.2.1 Summer Workshops

XSEDE co-sponsored five professional development workshops for faculty and one workshop focused on the development of new computational science educational materials. The workshops were also supported by the Shodor Education Foundation and the hosting institutions. The workshops are summarized in Appendix H.

The first five of the workshops in Table 8.2.1 were three to six day workshops focusing on the pedagogy, tools, and techniques for integrating computational science in each of the topic areas into the curriculum. Attendees were faculty from a wide range of colleges and universities along with a few graduate students. The workshops at Southern University and Montgomery College also included groups of faculty working toward the creation of formal programs in computational science at their institutions.

The PICUP workshop (Partnership for Integration of Computation into Undergraduate Physics) included seven physics faculty who focused on the creation of shareable computational physics packages for use in undergraduate introductory modern physics courses. Six packages were worked on at the workshop, four of which have been completed and posted on the PICUP website (http://helium.bradley.edu/PICUP/collection_modern_physics.php). The packages include background materials, example codes, and exercises that can be used in the classroom.

8.2.2 Workshops

8.2.2.1 Berkeley PARLAB

XSEDE also co-sponsored two workshops focused primarily on students. The first was the Berkeley PARLAB parallel programming bootcamp. This three-day workshop was offered both on site at Berkeley as well as via a web stream and attended by 393 people. Of those attending, 32% were students and 68% were faculty, staff, post-docs, or other professionals. Overall 55% of the attendees were from universities, 32% from research institutions and national labs, and 13% were from private corporations.

8.2.2.2 Online Course for Undergraduates

In addition, we continued to organize the effort to offer a formal, online version of the Berkeley parallel computing course for undergraduates as a full, online course. Lectures captured from the Spring 2012 offering of the course have been organized by the XSEDE training group along with a prototype, online module. The technologies that will be used to present the materials, gather and grade assignments, and provide support for students taking the course have been discussed and are in the process of being finalized. We have completed the installation of a Moodle server at OSC that can be used for this and other experimental courses. Authentication for the server has been tied to the XSEDE portal authentication system so that we can use the current XSEDE training site to register students. The course is targeted to be offered sometime in the first quarter of 2013.

8.2.2.3 3rd Annual EU-US HPC Summer School

From more than 230 applications, 60 graduate students and postdocs -- including 30 percent women -- were selected from higher education institutions across Europe and the United States to attend the 3rd Annual Summer School on Computational Challenges in High-Performance Computing, June 24-28, 2012. The event was hosted by the Partnership for Advanced Computing in Europe (PRACE) and the Extreme Science and Engineering Discovery Environment (XSEDE). The students met at the Royal Marine Hotel in Dublin, Ireland, where the Irish Centre for High-End Computing (ICHEC) -- the Irish member of PRACE, took care of local coordination and hospitality. Nationalities of the students spanned several continents including Asia, Europe, the Middle East, and Central and North America.

This was the third in an ongoing series of summer schools jointly organized by PRACE and XSEDE with funding from the European Commission (EC) and the United States National Science Foundation (NSF). The goals of the summer school series were to expand the knowledge of the attendees about high-performance computing (HPC) and its applications in multiple fields of science, technology, engineering and mathematics. The summer school stimulated international collaborations and friendships among the attendees and presenters through the unique global setup of the school.

Attendees were immersed in a mix of presentations and hands-on sessions led by more than 20 leading researchers and HPC professionals from both sides of the Atlantic. The program placed particular emphasis on how HPC is being applied to meet current and future computational challenges in various scientific disciplines, as well as the relevant tools and techniques for tackling different problems. Meals and social activities were coupled with mentoring to form an integral part of the school's program, which was designed and organized to promote interaction among the participants.

The goal was to expand the knowledge of the attendees about high performance computing (HPC) and it applications in multiple fields of science and engineering. The goal was also to foster new collegial friendships and partnerships (nationally and internationally) among the presenters and attendees. Additional information about the event is available at: https://www.xsede.org/web/summerschool12

Through a survey conducted at the end of the Summer School, 90% of the attendees, and 100% of the presenters and support staff, indicated that they found the summer school to be excellent or very good. Through the surveys, the respondents provided a number of suggestions for further improving the summer school in future years, along with a very strong vote for continuing to offer similar summer schools in the future. A full report of the Summer School is available upon request.

8.2.3 *Assisting with the Creation of Formal Programs*

Aside from the workshops at two of the institutions working toward formal program adoption, we continued to work with those and other institutions on their efforts to create a formal program. This included providing access to instructional materials that have been used in other undergraduate programs, gathering examples of course syllabi for more specialized graduate courses in bioinformatics, and consultation on possible program content with several institutions.

In addition, a presentation was made to the campus champions in September, making them aware of the range of services offered through the XSEDE education program. This has sparked interest from several other campuses in initial visits to discuss formal programs.

8.2.4 *XSEDE Conference*

We assisted with the solicitation and review of the presentations for the training, education, and outreach track at the XSEDE 2012 conference. We also chaired a session and participated in discussions with representatives of the minority serving institutions at a special session to discuss XSEDE programs.

8.2.5 *Introducing Modeling to Pre-Service Teachers*

During the past quarter, we have made significant progress in our work with College of Education at The Ohio State University to prepare modeling and simulation exercises that can be incorporated into the pre-service curriculum for science and math teachers. Five modules have been drafted for use in the methods class for those teachers. Each module contains background information on the topic, its relationships to the current science and math standards, and one or more exercises that can be incorporated into classroom use. The exercises use existing models and tools available on the web to illustrate problems in biology, chemistry, and earth science. They will be tested in the methods class at Ohio State during the Autumn semester of 2012. Following their evaluation, the revised models will be used to solicit participation from other education colleges.

8.2.6 *Creation of Repository of Education Materials*

Our final activity for the past quarter has been involved with the design of a repository for shared computational science training and education materials. We completed work on a comprehensive, draft ontology of materials that will allow faculty and students to search for materials based on subject areas as well as the competencies that have been created as part of our educational program activities. Working with the Shodor Education Foundation, we have been working to integrate the new ontology into the digital library hosted at the HPC University site.

The overall design of the system is complete and we expect a fully functional test system to be in place by November 2012. We expect to use the system to tag existing XSEDE training materials and a wide range of educational materials. We expect the system to be available for community use after the beginning of the year.

8.3 Outreach WBS 1.6.2

As expected, one of the most significant outcomes of Program Year One was the experience of implementing the Outreach portfolio. While a lot of detail was included in the proposal and initial designs, it is in the implementation that critical issues are often disclosed. This is especially true with Outreach Services, which are benefiting from a year of lessons learned. In particular, Campus Champions and the XSEDE Scholars Program are solid and scaling beyond the resources initially allocated to support them. One of the challenges being addressed is how to continue to support these successful programs and allow them their natural growth. It is also clear that other Outreach services, notably Student Engagement and the Campus Champions Fellowships (a joint project with ECSS) are in need of reevaluation to achieve their desired impact. These are the parameters which are key to Program Year Two.

8.3.1 Underrepresented Outreach

SURA's Program Year One efforts in deeper engagement with researchers and faculty at minority serving institutions is beginning to see tangible results. Mark Jack, a researcher at Florida A&M, has received an allocation on Ranger, and is continuing to receive support from SURA to transition his work to XSEDE services. Kofi Nyako, Morgan State University is using an XSEDE Education allocation to provide resources for his engineering class. Fisk University, as a result of the regional workshop held in Nashville in Program Year One, has joined the Campus Champions program. And travel support has been provided to seven researchers from MSIs to attend professional development events, including a TACC workshop, the American Indian Science and Engineering Society annual meeting, and the SC12 Broader Engagement program. Additional regional workshops are being planned for late winter/early spring at the University of Texas-El Paso, Florida International University, and in the Baltimore/DC area.

The Minority Research Community continues to grow, in size and activity level. Following a well-attended session at XSEDE'12, members of the MRC have begun drafting action plans for integrating XSEDE into their work. The monthly concall in August introduced Campus Bridging through an overview of the XSEDE Campus Bridging vision and a discussion of the Bridging pilot program. Four MRC members have expressed interest in Rocks Rolls and the Campus Bridging team is following up.

The XSEDE Scholars Program continues to engage students and is clearly having an impact on how they think about themselves, their careers, and computation. Following XSEDE'12, feedback from students includes this comment from Adolfo Escobedo (Texas A&M graduate student):

> *"This past week [at XSEDE12] was a very inspirational experience for me. A lot of times it is easy to feel alone because we think that there aren't others who know what it's like to be in our position at graduate school. With such a negative attitude, one can be continuously discouraged, and this causes inner doubts to mount to the point of attrition. However, this conference showed me that we have a sizeable community that is being strengthened by role models like yourself [Dr. Tapia], Dr. Castillo-Chavez, Dr. Velázquez, and many more. I am grateful for the opportunity to meet you."*

The Scholars are showing a hunger to learn more and more about computational STEM and its enabling technologies. While the program's budget is constraining the opportunities for the group to meet face-to-face, the program's leadership is answering the challenge in a number of ways:

- The webinar series for the second cohort is being strengthened with the inclusion of two new session types. In addition to the mentoring and professional development topics that were presented for Cohort One, Program Year Two sessions will include presentations from student researchers as well as technical session that will introduce students to computational tools and applications. The idea for the student research sessions came from a Cohort One Scholar, and was enthusiastically embraced by the current Scholars and their mentors. This set of sessions gives students experience presenting their work to a broader community of peers and professionals and will benefit the both the Scholars and the individual presenters.
- The Scholars program has teamed up with Campus Champions to put students in touch with their Champions wherever possible. While not all Scholars' campuses have Champions,

introductions are being brokered for students on the 12 campuses that do. This is not only improving both the Scholars and Champions experiences, but building interest and generating valuable input for the Student Champion program currently under discussion (see Campus Champions, below). In the upcoming quarter, students who do not have Champions will be introduced to Champions on nearby campuses, in anticipation of a more formalized Regional Champions Program.

Travel to attend national conferences, such as XSEDE'12, SC12, and the Tapia Celebration of Diversity in Computing is becoming increasingly challenging for the group as all costs continue to rise above the budget estimates. Upcoming evaluation will attempt to identify specific value and impact generated by these opportunities, to provide input into any reprioritization that may be necessary to meet the goals of the program.

The Minority Faculty Council held their first face-to-face meeting at XSEDE'12. Each member was asked to share a topic that s/he believes is critical to the efforts to broaden participation. After lively discussion, the group has decided to continue to meet as working groups to dive deeper into specific areas of concern, including education and training and how to make XSEDE resources more readily available and more useful to faculty. Council members are working on a document that will help guide XSEDE and the national community in addressing these critical issues. The group is preparing a work plan and timeline based on the understanding of XSEDE that they have developed through this quarter's activities.

8.3.2 Speakers Bureau

Efforts in the first quarter of Year 2 has been focused on evaluating the outcomes of XSEDE presence at national, professional, and society events, and planning for the effective use of the limited Program Year Two budget. Because of staffing changes, Campus Champion expenses (conference registration, group dinner) for the annual XSEDE conference have been shifted to the general Outreach budget. This necessitates a critical evaluation of the events that XSEDE Outreach will attend, and how XSEDE staff will be supported to attend and represent XSEDE. As of the end of this quarter, plans are being made for XSEDE to participate in the following conferences and events:

Dates	Event	Location
October 26-28	Southern Regional Education Board	Tampa, FL
February 7-10	Tapia Celebration of Diversity in Computing	Washington, DC
February 14-18	American Association for the Advancement of Science	Boston, MA
February 28-March 2	Emerging Researchers Network	Washington, DC
April 25-28	Humanities, Arts, Science and Technology Advanced Collaboratory	Toronto, Ontario, Canada
June 13-14	Joint Annual Meeting (NSF)	Washington, DC

XESDE staff did attend the SIGGRAPH and American Chemical Society conferences in August. These experiences made it clear that, to have impact at professional and discipline-specific events, it is critical to present material that is relevant to that specific audience. Very few STEM communities are aware of how services like XSEDE can transform their field, and XSEDE staff at these events needs to be well prepared to explain and demonstrate the value of these national resources. To that end, the Outreach teams are working with XSEDE External Relations to develop a more detailed set of materials that will highlight discipline-specific projects that are benefitting from computational tools and techniques. The first of these documents, Chemistry and

Chemical Engineering has been completed and will stand as a template for additional materials in other fields of science.

8.3.3 Student Engagement

During the previous quarter (Q2), twelve students were selected to participate in the first XSEDE Student Engagement Summer Immersion Experience. For ten weeks, from June 1 through August 3 they worked with XSEDE staff and researchers on a variety of projects. All of the students made summary presentations at the XSEDE'12 conference, and five also presented posters of their work as part of the XSEDE'12 Student Poster contest. While the formal evaluation is still underway, feedback from the students and their supervisors is generally positive. But there are a number of issues that need to be addressed for the second year of this program, including addressing the disparate needs of undergraduate versus graduate students, optimizing the use of a very limited and highly distributed participant support budget, and providing more substantial mentoring to the students throughout the year. The Student Engagement team is working with the XSEDE Scholars, XSEDE training and the Campus Champions to develop a more effective program for Program Year Two.

8.3.4 Campus Champions

New Campuses this Quarter	**Totals by the Numbers:**
University of Colorado at Colorado Springs	128 Institutions
University of Central Florida	67 Regular
Fisk University	43 ESPCoR
Florida State University	10 MSI
George Washington University	8 both EPSCoR and MSI
Mary Washington University	
Stanford University	172 Champions
Indiana University	81 present at XSEDE'12
Tufts University	
North Carolina Central University	

The Campus Champions' working groups, *Campus Outreach* and *User Assistance*, completed the drafts of material for Champions to use on their campuses. These documents were distributed to all of the Champions at the XSEDE'12 conference (and mailed to those who were unable to attend). The Working Groups are now receiving feedback from their peers as the Champions have returned to their campuses and have begun using the materials. Both Working Groups will continue to meet as needed to process feedback and keep the resources current.

Two new working groups are being formed to address initiatives to create programs for *Regional and Student Campus Champions*. Initial conference calls have been held, and the two groups are brainstorming what the roles and responsibilities would be for these new types of Champions. There is a lot of interest in both programs among the Champions, but the goals and objectives need to be defined carefully so that they can be effective additions to an already successful program, with clear metrics that can be evaluated and measured.

With the assistance of the Campus Outreach and User Assistance materials, Champions on five campuses are engaged in technology *Information Days* at their institutions. The University of Missouri Science and Technology, the University of Oklahoma, Ohio State, Michigan State University, and the University of Michigan will all be presenting computational STEM resource information to their faculty and researchers in the current academic period.

Training sessions, notably "New Champion Orientation" and "How to Write a Successful XRAC Proposal" were delivered in this quarter. Feedback from both has been positive, and there is a request that the XRAC session be added to the regular training calendar, at least on a quarterly basis. Much training was also provided at the XSEDE'12 conference, with Champions enthusiastically both delivering and consuming the offerings. The Champions have been proactive in identifying specific training needs, and a prioritized list has been sent to the XSEDE Training coordinator. Champions are also looking forward to working with the Training group to pilot the "*Train the Trainer*" program being developed during Program Year Two.

An overview presentation by the *Open Science Grid* to the Champions in June has met with unprecedented success. OSG is processing the requests for more information and for accounts and access that have come from Champions and their campuses and expect to be ready to begin actively recruiting new users and sites again sometime in the beginning of 2013.

The *Campus Champions Fellowship program* is finally under way, with four Fellows partnered with four ECSS consultants. Administrative coordination between the Fellows and the various XSEDE partners responsible for overseeing the program has proven to be complicated. Evaluation is currently investigating the recruiting, placement, and execution of the program, to provide actionable input prior to beginning the second cycle of implementation.

Challenges: The Campus Champions program is suffering from significant growing pains. Although there are no active efforts to recruit new Champions, more and more campuses are joining every quarter. This is taxing already lean budgets, both financially and with respect to the time and talents available to provide adequate support:

- According to the Memorandum of Understanding, signed by each Campus when they join the program, Champions are "required" to attend the annual XSEDE conference. While the Champions are expected to pay for their own travel expenses, XSEDE provides conference and tutorial registration. For the 81 Champions who attended, this totaled over $41,000 for XSEDE'12. Conference registration fees and the number of Champions attending are both increasing and the Outreach budget cannot support this expense if this trend continues. Outreach Services and Campus Champions Leadership are looking at ways to prioritize the limited budget so that the Campus Champions program will continue to support successful outcomes in the research and academic communities. Potential changes may include:
    - Dropping the conference attendance requirement (and associated complementary registration) from the Campus Champions Memorandum of Understanding;
    - Requiring a more involved presence at the annual conference (paper, poster, committee, etc.) in exchange for complementary registration;
    - Seeking additional NSF funding; and/or
    - Pursuing other non-XSEDE forms of support for the program.
- The time required to help new Champions get up to speed with XSEDE and Champion resources is beginning to exceed the time allotted to these functions. In addition to supporting Champions in getting started and helping their campuses, the XSEDE staff responsible for Champions are working on design and implementation of new programs (Regional Champions, Student Champions), providing support for campus events, and working with other XSEDE staff to provide enhanced services to Champions. To relieve some of this workload, ECSS is working with Outreach, using the flexible hiring process, to add additional staff to the Champions support team. As of the end of this quarter, a new staff position had been posted and applications were being collected. It is anticipated that this position will be filled by the end of the next quarter.

8.3.5 Extreme Scaling Workshop

The Extreme Scaling Workshop brought together 45 researchers and professionals from academia, industry and government to address algorithmic and applications challenges and solutions in large-scale computing systems with limited memory and I/O bandwidth.

This was the 6th in a series of workshops sponsored by Blue Waters and TeraGrid/XSEDE, held July 15-16, 2012 in Chicago. The workshop was held in cooperation with ACM SIGHPC. A call for papers was used to solicit submissions, and Irene Qualters (NSF) was invited to be the workshop keynote.

The workshop organizers were: Bill Kramer (NCSA), Ralph Roskies (PSC), Nick Nystrom (PSC), Sergiu Sanielevici (PSC), Scott Lathrop (Shodor). The workshop was organized to provide sets of two presentations of 30 minutes each followed by half hour for discussions about the presentations. The workshop details including the agenda and the presentation materials are publicly available at https://www.xsede.org/web/xscale/. The workshop proceedings, including eight papers, will be submitted to the ACM SIGHPC and the ACM Digital Library for broad dissemination. The total expenses were $10,250 and the total revenues (including $125 registration fees and contributions by Blue Waters and XSEDE) matched the expenses for a break-even set of costs for the workshop.

The workshop was organized to occur immediately before the annual XSEDE12 Conference that was also held in Chicago. The participants who planned to attend both events appreciated the ability to save on travel costs, but recommended not overlapping with the XSEDE tutorials in the future to reduce conflicts.

An external evaluation was conducted by the TEOS external evaluation team. The findings from the external evaluation include:

- Quality of Workshop: 82% of respondents reported the workshop fulfilled their expectations, and 93% rated their experience as successful and would recommend the workshop to others.
- Participant Knowledge Gain: 82% of the respondents agreed that the speakers stimulated their interest; 93% said the presentations improved their knowledge and understanding of the topics covered; and 86% are confident they can incorporate the information into their work.

The evaluation determined that workshop participants viewed this workshop as a unique opportunity to engage a small and specialized community. Blue Waters and XSEDE plan to continue to collaborate to offer future joint workshops, and look forward to working with ACM SIGHPC on future workshops.

8.3.6 XSEDE12

The Inaugural XSEDE conference – XSEDE12, was held 16-20 July in the Hotel Intercontinental on the Magnificent Mile of Chicago, IL. It was a tremendous success. This is not to say that there we did not make any mistakes or learn any lessons– but as an inaugural conference in a new series, and the first ever gathering of the community of XSEDE providers and XSEDE users, it was a great success.

8.3.6.1 Summary statistics

A total of 616 individuals registered for the conference, and a total of 586 people attended. There were a total of 104 talks presented in the technical tracks; of them, a total of 64 were represented in the conference proceedings by a full (peer reviewed) paper.

Acceptance rates were as follows for the technical tracks:

Technology:	48% (13/27)*
Science:	56% (23/41)*
Software:	72% (13/18)
EOT:	93% (14/15)
Total:	62% (63/101)*

*Note that Science and Tech track ended up inviting three talks that were accepted independent of the regular review process, so they were not included in these totals.

Tutorials also involved a much more rigorous and involved review process than was typical of most past TeraGrid conferences, with acceptances of 81% (17/21).

8.3.6.2 Highlights of the conference

The conference included an exciting lineup of speakers from around the world, presenting on a variety of topics. The conference program contains something of interest for almost everyone, including the keynote and plenary addresses from:

- Richard Tapia, mathematician, Rice University professor, diversity advocate, and recent National Medal of Science recipient (keynote speaker)
- Gayatri Buragohain, an award-winning electronics engineer from India who is the founder of Feminist Approach to Technology and co-founder of Joint Leap Technologies
- Thomas Eickermann, head of the communication systems division of the Julich Supercomputing Centre in Germany
- Jim Kinter III, director of the Center for Ocean- Land- Atmosphere Studies (COLA) and a professor at George Mason University
- Steven Reiner, Emmy Award winner, associate professor of journalism at Stony Brook University, and former“60 Minutes” producer.
- James Gutowski, speaking on behalf of the XSEDE12 Platinum level sponsorship by Dell and Intel. His talk focused on the innovative Stampede system, to be deployed by the Texas Advanced Computing Center, in partnership with Dell and Intel.

As the last major XSEDE event of the first year of the XSEDE project, this conference provided an opportunity to reflect on the work that has been accomplished, the impact that has been made on science and engineering, and the programs being established that promise future success. XSEDE12 offered the first opportunity to come together as a community dedicated to lowering the barrier to entry into the realm of advanced computation, achieving new scientific and engineering breakthroughs, and establishing new and improved methods of learning about, accessing, and using the resources of the National Science Foundation-funded project, XSEDE.

The XSEDE12 technical program provided an opportunity to present and discuss significant science achievements made possible through cutting-edge cyberinfrastructure, as well as the advancements in software, technology, and education that support those research efforts. This year’s program featured science papers drawn from a number of submissions on many topics, including the acceleration of molecular dynamics simulations, multi-scale simulations of blood--flow, mining of social media data, humanities supercomputing for large-scale video analysis, simulations involving storm interaction and tornado prediction, hybrid MPI/OpenMP simulation of DNS turbulence, and astronomy simulations of black hole binary spirals. The technology track, focused on systems and middleware, featured talks on software engineering best practices, technologies for efficient use of heterogeneous nodes, evaluation of data-intensive supercomputers, XSEDE parallel and distributed file system technologies, grid system software, and other technologies. In the software and software environments track, researchers presented work on improving bioinformatics software performance, a phylogenetics science gateway, parallel debugging, the parallel software programming tools, and Campus Bridging. The education, outreach and training track included discussion of science, technology, engineering, and mathematics (STEM) program evaluation; educational tools using cyberinfrastructure; XSEDE user and K- 12 outreach; and inclusion of minority students in computational research.

A student dinner Sunday night, a special track for student posters, and a student programming competition provided exciting activities that were designed for and enjoyed by student attendees.

The poster reception and visualization showcase brought together scientific staff, faculty, and student researchers for active, in- depth discussion, and sharing of research. In addition, Birds of a Feather and panel sessions provided the stage for discussion of opportunities and challenges surrounding big data and data-intensive computing, scientific cloud computing, cloud/HPC/grid educational activities, heterogeneous computing, improving accessibility of advanced computing resources, campus bridging, software sustainability, and security.

8.3.6.3 Diversity and accessibility

XSEDE12 was noteworthy for its focus on diversity – a tone set by the keynote and plenary speakers. Meeting diverse needs of participants was a priority, with sign language interpreters for the plenary sessions, large print programs, and physical accessibility for wheelchairs to all conference venues. The plenary talks will all be available on the web as video including within the viewing frame the sign language interpreters, making these talks easily accessible to people who understand best via sign language.

8.3.6.4 Evaluation and lessons learned

XSEDE12 General Chair Stewart set the following goals for the XSEDE12 conference when he agreed to take on this role:

- Have an excellent conference event that effectively exchanged information relevant to XSEDE12 and the communities it serves, highlighting its key role nationally and internationally (based on Stewart's personal view that XSEDE is currently the most important organizing function within US open research cyberinfrastructure and thus critical within the US and in US international relationships)
- Have XSEDE12 be operated in a way that promoted excellent organizational learning by
  - o Documenting through proposals and plans throughout the process of putting on XSEDE12 what we intended to do so that we could learn afterwards what we got right and not right, through plan and luck.
  - o Evaluating the conference effectively and formally
- Establishing new standards for IT conferences in diversity across all dimensions – diversity in attendance across racial, ethnic, and status (student, professional staff, faculty) dimensions; and new standards in accommodating differently abled individuals (physical accessibility, and sight and hearing enablement)
- Establish XSEDE as a 2nd-tier computing conference with excellence in presentation of technical, scientific, and education/outreach/education content at the conference and in the proceedings. [2nd tier was specifically the goal – in the belief that the TeraGrid conference series was largely viewed as a 3rd tier conference in terms of its proceedings output at least; and in the belief that becoming a 1st tier conference and joining SCxy and HPDC in that first tier takes years or decades).
- Have XSEDE12 break even, or at least come close.

A full formal public report will be produced about XSEDE12, along with considerable information related within the XSEDE organization. Overall, XSEDE12 achieved the goals set out above in a fashion that was good to excellent. Key highlights follow:

- Have an excellent conference event. Informal and formal evaluations were highly positive, particularly comments abou8t the general positive atmosphere. The one problem that stood out as an issue was networking, particularly in guest rooms in the oldest parts of the hotel.

We did as best we could to ameliorate this issue, but there is no doubt that this was the largest shortcoming in the execution of the conference.

- Have XSEDE12 be operated in a way that promoted excellent organizational learning by
  - The XSEDE12 team presented more than 10 individual proposals to XSEDE senior leadership for their advice, action and approval, keeping the operation of the conference well understood throughout the planning stages. The XSEDE12 team assembled and turned over to the XSEDE13 team more than 350 pages of planning and contract documentation.
  - The XSEDE evaluation team carried out IRB-approved, formal evaluations, which will be reported in detail in a separate document. On the whole, evaluations were highly positive.
- Establish XSEDE as a 2nd-tier computing conference with excellence in presentation of technical, scientific, and education/outreach/education content at the conference and in the proceedings. The quality of the conference, the talks, and especially the proceedings seems to have XSEDE well on its way solidly into the 2nd tier of information technology, computer science, and cyberinfrastructure conferences nationwide and worldwide.
- Have XSEDE12 break even, or at least come close. XSEDE12 will not close the books breaking even. We will come fairly close.

8.3.6.5 Acknowledgments

The program committee leaders of XSEDE12 contributed greatly to the success of the conference:

- Overall Leadership
  - General Chair: Craig Stewart, Indiana University
  - Deputy Chairs: Warren Froelich, SDSC; Kay Hunt, Purdue
  - Finance and Registration Chair: Jeff Gaede, NCSA
  - Communications Chair: Susan McKenna, NCSA
- Technical Program
  - Chair: Philip Blood, PSC
  - Deputy Chair: Amit Majumdar, SDSC
  - Science Track Chair: Carlos Rosales-Fernandez, TACC
  - Science Track Deputy Chairs: Jan Odegard, Rice; Frank Willmore, TACC
  - Technology Track (Systems and Middleware) Chair: Victor Hazlewood, NICS
  - Technology Track Deputy Chair: Thomas Hacker, Purdue
  - Software and Software Environments Track (Gateways, Bridging, applications developers) Chair: Jay Alameda, NCSA
  - Software and Software Environments Track (Gateways, Bridging, applications developers) Deputy Chairs: Suresh Marru, Indiana; Ewa Deelman, USC
  - Education, Outreach, and Training Track Chair: Sandie Kappes, NCSA
  - Education, Outreach, and Training Track Deputy Chairs: Renato Figueiredo, U Florida; Steven Gordon, OSC
  - Poster Track Co-Chairs: Amy Apon, Clemson; J. Barr von Oehsen, Clemson
  - Tutorials Chair: Mark Fahey, NICS
  - Tutorials Deputy Chairs: Galen Arnold, NCSA; Bilel Hadri, NICS
  - Proceedings Chair: Chander Sehgal, Open Science Grid and Fermilab
  - Proceedings Deputy Chair: Raj Kettimuthu, Argonne National Laboratory
- Logistics and Local Arrangements
  - Chair: Warren Froelich, SDSC

- Deputy Chair: Kay Hunt, Purdue
- Vendors Liaison: Donna Hunt-Caraballo, HMS Meeting Services
- Networking and Security Chair: Randy Butler, NCSA
- Networking and Security Deputy Chair: Tom Hutton, SDSC
- Visualization Showcase Chair: Amit Chourasia, SDSC
- Visualization Showcase Deputy Chair: Sean Ahern, NICS
- Social Events Chair: Amit Chourasia, SDSC
- Social Events Deputy Chair: Diane Baxter, SDSC
- Birds of a Feather Sessions Co-Chairs: Susan Mehringer, Cornell; David Lifka, Cornell
- Awards Chair: Tom Furlani, Buffalo
- Awards Deputy Chair: Gregor von Laszewski, Indiana
- Student Volunteers and Program Chair: Jenett Tillotson, Indiana
- Student Volunteers and Program Deputy Chair: Ange Mason, SDSC
- Sponsorships and Exhibits Chair: Kay Hunt, Purdue
- Sponsorships and Exhibits Deputy Chair: Therese Miller, Indiana
- Campus Champions Chair: Philip Blood, PSC
- Campus Champions Deputy Chair: Jeff Pummill, Arkansas
- XSEDE Working Group Chair: Tim Cockerill, NCSA

Everyone involved worked particularly hard. Chander Sehgal deserves special thanks for his role as Proceedings Chair. An unanticipated side effect of the success we had in getting full papers submitted to and accepted into the proceedings was a tremendous gap between the amount of work that Chander had been told his role would involve and the amount of work he ended up actually investing. The quality of the proceedings is strong testament to the quality of Chander's work.

Our partners in putting on the conference deserve great thanks: Greg Brice, Kenny Armstrong, and their colleagues of AVI; Amy Watts, Alana Zeiger, John Barbier, and their colleagues at Hotel Intercontinental Chicago Miracle Mile; and most especially Donna Hunt (President of HMS Meeting Services), Yvonne Bean (Director of Global Accounts at HelmsBriscoe), and their team (Dianne Matthews, Christine Moore, Jack Williams, and LaKeenya Young). Donna, Yvonne, and their staff deserve tremendous credit for their critical roles in the success of the conference. Thanks also go to John Towns, XSEDE PI, and co-PIs Jay Boisseau (TACC), Ralph Roskies (PSC), and Nancy Wilkins- Diehr, as well as the National Science Foundation and Barry Schneider. Thanks go also to staff at IU worked to support and organize XSEDE12:

Nina Paine, Rudeana Honeycutt, Daphne Siefert-Herron, Karen Garrett (Office of the VP for IT); Richard Knepper, Therese Miller, Julie Wernert, Malinda Husk, (Research

Technologies and Pervasive Technology Institute); and Beth Plale (Professor in the IU School of Informatics and Computing and Managing Director of the IU Pervasive Technology Institute).

A conference the scope of XSEDE12 would not exist without the generous contributions of sponsors. We are especially appreciative of the considerable support from: Appro International, Inc.; the Coalition for Academic Scientific Computation (CASC); the Computation Institute; Cray; Dell and Intel; FutureGrid; NVIDIA; Penguin Computing; the San Diego Supercomputer Center, and the Indiana University Pervasive Technology Institute. These organizations were both willing and able to support the first XSEDE conference. We deeply appreciate their generosity and faith that the conference would prove meritorious of their support. Three grant awards have directly aided the planning and execution of this conference. NSF award 1053575 (John Towns, National Center for Supercomputing Applications, PI; and Ralph Roskies, Pittsburgh Supercomputing Center; John Boisseau, Texas Advanced Computing Center; and Nancy Wilkins-

Diehr, San Diego Supercomputer Center, Co- Principal Investigators) funded much of the cost of planning this conference and some of the cost of the conference execution. NSF award 1237393 (Jennet Tillotson, Indiana University Pervasive Technology Institute, Principal Investigator; Philip Blood, Pittsburgh Supercomputing Center, and Timothy Cartwright, University of Wisconsin, Co-Principal Investigators) supported participation of some of the students and Campus Champions who participated in this conference. The time of Nina Paine and some of the time of Craig Stewart dedicated to planning this conference was funded by a grant from the Lilly Endowment to Indiana University to create the Indiana University Pervasive Technology Institute. The contributions in this proceedings volume each indicate the many sources of support that have enabled the scientific, technical, and educational achievements described in this conference.

The Association for Computing Machinery, Inc., deserves thanks for allowing XSEDE to host this event in cooperation with the ACM SIGAPP and publish this record of the intellectual material that is the core of the conference. We especially thank the leadership of SIGAPP — Chair Sung Shin and Vice Chair Richard Chbeir —and hope that the XSEDE12 conference marks the beginning of a long and productive collaboration between XSEDE and ACM SIGAPP.

8.4 Community Requirements and External Evaluation WBS 1.6.3

8.4.1 Community Requirements Highlights

The TEOS community requirements activities proceeded on track. Level 3 Managers' gave updates and responses to the Community Needs Survey summary at the face-to-face meeting last quarter. In response, the TEOS Advisory Committee (AC) generated a brief set of recommendations for the TEOS Level 3 managers. TEOS managers also received recommendations from the NSF review in June. The Community Requirements Manager synthesized the major points of these recommendations for a TEOS management team meeting at XSEDE 12, and a condensed synthesis is posted to the wiki.

Level 3 Managers have drafted responses to both reviews. Their responses to the AC review will be discussed at the upcoming AC meeting. Upon the recommendation of the TEOS AC, we have scheduled a Strategic Planning Retreat for just prior to the next quarterly meeting in December. At that meeting, TEOS leadership staff will discuss both reviews and their impact on future plans.

The TEOS Advisory Committee membership has been expanded to include Kevin Franklin of UIUC, in an effort to provide further breadth of background in the Humanities, Arts and Social Sciences communities. The TEOS Advisory Committee current membership includes:

- Carlos Castillo-Chavez, Arizona State University
- Kevin Franklin, UIUC
- Roscoe Giles, Boston University
- Gwen Jacobs, Montana State University
- Rubin Landau, Oregon State University
- Wilf Pinfold, Intel
- Nora Sabelli, SRI
- Valerie Taylor, Texas A&M University

Valerie Taylor and Kevin Franklin both serve on the XSEDE Advisory Board (XAB) to foster communications between the XAB and the TEOS AC.

8.4.1.1 Next Quarter Focus:

The quarterly conference call of TEOS Advisory Committee and Level 3 Managers has been scheduled for October 18, 2012. Brief summaries of the major TEOS services for marketing purposes have been drafted for sharing prior to the AC meeting, and we will seek creative ideas from the Advisory Committee for increasing the effectiveness of TEOS marketing to ensure strong, positive, impact among the community. The Community Requirements Manager will report on the strategic planning retreat and TEOS actions resulting from that meeting.

8.4.1.2 *Risks*

With any proposed program or activity changes that result from the TEOS Strategic Planning Retreat are risks of changes in scope and budgets to partner activities, and any confusion that may cause. The Community Requirements Manager will work with Scott Lathrop on a communication plan to extend across TEOS and XSEDE to mitigate that risk.

8.4.2 *External Evaluation Highlights*

The external evaluation team has been very active working across all TEOS team to conduct formative evaluations of the programs and activities. These evaluations are proving to be very effective providing the TEOS programs with advice for improving resources and services.

8.4.2.1 *Training*

The external evaluation team continued to explore the feasibility of tracking users longitudinally through the XSEDE User Portal (XUP). The team identified and presented risks for the Training evaluation to XSEDE and TEOS leadership at the XSEDE Quarterly Meeting in September 2012. The risks included (1) low survey response rates (below 16%) on the XSEDE User Portal (XUP) and (2) threats to longitudinally tracking users through the XUP. The evaluation team attributes the identified risks to multiple means of registration for Training activities outside of the XUP as well as the generation of multiple XUP usernames by TEOS participants. Currently, XUP registered Training participants receive a post-training session survey through the XUP upon return to the registration system. The registration system also collects vital demographic data for evaluation and reporting purposes. Alternative forms of Training registration vary greatly and the data gathered cannot be linked.

The next steps for the external evaluation team and TEOS leadership are to determine policies and/or alternatives for Training registration and methods for data collection.

8.4.2.2 *Education*

In August 2012 the external evaluation team administered an online survey for the 2012 Short Course on Parallel Programming at the University of California at Berkeley. 23% (88/375) of the registrants responded to the online survey. 42% (37/88) of the respondents identified themselves as graduate students and 21% (18/85) of all respondents claimed to have an XSEDE Portal username. 52.9% (46/87) reported that they have a better understanding of parallel computing as a result of this experience and 50.6% (44/87) would recommend this course to others. Respondents were asked to rate the workshop activities on a 5 point scale from not at all useful = 1 to very useful =5. Tim Mattson’s presentations were ranked the highest by respondents: OpenMP-Basics (M = 4.43, SD = 0.65), Distributed Memory Programming in MPI (M = 4.35, SD = 0.74), and OpenMP – New Features (M = 4.34, SD = 0.68). Suggestions were also made for additional topics to be covered in future workshops. For more detailed findings, please refer to the interim evaluation report submitted to Scott Lathrop, Steve Gordon, and James Demmel in September 2012.

Sinte Gleska University hosted an onsite XSEDE Workshop on October 12, 2012. The external evaluation team drafted a short paper and pencil survey to be administered and collected at the event. The survey included four demographic questions and five open-ended items. The open-ended items did not focus on presentation content, but probed feedback on the process of adoption and implementation of XSEDE services by participants. Steve Gordon will administer, collect, and send the surveys to the external evaluation team for analysis and reporting. An interim evaluation report will be generated and submitted to Steve Gordon and Scott Lathrop following data analysis.

Identification of potential case study institutions continues to be an objective of the external evaluation team. Plans are currently being formulated to evaluate the Spring 2013 seminar being offered by Montgomery College.

8.4.2.3 Outreach

Student Engagement: A post-participation online survey was administered to student participants of the 2012 XSEDE Student Engagement Program. The survey included four demographic items and a combination of 9 open- and closed-items. The questions probed feedback on outcomes related to participation in the program as well as overall experience. An interim evaluation report will be generated after the closing of the survey and submitted to Scott Lathrop and Laura McGinnis. Program supervisors will also receive a post-participation survey to determine the added-value of participation and offer suggestions to improve the program. These data will be analyzed and compiled into an interim evaluation report for Laura McGinnis and Scott Lathrop.

Campus Champions: The evaluation team is currently working with the Outreach program manager to finalize evaluation plans for the Campus Champions Fellows Program. This group is also coordinating an assessment for the overall Campus Champions Program in order to better define and assist its members. Topics of interest include Champion demographics, specific roles, number of users, level of support, and interest in the Campus Champions Fellows Program. Evaluators participate in regular Campus Champions phone call to inform evaluation plans.

SURA: Evaluators are currently engaged in the planning of SURA's upcoming regional events. Data from the Nashville Regional Event (May 2012) is being utilized to inform program planning and decision-making. Evaluators participate in regular SURA Minority Research Council phone calls to inform evaluation plans.

8.4.2.4 Campus Bridging

Evaluators continue to work with the Campus Bridging team to formalize the evaluation plans. Lorna Rivera has attended regular Campus Bridging phone calls to inform evaluation plans. An Indiana University site visit on October 29, 2012 has been scheduled.

8.4.2.5 XSEDE12

The external evaluation team submitted interim evaluation reports pertaining to the XSEDE12 conference evaluation for the following evaluation activities; overall conference survey, student survey, tutorial survey, XSEDE staff survey, and sponsor interviews. To view the reports, please contact Craig Stewart, Nancy Wilkins-Diehr, and Scott Lathrop.

8.4.2.6 Key Trends

The evaluation has identified the following key trends from the last quarter within TEOS:

- High Campus Champion engagement and satisfaction as evidenced by their interaction on the Campus Champions listserv, formulation of working groups, involvement at XSEDE12, and responses to evaluation activities.
- High number of very novice users in all parts of the TEOS branch (i.e. Training, Campus Champions, SURA, student programs, etc.). Novice members of the community are primarily expecting the following at Outreach events: (1) detailed and introductory training content; (2) educational materials that can be easily incorporated at the local level; and (3) step by step instructions for accessing XSEDE resources.
- Student groups are showing a heightened interest for developing professional learning communities. Some outreach programs are beginning to explore ways to exploit this.

8.4.2.7 Plans for Next Quarter

In addition to the aforementioned plans, evaluators will continue to compile data for the annual evaluation report to be generated and disseminated prior to the TEOS December 2012 Retreat. The evaluation team will also explore additional potential case studies for Campus Bridging, Campus Champions, Education, and SURA to present and discuss at the TEOS retreat.

8.5 E&O Infrastructure WBS 1.6.4

Forty-two distinct events were added to the Education & Outreach Blog on the XSEDE web site. Ange Mason (SDSC) collects and vets events for their suitability for various components of our audiences, and modifies the introductions to be appropriate for those audiences.

Mason and Jim Ferguson (NICS) have been working with the Blue Waters project and the HPC University effort to re-design the site and feature a feed from the E&O Blog directly to the HPC University front page. This effort began in the summer with an XSEDE-sponsored student intern at Shodor and has moved on to regular web staff at Shodor. We are also planning to push out many of these events on the Blog via an independent Facebook presence from the main XSEDE Facebook presence, which focuses on project-wide external relations items.

Ferguson and Mason have begun a process to reorganize the TEOS web presence at XSEDE with calls for comment to the other TEOS area leads. In the interim, text for each subproject is undergoing review and update following accomplishments and changes in plan after the first year of the XSEDE project.

8.6 Campus Bridging WBS 1.6.5

The highlight for the campus bridging team was one talk and two panels presented at XSEDE12. “What is campus bridging and what is XSEDE doing about it” was really the culmination of more than a year of work in campus bridging with XSEDE, and is the clear enunciation of scope and planned tasks for the remainder of the initial XSEDE award. In addition, panels on the pilot projects and campus bridging and security were all well attended and led to lively discussion.

The Campus Bridging team created a video of the “What is campus bridging” for streaming and podcast purposes. The video describes the general concepts of campus bridging and XSEDE Campus Bridging initiatives and generally conforms to the talks delivered by the Campus Bridging Team at Internet 2 Members' Meetings, XSEDE11, and SC11. This video will be made available before SC12 begins.

Also, at the September quarterly meeting, the XSEDE campus bridging team met with other key stakeholders and arrived at a prioritization of activities related to campus bridging for XSEDE as a whole.

The Campus Bridging team discussed team initiatives with the XSEDE Operations team and the Software Development and Integration team on a regular basis in order to determine the correct course of action for both the GFFS Pilot Project work and the software packages to be included in the Campus Bridging Rocks Rolls, as well as the Level 3 decomposition of use cases created by the Architecture and Design team.

The Campus Bridging team also met with the Minority Research Community in August in order to describe Campus Bridging initiatives to the community and gather input on directions. Significant interest was expressed in the community about both the Campus Bridging team's Rocks Roll packages and in training and documentation initiatives, as well as the propagation of the GFFS and Globus Online tools for data management.

8.6.1 *Definition of use cases and quality attributes for XSEDE's Campus Bridging efforts*

The Architecture and Design teams have completed the Level 3 Decomposition for Campus Bridging Use Cases and Quality Attributes. Familiarity with the process of creating use cases and quality attributes has been passed on to teams who are currently going through the process with the Architecture and Design teams.

8.6.2 *GFFS Pilot Project*

The GFFS Pilot project sites have completed a training course with the Genesis II developers and have installed GFFS clients and client containers locally. The Operations team has completed installation of the GFFS root container (beta version) for XSEDE and is expected to implement GFFS on XSEDE SP resources in series over the following weeks. Pilot sites are to begin testing at the end of October.

8.6.3 *Campus Bridging Software Packages*

The Campus Bridging team has, in concert with Operations and Software Development and Integration teams, put together a list of XSEDE software which is approved for inclusion in the XSEDE Campus Bridging Rocks Rolls and packaged software. Campus Bridging is working to establish milestones for the packaging of the software and a distribution mechanism for users.

8.6.4 *Challenges in Program Year Two*

The Campus Bridging team anticipates that there may be some challenges in getting pilot sites "completed" with their testing in the 2-4 weeks allocated in the operational calendar. Pilot sites should be able to complete at least minimal functionality tests in the beta environment and get their responses around that time period.

9 TAIS/Audit Services 1.7

9.1 Technical Progress

9.1.1 Additional Data Sources

The data addressed by XDMoD (**X**SE**D**E **M**etrics **o**n **D**emand) has been expanded to include more than processor utilization data (CPU cycles, jobs, wait times, etc). This has led to adding support for a number of new data realms to the XDMoD data warehouse. Realms within XDMoD are used to group distinct types of data and metrics. Each realm consists of a set of data and a number of metrics derived mainly from that data. With the recent addition of the Performance realm, six realms are currently supported as shown in Table 1 below. XDMoD populates these realms with ingested data from both the XSEDE centralized database (XDcDB) and POPSdatabases.

Table 1 Data realm descriptions

Realm	**Description**
Jobs[1]	Provides data and associated metrics for jobs run on XSEDE resources. Metrics provide details on many aspects of user jobs including wait times, job sizes, SUs consumed, resource utilization, and queue expansion factor. Data can be aggregated by user, PI, institution, resource, service provider, field of science, NSF directorate, gateway, queue, and allocation.
Allocations[1]	Provides data and associated metrics for active and expired allocations across XSEDE. Metrics provide details on burn rate, usage rate, total SUs allocated and total SUs used. Data can be aggregated by PI, resource, field of science, NSF directorate, field of science, and allocation type.
Accounts[1]	Provides general account metrics such as number of accounts created, opened, and closed for any given time period.
Grants[2]	Provides general information regarding grants awarded in support of XSEDE allocations including number of awards and total amount awarded. Data can be aggregated by field of science, funding agency, and NSF directorate.
Proposals[2]	Provides basic information regarding awarded XSEDE projects and proposals. Metrics associated with the proposals realm can be aggregated by field of science and NSF directorate.
Performance[3]	Uses application kernel data to provide metrics on cpu, I/O, memory and network performance as a function of time and across different resources.

1: Data for this realm comes from the XSEDE Central Database (XDcDB)

2: Data for this realm comes from the POPS database

3. Data for this realm comes from the application kernels

9.1.2 XDMoD Portal Progress:

The XDMoD portal provides a role-based web interface for mining XSEDE metrics data and performing statistical analysis of XSEDE usage. During the previous quarter, substantial progress was made on XDMoD including: addition of numerous features to the Usage Explorer and the Application Kernel Explorer tools, and preparation for release of XDMoD 2.0. Please note that for the general public and those users lacking a current XSEDE allocation, the functionality of the public role, which requires no XDMoD account, has been greatly expanded (see Appendix 1). The remainder of this section provides greater detail on features in development.

Usage Explorer:

The Usage Explorer has been greatly improved both in capability and usability. The charting capability of XDMoD has been dramatically improved through the implementation of Highcharts (http://www.highcharts.com/), a new open-source charting package, as shown in Figure 1. This allows for clearer charts with improved scaling and support for inclusion in additional document types. The font size is also adjustable and additional export options such as SVG allow the user more control over exported plots. Figure 2 shows an exported plot from the upgraded Usage Explorer.

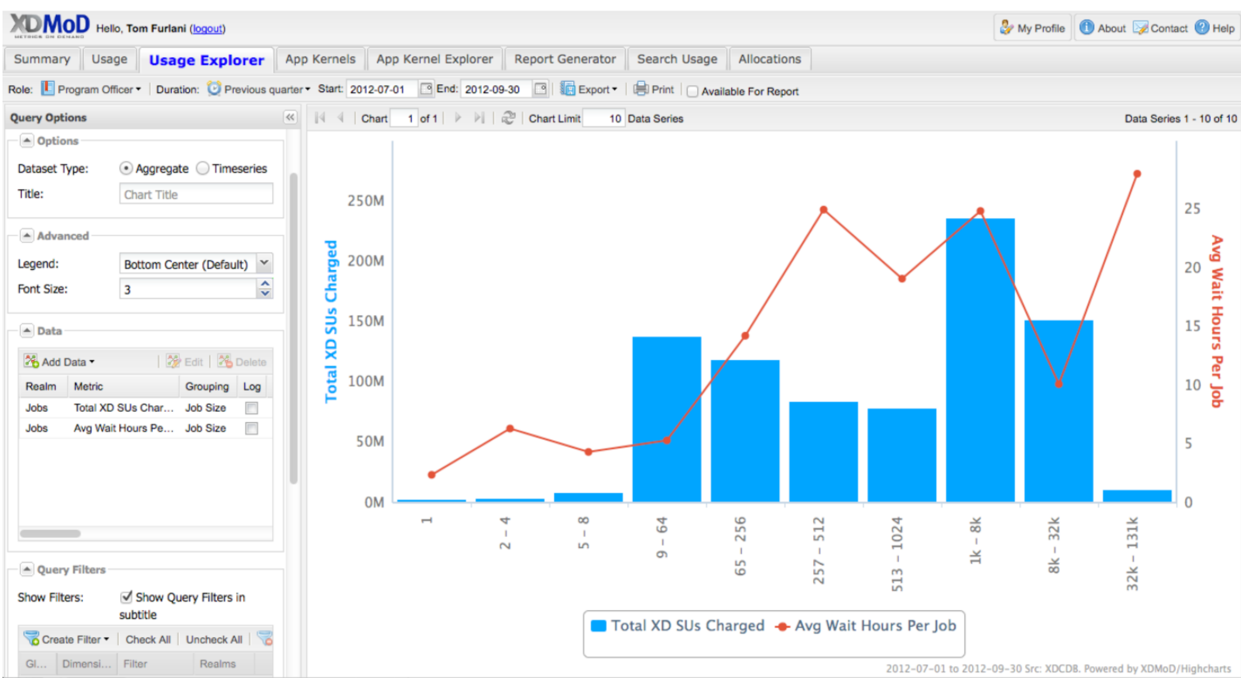


Figure 1. The XDMoD Portal display of the Usage Explorer. A plot of the total XSEDE usage broken out by job size for the third quarter of 2012 is shown on the primary axis (left-hand axis) and the average wait hours per job versus job size is shown on the secondary axis (right-hand axis).

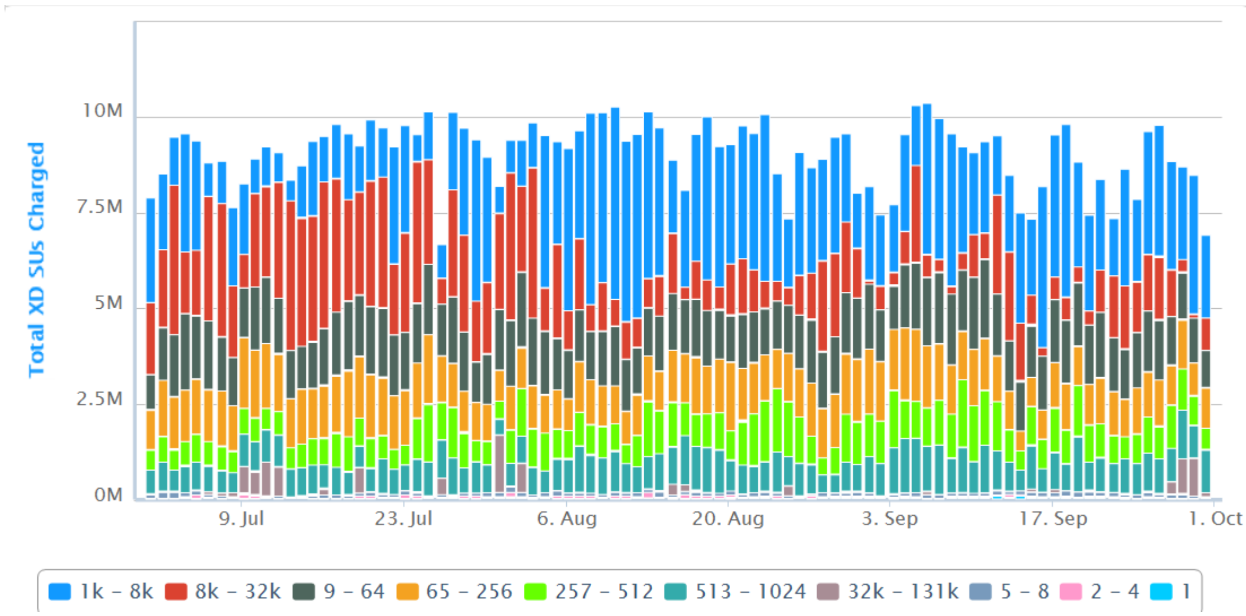


Figure 2. The XDMoD Usage Explorer. An exported time series plot of the total usage by job size for the third quarter of 2012 is shown.

Another new feature under development is the addition of the Performance realm to the Usage Explorer. This is still a work in progress and has not yet been added to the production version of XDMoD but will be available for V2.0 following its release at SC12. Figures 3-6 show a preliminary preview of some plots from this realm for a few selected resources. They are based upon the 64 core application kernel data on the selected resources. Although these indices are still under development, Table 2 below shows which application kernels contribute to each performance index. For all cases below, the desired result is for average values for each resource to remain constant over time. Large variations in a given average would be indicative of a potential problem. Details of this will be described after finalization and release.

Table 2 Performance Index composition

Index	**Application Kernel**	**metric**
CPU performance	graph500	wall clock
	hpcc	linpack floating point performance
	osjitter	mean noise
	npb	floating point performance
	nwchem	wall clock
IO performance	ior	read- and write aggregate
	mpi_tile_io	read and write throughput
	nwchem	wall clock
Memory performance	hpcc	linpack floating point performance
Network performance	graph500	median TEPS
	hpcc	linpack floating point performance
	npb	floating point performance
	mpi_tile_io	read and write throughput

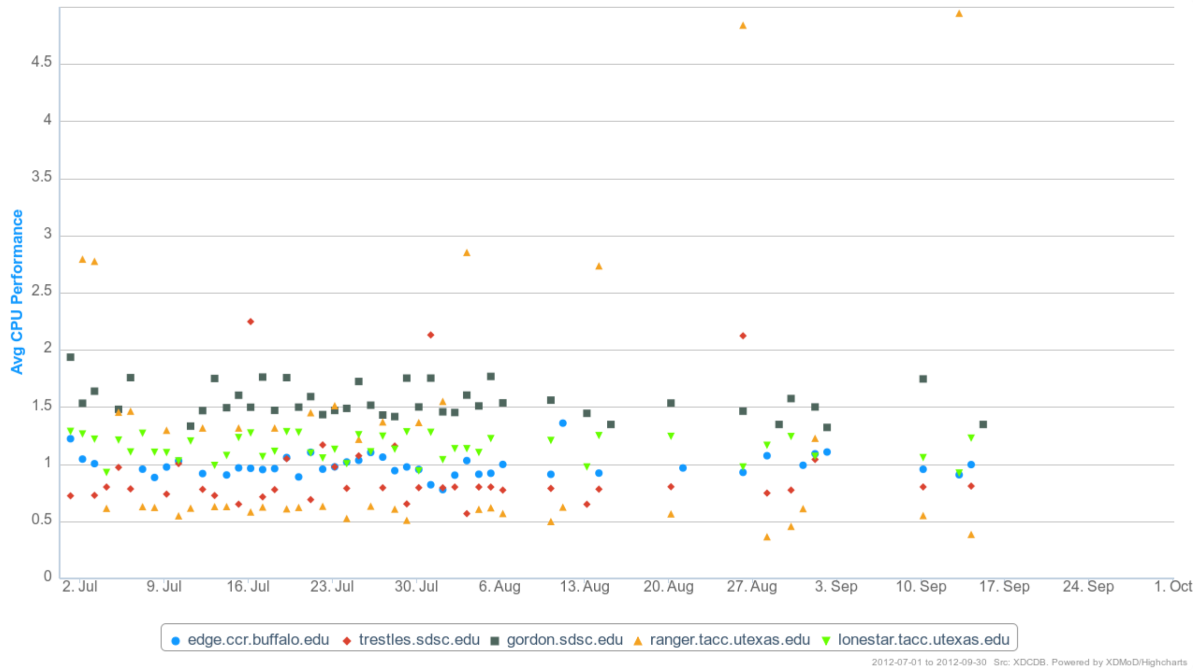


Figure 3. CPU_performance for 5 selected resources based upon application kernel data. The average CPU performance for each resource and at each time point is obtained by averaging the results of the relevant application kernels on that resource.

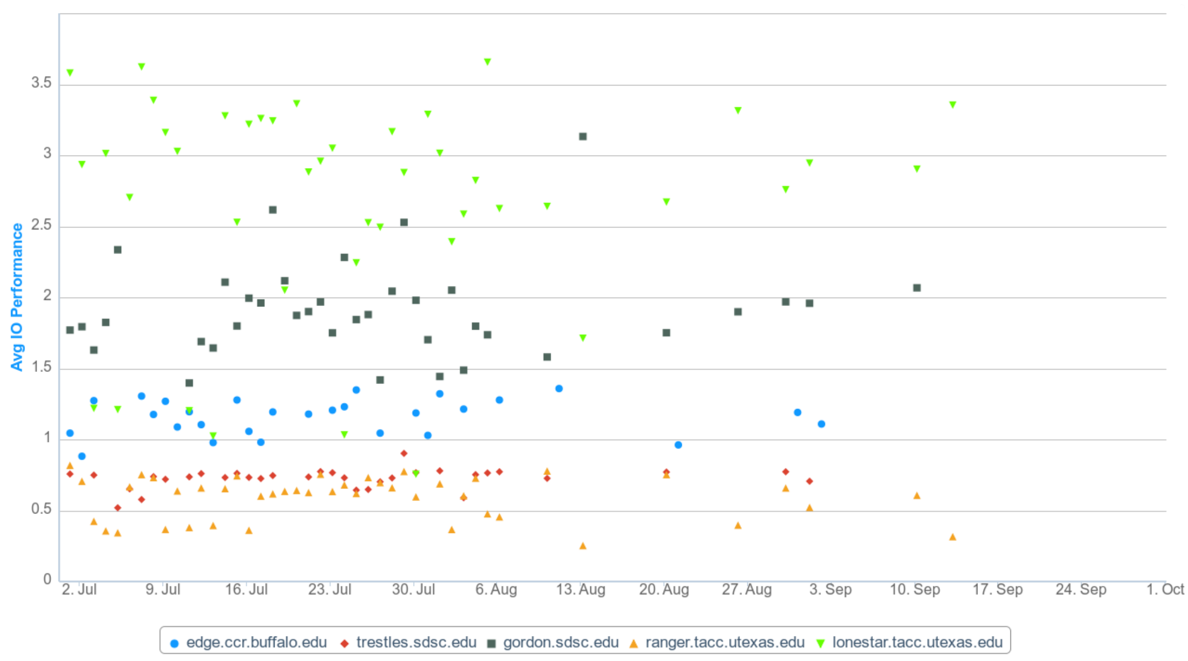


Figure 4. I/O_performance for 5 selected resources based upon application kernel data. The average I/O performance for each resource and at each time point is obtained by averaging the results of the relevant application kernels on that resource.

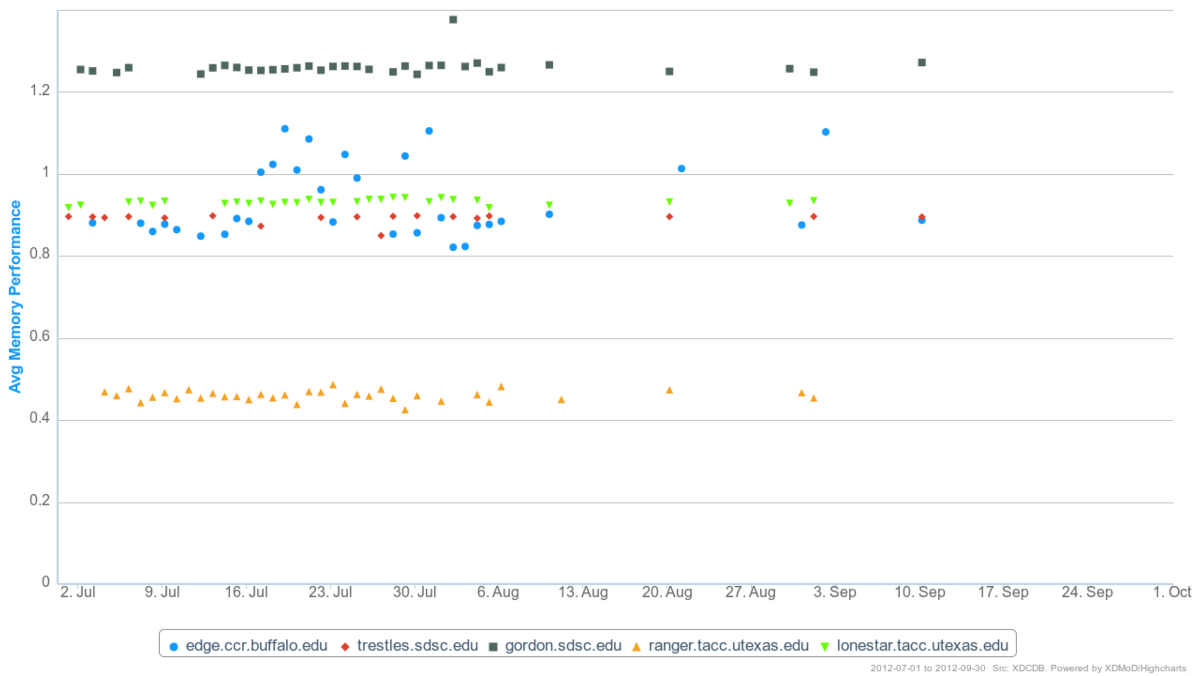


Figure 5. Memory_performance for 5 selected resources based upon application kernel data. The average memory performance for each resource and at each time point is obtained by averaging the results of the relevant application kernels on that resource.

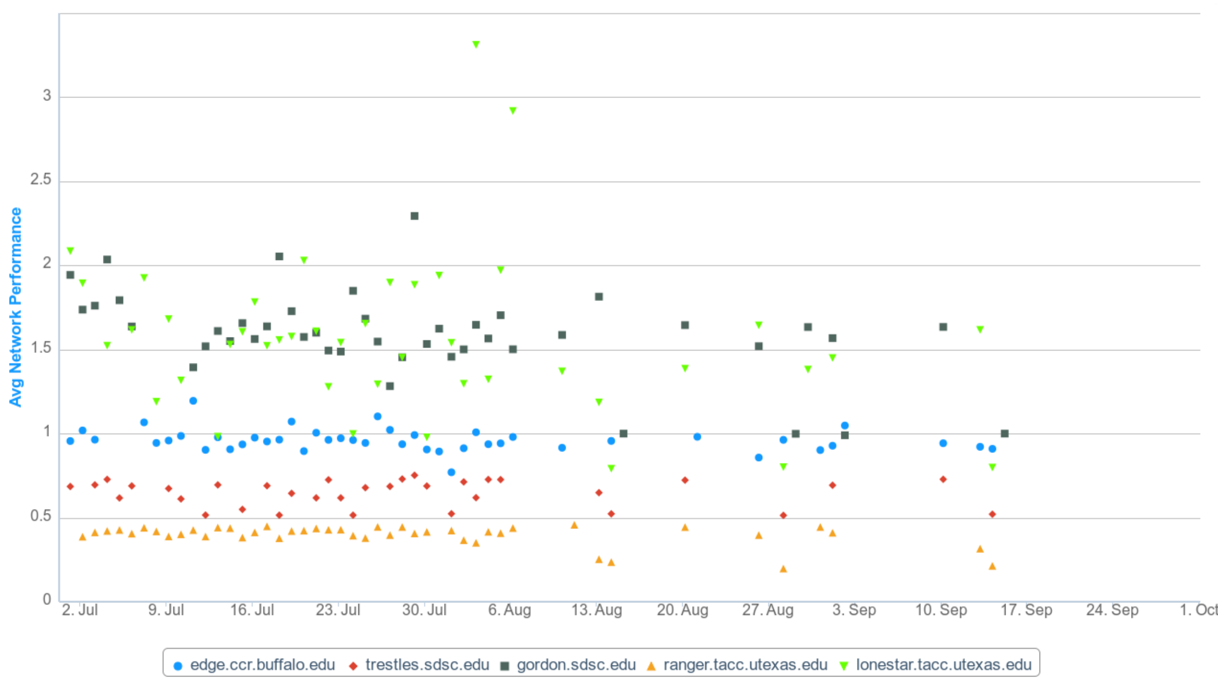


Figure 6. Network_performance for 5 selected resources based upon application kernel data. The average network performance for each resource and at each time point is obtained by averaging the results of the relevant application kernels on that resource.

The XDMoD summary page has been improved in design, layout, and with the addition of "Highcharts" to give it improved functionality and appearance. Figure 7 below shows a screen shot of the new summary page.

Figure 7. New XDMoD summary page utilizing new Highcharts charting package.

Custom Report Builder:

The Custom Report Builder has also undergone substantial improvement to enhance usability. Additional instructions have been added to guide users through the process of generating and tracking reports under multiple roles. A powerful new report template feature has been added that will facilitate the generation of charts for inclusion in the SP quarterly reports. For example, the director of a service provider can generate the entire series of quarterly report charts for each of his resources with a single mouse click on the "Template: SP Quarterly Report" button, as shown in Figure 8. The user now has the option to export the report as a PDF or MS Word file. With the recently added feature to customize the dates on existing plots in existing reports, users easily can generate a complete custom report on his resources for any given desired time frame.

Application Kernel Process Control:

Running the application kernels continuously on the XSEDE (or other) resources generates a tremendous amount of performance data that makes manual oversight of the data to identify underperforming hardware or software impractical. Accordingly, we have been exploring the development of automated processes to monitor application kernel performance. A preliminary model is being developed to use the application kernel data to assess quality of service. Figure 9 shows a representative plot of this effort. A region is automatically selected as the control region. The control region is by definition considered to be the normal operating envelope of the given application kernel. The process, in this case the performance of a given application kernel, is assumed to be nominally in control in this region. If the 5-point running average at a given point beyond the control region exceeds a specified tolerance (based upon the data range in the control region) the process is flagged as out of control. In figure 9 the region where the file close time exceeds 0.2 seconds is considered out of control. The details of when to automatically readjust the control region to account for system upgrades or normal changes, when to flag a process as out of control, etc., are still being finalized.

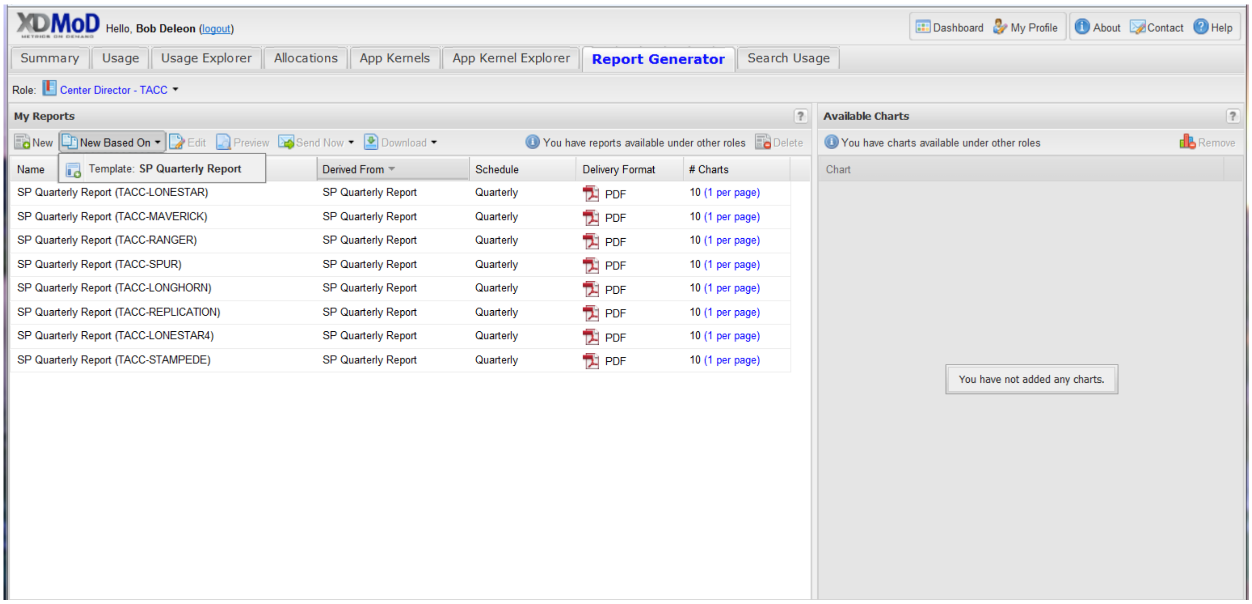


Figure 8. The XDMoD Custom Report Builder. Note that this series of 8 quarterly reports for TACC was generated by a single mouse click on the SP Quarterly Report template in the Custom report builder.

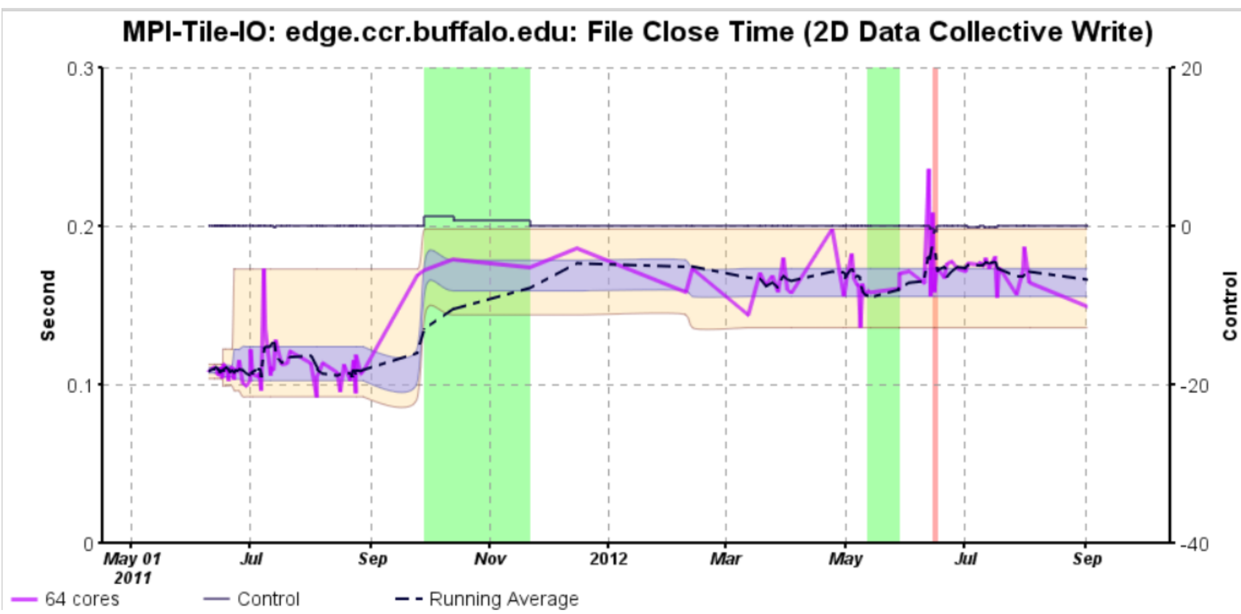


Figure 9. Application Kernel process control. The purple line is the data, the dotted line is a 5-point average, the blue shading indicates the control zone range, the tan shading is the range for the particular zone. The red zones indicate that the process is out of control in an unfavorable sense while the green zones indicate superior performance compared to the in control performance.

9.2 Subaward to National Institute for Computational Science (NICS):

A subaward to Dr. Haihang You of the National Institute for Computational Science was executed. This subaward will leverage Dr. You's expertise and prior work in developing a framework, called the Performance Environment Autoconfiguration frameworK (PEAK) ["Achieve better performance with PEAK on XSEDE resources", B. Hadri, H. You, S. Moore, XSEDE'12 proceedings], to automatically help developers and users of scientific applications select the optimal configuration for their application on a given platform and to update that configuration when changes in the underlying hardware and systems software occur. The configuration options considered for the performance optimization include the compiler with its settings of compiling options, the numerical libraries and settings of library parameters, and settings of other environment variables. The PEAK framework has been demonstrated to select the optimal configuration to achieve significant speedup for some scientific applications executed on XSEDE platforms such as Kraken and Nautilus. We seek to leverage this technology for the benefit of the Technology Audit Service award for XSEDE by incorporating a version of it into our application kernel development work.

The benefit for TAS will be substantial. Implementing the PEAK technology will help XSEDE service providers and HPC centers produce optimal application builds and to ensure that they remain optimal through system upgrades. Under the subaward, Dr. Haihang You will oversee software development activities for the Technology Audit Service Tasks. In particular, under this sub-award the National Institute for Computational Sciences (NICS) will;

1. Build and benchmark computational-intensive kernels (e.g., HPC Challenge Benchmarks, key numerical LAPACK and FFT routines) and top-used HPC applications on NICS's "Kraken" supercomputer and other applicable XSEDE systems (potentially including Ranger, Lonestar, Gordon, Trestles, and new XSEDE systems, subject to availability), with the aim to assess the impact of different compilers, libraries, tuning options, and user environments on HPC application performance. NICS will leverage the prior activities and expertise in this effort (i.e. the **P**erformance **E**nvironment **A**utoconfiguration frameworK [PEAK]) and work with the Buffalo Team to incorporate the measured metrics in XDMoD web interface. In the long term NICS could expand the efforts to GPU accelerators on the "Keeneland" supercomputer.

2. Explore the idea of I/O auto-tuning for optimal Lustre filesystem performance using both simulation and micro-benchmarks (e.g., the IOR and MPI-Tile-IO benchmarks currently used in the TAS application kernels) on the "Kraken" supercomputer and other applicable XSEDE systems. The results will benefit the audience and stakeholders of TAS as well as HPC users who work in I/O intensive areas such as climate sciences and Big Data. NICS will work with the Buffalo Team to write research papers about the findings and make the results available in XDMoD.

Qualifications of Dr. You: Dr. Haihang You is a computational scientist at National Institute for Computational Sciences (NICS) at University of Tennessee. Prior to joining NICS, Dr. You was a research associate at the Innovative Computing Laboratory, Dept. of Electrical Engineering and Computer Science, University of Tennessee, where he had worked on various high-profile computational science projects such as PAPI, Dynaprof, ATLAS, and GCO led by the world-famous High-Performance Computing expert Dr. Jack Dongarra. His research interests include high performance computing, performance analysis, compiler & automatic tuning and optimization system, linear algebra, iterative adaptive discontinuous Galerkin finite element methods, parallel I/O tuning, and system utilization analysis and improvement of supercomputer systems. These are the exact areas of interest for UB on the NSF TAS award and accordingly, Dr. You is uniquely qualified to carry out this joint research project.

9.3 IU Sub contract: Practical Impacts on a Strategy for Scientific Impact Assessment:

We analyzed practical tests traditional and popular metrics including the count of publications, citations, H-index, G-index, and other information found outside of the XSEDE portal. The result can be summarized as follows:

1. We investigated automated ways of identifying this information via third party tools such as IU's Scholarmeter using indirectly Google Scholar, Microsoft Academic search API, and Arnetminer. We identified that the result for the top users of XSEDE are very inconsistent. This is based on the fact that data about publications is incomplete for these users, and that the systems are not able to handle the name ambiguities.
2. In order to circumvent these issues, we experimented by managing publications in an alternative fashion while using services from Google, Mendeley, and Zotero. We integrated in a test case of Mendeley and Zotero to allow easy management of references by the user. We found that such a combination is in fact a very good model for managing ones publications. In fact we came to the conclusion that it would be better to have the users manage their publications in a system such as Mendeley or Zotero and have the data managed through them uploaded indirectly through an XSEDE database. An upload of data to an XSEDE publication database, should be possible through a tagged library in either Zotero or Mendeley. The XSEDE team came to a similar conclusion in which they want to allow upload of references through Mendeley and Zotero. Our solution however, would project a distributed database that is managed in Zotero/Mendeley directly and not in the centralized XSEDE database. In the next period we will analyze the advantages and disadvantages about these approaches. We will continue to regularly communicate with the XSEDE portal team in order to leverage our experiences.
3. We looked at the data currently in the XDcDB and will identify how to best utilize them. One of the preliminary results we have from the few entries in it is that many of the coauthors in publications associated with XSEDE do not have portal accounts. This verifies the need to conduct analyses outside of the XSEDE publication database.
4. A big issue with all of the approaches we have is that the accuracy is strongly dependent on the users' input.
5. We have reached the conclusion together with the XD portal team that it is best to integrate the upload of publications into the XRAC process so that sufficient motivation is given for uploading the publication data. The communication with the POPS team regarding to this issue is yet to be done. To simplify entry we suggest that a way to automatically suggest a list of publications to users should be provided.
6. We started to experiment with using a WordPress to create a "personal" web page for users to manage their publications via Mendeley and Zotero.

9.4 XDMoD Usage:

XDMoD 1.6 (https://xdmod.ccr.buffalo.edu), which was released during the first quarter of 2012, is the first version providing access to all XSEDE users with an active XSEDE allocation as well as a public view with substantial functionality. Appendix 1 contains a summary of the data available through each of the XDMoD roles (Public, User, PI, Campus Champion, Program Officer, Center Director/Staff). Current XDMoD usage during the present reporting period is shown in Figure 10. While the usage is substantial, we anticipate increased usage in the future as more users become aware of its availability and capability.

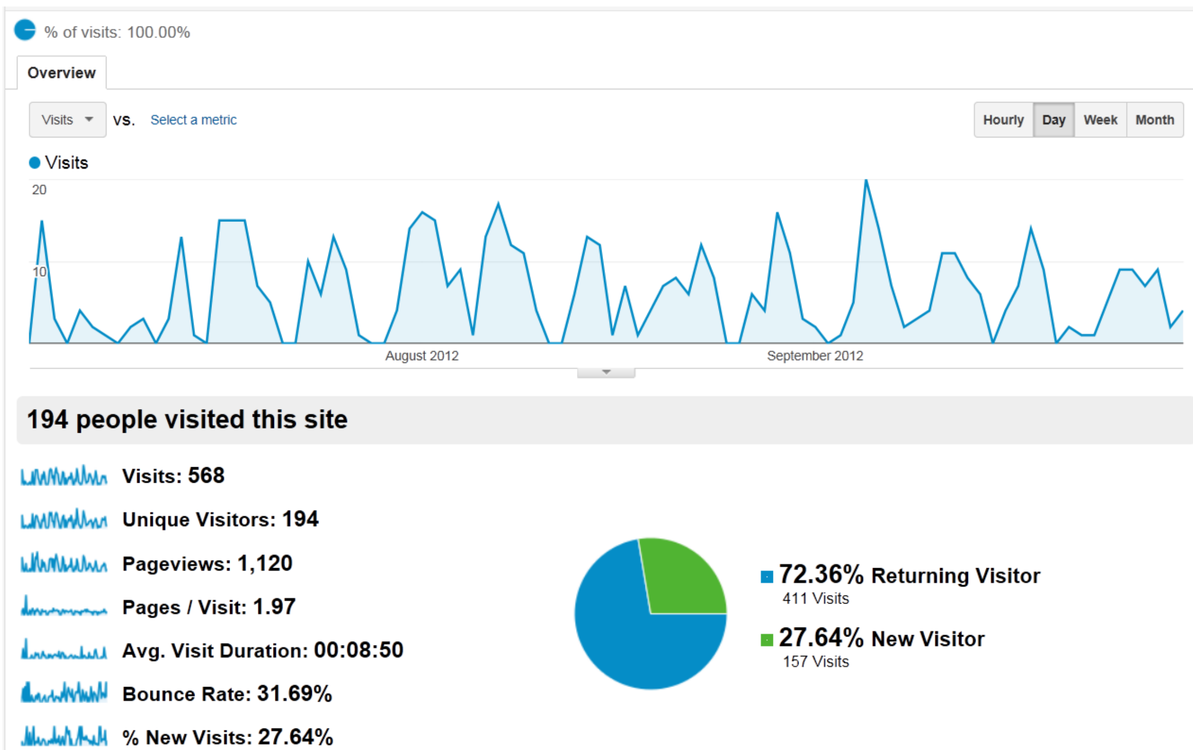


Figure 10. Google analytics overview of XDMoD usage for July 1, 2012 to September 30, 2012.

9.5 Coordination with External Projects and Agencies

TAS has been in active coordination with TACC concerning addition of XSEDE user publications to the XDCDB through the XSEDE User Portal.

FutureGrid has for the last two years made available to its users the ability to upload bibliography entries as part of its sophisticated project management service exposed to its users. We got feedback from TACC that the newly developed feature in the XSEDE portal is similar to what we have been offering in FutureGrid. As we targeted to add the upload feature into the TAS portal, we have revised our strategy and will leave that task up to the core XSEDE portal team. However we continue to explore the analysis and identification of data that results from these uploads. As Gregor von Laszewski is the Software Architect in FutureGrid and plays a role in TAS, this collaboration is beneficial and shows the value FutureGrid has had on TAS and also XSEDE.

9.6 Meetings, Events Publications and Presentations

TAS team members attended XD12 in Chicago, IL (July 2012).

TAS XD12 Attendees included: Dr. Thomas Furlani, Dr. Matthew Jones, Mr. Steven Gallo, Mr. Ryan Gentner, Mr. Amin Ghadersohi, Dr. Abani Patra, Dr. Charng-Da Lu, Dr. Robert L. DeLeon, Dr. Gregor von Laszewski (IU), Dr. Fugang Wang(IU) and Mr. Jonathan Brier (UM).

XD12 presentations made by TAS:

- "Comprehensive Resource Measurement and Analysis for HPC Systems" Charng-Da Lu*, Jim Browne ‡, Robert L. DeLeon*, John Hammond†, Bill Barth†, Thomas R. Furlani*, Steven M. Gallo*, Matthew D Jones*, Abani K. Patra*. (*Center for Computational Research, SUNY at Buffalo, †Texas Advanced Computing Center, University of Texas, Austin, TX, ‡Department of Computer Science, University of Texas, Austin, TX)
- "XDMoD 2.0: Performance Metrics and Auditing Framework for High Performance Computer Systems" Amin Ghadersohi*, Ryan J. Gentner*,Thomas R. Furlani*, Matthew D. Jones*, Steven M. Gallo*,Charng-Da Lu*, Abani Patra*, Robert L. DeLeon*, Gregor von Laszewski[+] and Fugang Wang[+] (*Center for Computational Research, SUNY at Buffalo, [+] Indiana University)

Appendix 1: XDMoD Role Definitions

1. **Public Role (no account is required)**
    - Overall XSEDE utilization broken down by resource, field of science, time, etc.
    - Performance data across SPs – performance of the TAS application kernel suite
    - User Like Me (tool to assist users in identifying the resources for their needs)
    - No user specific data
    - Access to resource specific application kernel data

2. **User Role – extends Public role and adds the following data (requires an active XSEDE account)**
    - Personal utilization information for the authenticated user
    - Drill down to user's individual job details and allocation information
    - Aggregated resource utilization data only
    - Access to resource specific application kernel data

3. **PI (co-PI, and PI-delegates) Role – extends User role and adds the following data (requires an active XSEDE account)**
   - Provide detailed utilization information for any/all users under the PI's allocations
   - User specific data limited to PI and users under their allocation(s)
   - Aggregated resource utilization data only
   - Access to resource specific application kernel data

4. **Center Director/Staff Role**
   - Utilization data specific to the user's associated center/resource
   - Performance data specific to the user's associated center/resource
   - Access to resource specific application kernel data

5. **Program Officer Role (XSEDE management, XSEDE delegates, PO delegates)**
   - No restrictions on data access
   - XSEDE utilization
   - Ability to search all data for a specific user
   - Performance data across all SPs

6. **Campus champion Role (also a PI)**
   - Access to user-specific data for users under their allocation (may be sensitive if sharing specific PI data from other PIs on campus, use a generic user/PI profile for those not on their allocation)
   - Utilization data specific to the champion's associated university/center
   - Performance data specific to the champion's associated university/center
   - Ability to view detailed job-level information for users of the university/center (under their allocation rather than university/center?)
   - Resource specific utilization data limited to one university/center under their purview
   - Access to resource specific application kernel data

Definitions of terms:

Generally the roles are hierarchical in terms of the managerial responsibilities, and therefore the data to which they have default access (assuming that some user and resource-specific data is access restricted).

Public: anyone, not restricted to people with an XSEDE account.

User: person who has an XSEDE account and can use XSEDE services, but does not manage a research group/allocation (PI), direct a resource center (RP/SP) or have XSEDE or NSF managerial responsibilities.

PI or co-PI: person who has an XSEDE account and also is the designated PI or co-PI on XSEDE allocation(s)., and therefore manages such allocations and the associated usage. This role does not direct a resource/service provider or have XSEDE or NSF managerial responsibilities.

RP: resource/service provider, an entity that provides services to XSEDE such as computational or storage resources.

User specific data: usage data for a specified user. That is, the users name is associated with the XSEDE usage.

Resource specific utilization data: usage and/or performance data for a given resource, often associated by name with the user.

Delegates: persons designated by a data manager to have the same data access as themselves. For example, PI delegates, RP/SP center director delegates, XSEDE management delegates or program officer delegates.

Job-level information for users: specific usage (jobs) that are associated with a named user.

Performance data specific to associated center/resource: Right now we have no specific examples that would fit in this category. Performance of the TAS application kernels are available to all.

10 TAIS/Technology Investigation Service 1.7

10.1 Overview

During this quarter, the TIS team was actively involved in several organizational functions.

We worked on the integration of TIS into the overall XSEDE project. XSEDE '12. Many members of the TIS attended the XSEDE '12 meeting in Chicago. J Ray Scott gave several presentations about TIS at the meeting to other XSEDE groups such as ECSS. A group meeting was held at the end of the week. J Ray has initiated discussions with the leads of Operations and SD&I to explore how the three groups can work together now that TIS is in XSEDE. TIS Program Manager, Martin Biernat, has created and filed a Program Change Request, PCR, for the TIS merger into XSEDE. The group has begun to identify risks as required by the XSEDE project. Martin is preparing these risks to be entered into the risk database. The Level 2 and Level 3 TIS managers as well as the Program Manager attended the XSEDE Quarterly Meeting and presented status reports.

As requested by the XSEDE leadership, the L3 managers reviewed the XSEDE User Survey. Examination of the user survey shows nothing specific to be evaluated for user requirements. Users with unmet requirements either requested the deployment of a specific application and therefore no evaluation is needed or they requested operational changes from SP's. We suggest that we add an appropriate question to the survey to see what unmet requirements might be met by an unspecified application.

Internally, TIS was reorganized to streamline the group and focus more on two key areas. The Technology Identification group will be led by Maytal Dahan. This group will keep the XTED technology database operational and enhance its capabilities. Dan LaPine will head the Technology Evaluation group, folding in staff from formerly separated groups within TIS. This reorganization will strengthen the evaluation component of TIS.

10.2 Technology Identification 1.7.1

The focus for Technology Identification was to expand the capabilities of reviewing technologies by decoupling reviews from the Technology entities so we can support multiple Reviews per technology. Development of this release (v 0.7.1) was completed. However, pushing to production is put on hold until migration from TIS to XSEDE infrastructure is completed. This quarter we have also completed the migration plan for moving TIS services to XSEDE. The plan was approved and the migration was started this quarter and is expected to be completed in early next quarter. After migration efforts are complete and the release of 0.7.1 to production, the plan is to re-evaluate the supplied versus missing features in order to prioritize new functionality development moving forward. No action required for the user survey but we will make sure to have TIS addressed in future user surveys.

10.3 Technology Evaluation 1.7.2

Evaluations for Unicore and Pegasus continue. We are integrating the resources from the Tech Evaluation Laboratory and Tech Insertion Support in one area under Technology Evaluation. Jesse Hanley (NICS) and Chris Koeritz (UvA) joined the group.

Areas we made progress on:

Integrating all the missions and personnel of the other 2 areas under the Technology Evaluation area PCR. Integrating the new members Jesse and Chris into the work flow. Final test runs were started on the Pegasus Evaluation.

Areas we are behind in:

We have not finished the ongoing evaluations nor have we started testing Evaluations Six and Seven. We have not yet produced a consistent process to determine the next evaluation's application and requirements. The turnover in staff and changes in organization have not helped us finish the current evaluations.

Review of the User Survey:

Examination of the user survey shows nothing specific to be evaluated for user requirements. Users with unmet requirements either requested the deployment of a specific application (no need for evaluation) or requested operational changes from SP's. Suggest that we add an appropriate question to the survey to see what unmet requirements might be met by an unspecified application. Will follow-up with Glen Brook for user survey changes in Q2PY3.

Goals:

Finish the current evaluations. Start 2 new evaluations. Create a training package for new members and use it. Get a defined process to determine new evaluations and requirements.

10.4 TIS user advocate's team

As of August, 2012, the TIS user advocate's team has joined the Feedback team in the user engagement area of User Services (section 5.4).

The Feedback team conducted a BoF entitled "XSEDE – Review and Directions after One Year" at the XSEDE 12 conference. The BoF examined developments within XSEDE during the first year of the project and solicited associated feedback. Preliminary results from the PY1 XSEDE User Survey were used to motivate discussion about potential improvements to XSEDE, and associated feedback was collected, as well. A report documenting the event is posted on the XSEDE Staff Wiki for reference. The Feedback team completed data mining on the tickets submitted to help@xsede.org during the previous quarter. A report documenting the results of the quarterly data mining activities is posted on the XSEDE Staff Wiki for reference. The team worked with users to submit suggestions to feedback@xsede.org and made the Systems Engineering team aware of them.

The 2012 XSEDE Annual User Survey was designed to gather information about user satisfaction with XSEDE services and to determine if XSEDE users are better provisioned with cyber infrastructure services than researchers who are not users of XSEDE. On May 1, 2012, the survey was sent to 5000 current XSEDE users and to 5,000 NSF principal or co-principal investigators funded between 2007 and 2011 who were not current XSEDE users. The final report is based on data from 734 respondents that completed at least 50% of the survey before it closed on June 11, 2012. The user advocate's team is evaluating the respondents' comments concerning the provisioning of XSEDE researchers with cyber infrastructure technologies.

11 ExTENCI

XSEDE and Open Science Grid have been working together to support science that can make use of both cyberinfrastructure platforms.

11.1 Overview

The Extending Science Through Enhanced National Cyberinfrastructure (ExTENCI) Project is a joint Open Science Grid (OSG) and TeraGrid/XSEDE project, funded by OCI. The PIs are Paul Avery (U. Florida) and Ralph Roskies (PSC). The planned two year project began in August 2010 and has received a no-cost extension through July 2013.

The goal of ExTENCI is to develop and provide production quality enhancements to the national cyberinfrastructure that will enable specific science applications to more easily use both OSG and XSEDE/TeraGrid or broaden access to a capability to both XSEDE/TeraGrid and OSG users.

Overall, the project has completed 96 of the 126 total deliverables, counting new deliverables defined at the end of year 2. ExTENCI has four primary areas of work, each of which is discussed in the sections below.

11.2 ExTENCI – Distributed File System

- Completed and delivered an XSEDE '12 talk on ExTENCI Distributed File System work
- Ongoing upgrade of UF Server Software to Lustre pre-2.2
- Collaborated with Peter Braam / Xyratex with Kerberos Lustre. With his help, three problems that caused intermittent crashing of the Kerberized Lustre clients were resolved.
- Completed GSISSH work for PKINIT deployment
- Upgraded clients to latest kernel / lustre (2.6.18_308.12.1.3l5xen)
- Tested kerberized lustre NFS mounts on VM clients (NFS kerberos both on/off)
- FIU/UF successfully implemented a kerberized lustreWAN+XRootD solution with 25 XRootD compute node clients.
- Two papers (previously submitted to CHEP2012) were submitted and accepted for publication in Journal of Physics: Conference Series

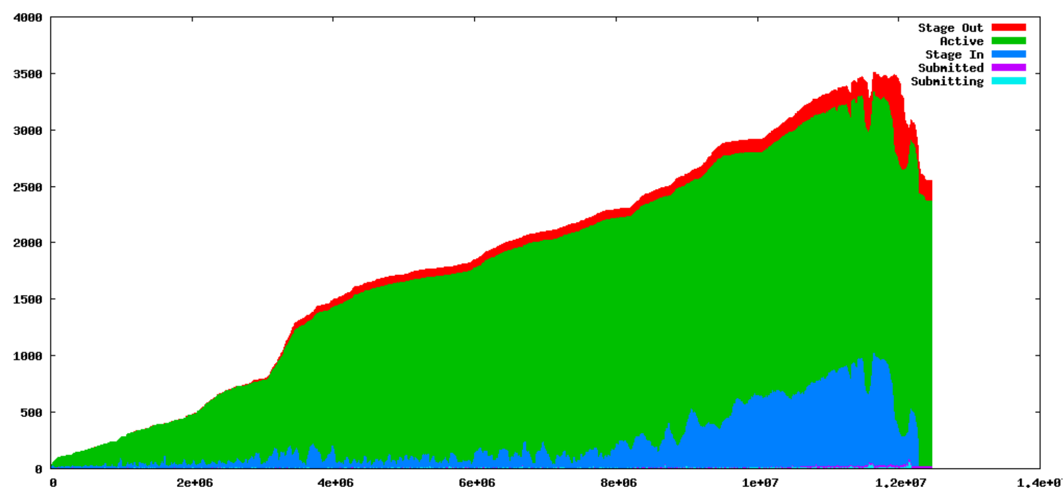
11.3 ExTENCI – Virtual Machines

- Purdue Wispy hardware upgrade completed. Updated to 8 nodes of Intel Sandy Bridge processors (16-core per node). There was one issue with accessing VMs from outside IPs after they run. The Purdue staff resolved the problem and Wispy is working.
- The GlideinWMS team tested CMS VMs but ran into a problem with Nimbus on Wispy. The Nimbus team determined that it was a bug in the Nimbus software (https://github.com/nimbusproject/nimbus/issues/110). The bug has been fixed for the next Nimbus release. Purdue obtained a patch from the Nimbus team and applied it. It fixed the problem and the GlideinWMS team was informed of this progress.
- Purdue gave a Dashboard demonstration to FutureGrid staff in early August. Stephen Harrell now has a new version of the Cloud Dashboard with the HUBzero specific code removed and with additional GUI elements for FutureGrid to test. Waiting to hear about their experience.

- Defined four new deliverables for the Clemson team with the addition of a new Clemson PI, Amy Apon.
- Purdue began collaborating with Amy Apon and her students to get some Real Science™ VMs running.

11.4 ExTENCI – Workflow & Client Tools

- Trained RDCEP grad student Michael Glotter on using Swift-GWMS-OSG toolkit for running DSSAT.
- Problems with running Swift on Nimbus on Wispy have been resolved. Next step to complete this task is to start using Wispy for RDCEP DSSAT runs.
- In the meantime we tested a DSSAT run on FutureGrid.
- Several Swift bugs affecting cloud and OSG runs were fixed.
- Swift was enhanced to support unique X509 credentials per-storage-site, so that we can use data in OSG runs from XSEDE, ALCF, campus, and other locations.
- Demonstrated Swift over Nimbus/Phantom on FutureGrid at XSEDE Science Cloud tutorial and at XSEDE summer online training workshop. Showed ability to recover from lost nodes and to adjust resource level in the middle of a workflow.
- Started discussion with Phil Maechling of SCEC on refining goals and tool sets for the ExTENCI SCEC workflow tasks.
- The RDCEP project has completed it first large-scale production run on OSG. It used ~1,000 OSG cores and ran for about 3 hours (~50K DSSAT simulations). The run is shown in the following utilization plot (but the Y axis is incorrect: the run peaks at ~1,000 cores). Subsequently, this project completed DSSAT simulations in production runs of 140,000 hours on OSG.
- http://www.ci.uchicago.edu/~davidk/cps-2012-09-06_23-03-06.log.jobs.png



11.5 ExTENCI – Job Submission Paradigms

- Finished migration away from RENCI OSG gateway. Instead of using the OSG-XSEDE gateway, we have set up and tested our own OSG submit host VM (with the help of Tanya Levshina and Mats Rynge). This makes it much easier for us to connect the science portal with OSG. Job submission and file staging seems to work fine; however, Gratia probes don't seem to work properly yet. With the OSG submit host, accounts, basic software stack, etc. in place, we are about to start with BigJob testing.

- Engaged with Chander Sehgal, Tanya Levshina and Mats Rynge to hammer out a plan to support large data volumes on OSG. A rough roadmap and follow-up meetings were established. A genomics application will be the first SAGA use of the new iRODS capability for distributing data to OSG sites where jobs will run.
- Having some problems compiling and deploying Cactus on OSG.
- Our science portal designer is finally back on track - he's been working on a re-design (http://gw68.quarry.iu.teragrid.org/) using the Django web framework. Google/Yahoo o-Auth has been implemented to make user management easier. A toy simulation has been successfully submitted by the Cactus guys via the portal.
- "Pilot Abstractions for Clouds" has been submitted for a special issue of *Concurrency and Computation Practice and Experience.*

12 XD Service Provider Reports

2012 Q3: July 1, 2012, through September 30, 2012

XD Service Provider Forum Leadership

Carol Song, Chair	Purdue University
David Y. Hancock, Vice Chair	Indiana University

XD Service Provider Principal Investigators

Sean Ahern	U Tennessee – National Institute for Computational Science
Jay Boisseau	U Texas - Texas Advanced Computing Center
Geoffrey Fox	Indiana University
Kelly Gaither	U Texas - Texas Advanced Computing Center
Michael Levine	Pittsburgh Supercomputing Center
Miron Livny	U Wisconsin-Madison
Richard Loft	National Center for Atmospheric Research
Richard Moore	U California San Diego - San Diego Supercomputer Center
Michael Norman	U California San Diego - San Diego Supercomputer Center
Manish Parashar	Rutgers University
Gregory D. Peterson	U Tennessee – National Institute for Computational Science
Carol Song	Purdue University
Craig Stewart	Indiana University
John Towns	U Illinois - National Center for Supercomputing
Jeffrey Vetter	Georgia Institute of Technology

12.1 Overview

The XD Service Provider Forum is the representative body of federated providers of leading-edge computational, storage and visualization resources, software and associated services to the open science community. In partnership with the XSEDE project, the SPs have delivered more than 833 million service units (SUs) to the XSEDE user community in the last quarter. Approximately 1 billion SUs were requested and 493 million SUs were awarded for the quarter.

In August, the SP Forum accepted its first new member, Rutgers University, as it became a Level 3 XSEDE Service Provider. RDI^2 is an advanced computation institute that provides academic and industry researchers with the resources, skills, and expert support necessary to leverage advanced computation technology for computational and data-enabled science and engineering. The institute has an IBM Blue Gene®/P supercomputer, "Excalibur", installed in March 2012, and additional racks of IBM's Blue Gene®/Q, a Linux cluster, visualization resources to be acquired in 2012, all located in an expanded facility on the university's Livingston Campus in Piscataway, New Jersey. Its initial interaction with XSEDE will be through co-branding as stated in the Rutgers' application. The SPF voted to approve Rutgers membership in August 2012.

The SP Forum has also received formal applications from all the interim members, as well as from the Blue Waters project, and plan to complete the review and approval process by early November.

The SP forum has worked with the XSEDE project to define and formalize the storage allocations policy and implementation by collecting information about storage resources that will be allocated through the POPS system starting in 2013 and provided input to the implementation process. The SPF worked with the XSEDE project, especially the User Services group, on initial concepts regarding the tiers of the storage resources and how they should be allocated based on their interactions with users. SPs provided feedback on the proposed implementation plan, and worked on the storage allocation plan through discussions, edits and comments. The SPF also surveyed the SPs about the storage systems that will be allocated through XSEDE (survey result can be found at the SPF wiki under "Other documents"). The survey result is a collection of system characteristics and SP plans regarding a few critical implementation issues. The spreadsheet is available at:

https://www.xsede.org/c/wiki/get_page_attachment?p_l_id=254074&nodeId=242671&title=Other+Documents&fileName=Other+Documents%2FSP-Storage-Resource-Input-1019.xls.

In response to the recent NSF reorganization in which the Office of Cyberinfrastructure (OCI) will be merged back into the CISE directorate, the SPF decided to send a letter to the NSF Advisory Committee for Cyberinfrastructure outlining the concerns and recommendations of its members. The text of the letter is available at:

https://www.xsede.org/c/wiki/get_page_attachment?p_l_id=254074&nodeId=242671&title=Other+Documents&fileName=Other+Documents%2FSPF+response+to+NSF+reorg+-+Letter+to+ACCI.pdf

The SP Forum held its first face to face meeting in July at the XSEDE 2012 conference, most of which was devoted to the discussion of the storage allocation policy and implementation plan. The SPF conducts its business and coordination through regular conference calls on Tuesdays at 11am Eastern Time. Presentations to the SPF this quarter include:

- An overview of the SUPREMM project (Integrated HPC Systems Usage and Performance of Resources Monitoring and Modeling) by the PIs (Abani Patra and Jim Browne). Draft documents of the project, including data requirements, were provided to the SPF members. The project will request help from the SPs in collecting and analyzing system and application usage statistics.

- Overview of the XSEDE Software Development and Integration (SD&I) activities by the group's leader JP Navarro.
- Overviews of the current and planned activities by XSEDE Operations lead Victor Hazlewood.

The SP quarterly report template has been revised to provide more clear guidance on reporting staff publications and EOT events. The changes are also intended to be consistent with the XSEDE report format.

13 XSEDE Quarterly Report: FutureGrid Service Provider (July 1, 2012 – September 30, 2012)

13.1 Executive Summary

- Awarded new ScaleMP cluster to International Computer Concepts (ICC), Lake Zurich, IL. The new system will be named "Echo" and will be built with new Intel Sandy Bridge technology. ScaleMP will certify their software on the new cluster as part of the implementation.
- Conducted the Science Cloud Summer School July 30 – August 03 (see TEOS Highlights)
- Implemented "Lima," a new 8-node cluster, at SDSC to experiment with SSD disks. Lima will be used to compare performance of HPC applications and virtualization on SDD vs HDD disk.
- Installed new switches on *india* to support tagged VLANs and PXE booting for multiple cloud provisioning systems on a single switch.

13.1.1 Resource Description

FG Hardware Systems

Name	System type	# Nodes	# CPUs	# Cores	TFLOPS	Total RAM (GB)	Secondary Storage (TB)	Site
	Operational							
india	IBM iDataPlex	128	256	1024	11	3072	335	IU
hotel	IBM iDataPlex	84	168	672	7	2016	120	UC
sierra	IBM iDataPlex	84	168	672	7	2688	96	SDSC
foxtrot	IBM iDataPlex	32	64	256	3	768	0	UF
alamo	Dell PowerEdge	96	192	768	8	1152	30	TACC
xray	Cray XT5m	1	168	672	6	1344	335	IU
bravo	Large Disk / Large Memory	16	32	128	1.5	3072	192	IU
delta	Large Disk / Large Memory With Tesla GPUs	16	32 CPU 32 GPU	192 14336	9	1536	192	IU
Total				**4384**				
	On order							
echo	Large Disk / Large Memory (for ScaleMP software)	16	32	192	2	6144	192	IU
lima	SSD		16	128	1.3	512	3.8 (SSD) 8 (disk)	SDSC

FG Storage Systems

System Type	Capacity (TB)	File System	Site
Xanadu 360	180	NFS	IU
DDN 6620	120	GPFS	UC
SunFire x4170	96	ZFS	SDSC
Dell MD3000	30	NFS	TACC
IBM dx360 M3	24	NFS	UF

Also, substantial backup storage at IU: Data Capacitor and HPSS.

13.2 Science Highlights

V3VEE Project

Peter Dinda
Department of EECS
Northwestern University

Abstract

We plan to use FutureGrid to help to evaluate virtualization technologies for high performance computing. In particular we seek a testbed for scaling studies involving our Palacios VMM and its components (e.g. the VNET/P overlay).

Intellectual Merit

The V3VEE project (v3vee.org) is creating a virtual machine monitor framework for modern architectures (those with hardware virtualization support) that will permit the compile-time creation of VMMs with different structures, including those optimized for computer architecture research and use in high performance computing. V3VEE began as an NSF-funded collaborative project between Northwestern University and the University of New Mexico. It currently involves five DOE-funded partner institutions: Northwestern University, the University of New Mexico, the University of Pittsburgh, Sandia National Laboratories, and Oak Ridge National Laboratory. V3VEE is a community resource development effort that anyone can contribute to.

Broader Impacts

The infrastructure developed in the V3VEE project is used extensively in research and education. The codebase is freely available and BSD licensed. Underrepresented groups are impacted through Northwestern's AGEP program and through U NM, a minority serving university. More information on the project can be found at http://v3vee.org.

Use of FutureGrid

We want to run scaling studies of Palacios combined with its VNET/P overlay network on 1-10 Gbps Ethernet configurations and/or Infiniband configuration. That is, to run on as many nodes as possible and see the effects.

Results

All V3VEE project papers, presentations, and the Palacios codebase are available from v3vee.org. The most relevant papers for this proposal are:

1.L. Xia, Z. Cui, J. Lange, Y. Tang, P. Dinda, P. Bridges, VNET/P: Bridging the Cloud and High Performance Computing Through Fast Overlay Networking, Proceedings of the 21st ACM Symposium on High-performance Parallel and Distributed Computing (HPDC 2012), accepted, to appear. (also TR version) J. Lange, P. Dinda, K. Hale, L. Xia, An Introduction to the Palacios Virtual Machine Monitor---Version 1.3, Technical Report NWU-EECS-11-10, Department of Electrical Engineering and Computer Science, Northwestern University, November, 2011.

2.J. Lange, K. Pedretti, P. Dinda, P. Bridges, C. Bae, P. Soltero, A. Merritt, Minimal Overhead Virtualization of a Large Scale Supercomputer, Proceedings of the 2011 ACM SIGPLAN/SIGOPS International Conference on Virtual Execution Environments (VEE 2011), March, 2011.

3.J. Lange, K. Pedretti, T. Hudson, P. Dinda, Z. Cui, L. Xia, P. Bridges, A. Gocke, S. Jaconette, M. Levenhagen, R. Brightwell, Palacios and Kitten: New High Performance Operating Systems for Scalable Virtualized and Native Supercomputing, Proceedings of the 24th IEEE International Parallel and Distributed Processing Symposium (IPDPS 2010), April, 2010.

Investigation of Data Locality and Fairness in MapReduce

Zhenhua Guo
Pervasive Technology Institute
Indiana University

Abstract

Traditional High-Performance Computing (HPC) environments separate compute and storage resources and adopt "bring data to compute" strategy. MapReduce is a data parallel model that makes use the same set of nodes for both compute and storage. As a result, data affinity is integrated into the scheduling algorithm to bring compute to data. In data-intensive computing, data locality becomes more important than before because it can potentially reduce network traffic significantly. In this project, we try to investigate the data locality of MapReduce in detail, and do the following things: 1) we summarize important system factors and theoretically deduce the relationship between those factors and data locality; 2) we analyze the state-of-the-art Hadoop scheduling algorithms to investigate their performance; 3) we propose new scheduling algorithms that yield optimal data locality; 4) we integrate data locality and fairness; 5) we compare our algorithms with the default Hadoop scheduling algorithm

Intellectual Merit

This project tries to address an important issue in MapReduce : data locality. Our proposed algorithms yield optimal data locality and can dramatically reduce the time of data movement. The integration of data locality and fairness allows users to make the best tradeoff based on their environments and requirements.

Broader Impacts

In the era of data-intensive computing, we all know data locality is critical because it is not efficient to move extreme amount of data during data processing. This project can help researchers to better understand MapReduce data locality in a quantitative way. In addition, this project produces some insightful conclusions and results that pave the foundation for further research on data parallel systems.

Use of FutureGrid

We ran extensive simulation experiments on FutureGrid bare metal machines.

Results

Our experiment results show that our proposed algorithms improve data locality and outperform the default Hadoop scheduling substantially. For example, the ratio of data-local tasks is increased by 12% - 14% and the cost of data movement is reduced by up to 90%. The detailed results of this project have been presented in two papers:

1.[Guo:2012:IDL:2287016.2287022] Guo, Z., G. Fox, and M. Zhou, "Investigation of data locality and fairness in MapReduce", Proceedings of third international workshop on MapReduce and its Applications Date, Delft, The Netherlands, ACM, pp. 25–32, 2012.

2.[Guo:2012:IDL:2310096.2310222] Guo, Z., G. Fox, and M. Zhou, "Investigation of Data Locality in MapReduce", Proceedings of the 2012 12th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing (ccgrid 2012), Ottawa, Canada, IEEE Computer Society, pp. 419–426, 2012.

Hadoop-GIS: a High Performance Query System for Analytical Medical Imaging

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Abstract

Querying and analyzing large volumes of spatially oriented scientific data becomes increasingly important for many applications. For example, analyzing high-resolution digital pathology images through computer algorithms provides rich spatially derived information of micro-anatomic objects of human tissues. The spatial oriented information and queries at both cellular and sub-cellular scales share common characteristics of "Geographic Information System (GIS)", and provide an effective vehicle to support computer aided biomedical research and clinical diagnosis through digital pathology. The scale of data could reach a million derived spatial objects and hundred million features for a single image. Managing and querying such spatially derived data to support complex queries such as image-wise spatial cross-matching queries poses two major challenges: the high complexity of geometric computation and the "big data" challenge. In this paper, we present a system Hadoop-GIS to support high performance declarative spatial queries with MapReduce. Hadoop-GIS provides an efficient real-time spatial query engine RESQUE with dynamically built indices to support on the fly spatial query processing. To support high performance queries with cost effective architecture, we develop a MapReduce based framework for data partitioning and staging, parallel processing of spatial queries with RESQUE, and feature queries with Hive, running on commodity clusters. To provide a declarative query language and unified interface, we integrate spatial query processing into Hive to build an integrated query system. Hadoop-GIS demonstrates highly scalable performance to support our query cases

Intellectual Merit

Hadoop-GIS is a unique system that integrates DBMS technologies into MapReduce technologies to provide a hybrid architecture to support high performance complex spatial queries with expressive query languages. This also drives the research direction on marrying DBMS and MapReduce technologies. Hadoop-GIS takes a GIS-like approach by mapping pathology imaging problems into GIS problems, a highly innovative approach in the field. The approach provides significant new insights for biomedical research with digital pathology, and creates many new opportunities.

Broader Impacts

Hadoop-GIS is a system for interdisciplinary biomedical research, which accelerates the diagnosis and understanding of brain tumor for better cure. The technologies also help to train computer science researchers and students to learn the state-of-the-art of MapReduce technologies, and the system is used for an advanced graduate course for lectures and projects (https://web.cci.emory.edu/confluence/display/CS730R/). The technologies could also be generalized for similar problems in different domains, such as cross-matching problems in digital sky survey projects, and oil exploration problems..

Results

1. We have provided scalability testing on the FutureGrid platform with 320 cores based on Hadoop. Technical report: http://confluence.cci.emory.edu:8090/confluence/download/attachments/403

2. We have developed an open source system Hadoop-GIS by extending Apache Hive project with spatial querying capabilities. The URL for its website is forthcoming.

Metagenome analysis of benthic marine invertebrates

Jason Kwan
Department of Medicinal Chemistry
University of Utah

Abstract

We are carrying out deep sequencing of environmental DNA from benthic marine organisms that are important components of their community but that have not been extensively examined genomically. In these organisms, symbiotic bacteria are demonstrably critical to host survival. The metagenomes are extremely complex, yet robust assemblies can sometimes be achieved. These properties make benthic marine invertebrates excellent models for NGS technology. In this project, we will use Future Grid resources to carry out de novo assembly of marine invertebrate metagenomic sequence data, a process that requires large amounts of memory and CPU power due the volume of data.

Intellectual Merit--

This work will help determine the potential utility of NGS technology, which produces a large amount of data but as relatively short reads, in metagenomics.

Broader Impacts

In the course of our work we will determine the practical aspects of processing large and complex Illumina sequencing data to obtain de novo genome assemblies of very minor members of the metagenome. This will be of great use to the metagenomics community.

Use of FutureGrid

Future Grid will be used for de novo assembly of metagenomic sequence data generated by Illumina technology. FG will also be used for the analysis of the assembled data - including automatic annotation and large scale BLAST searches

Results

We have been able to successfully assemble the complete genome of a previously unknown endosymbiotic bacterium from metagenomic sequence data obtained from a marine invertebrate (even though the bacterium only accounted for ~0.6% of the data). The complete genome afforded many insights into the symbiotic relationship, which will be reported in a paper that we have submitted (currently under review). The insights gained in this effort have allowed us to develop new methods in data processing and assembly which we are currently refining and will be the subject of future publications. We will continue to use Future Grid in these efforts to gain insight into other symbiotic systems. The scientific broad impact of this work is twofold. First, these symbiotic relationships are a key, yet poorly understood aspect of coral reef biodiversity. Second, these symbioses lead to the production of bioactive small molecules. By understanding the origin of compounds, we are developing new methods to tap biodiversity for potential application in medicine, agriculture, and other areas.

Co-Resident Watermarking

Adam Bates
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University of Oregon

Abstract

Virtualization is the cornerstone of cloud computing, allowing providers to instantiate multiple virtual machines on a single set of physical resources. Customers utilize cloud resources alongside unknown and untrusted parties, creating the co-resident threat: there is a possibility of unauthorized access to sensitive customer data through the exploitation of covert channels. Previous approaches to determining and exploiting co-residency require the ability to examine and manipulate internal hardware on these machines, behavior that can be patched or otherwise defended. We describe a new attack called co-resident watermarking that allows co-residents to inject a watermark into the network flow of a target instance. This watermark can be used to exfiltrate and broadcast co-residency data from the physical machine, compromising isolation without reliance on internal side channels. We evaluate co-resident watermarking under various network conditions and system configurations, showing co-residency can be determined in under 60 seconds and that a covert channel bitrate of 1.91 bps can be achieved. This work represents a first step in characterizing the co-resident watermarking threat.

Intellectual Merit

Our approach uses concepts previously explored in network flow watermarking. Watermarking is a method of breaking anonymity by tracing the path of a network flow. A target's traffic is subjected to controlled packet delay at an institutional boundary in order to give it a distinct and recognizable pattern. When the traffic exits the institutional boundary, that pattern is still present and can be decoded. Watermarking is of great interest because of its ability to detect stepping stone relays and to compromise anonymity services.

Broader Impacts

Through third party clouds, businesses are able to avoid overprovisioning and pay for only the exact amount of computing that they require. The key to allowing the rollout of these services is virtualization, where physical resources and multiple guest virtual machines can be multiplexed on a single physical machine. However, new security challenges come forth as users are now potentially vulnerable to the actions of others allocated to their same physical machine: they no longer solely control resources. Researchers have already demonstrated attacks against virtualization middleware that allow for the detection and exploitation of co-residency. However, systems-level vulnerabilities such as these could eventually be resolved by patching the hypervisor. We are attempting to demonstrate that even if other channels for establishing co-residency are removed, we can determine whether an adversarial guest is co-resident with a targeted server through observation of network traffic.

Results

Our use of Futuregrid led to an accepted paper at the 2012 ACM Cloud Computing Security Workshop entitled "Detecting Co-Residency with Active Traffic Analysis Techniques". This work will be presented on 19 October, 2012. Futuregrid is featured in the acknowledgements section. A copy of the paper is available at: http://ix.cs.uoregon.edu/~amb/documents/Bates_Ccsw12.pdf

13.3 User-facing Activities

13.3.1 System Activities

13.3.1.1 Hardware

- IU iDataPlex ("*india*"). Installed new switches to support tagged VLANs and PXE booting for multiple cloud provisioning systems on a single switch.
- IU Cray ("*xray*"). System operational for production HPC users. A new software release is available.
- IU HP ("*bravo*"). System operational for production users. 50% of the nodes being used for testing with the Network Impairment Device. HDFS available on remaining nodes. Swift test implementation installed.
- IU GPU ("*delta*"). 16 nodes available for production HPC jobs; cloud software not yet integrated.
- SDSC iDataPlex ("*sierra*"). Upgrade of two nodes to RHEL6 done in ppreparation for upgrades of sierra and india. System operational for production Eucalyptus, Nimbus, and HPC users.
- UC iDataPlex ("*hotel*"). System operational for production Nimbus and HPC users. Successfully tested using AuthZ plugin to call LDAP with the Globus toolkit 5.0x and 5.2x.
- UF iDataPlex ("*foxtrot*"). System operational for production Nimbus users. Jumbo frames enabled resulting in improved WAN data transfer rates.
- TACC Dell ("*alamo*"). System operational for production Nimbus and HPC users. Nimbus moved to CentOS 6. OpenStack installation in progress. Test nodes for XWFS have been released.
- SDSC SSD (*"lima"*). Implemented "Lima," a new 8-node cluster, at SDSC to experiment with SSD disks. Each node has two 2.6 GHz AMD Opteron 8-core CPUs, 64 GB RAM, one 480 GB Intel 520 SSD drive, and one 1 TB HDD disk. In total, it has 128 cores for 1.3 TFlops of compute power, 512 GB RAM, 3.8 GB SSD disk, and 8 TB HDD disk. Lima will be used to compare the performance of HPC applications and virtualization on SDD versus HDD disk.

All system outages are posted at https://portal.futuregrid.org/outages_all.

13.3.2 Services Activities (specific services are underlined in each activity below)

Accounting

An initial set of real-time metrics have been added to the Cloud Metrics reports (https://portal./futuregrid.org/metrics). The total number of running VMs on *india* and *sierra* for Eucalyptus and OpenStack are displayed via a dynamic chart, which is refreshed every 5 seconds. In addition, the number of running VMs per user has bee nadded via a jQuery Sparkline plugin. This displays which user uses/launches how many VMs recently and identifies resource overuse. This was tested throughout the VSCSE Science Cloud Summer School and was able to identify not only users using too many resources, but also users who did not follow their respective tutorials.

Cloud Services and Support Software

Eucalyptus. Started the deployment of new version of Eucalyptus, which will be based on RedHat 6.

Nimbus. Improvements made to current usage metric tools. Began work with the "galaxy" community, which has great potential of using FutureGrid. Implemented Nimbus 2.10 on *sierra* and *hotel*.

OpenStack. Created a new tool and documentation that allows users to change their own password for the OpenStack dashboard.

ViNe. Continjued improvement of ViNe2 management capabilities in order to support automatic overlay tuning. The goal is to dynamically adjust ViNe overlay routes as network conditions change (e.g. network congestion, network outages, changes in physical network connections of laptops where ViNe routers are deployed, etc.).

Experiment Management

Experiment Harness. Beta versions of the TeraGrid/XSEDE glue2 software installed on *alamo* and *foxtrot*. RabbitMQ now running with ALamo host certificates, FutureGrid Nimbus certificates, and other FutureGrid certificates.

Pegasus. Pegasus is now visible on the FutureGrid portal, complete with documentation in the User Manual (https://portal.futuregrid.org/manual/pegasus) and an updated tutorial (http://pegasus.isi.edu/futuregrid/tutorials).

Image Management. Created FG Move documentation. Implementation planning for FG Move on *sierra* to support Eucalyptus and HPC.

HPC Services

Implemented a Cygwin executable to simplify access to FutureGrid resources from Windows.

Performance

Inca. Deployed enhancement to publish Inca monitoring data into the FutureGrid messaging system based on AMQP. Deployed a new Inca test to verify the CUDA environment on *delta*.

Vampir. Continued work on collecting usage data for Vampir and other HPC client programs using Modules data. Currently logging Module data on *sierra*.

PAPI. Implementation planning for PAPI-V, In aneffort to deliver in a package that can be deployed and tested across all FutureGrid platforms. This is the first version of PAPI with initial support for virtual environments. It also introduces a VMware component that pioneers the capability of exposing specific VM environment parameters through its own PAPI interface. A configuration document is in progress.

perfSONAR. Monitoring systems in place and recording data throughput between sites. 10Gbps upgrade order has been placed.

FutureGrid Portal

13.4 Security

No security issues occurred during this period.

13.5 Education, Outreach, and Training Activities

- Hired three (3) new part-time hourly students to supplement user support

- FutureGrid at XSEDE'12 in Chicago:

Monday July 16			
1:00pm - 5:00pm	Tutorial: Infrastructure Clouds for Science and Education	John Bresnahan Kate Keahey Renato Figueiredo	University of Chicago University of Chicago University of Florida
Tuesday July 17			
3:45pm - 4:15pm	EOT: FutureGrid Education: Using Case Studies to Develop Curriculum for Communicating Parallel and Distributed Computing Concepts	Jerome Mitchell	Indiana University
4:45pm - 5:45pm	BOF: Hosting Cloud, HPC and Grid Educational Activities on FutureGrid	Renato Figueiredo Barbara O'Leary	University of Florida Indiana University
Wednsday July 18			
5:30pm - 6:30pm	BOF: Cloud Computing for Science: Challenges and Opportunities	Kate Keahey Manish Parashar	University of Chicago Rutgers University
5:30pm - 6:30pm	BOF: MapReduce and Data Intensive Applications	Judy Qiu	Indiana University

- Science Cloud Summer School. Completed July 30 – August 3, 2012.

The Science Cloud Summer School targets education and training of graduate students and the fostering of a community around a topic that has increasing interest and relevance: the use of cloud computing technologies in science - including infrastructure-as-a-service and platform-as-a-service. Because cloud computing systems and technologies provide a considerable departure from traditional models and evolve at a rapid pace, this event would provide a basis for students to immerse in a focused, intensive curriculum to learn fundamentals and experiment with these technologies in practice.

Science Cloud Summer School is part of the Virtual School of Computational Science and Engineering's (VSCSE) 2012 Summer School. There were ten (10) participating sites with high end video linkage:

- Indiana University, Bloomington, IN (*host institution*)
- Louisiana State University, Center for Computation& Technology, Baton Rouge, LA
- Michigan State University, Institute for Cyber Enabled Research, East Lansing, MI
- Pennsylvania State University, State College, PA
- Princeton University, Princeton, NJ
- Rutgers University, Piscataway, NJ
- University of California Los Angeles, Los Angeles, CA
- University of Michigan, Ann Arbor, MI
- University of Wisconsin - Milwaukee, Milwaukee, WI

A dedicated Tumblr web site was created to support the summer school. See: http://sciencecloudsummer2012.tumblr.com

Students were expected to provide their own laptops. The curriculum covered both technology (computer science) and use of clouds (informatics, computational science). See below:

Day 1: Monday July 30 INTRODUCTION			
11:00am - 12:00pm	Introduction	Geoffrey Fox	Indiana University
12:00pm - 1:00pm	Application: Biology on the Cloud	Michael Schatz	Cold Spring Harbor
1:00pm - 1:30pm	Infrastructure Used: FutureGrid	Geoffrey Fox	Indiana University
1:30pm - 2:30pm	*Lunch Break*		
2:30pm - 3:30pm	Introduction to virtual high performance computing clusters	Thomas J. Hacker	Purdue University
3:30pm - 4:30pm	Nimbus: Infrastructure Cloud Computing for Science	Kate Keahey	University of Chicago
	Resources used:		
	hotel, 40 servers		
	sierra, 17 servers		
4:30pm - 5:00pm	*Afternoon Break*		
5:00pm - 5:45pm	Nimbus Infrastructure: Hands-on Using Infrastructure Clouds	John Bresnahan	University of Chicago
	Resources used:		
	hotel, 40 servers		
	sierra, 17 servers		
5:45pm - 6:45pm	Nimbus Platform: Managing Deployments in Multi-Cloud	John Bresnahan	University of Chicago
	Resources used:		
	hotel, 40 servers		
	sierra, 17 servers		
6:45pm -	Wrap-Up Session		
Day 2: Tuesday July 31			
11:00am -	Running MapReduce in Non-Traditional Environments	Abhishek Chandra	University of
12:00pm - 1:30pm	Virtual Clusters Supporting MapReduce in Cloud	Jonathan	Indiana University
	Lab Session: Reproducible Environment for Scientific Applications	Tak-Lon Wu	
	Resources used:		
	laptop, virtualbox, india, eucalyptus		
1:30pm -	*Lunch Break*		
2:30pm - 4:30pm	MapReduce and NOSQL Cloud Storage	Jerome Mitchell Xiaoming Gao	Indiana University
	Resources used:		
	laptop, virtualbox, india, eucalyptus		
4:30pm -	*Afternoon Break*		
5:00pm -	Data Mining with Twister Iterative MapReduce	Judy Qiu	Indiana University
6:45pm -	Wrap-Up Session		
Day 3: August 1, *ACADEMIC AND COMMERCIAL CLOUD INFRASTRUCTURE*			
11:00am - 1:00pm	Building Scalable Data Intensive Applications on the Cloud with Makeflow and WorkQueue	Douglas Thain	Notre Dame
1:00pm - 2:00pm	*Lunch Break*		
2:30pm - 3:30pm	Commercial IaaS/PaaS I: AWS for Scientists	Jamie Kinney	Amazon Web Services
3:30pm - 4:30pm	Commercial IaaS/PaaS II: Azure and Twister4Azure	Thilina Gunarathne	Indiana University
4:30pm - 5:00pm	*Afternoon Break*		
5:00pm - 5:45pm	Networking and Clouds	Martin Swany	Indiana University
5:45pm - 6:45pm	IaaS in Action II: OpenStack	Gregor von Laszewski Javier Diaz	Indiana University
	IaaS in Action II: FutureGrid RAIN: Dynamic Provisioning on Bare Metal and IaaS in a Federated Cloud		
	Follow allong demos, lab can be done in self study		
6:45pm - 7:00pm	Wrap-Up Session		

Day 4: August 2, *CYBERINFRASTRUCTURE/HPC AND CLOUDS: TECHNOLOGY AND APPLICATIONS*			
11:00am - 1:15pm	Federating HPC, Cyberinfrastructure and Clouds using	Manish Parashar	Rutgers University
	Resources used:		
	hotel, 40 servers		
	sierra, 17 servers		
1:15pm - 2:15pm	*Lunch Break*		
2:30pm - 4:15pm	Federating HPC, Cyberinfrastructure and Clouds using	Manish Parashar	Rutgers University
	Resources used:		
	hotel, 40 servers		
	sierra, 17 servers		
4:15pm -	*Afternoon Break*		
4:45pm -	Magellan: Evaluating Cloud Computing for Science	Lavanya	LBNL
5:45pm - 6:45pm	Scientific Workflows in the Cloud	Gideon Juve	USC
6:45pm - 7:00pm	Wrap-Up Session		
Day 5: August 3, *EDUCATION APPLICATIONS AND ADVANCED TECHNOLOGY*			
11:00am - 12:00pm	Cloud Technology: Virtual Private Clusters: Virtual Appliances and Networks in the Cloud	Renato Figueiredo	University of Florida
12:00pm -	Applications of Cloud: DOE Systems Biology Knowledgebase	Rick Stevens	Argonne National
1:00pm - 1:30pm	Survey		
1:30pm - 2:30pm	*Lunch Break*		
2:30pm - 3:30pm	Cloud Technology: Cloud Security: New Challenges and New Opportunities	XiaoFeng Wang	Indiana University
3:30pm - 4:30pm	Applications of Cloud: The iPlant Collaborative: Science in the Cloud for Plant Biology	Dan Stanzione	TACC
4:30pm - 5:00pm	*Afternoon Break*		
5:00pm - 5:45pm	Cloud Technology: GPU on Clouds	Andrew J. Younge	Indiana University
5:45pm - 6:00pm	END SUMMER SCHOOL		

Events this quarter (in order of most recent):

Type	Title	Location	Date(s)	Hours	Number of Participants	Number of Under-represented people	Method
Indiana University							
Presentation	Panda: MapReduce Framework on GPUs and CPUs	Indiana University	08/10/2012				Live
Presentation	Scalable Deep Analytics on Cloud and High Performance Computing Environments	NASA SACD Lecture Series on Complex Systems and Deep Analytics, NASA Langley Research Center, Hampton, VA	08/08/2012				Live
Presentation	Science Clouds and CFD	NIA CFD Conference: Future Directions in CFD Research, A Modeling and Simulation Conference, Hampton, VA	08/6/2012				Live
Presentation	GPUs on Clouds	VSCSE Summer School on Science Clouds	08/03/2012	0.45			Live and Webcast
Presentation	FutureGrid Move	VSCSE Summer School on Science Clouds	08/01/2012	0.45			Live and Webcast
Presentation	FutureGrid Image Management and RAIN	VSCSE Summer School on Science Clouds	08/01/2012	0.45			Live and Webcast
Presentation	OpenStack and Eucalyptus on FutureGrid	VSCSE Summer School on Science Clouds	08/01/2012	0.45			Live and Webcast
Presentation	Twister4Azure: Iterative MapReduce for Windows Azure Cloud	VSCSE Summer School on Science Clouds	08/01/2012	1.0			Live and Webcast
Presentation	Windows Azure Cloud	VSCSE Summer School on Science Clouds	08/01/2012	1.0			Live and Webcast

Presentation	Twister Tutorial	VSCSE Summer School on Science Clouds	07/31/2012	1.5			Live and Webcast
Presentation	High Level Language: Pig Latin	VSCSE Summer School on Science Clouds	07/31/2012	1.0			Live and Webcast
Presentation	Apache Hbase	VSCSE Summer School on Science Clouds	07/31/2012	1.0			Live and Webcast
Presentation	Good O'le Hadoop! How We Love Thee!	VSCSE Summer School on Science Clouds	07/31/2012	1.0			Live and Webcast
Presentation	Reproducible Environment for Scientific Applications (Lab Session)	VSCSE Summer School on Science Clouds	07/31/2012	1.0			Live and Webcast
Presentation	Virtual Clusters Supporting MapReduce in the Cloud	VSCSE Summer School on Science Clouds	07/31/2012	1.0			Live and Webcast
Presentation	FutureGrid Overview	VSCSE Summer School on Science Clouds	07/30/2012	1.0			Live and Webcast
Presentation	Introduction to Clouds and the VSCSE Summer School on Science Clouds	VSCSE Summer School on Science Clouds	07/30/2012	1.0			Live and Webcast
Keynote	Cyberinfrastructure for eScience and eBusiness from Clouds to Exascale	ICETE 2012 Joint Conference on e-Business and Telecommunications, Rome, Italy	07/27/2012				Live
Panel	Clouds and Security	ICETE 2012 Joint Conference on e-Business and Telecommunications, Rome, Italy	07/24/2012				Live
Workshop	Computing Testbeds as a Service	NSF INCOSE2 Workshop on Instrumentation for Computer Science, Snowbird, UT	07/21/2012				Live
Presentation	MapReduce and Data Intensive	BoF Session, XSEDE'12, Chicago, IL	07/18/2012	1.0			Live

	Applications						
Panel	Use of Clouds to Support The Long Tail of Science	Panel on the Long Tail of Science, XSEDE'12, Chicago, IL	07/18/2012	1.5			Live
Presentation	FutureGrid Education: Using Case Studies to Develop Curriculum for Communicating Parallel and Distributed Computing Concepts	EOT Session, XSEDE'12, Chicago, IL	07/17/2012	0.5	~25		Live
Presentation	Hosting Cloud, HPC, and Grid Educational Activities on FutureGrid	BoF Session, XSEDE'12, Chicago, IL	07/17/2012	1.0			Live
Presentation	FutureGrid Overview	FutureGrid User Advisory Board, XSEDE'12, Chicago, IL	07/16/2012	0.5	~20		Live
Keynote	Science Clouds and Their Use in Data Intensive Applications	10th IEEE International Symposium on Parallel and Distributed Processing with Applications ISPA2012 Leganes, Madrid, Spain	07/10/2012 to 07/13/2012				Live
Workshop	Science Clouds and Their Innovative Applications	FICC2012, Tsinghua University, Beijing, China	07/09/2012 to 07/10/2012				Live
Presentation	Digital Science Center Overview	Beihang University, Beijing, China	07/08/2012				Live
University of Chicago							
Presentation	Nimbus Platform: Managing Deployments in Multi-Cloud	VSCSE Summer School on Science Clouds	07/30/2012	1.0			Live and Webcast
Presentation	Nimbus Infrastructure: Hands-On Using Infrastructure	VSCSE Summer School on Science Clouds	07/30/2012	1.0			Live and Webcast

	Clouds						
Presentation	Nimbus: Infrastructure Cloud Computing for Science	VSCSE Summer School on Science Clouds	07/30/2012	1.0			Live and Webcast
Presentation	Cloud Computing for Science: Challenges and Opportunities	BoF Session, XSEDE'12, Chicago, IL	07/18/2012	1.0			Live
Tutorial	Infrastructure Clouds for Science and Education	XSEDE'12, Chicago, IL	07/16/12	4.0			Live
University of Florida							
Presentation	Hosting Cloud, HPC, and Grid Educational Activities on FutureGrid	BoF Session, XSEDE'12, Chicago, IL	07/17/2012	1.0			Live
Tutorial	Infrastructure Clouds for Science and Education	XSEDE'12, Chicago, IL	07/16/12	4.0			Live
University of Southern California							
University of Tennessee at Knoxville							
University of Texas at Austin							

13.6 SP Collaborations

No new collaborations this quarter.

13.7 SP-Specific Activities

See 1.3.2 Services Activities.

13.8 Publications

Guo, Z., G. Fox, and M. Zhou, "**Investigation of data locality and fairness in MapReduce**", *Proceedings of third international workshop on MapReduce and its Applications Date*, Delft, The Netherlands, ACM, pp. 25–32, 2012.

Wolinsky, D. I., P. Chuchaisri, K. Lee, and R. J. Figueiredo, "**Experiences with self-organizing, decentralized grids using the grid appliance**", *Cluster Computing*, 2012.

Guo, Z., G. Fox, M. Zhou, and Y. Ruan, "**Improving Resource Utilization in MapReduce**", *the 2012 IEEE International Conference on Cluster Computing*, Beijing, China, IEEE Computer Society, 2012.

Fox, G., G. von Laszewski, J. Diaz, K. Keahey, J. Fortes, R. Figueiredo, S. Smallen, W. Smith, and A. Grimshaw, "**FutureGrid - a reconfigurable testbed for Cloud, HPC and Grid Computing**", *Contemporary HPC Architectures*, 2012.

Chen, W., and E. Deelman, "**Integration of Workflow Partitioning and Resource Provisioning**", *The 12th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing (CCGrid 2012)*, Ottawa, Canada, 05/2012.

William, T., D. K. Berry, and R. Henschel, "**Analysis and Optimization of a Molecular Dynamics Code using PAPI and the Vampir Toolchain**", *Cray User Group 2012*, Stuttgart, CUG, 05/2012

Furlani, T. R., M. D. Jones, S. M. Gallo, A. E. Bruno, C. - D. Lu, A. Ghadersohi, R. J. Gentner, A. Patra, R. L. DeLeon, G. von Laszewski, et al., "**Performance metrics and auditing framework using application kernels for high performance computer systems**", *Concurrency Experience and Practice*, issue to be published, 05/2012

Guo, Z., G. Fox, and M. Zhou, "**Investigation of Data Locality in MapReduce**", *Proceedings of the 2012 12th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing (ccgrid 2012)*, Ottawa, Canada, IEEE Computer Society, pp. 419–426, 05/2012. Abstract

Lee, K., D. I. Wolinsky, and R. Figueiredo, "**PonD : Dynamic Creation of HTC Pool on Demand Using a Decentralized Resource Discovery System**", *Proceedings of the 21st international symposium on High Performance Distributed Computing (HPDC)*, Delft, the Netherlands, ACM, 06/2012.

Diaz, J., G. von Laszewski, F. Wang, and G. Fox, "**Abstract Image Management and Universal Image Registration for Cloud and HPC Infrastructures**", *IEEE CLOUD 2012, 5th International Conference on Cloud Computing*, Honolulu, Hawaii, IEEE, 06/2012.

Yin, W., Y. Simmhan, and V. Prasanna, "**Scalable Regression Tree Learning on Hadoop using OpenPlanet**", *International Workshop on MapReduce and its Applications (MAPREDUCE)*, 06/2012.

von Laszewski, G., J. Diaz, F. Wang, and G. Fox, "**Comparison of Multiple Cloud Frameworks**", *IEEE CLOUD 2012, 5th International Conference on Cloud Computing*, Honolulu, Hawaii, IEEE, 06/2012.

Peluso, S., P. Ruivo, P. Romano, F. Quaglia, and L. Rodrigues, "**When Scalability Meets Consistency: Genuine Multiversion Update-Serializable Partial Data Replication**", *The 32nd International Conference on Distributed Computing Systems*, Macau, China, IEEE, 06/2012.

von Laszewski, G., H. Lee, J. Diaz, F. Wang, K. Tanaka, S. Karavinkoppa, G. C. Fox, and T. Furlani, "**Design of a Dynamic Provisioning System for a Federated Cloud and Bare-metal Environment**", *Workshop on Cloud Services, Federation, and the 8th Open Cirrus Summit*, San Jose, CA, IEEE, 09/2012.

Bosin, A., M. Dessalvi, G. M. Mereu, and G. Serra, "**Enhancing Eucalyptus Community Cloud**", *Intelligent Information Management*, vol. 04, issue 03, pp. 52 - 59, 2012

13.9 Metrics

13.9.1 Standard systems metrics

Top 70 FutureGrid Users #Jobs run (Jul-Sep 2012) - largest to smallest

Area	User	# Jobs	Avg Job Size (cpus)	Avg Wait Time (h)	Wall Time (d)	Avg Mem (MB)
University of Virginia (Project #118)	kasson	702700	1	0	165.2	1.4
University of Virginia (Genesis)	xcguser	49957	1	4.7	6369.4	93.6
University of Buffalo	charngda	17745	26.4	7.8	1509.9	118.7
SDSC - INCA	inca	4972	6.7	3.6	37.2	10.9
University of Massachusetts (Project #237)	dshrestha	1787	42.9	4.5	1931.2	661.3
University of Virginia (Project #118)	pela3247	1673	28.4	21.9	52731.2	851.1
Emory University (Project #141)	sagravat	1581	1	0	0.6	148.7
University of Notre Dame (Project #234)	dthain	1290	1	0	24.4	5.8
University of Utah (Project #149)	jasonkwan	672	7.4	4.5	2727.6	66451.9
University of Notre Dame (Project #234)	pdonnelly	461	1	0	1.8	6.6
University of Notre Dame (Project #234)	dpandiar	349	1	0	18.1	11.7
University of Virginia (UNICORE)	unicore	298	7.7	0.3	12.3	3.1
Juelich Supercomputing Centre (Project #170)	msmemon	173	3.5	0	0.1	2.9
University of Florida (Project #140)	zincum	138	16.6	0.4	2.4	1301.7
USC (Project #132)	cwickram	121	23.1	0	48.2	11318.5
LSU (SAGA)	sagaproj	120	1	0.2	0	0.4
Indiana University	lihui	104	8.4	12.6	356.7	388.3
University of Chicago	leggett	101	17.8	0.1	2.7	276.4
Indiana University	bsaha	99	3	0.6	0.2	23.8
University of Florida (graduate class)	zhiyikang	77	25.9	1.7	0.2	11.5
LSU (graduate class)	nykim	75	25.2	0.4	70.2	276.4
University of Notre Dame (Project #234)	iekechukwu	71	1	0	0.4	4.9
TACC (multiple projects)	wsmith	56	2.4	0	0	1.5
University of Arizona (Project #243)	jeffk	55	1	0.1	0.2	4.7
Indiana University (multiple projects)	gaoxm	54	78.6	3.7	308	352.9
LSU (SAGA)	oweidner	51	13	0.8	11.6	444.8
University of Arizona (Project #243)	evan	49	1	0	0.4	4.7
Indiana University (multiple projects)	claydavi	46	1	0	0.1	5.8
University of Florida (multiple projects)	navina	45	9	0	0.2	240.6
LSU (SAGA)	pmantha	44	15.3	0.1	10.1	112.1
Indiana University (Project #183)	crajacks	44	2.4	1.2	11.8	2336.5
University of Arizona (Project #243)	jrcresawn	44	1	0.4	0.1	6.2
Indiana University (Project #231)	upitamba	43	11.2	0	27.2	23474.3
University of Notre Dame (Project #234)	malbrec2	41	1	0	0.2	8
Rutgers University (Science Cloud Summer Scl	yunjiang	35	1	0	1.7	10.3
UCLA (Science Cloud Summer School)	kchan	31	1	0	2.4	10.9
Michigan State University (Science Cloud Sum	piwarsk1	31	1	0	2	10.5
University of South Carolina (Science Cloud Su	sjohnson	31	1	0	0.2	8

Area	User	# Jobs	Avg Job Size (cpus)	Avg Wait Time (h)	Wall Time (d)	Avg Mem (MB)
Indiana University (Science Cloud Summer Scl	raminder	29	1	0	0.3	7
University of Michigan (Science Cloud Summe	trbarrette	29	1	0	0.1	5.9
Indiana University (Project #203)	adnanozsoy	28	1	10.5	1.7	495.5
Indiana University (Science Cloud Summer Scl	thomlee	27	1	0	0.2	8.7
University of Notre Dame (Project #234)	psempoli	27	1	0	0.1	6.6
Indiana University (multiple projects)	ktanaka	26	4.6	0.2	0	3
Indiana University (Science Cloud Summer Scl	jayesh1511	26	1	0	0.2	9.7
University of Notre Dame (Project #234)	cbauschk	26	1	0	0	4.8
UCLA (Science Cloud Summer School)	huqy	25	2.2	0	0.2	21.9
Michigan State University (Science Cloud Sum	hezq06	25	1	0	0.1	9.7
LSU (Science Cloud Summer School)	xawx	25	1	0	0.7	8.5
University of Arizona (Project #243)	sjmiller	24	1	0	0	4.1
University of Arizona (Project #243)	cwvh	23	1	0	0.1	6.6
UCLA (Science Cloud Summer School)	elnaz	22	1	0	0.9	7.2
Michigan State University (Science Cloud Sum	chenchunyu	21	1	0	0.3	10.3
Indiana University (Science Cloud Summer Scl	smccaula	21	1	0	0.4	9.9
University of South Carolina (Science Cloud Su	adelecho	21	1	0	0.9	9.8
Indiana University (Science Cloud Summer Scl	viknesb	21	1	0	0.2	9.7
Princeton University (Science Cloud Summer S	shilei8583	21	1	0	1.3	9.5
Penn State University (Science Cloud Summer	elena	21	1	0	0.1	9.3
University of Oklahoma (Science Cloud Summ	bstamps	21	1	0	0.4	8.6
Indiana University (Science Cloud Summer Scl	kongch	21	1	0	0.9	8.2
University of D.C. (Science Cloud Summer Sch	tensae	21	1	0	0.6	8.2
Milwaukee School of Engineering (Science Clo	bojungx	21	1	0	0.1	6.4
LSU (Science Cloud Summer School)	apacheco	20	1	0	0.1	8
Indiana University (Science Cloud Summer Scl	prameshb87	20	1	0	0.1	7.9
LSU (Science Cloud Summer School)	rod	20	1	0	0	7.8
University of Wisconsin - Milwaukee (Science	mattq	20	1	0	0	5.9
University of Arizona (Project #243)	natfitz	19	1	0	0	6.6
University of Arizona (Project #243)	icj	19	1	0	0.1	6.1
University of South Carolina (Science Cloud Su	crotwell	19	1	0	0	5.7
University of Arizona (Project #243)	trr	19	1	0	0	5.7

13.9.2 Standard systems metrics (continued)

Top 30 (Average) Memory Users - Largest to Smallest

Area	User	# Jobs	Avg Job Size (cpus)	Avg Wait Time (h)	Wall Time (d)	Avg Mem (MB)
University of Utah (Project #149)	jasonkwan	672	7.4	4.5	2727.6	66451.9
Indiana University (Project #231)	upitamba	43	11.2	0	27.2	23474.3
USC (Project #132)	cwickram	121	23.1	0	48.2	11318.5
Indiana University (Project #183)	crajacks	44	2.4	1.2	11.8	2336.5
University of Florida (Project #140)	zincum	138	16.6	0.4	2.4	1301.7
Indiana University (multiple projects)	yangruan	5	66.4	663.5	1.2	1104.2
University of Virginia (Project #118)	pela3247	1673	28.4	21.9	52731.2	851.1
University of Massachusetts (Project #237)	dshrestha	1787	42.9	4.5	1931.2	661.3
Indiana University (Project #203)	adnanozsoy	28	1	10.5	1.7	495.5
LSU (SAGA)	oweidner	51	13	0.8	11.6	444.8
Indiana University	lihui	104	8.4	12.6	356.7	388.3
Indiana University (multiple projects)	gaoxm	54	78.6	3.7	308	352.9
USC (Project #132)	zyfo2	1	32	0	0	285.1
University of Chicago	leggett	101	17.8	0.1	2.7	276.4
LSU (graduate class)	nykim	75	25.2	0.4	70.2	276.4
University of Florida (multiple projects)	navina	45	9	0	0.2	240.6
University of Florida (graduate class)	dstoker	10	32	0	0.4	240
University of Florida (graduate class)	idfree	2	32	25.1	0.1	226.1
University of Florida (graduate class)	vikrant	2	32	3.7	0.1	201.4
USC (Project #132)	weiyin	2	64	45.2	0.2	173.1
University of Florida (graduate class)	oucfei	16	32	0	0.2	172.9
University of Florida (graduate class)	xiaobai07	16	32	0	0.5	166.4
USC (Project #132)	chen60	5	28.8	3.2	5.4	149.7
Emory University (Project #141)	sagravat	1581	1	0	0.6	148.7
University of Buffalo	charngda	17745	26.4	7.8	1509.9	118.7
LSU (SAGA)	pmantha	44	15.3	0.1	10.1	112.1
University of Virginia (Genesis)	xcguser	49957	1	4.7	6369.4	93.6

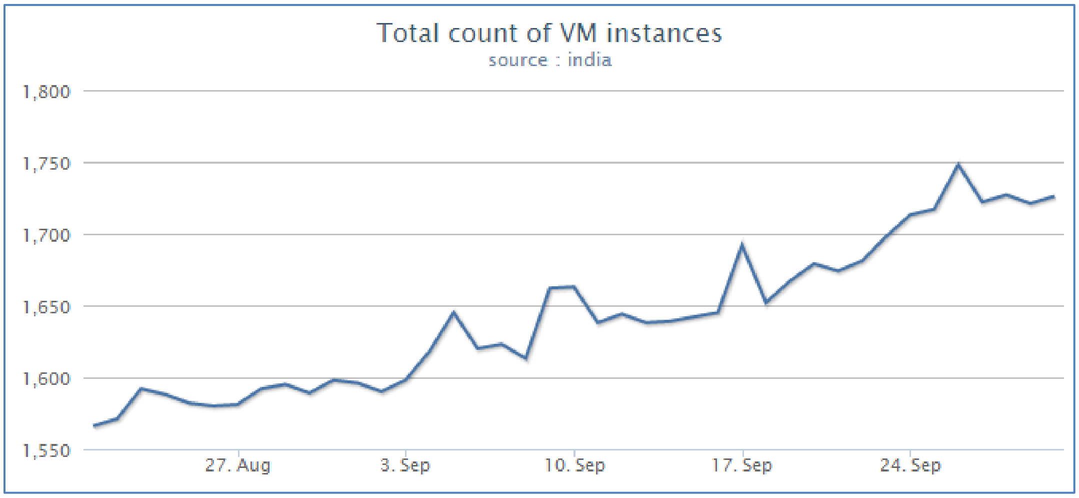
13.9.3 *Standard systems metrics (continued)*

Top 25 (Average) Job Size Users - Largest to Smallest

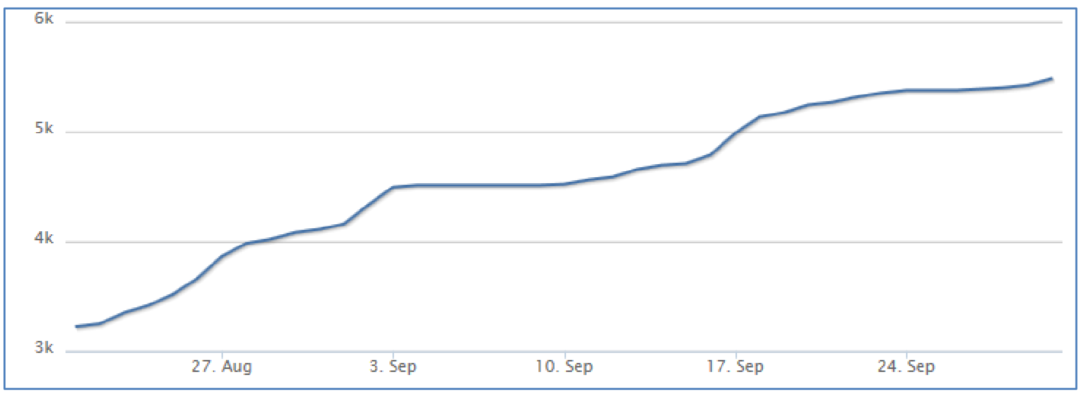
Area	User	# Jobs	Avg Job Size (cpus)	Avg Wait Time (h)	Wall Time (d)	Avg Mem (MB)
Indiana University (multiple projects)	weng	2	120	7	201.3	10.9
Indiana University (multiple projects)	gaoxm	54	78.6	3.7	308	352.9
Indiana University (multiple projects)	yangruan	5	66.4	663.5	1.2	1104.2
USC (Project #132)	weiyin	2	64	45.2	0.2	173.1
University of Massachusetts (Project #237)	dshrestha	1787	42.9	4.5	1931.2	661.3
Indiana University (multiple projects)	zhguo	5	35.2	9.2	1014.7	3.6
University of Florida (graduate class)	oucfei	16	32	0	0.2	172.9
University of Florida (graduate class)	xiaobai07	16	32	0	0.5	166.4
University of Florida (graduate class)	dstoker	10	32	0	0.4	240
University of Florida (graduate class)	sandeepnl	5	32	0	0.1	83.6
Binghamton University (Project #40)	rdelval1	3	32	0	2.4	43.1
University of Florida (graduate class)	idfree	2	32	25.1	0.1	226.1
University of Florida (graduate class)	vikrant	2	32	3.7	0.1	201.4
YunNan University, China (Project #238)	anny	2	32	17.4	0	0.7
University of Florida (graduate class)	zyfo2	1	32	0	0	285.1
USC (Project #132)	chen60	5	28.8	3.2	5.4	149.7
University of Virginia (Project #118)	pela3247	1673	28.4	21.9	52731.2	851.1
University of Buffalo	charngda	17745	26.4	7.8	1509.9	118.7
University of Florida (graduate class)	zhiyikang	77	25.9	1.7	0.2	11.5
LSU (graduate class)	nykim	75	25.2	0.4	70.2	276.4
USC (Project #132)	cwickram	121	23.1	0	48.2	11318.5
USC (Project #132)	simmhan	17	22.4	0	0	3.2
University of Chicago	leggett	101	17.8	0.1	2.7	276.4
University of Florida (Project #140)	zincum	138	16.6	0.4	2.4	1301.7
University of Arizona (Project #243)	nirav	2	16.5	0	0	17.3
Independent Consultant (Project #259)	leg	7	16	0	0	4.9

13.9.4 Standard systems metrics (continued)

Total Count of VM Instances on *india*



Total Count of VM Instances on *sierra*



13.9.5 Standard User Assistance Metrics

RT Ticket System

Created tickets in period, grouped by status:

Status	Tickets
deleted	0
new	2
open	21
rejected	15
resolved	168
stalled	0
Total	206

Resolved tickets (223) in period, grouped by queue (category):

a) 017 FutureGrid account requests
b) 023 Portal account requests
c) 011 Eucalyptus issues
d) 033 Nimbus issues
e) 011 OpenStack issues
f) 004 Portal issues
g) 081 General issues
h) 016 *hotel* issues
i) 003 *alamo* issues
j) 021 User Support issues
k) 003 Systems issues

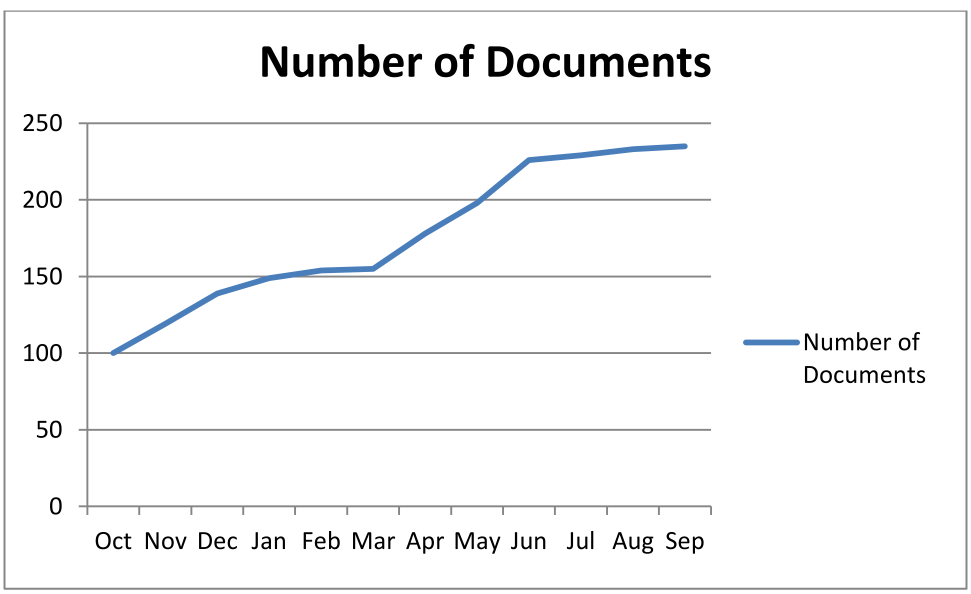
New/Open tickets (23) in period, grouped by queue (category):

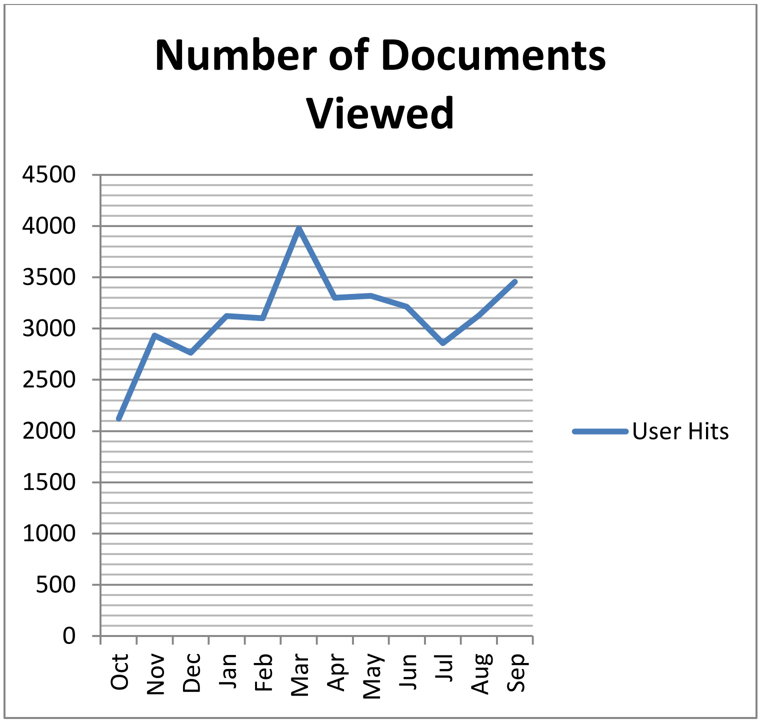
a) 001 FutureGrid account requests
b) 003 Eucalyptus issues
c) 002 Nimbus issues
d) 002 OpenStack issues
e) 010 General issues
f) 003 User Support issues
g) 002 Alamo issues

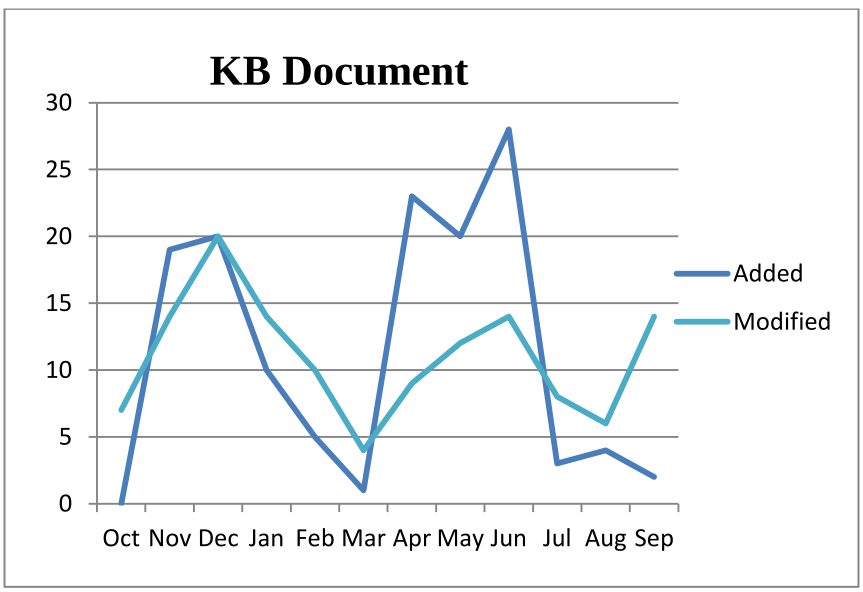
13.9.6 SP-specific Metrics

Knowledge Base:

Analysis FutureGrid Knowledge Base PY2 2011-2012					
	Hits		Documents		
	Total Hits	User Hits	Added	Modified	Total Docs
October 2011	2541	2121	0	7	100
November 2011	3695	2933	19	14	119
December 2011	3517	2764	20	20	139
January 2012	6581	3123	10	14	149
February 2012	6609	3101	5	10	154
March 2012	9241	3977	1	4	155
April 2012	4813	3300	23	9	178
May 2012	4600	3319	20	12	198
June 2012	4474	3212	28	14	226
July 2012	4344	2856	3	8	229
August 2012	5076	3130	4	6	233
September 2012	6333	3457	2	14	235




Number of Documents Viewed
4500
4000
3500
3000
2500
2000
1500
1000
500
0
Oct
Nov
Dec
Jan
Feb
Mar
Apr
May
Jun
Jul
Aug
Sep
User Hits


KB Document
30
25
20
15
10
5
0
Oct Nov Dec Jan Feb Mar Apr May Jun Jul Aug Sep
Added
Modified

Projects:

- Thirty-one (31) new projects added this quarter
- Categorization of projects to date:

a) Project Status:
Active Projects: 237(89.1%)
Completed Projects: 17(6.4%)
Pending Projects: 3(1.1%)
Denied Projects: 8(3%)

b) Project Orientation:
Research Projects: 217(81.6%)
Education Projects: 46(17.3%)
Industry Projects: 2(0.8%)
Government Projects: 1(0.4%)

c) Project Primary Discipline (large to small count):
Computer Science (401): 216(81.2%)
Biology (603): 11(4.1%)
Industrial/Manufacturing Engineering (108): 4(1.5%)
Not Assigned: 10(3.8%)
Genetics (610): 2(0.8%)
Physics (203): 2(0.8%)
Aerospace Engineering (101): 1(0.4%)
Statistics (403): 1(0.4%)
Engineering, n.e.c. (114): 2(0.8%)
Biosciences, n.e.c. (617): 1(0.4%)
Biophysics (605): 1(0.4%)
Economics (903): 1(0.4%)
Electrical and Related Engineering (106): 3(1.1%)
Pathology (613): 1(0.4%)
Civil and Related Engineering (105): 1(0.4%)
Biochemistry (602): 1(0.4%)
Atmospheric Sciences (301): 1(0.4%)
Microbiology, Immunology, and Virology (611): 2(0.8%)
Earth, Atmospheric, and Ocean Sciences, n.e.c. (304): 2(0.8%)
Geosciences (302): 1(0.4%)
Mechanical and Related Engineering (109): 1(0.4%)
Social Sciences, n.e.c. (910): 1(0.4%)

d) Project Service Request/Wishlist:
High Performance Computing Environment: 132(49.6%)
Eucalyptus: 132(49.6%)
Nimbus: 140(52.6%)
OpenStack: 87(32.7%)
OpenNebula: 59(22.2%)
Hadoop: 95(35.7%)
Twister: 40(15%)
MapReduce: 91(34.2%)
Genesis II: 31(11.7%)

XSEDE Software Stack: 49(18.4%)
Unicore 6: 17(6.4%)
gLite: 19(7.1%)
CUDA(GPU Software)): 6(2.3%)
Vampir: 13(4.9%)
Globus: 16(6%)
Pegasus: 15(5.6%)
PAPI: 14(5.3%)
MPI: 9(3.4%)
ScaleMP: 2(0.8%)
SAGA: 1(0.4%)

14 Indiana University Pervasive Technology Institute - Service Provider Quarterly Report

14.1 Executive Summary

Indiana University was approved as a Level 2 Service Provider for PY2, through the delivery of capability computing and capacity computing infrastructure, networking and software services. During this project year, we plan on offering Mason as an XSEDE resource through the NSF-funded National Center for Genome Analysis Support (NCGAS). This system targets researchers using genome assembly software, large-scale phylogenetic software, or other genome analysis applications requiring a large amount of computer memory.

Integrating these resources aids XSEDE in its support of non-traditional researchers using science gateways as well as investigators in the life sciences. Additionally, offering Mason and associated NCGAS expertise allows IU to support researchers in an environment that is consistent with other national cyberinfrastructure by leveraging common allocations and software.

14.1.1 *Indiana University Level 2 Service Provider Systems: Resource Descriptions*

Level 2 - Quarry (Virtual Machines) - The Quarry Gateway Web Services Hosting resource at Indiana University consists of multiple Intel-based HP systems geographically distributed for failover in Indianapolis and Bloomington, IN. Currently there are four HP DL160 front-end systems at each site, all configured with dual quad-core Intel E5603 processors, 24 GB of RAM, and a 10 gigabit Ethernet adapter. There are a total of 48 XSEDE Virtual Machines. The front-end systems host the KVM-based virtual machines. Virtual Machine (VM) block storage is provided by two HP DL180 servers at each site configured with a quad-core Intel X5606 processor, 12 GB of RAM, a 10 gigabit Ethernet adapter, and a RAID controller attached to an HP storage array. Quarry is used solely for hosting Science Gateway and Web Service allocations, or services to support central XSEDE infrastructure. Requests are restricted to members of approved projects that have a web service component.

Level 3 (Pending) - Rockhopper - Rockhopper is a collaborative effort between Penguin Computing, IU, the University of Virginia, the University of California Berkeley, and the University of Michigan to provide supercomputing “cluster on demand” services in a secure US facility. Researchers at US institutions of higher education and federally funded research centers can purchase computing time from Penguin Computing and receive access via high-speed national research networks operated by IU. It takes just minutes to go from holding a credit card in one’s hands and filling out a web form to being computing on Rockhopper (the system itself is owned by Penguin; cycles on Rockhopper are purchased from Penguin). Rockhopper is a 4.4 TFLOPS system based on AMD processors.

14.2 Science Highlights

Indiana University Participation in STEAM Innovation Fair at Conner Prairie, September, 2012.

Indiana University was invited to participate in the STEAM Innovation Fair at Conner Prairie in Indianapolis, Indiana in September 2012. This is the second year for this two-day event that showcases university and business innovations across the state. The mission of this event is to focus not only on the historic innovators of the past, but also on current innovators and how their sense of discovery is important to the future advancement of our society. Approximately 4,260 attended the festival.

The Indiana University booth had four main components for engaging the public: mineral finding robots; password cracking on a home grown computer cluster; bending light using laser light refraction; and 3D science videos produced by our Advanced Visualization group with funding from the TeraGrid grant. These hands-on demonstrations allowed the lay audience to engage with technology to see how it benefits society, from bending light as an example of how data travel over fiber optic cable at the speed of light, to programming robots to find minerals on Mars. These examples show the importance of how technology has allowed scientific innovation and discovery to happen at an accelerated pace.

Figure 5. Photo of Indiana University booth at STEAM Innovation Fair.

Education, outreach, and training are important to the mission of the Pervasive Technology Institute. Staff working in the Institute are always looking for ways to reach out to the public and in particular K-12 students. This engagement has a positive impact in not only demonstrating the important contribution of the university to the state, but also in encouraging young students to pursue science and technology tracks in their education.

14.3 User-facing Activities

14.3.1 System activities

14.3.1.1 Level 2 – Quarry (virtual machines)

During Q1 of PY2, administrators completed reconfiguration of the Quarry VM hosting environment storage. The new configuration uses DRBD to synchronously mirror ZFS volumes between the Bloomington and Indianapolis campuses, with iSCSI connectivity to the hosted

VMs. Migration to the new KVM environment, begun during PY1, will resume once the OpenVZ data have been moved to this new storage. A handful of VMs, including a backup system for Inca, were moved during the first quarter.

Outages during this quarter were minimal, totaling less than four hours, and resulting only from requested VM image snapshots or required migrations from OpenVZ to KVM.

14.3.1.2 Level 3 (pending) – Rockhopper (Penguin on Demand commercial cluster as a service)

There were no issues with Rockhopper during this quarter.

14.3.2 Services activities

14.3.2.1 Level 2 – Quarry

No changes were made to the Quarry VM service this quarter.

Quarry continues to be used solely for hosting science gateway and web service allocations, or services to support central XSEDE infrastructure. Requests are restricted to members of approved projects that have a web service component. An external request form can be found at: http://pti.iu.edu/hps/vm-account-request.

14.3.2.2 Level 3 (pending) – Rockhopper

The Rockhopper service saw a significant increase in usage during the Q1 of PY2. There were 1,746 user logins recorded, and 30,875 jobs were run. These numbers represent an increase of 26% and 6% respectively over the entire first project year. In addition, eight new users were added to the system, increasing the total to 40.

14.4 Security

There were no security issues.

14.5 Education, Outreach, and Training Activities

Type	Title	Location	Date(s)	Hours	Number of Participants	Number of Under-represented people	Method
Conference talk/presentation/panel	Celebrate Science Indiana	Indianapolis, IN	6-Oct-12	7 hours	3000	500	S
Conference talk/presentation/panel	STEAM Innovation Fair at Conner Prairie	Indianapolis, IN	15-16 Sept -12	14 hours	4500	800	S
Conference talk/presentation/panel	New Faculty Orientation at IUPUI	Indianapolis, IN	15-Aug-12	4 hours	100	15	S
Conference talk/presentation/panel	XSEDE12	Chicago, IL	19 July-12	24 hours	80	30	S
Conference talk/presentation/panel	OVPIT Annual Statewide Conference	Bloomington, IN	24-25 Sept-12	12 hours	620	100	S
Workshop	Minority Engineering Advancement Program	Indianapolis, IN	9 & 12-13 July 12	16 hours	20	20	S
Conference talk/presentation/panel	Indiana Clinical Translational Science Annual Meeting	Indianapolis, IN	31-Aug-12	8 hours	150	90	S

Type	Title	Location	Date(s)	Hours	Number of Participants	Number of Under-represented people	Method
Tutorial	XSEDE12-Developing Science Gateways using Apache Airavata	Chicago, IL	16 July-12	4 hours	25		S
Tutorial	XSEDE 12-Hands-on Tutorial for Building Science Gateway Applications on Cyberinfrastructure	Chicago, IL	16 July-12	4 hours	25		S
Tutorial	SDSC Summer Institute Science Gateways Tutorial	San Diego, CA	9 Aug-12	8 hours	30		S
Conference talk/presentation/panel	Smithsonian Institution Folklife Festival 2012, Washington D.C.	Washington, D.C.	1 & 4- 8 July-12	48 hours	6096		S
Workshop	Introductory Parallel Programming Workshop	Indianapolis, IN	25-Sep-12	8 hours	12		S
Workshop	Introductory Parallel Programming Workshop	Bloomington, IN	27-Sep-12	8 hours	32		S

Table 5. EOT activities for Q1.

14.6 SP Collaborations

There were no collaborations to report this quarter.

14.7 SP-Specific Activities

Data Services (WBS 1.2.2)

Since its deployment in August of 2010, Justin Miller has been the administrator of Indiana University's portion of the XSEDE-wide Albedo file system. He has looked after those servers and will oversee IU's participation in Albedo's retirement.

In addition, Justin has been supporting XSEDE users who are using Data Capacitor resources primarily through gateway allocations.

Systems Operational Support (WBS 1.2.6)

14.7.1 Virtual machines

IU staff provided ongoing operational support for VMs hosted on the IU Quarry system.

14.7.2 XD Operations Center Fail-over

In the event of an emergency and/or an extended outage, Indiana University GNOC will serve in the role of a backup XNOC. GNOC is located in Indianapolis on the IUPUI campus, which houses the Global Research Network Operations Center (GRNOC). GRNOC will be prepared to receive/send emails that are directed to help@xsede.org. In addition, GRNOC has set up a dedicated phone line at (317) 274-7782 and is prepared to take phone calls directed to XNOC should the primary XSEDE Operations Center at NCSA be unreachable due to an emergency and/or an extended outage.

The list below includes items that are close to being completed:

- Phones: XSEDE NOC greeting on IU phone system was added and we are waiting on the pending toll free provider redirecting the number and process. Few more details are still being worked out as far as whom should be authorized to request a pull of the phone to be answered by GNOC. XNOC will initiate a push for all the incoming calls if need be during an emergency and or an outage.
- Email: Setup of email acceptance for failover on the IU GNOC side. This is awaiting XSEDE/NCSA setup, policy and procedures, documentation before we continue. An in-box is already setup but process/procedure is still in the works to determine who/how can emails be pushed to be sent to GNOC.

The list below includes items that are still in the works:

- Ticketing: GNOC awaits announcement of a final decision on a new trouble ticket system for XNOC. A shared account has been created for GNOC to have access to the ticketing system once a decision is made.
- Monitoring: Still pending; we are waiting on a setup to access current XNOC monitoring.
- Process and Procedure Documentation: GNOC is still waiting on centralizing all XSEDE documentation to XSEDE Staff Wiki.
- Fail-over Documentation: If process/procedure documentation is centralized into the staff wiki, then the fail over process (for documentation) will become part of the overall fail-over process.
- Training: GNOC staff need to receive training from XNOC on trouble ticket system usage and or other tools that will be needed during an emergency and/or an extended outage.
- XNOC Staff relocation: This item is still in the works. If need be, XNOC staff can relocate to GNOC to work at Indianapolis during an extended XNOC outage.

14.8

User Engagement (WBS 1.3.3)

The final report of the 2012 XSEDE User Satisfaction Survey was delivered to leadership in July 2012. It can be found at:

https://xsedewiki.uits.indiana.edu/wiki/index.php/IU_Specific_XSEDE_Documents
To obtain a copy of the final report, please contact Julie Wernert, jwernert@iu.edu.

Major findings of the survey were reported in the previous quarterly report. Overall response to the survey has been positive, but we have made several recommendations to improve participation, as well as the planning process:

- Future surveys should be much shorter in length, allowing respondents to complete the survey in 10 minutes or less. The *average* time to take the 2012 survey was 25 minutes.
- The annual survey should largely be confined to broad issues that are of interest to all users. Alternatively, allow respondents to either opt out after the general questions, or opt into going on to more granular service- or resource-specific questions.
- To gauge satisfaction with specific resources and services used by smaller subsets (e.g., ECSS), consider short, targeted "point-of-service" surveys.

- Make known to the user community those priorities that were set – and subsequent actions that were taken – as a result of survey results. This will increase engagement in and "ownership" of the process by the user base.
- Make well known to the service provider community (SP Forum, et al) the members of the survey development committee, venues for review and commentary, and timeline.
- Consider a separate survey to gather staff input specifically geared toward staff concerns/issues. A formal mechanism for staff to provide input would likely result in invaluable, actionable data.
- To the extent possible, be mindful of major NSF deadlines that may conflict with the survey deployment.

Indications are that many of these recommendations will be adopted, with the annual survey process expected to transition to a yearlong feedback "campaign." In addition to the annual survey aimed at gathering general feedback, several additional surveys (approximately one per quarter) will be added to complement and augment data gathered through the annual survey. Additional surveys proposed include targeted, "real-time" surveys for (1) Extended Collaborative Support Services, (2) New and Innovative Projects, (3) each major XSEDE resource (e.g., Stampede, Kraken, etc.), and (4) XSEDE staff. These additional surveys will be more granular in nature, targeted toward specific users, and more proximate in time to the point of service. Future surveys cycles will also allow more time for broader XSEDE engagement and in-depth data analysis.

Planning for the 2013 User Satisfaction Survey will begin in November or December 2012, with the goal of launching in early 2013.

Novel & Innovative Projects (WBS 1.4.2)

The IU Science Gateways group has initiated a project to enable the UCI OpenCourseWare project and Professor Emeritus Douglas R. White from University of California Irvine to develop a social science gateway. The gateway will enable courses available on the open source Moodle and Apache Airavata tools. The gateway will provide access to student assignments and other Social Science analytic problems that are hosted through the San Diego Supercomputer Center Trestles Cluster.

IU Science Gateway Group team members also attended the HathiTrust Uncamp (http://www.hathitrust.org/htrc_uncamp2012, September 10-11) to discuss their computational humanities requirements.

Extended Support for Science Gateways (WBS 1.5.2)

Gateway Leadership

The Extended Support for Science Gateways (ESSGW) is tasked to provide assistance to researchers wishing to access XSEDE resources through web portals and science gateways. The group assists both new and advanced groups and has experience in the use of web technologies, grid software, fault tolerance, complex workflows, and security and accounting aspects of the program.

This quarter, Suresh Marru coordinated efforts of the ECSS Science Gateways group including:

- Leading gateway community engagement.
- Coordinating gateway support personnel across all the sites.
- Working with the Architecture and Design team and finalizing three gateway use cases. This exercise is resulting in an extensive survey of gateway architecture in regards to XSEDE integration. The effort was coordinated through contributed use cases from teleconferences.
- Planning to conduct a two-month workshop with four biweekly calls in running down various layers of the gateway architecture and conducting technology knowledge sharing sessions.
- Participating in an XSEDE12 panel discussing Security for Science Gateways and Campus Bridging.

UltraScan Science Gateway

The Ultrascan Laboratory Information Management System provides a user friendly web interface for evaluation of experimental analytical ultracentrifuge data using the UltraScan modeling software.

Efforts during the quarter focused on working with Ultrascan developers and SDSC admins to deploy the code on Trestles and Gordon.

The Ultrascan SOMO work was published and presented at the XSEDE 12 conference.

Dark Energy Survey Simulation Working Group

The simulation working group for the Dark Energy Survey is developing a high throughput workflow environment for cosmological simulations. The simulations provide support for analysis of systematics in the three methods associated with large-scale astronomical structures.

This quarter the ECSS support focused on developing workflow solutions for N-body production process executing 2LPT and L-GADGET codes using the Apache Airavata software suite. The support continued on running the production workflow for N-body simulation on TACC Ranger cluster; migrating the DES code and Workflow to SDSC Trestles; exploring file transfer mechanisms to archival systems and post processing environments; and providing automatic processing steps within the workflow.

Petascale computations in mineral physics with Quantum ESPRESSO (VLAB)

The VLAB project provides petascale computations in mineral physics with the Quantum ESPRESSO codes. The ESSGW suport is helping the VLAB project team to build workflow infrastructure to perform first principles calculations of unprecedented magnitude and scope in mineral physics. The project is focusing on optimizing the execution of the Quantum ESPRESSO software for materials simulations in XSEDE systems. This quarter, gateway support focused on working with VLab Gateway developers in porting Quantum ESPRESSO to the XSEDE Ranger Cluster, enabling job submission through the Apache Airavata gateway-building framework.

Extended Support for Training, Education, and Outreach (WBS 1.5.3)

Gateway Training and Outreach

Science Gateways simplify access to XSEDE by providing easy-to-use, familiar interfaces. Gateway developers are challenged in building and maintaining gateways and are often overwhelmed in choosing middleware. Often these middleware solutions are black boxes to the developers that make them expend valuable man-hours in debugging real-time problems.

At XSEDE12, the Science Gateway Group and its collaborators spearheaded two tutorials: “Developing Science Gateways using Apache Airavata API” with Sudhakar Pamidighantam (NCSA), Ye Fan (NCSA), and Matt McKenzie (NICS); and “Hands-on Tutorial for Building Science Gateway Applications on Cyberinfrastructure” with Yan Liu (NCSA) and Nancy Wilkins-Diehr (SDSC).

Through these tutorials audience members were presented with hands-on practical insights into gateway building aspects. The tutorials also provided insights into aspects of open community software development practices – not just using open software but how to contribute, get recognized, and also have a say in future directions.

The morning tutorial focused on providing insights into introducing XSEDE capabilities: account access, data resources, HPC clusters and job management services, the software environment, and information services. The tutorial provided exercises for programmatically developing XSEDE-enabled applications using the SimpleGrid Application Programming Interface (API). The tutorial demonstrated developing web applications using Web 2.0 technologies (JavaScript, AJAX, and Ext JS) to enable community-wide shared access to deploy an iGoogle-like web app gadget using Apache Rave.

The afternoon tutorial taught lessons on executing compute jobs and workflows on XSEDE resources through grid interfaces; wrapping command line applications and turning them into web accessible programmable interfaces; and learning about the open community development process to contribute to existing software with proper contribution governance models. The tutorial was based on Apache Airavata, a software toolkit to build science gateways. Using Airavata the participants composed and executed monitoring applications and workflows on the XSEDE Ranger Cluster.

Campus Bridging (WBS 1.6.5)

Discussion of campus bridging within XSEDE and within the national cyberinfrastructure community

In Q1 of PY2, the Campus Bridging team discussed team initiatives with the XSEDE Operations team and the Software Development and Integration team on a regular basis in order to determine the correct course of action for both the GFFS Pilot Project work and the software packages to be included in the Campus Bridging Rocks Rolls, as well as the Level 3 decomposition of use cases created by the Architecture and Design team.

The Campus Bridging team also met with the Minority Research Community in August in order to describe Campus Bridging initiatives to the community and gather input on directions. Significant interest was expressed in the community about both the Campus Bridging team's Rocks Roll packages and in training and documentation initiatives, as well as the propagation of the GFFS and Globus Online tools for data management.

The Campus Bridging team created a video for streaming and podcast purposes. The video describes the general concepts of campus bridging and XSEDE Campus Bridging initiatives and generally conforms to the talks delivered by the Campus Bridging Team at Internet 2 Members' Meetings, XSEDE11, and SC11. This video will be made available before SC12 begins.

Definition of use cases and quality attributes for XSEDE's Campus Bridging efforts

The Architecture and Design teams have completed the Level 3 Decomposition for Campus Bridging Use Cases and Quality Attributes. Familiarity with the process of creating use cases and quality attributes has been passed on to teams who are currently going through the process with the Architecture and Design teams.

GFFS Pilot Project

The GFFS Pilot Project sites have completed a training course with the Genesis II developers and have installed GFFS clients and client containers locally. The Operations team has completed installation of the GFFS root container (beta version) for XSEDE and is expected to implement GFFS on XSEDE SP resources in series over the following weeks. Pilot sites are to begin testing at the end of October.

Campus Bridging Software Packages

The Campus Bridging team has, in concert with the Operations and Software Development and Integration teams, put together a list of XSEDE software that is approved for inclusion in the XSEDE Campus Bridging Rocks Rolls and packaged software. Campus Bridging is working to establish milestones for the packaging of the software and a distribution mechanism for users.

Challenges in Program Year Two

The Campus Bridging team anticipates that there may be some challenges in getting pilot sites "completed" with their testing in the 2-4 weeks allotted by the operational calendar. Pilot sites should be able to complete at least minimal functionality tests in the beta environment and get their responses around that time period.

14.9 Publications

Conference Papers

Pamidighantam, S., S. Marru, and M. Pierce, GridChem and ParamChem: Science Gateways for Computational Chemistry (and More), Sep 25, 2012.

Falk-Krzesinski, H., and W. K. Barnett, "Promoting Collaboration and Team Science Across the CTSA Consortium OR Now that you've VIVOed, what Next? " VIVO Conference 2012, Miami, Fla., Aug 2012.

Basney, J., R. Butler, D. Fraser, S. Marru, and undefined, Security for science gateways and campus bridging: XSEDE12 panel (extended abstract), Salt Lake City, UT, ACM, Jul 2012.

Basney, J., R. Butler, D. Fraser, S. Marru, and C. A. Stewart, "Campus Bridging Security Challenge" XSEDE12, Chicago, IL, Jul 2012.

Boyles, M., A. William, C. Frend, and C. Eller, "Using Stereoscopic 3D Videos to Inform the Public about the Benefits of Computational Science" XSEDE 2012, Chicago, Illinois, Jul 2012.

Brookes, E., R. Singh, M. Pierce, S. Marru, B. Demeler, and M. Rocco, "Ultrascan solution modeler: integrated hydrodynamic parameter and small angle scattering computation and fitting tools" XSEDE12, Chicago, IL, ACM, Jul 2012.

Erickson, B. M. S., R. Singh, A. Evrard, M. R. Becker, M. Busha, A. V. Kravtsov, S. Marru, M. Pierce, and R. H. Wechsler, "A high throughput workflow environment for cosmological simulations" XSEDE12, Chicago, IL, ACM, Jul 2012.

Stewart, Craig, A., "XSEDE Opening Remarks" XSEDE 012 (eXtreme Enviroment for Science and Engineering Discovery), Chicago, IL, Jul 2012.

Stewart, C. A., "XSEDE12 Closing Remarks" XSEDE 012 (eXtreme Enviroment for Science and Engineering Discovery), Chicago, IL, Jul 2012.

Zhang, H., H. Li, M. Boyles, R. Henschel, E. K. Kohara, and M. Ando, "Exploiting HPC Resources for the 3D-Time Series Analysis of Caries Lesion Activity" XSEDE 2012, Chicago, Illinois, Jul 2012.

Conference Proceedings

Mukherjee, R., A. Thota, H. Fujioka, T. C. Bishop, and S. Jha, "Running many molecular dynamic simulations on many supercomputers" XSEDE (eXtreme Enviroment for Science and Engineering Discovery), Chicago, Il, Jul 2012.

Presentations

Pierce, M., S. Marru, and S. Pamidighantam, https://scholarworks.iu.edu/dspace/handle/2022/14703, Hubbub 2012, Indianapolis, IN, Sep 25, 2012.

Simms, S., and K. Seiffert, Empowering Bioinformatics Workflows Using the Lustre Wide Area File System across a 100 Gigabit Network, Sep 2012.

14.10 Metrics

14.10.1 Standard User Assistance Metrics

14.10.1.1 User Information and Interfaces (WBS 1.3.2)

Knowledge Base

Summary statistics for the XSEDE Knowledge Base:

Metric	For current quarter
Number of KB documents available at end of quarter	538
Number of new KB documents added	62
Total number of retrievals	174,212
Total number of retrievals minus bots	87,987

Table 6. High-level XSEDE Knowledge Base metrics for current quarter.

Metric	PY to date (when applicable)
Number of KB documents available at end of quarter	538
Number of new KB documents added	62
Total number of retrievals	174,212
Total number of retrievals minus bots	87,987

Table 7. High-level XSEDE Knowledge Base metrics for current period and project year to date.

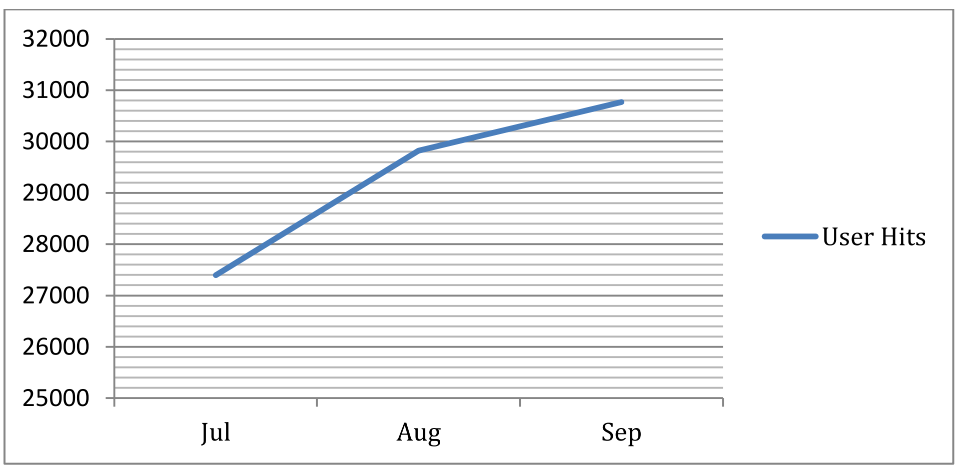


Figure 6. Total Knowledge Base accesses by month, current program year to date.

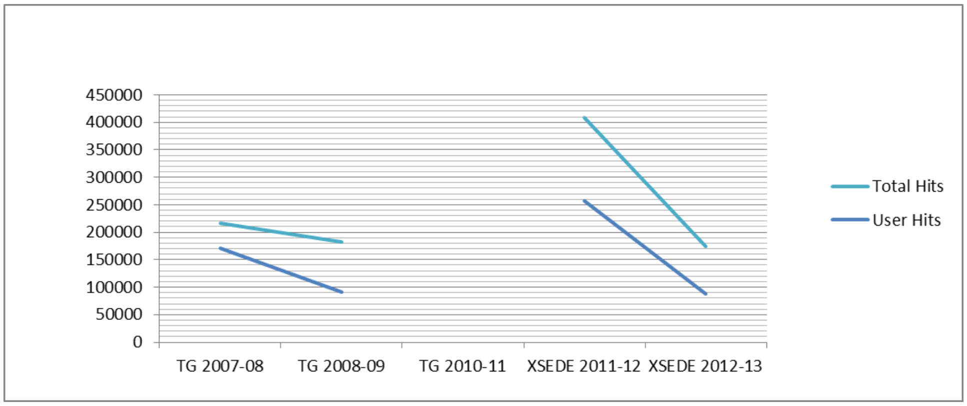


Figure 7. XSEDE and TeraGrid Knowledge Base annual accesses. (Data are unavailable for 2009/2010.)

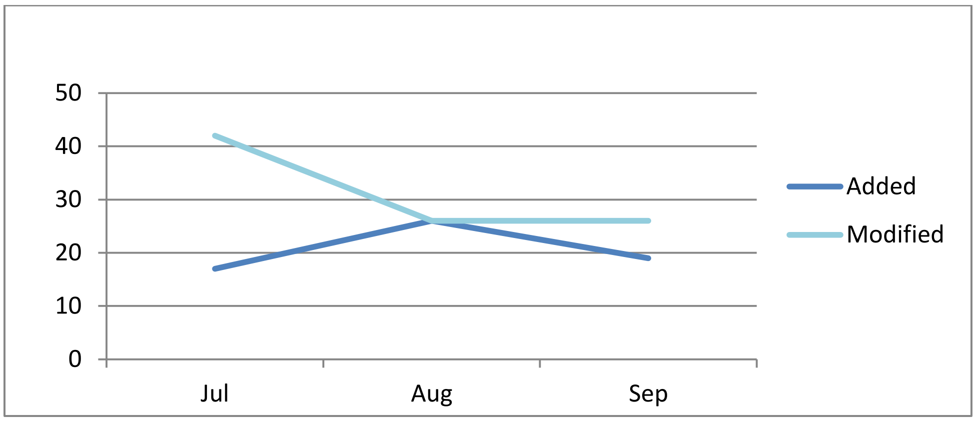


Figure 8. Knowledge Base editing activity (new entries added; existing entries modified or removed) by month, current program year to date.

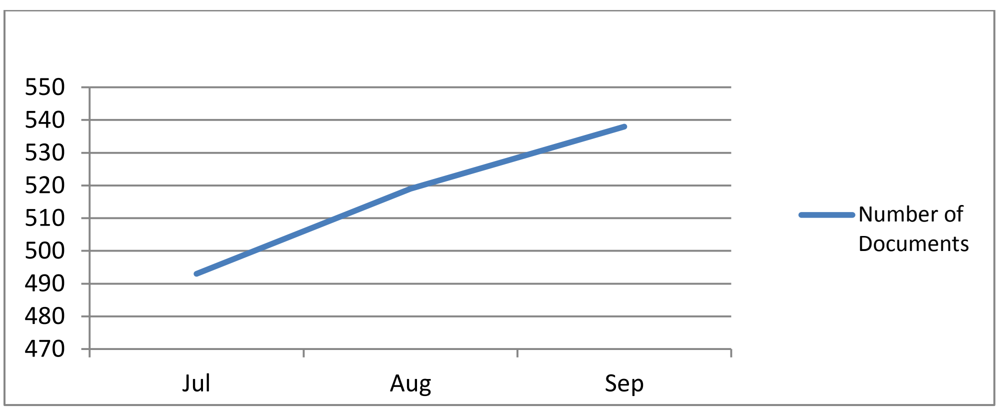


Figure 9. Total number of documents in XSEDE Knowledge Base by month, current program year to date.

Time to Resolution	account issues	file systems	grid software	jobs/batch queues	login/access issues	mss/data issues	network issues	software/apps	system issues	other
0-1 hr										
1-24 hr										
1-7 d										
1-2 wk										
> 2 wk						1			1	1
Still Open										

Table 8. IU Ticket resolution times by category from XSEDE Ticket System.

14.10.2 SP-specific Metrics

14.10.2.1 Usage metrics – current quarter

	# Allocations	# VMs allocated	# TB allocated	System	Storage high water mark	TB written	TB read
Quarry VM	25	54					
Rockhopper				1,746			
Data Capacitor WAN	47		2.25	36B	316	135	209
Scholarly Data Archive – HPSS							

Table 9. Service Provider system key usage metrics for the current quarter (Q1 of PY2 –July-September 2012).

System	Overall % uptime	# planned downtimes	Planned downtime duration total (minutes)	# unplanned downtimes	Unplanned downtime duration total (minutes)	Total minutes in reporting period
Quarry VM	99.8%	1	210	1	18	131,040
Rockhopper						
Data Capacitor WAN	99.78	1	240	1	52	132,480
Scholarly Data Archive – HPSS						

Table 10. Service Provider system key usage metrics for the current quarter (Q1 of PY2 –July-September 2012).

14.10.2.2 Usage metrics – project year 2

System	# Allocations	# VMs allocated	# TB allocated	# accesses	Storage high water mark	TB written	TB read
Quarry VM	25	54					
Rockhopper				1,746			
Data Capacitor WAN	47		2.25	36B	316	135	209
Scholarly Data Archive – HPSS							

Table 11. Service Provider system key usage metrics for PY2 (July 2012–September 2012).

System	Overall % uptime	# planned downtimes	Planned downtime duration total (minutes)	# unplanned downtimes	Unplanned downtime duration total (minutes)	Total minutes in reporting period
Quarry VM						
Rockhopper						
Data Capacitor WAN	99.78	1	240	1	52	132480
Scholarly Data Archive – HPSS						

Table 12. Service Provider system key usage metrics for PY2 (July 2012–September 2012).

14.10.3 Standard systems metrics

N/A.

15 NCSA - Service Provider Quarterly Report

15.1 Executive Summary

NCSA's *Forge* GPU computing system retired September 30, 2012. Users were sent a notice to prepare them for the transition to other systems, and notifying them of the availability of the new Keeneland GPU computing resource. NCSA will provide read-only access to the tape archive beyond September 30, 2012. This will serve as the last NCSA Service Provider report.

15.1.1 Resource Description

Forge consists of 36 Dell PowerEdge C6145 quad-socket nodes with dual 8-core AMD Magny-Cours 6136 processors and 64 GB of memory. Each node supports 6 NVIDIA Fermi M2070 GPUs.

NCSA's hierarchical archival storage system is available for permanent storage of data. Access is via FTP- and SSH-based transfer clients, including GridFTP clients. NCSA's mass storage now holds more than six petabytes of data and has the capacity to archive ten petabytes of data.

15.2 Science Highlights

Geography and Regional Science: Extending and Sustaining CyberGIS Discovery Environment (Shaowen Wang, University of Illinois at Urbana-Champaign)

Viewshed analysis, often supported by Geographic Information Systems (GIS), is widely used in many application domains. A viewshed is created from a digital elevation model by using an algorithm that estimates the difference of elevation from one cell (the viewpoint cell) to the next (the target cell).

However, as terrain data continue to become increasingly large and available at high resolutions, data-intensive viewshed analysis poses significant computational challenges. General-purpose computation on graphics processing units (GPUs) provides a promising means to address such challenges. The work of Shaowen Wang and his team at the University of Illinois at Urbana-Champaign has established a parallel computing approach to data-intensive viewshed analysis of large terrain data using GPUs. Their approach exploits high-bandwidth memory of GPUs and parallelism of massive spatial data to enable memory-intensive and compute-intensive tasks while CPUs (central processing units) are used to achieve efficient Input/Output (I/O) management. Furthermore, a two-level spatial domain decomposition strategy was developed to mitigate a performance bottleneck caused by data transfer in the memory hierarchy of GPU-based architecture. A suite of experiments was conducted using NCSA's Forge cluster to evaluate computational performance of the approach. The experiments demonstrated significant performance improvement over a well-known sequential computing method, and enhanced ability of analyzing

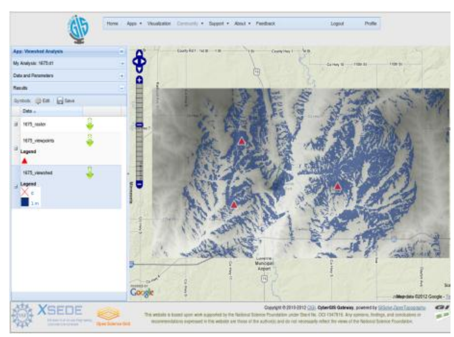


Figure 1 The viewshed app in the CyberGIS Gateway. The viewshed app uses GPUs for large-scale and data-intensive viewshed analysis. Gateway provides an online problem-solving environment for community users to conduct cyberinfrastructure-empowered (currently we use XSEDE, OSG, and local resources) spatial analysis and enable scientific collaborations.

sizable datasets that the sequential computing method cannot handle. This work was presented at several conferences and was published in the *International Journal of Geographical Information Science*.

Atmospheric Sciences: Investigations of Atmospheric Turbulent Flows over Complex Terrain using GPU Clusters, (Inanc Senocak, Boise State University)

There is a growing interest to increase the utilization of wind energy resources for electricity production. But increasing the percentage of wind energy in overall energy production is much more complex than simply installing wind farms in windy areas with flat terrains. The overall goal of the research of Inanc Senocak Of Boise State University is to better understand the characteristics of turbulent flows in complex terrain with canyons under different atmospheric stability conditions using a multi-scale modeling approach, so that these wind energy resources can be reliably harnessed for the production of electricity. Using an MPI-CUDA incompressible solver (GIN3D) that has been developed in Senocak's research group, the team used NCSA's Forge to concurrently execute meso and micro scale models to forecast winds over complex terrain for wind energy production. Simulation results then are used to perform turbulent kinetic energy budget analysis, which helps identify and understand the primary source of turbulence production in complex terrain environment under different stability conditions. Standard deviations of the wind velocity is examined and compared against existing correlations. Simulations are validated against measurements obtained from a test area in the state of Idaho in a complex terrain area instrumented with weather stations. Both experimental and computational data are studied to find appropriate scaling parameters to characterize the flow structure within canyons and along ridges. The terrain and urban domains can extend up to 10 km in the horizontal plane. This research has been presented at numerous conferences and published in *The Journal of Supercomputing*, *Computing in Science & Engineering*, and *Environmental Fluid Mechanics*.

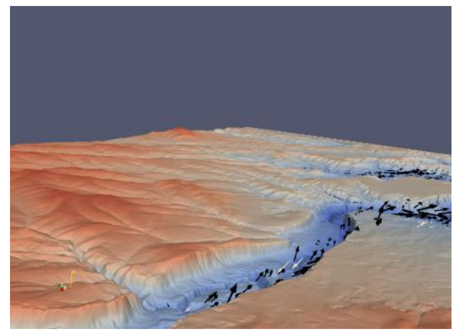


Figure 2 Simulations on Forge help to better understand the characteristics of turbulent flows in complex terrain with canyons in different atmospheric stability conditions, so that the wind can be reliably harnessed for electricity production.

15.3 User-facing Activities

15.3.1 System Activities

Filesystems and Storage:

Continued support of NCSA's Dell NVIDIA Cluster Forge and the archival system MSS.

Networking:

NCSA continues to manage the DNS services for XSEDE which includes the teragrid.org and xsede.org domains. We delegate subdomains to other SP sites and make DNS adds and deletions as requested by project groups. We setup and manage the dynamic dns system. We also acquire certificates for the various web services being deployed on XSEDE.

Systems:

NCSA's *Forge* GPU computing system retired September 30, 2012. Users were sent a notice to prepare them for the transition to other systems.

15.3.2 *Services Activities*

Continued support of NCSA's Dell NVIDIA Cluster Forge and the archival system MSS.

15.4 Security

The NCSA security team did not have any incidents involving XSEDE users or resources for the third quarter 2012. There were also no changes to the security monitoring during the quarter.

15.5 Education, Outreach, and Training Activities

NCSA provides online training via CI-Tutor. Course usage statistics are captured in the following table:

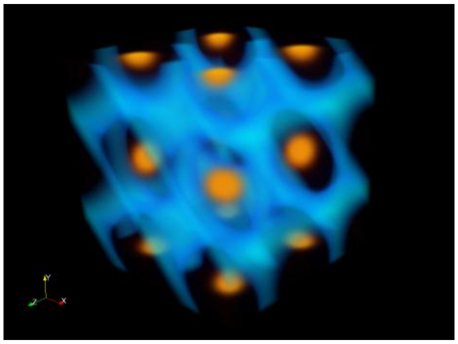
Course Title	Jul-12	Aug-12	Oct-12	Total
Access Grid Tutorials	1	2	6	9
BigSim: Simulating PetaFLOPS Supercomputers	1	2	6	9
Debugging Serial and Parallel Codes	6	9	10	25
Getting Started on theTeraGrid	0	4	6	10
Getting Started on XSEDE	0	0	0	0
Intermediate MPI	12	12	11	35
Introduction to MPI	43	63	57	163
Introduction to Multi-core Performance	7	18	9	34
Introduction to OpenMP	21	17	36	74
Introduction to Performance Tools	5	7	8	20
Introduction to Visualization	7	9	8	24
Multilevel Parallel Programming	5	13	6	24
Parallel Computing Explained	25	30	29	84
Parallel Numerical Libraries	2	8	5	15
Performance Tuning for Clusters	2	10	5	17
Tuning Applications for High Performance Networks	4	4	2	10
Using the Lustre File System	13	11	5	29
XSEDE Cybersecurity	3	2	1	6
Total	157	221	210	588

15.6 SP Collaborations

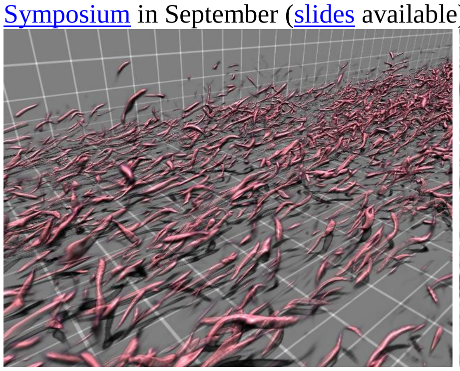
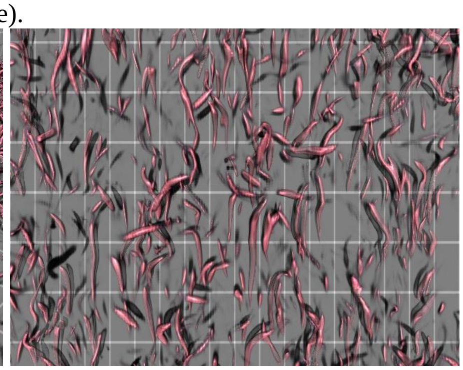
Nothing to report.

15.7 SP-Specific Activities

Continued visualization work on Asymptotic Scaling of Heat Transport in Infinite Prandtl Number Fluids at Very High Resolution with PI Benson Muite of the University of Michigan. Instrumented CUDA Fortran code to use ParaView CoProcessing. Provided training materials to project team for implementing in similar code bases. Started instrumenting MPI codes to use same automated visualization processes (example images below).



Continued visualization work with A. Ferrante, University of Washington, on DNS of Spatially Developing Turbulent Boundary Layers. Completed scene construction and rendering full-resolution sequences for production runs (example images shown below). Presented work with D. Adams (NCSA) at XSEDE ECSS Symposium in September (slides available).

Continued visualization work with V. Kuhn, University of Southern California, on Interactive Large Scale Media Analytics. Co-authored paper and poster accepted and presented at 8th IEEE International Conference on eScience.

15.8 Publications

Papers

None to report this quarter.

15.9 Metrics

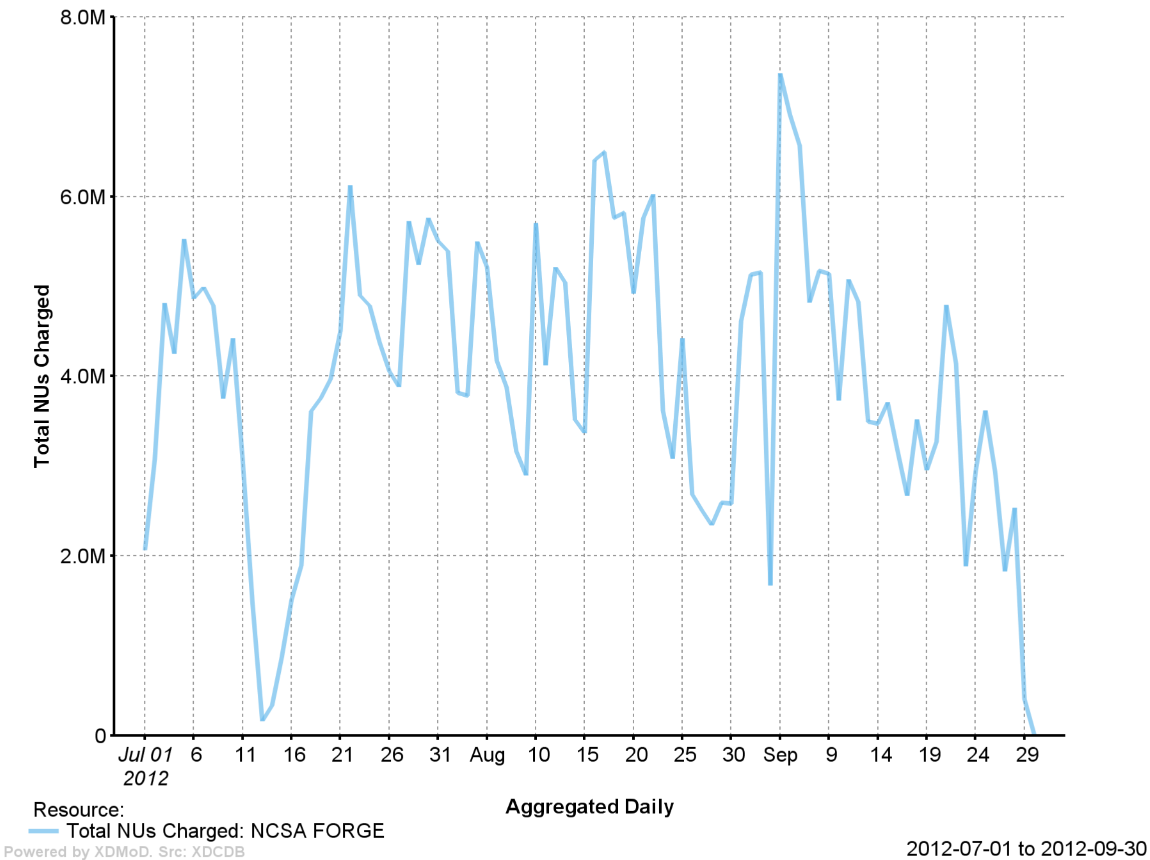
NCSA Ticket resolution times by category from XSEDE Ticket System

Time to Resolution	account issues	file systems	grid software	jobs/batch queues	login/access issues	mss/data issues	network issues	software/apps	system issues	other
0-1 hr				1						
1-24 hr										
1-7 d								1	17	5
1-2 wk						1			10	4
> 2 wk						5		3	30	2
Still Open						1			1	

Total NUs Charged by Resource

Service Provider = NCSA

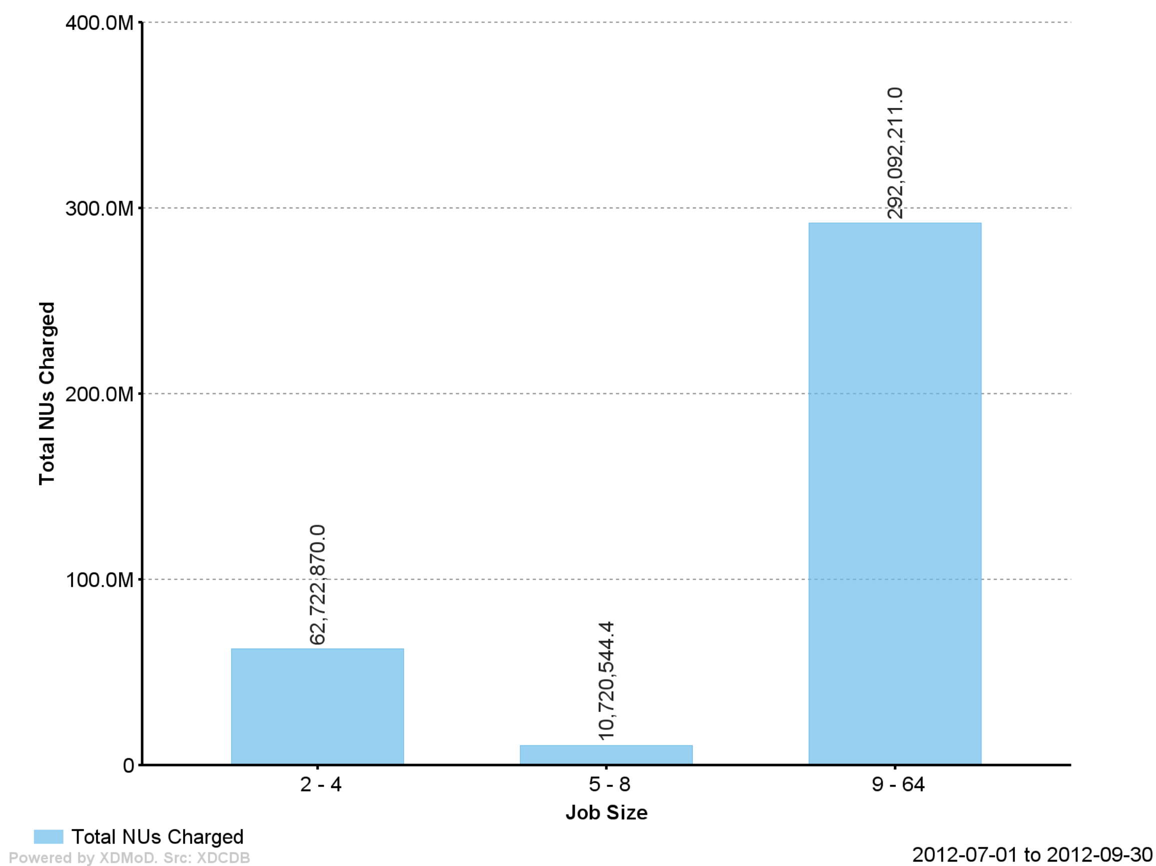
2012-07-01 to 2012-09-30



Total NUs Charged by Job Size

Resource = NCSA-FORGE

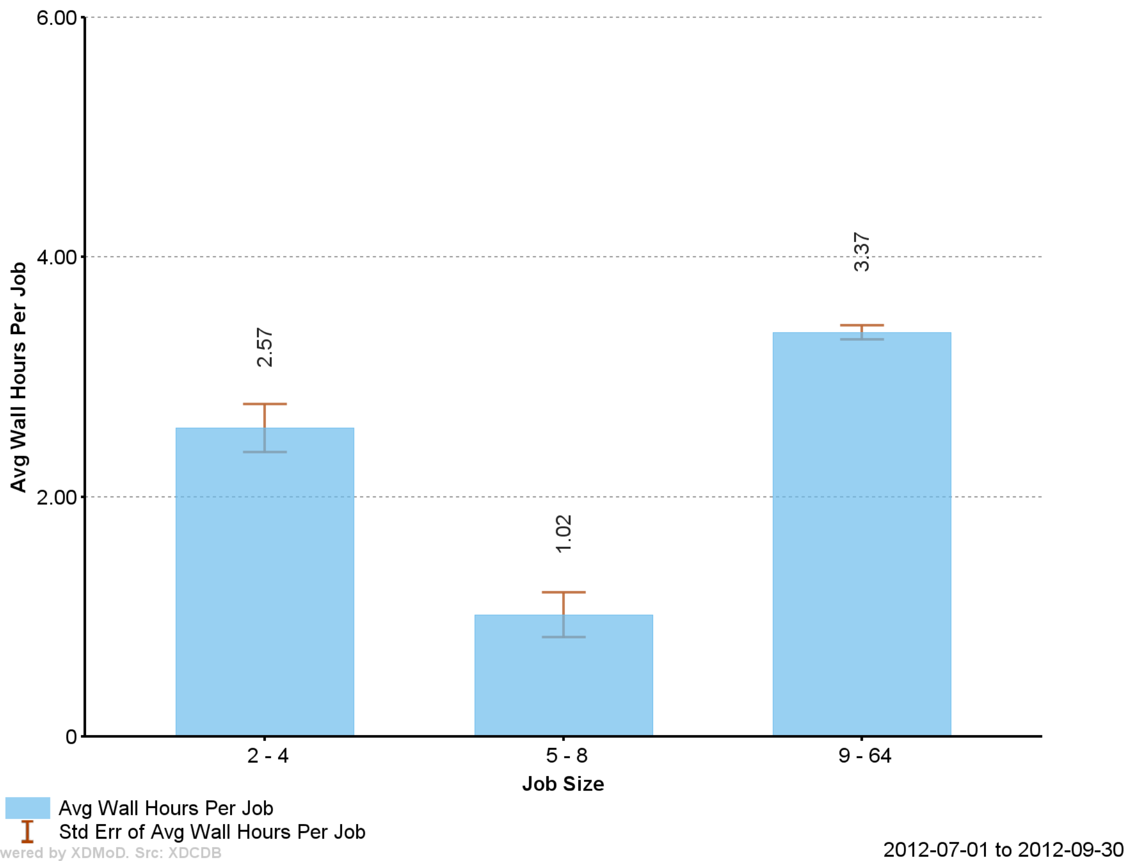
2012-07-01 to 2012-09-30



Avg Wall Hours Per Job by Job Size

Resource = NCSA-FORGE

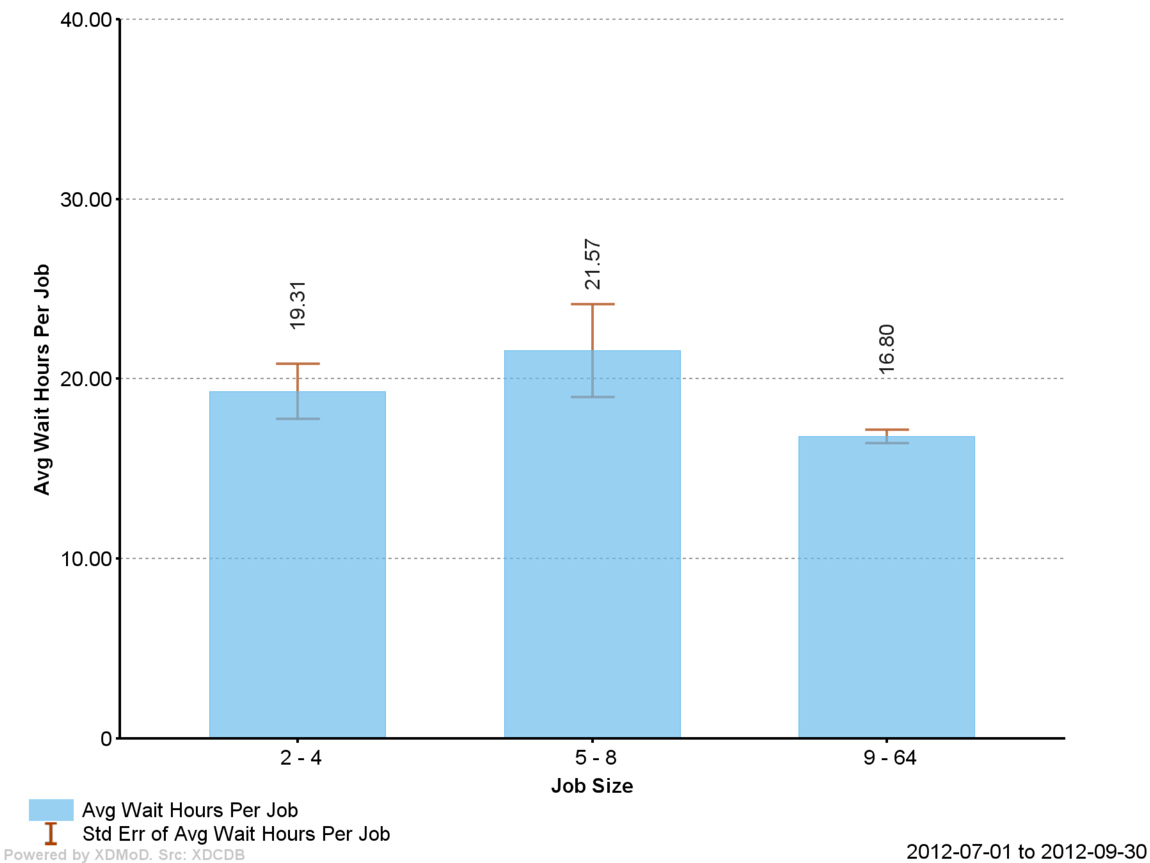
2012-07-01 to 2012-09-30



Avg Wait Hours Per Job by Job Size

Resource = NCSA-FORGE

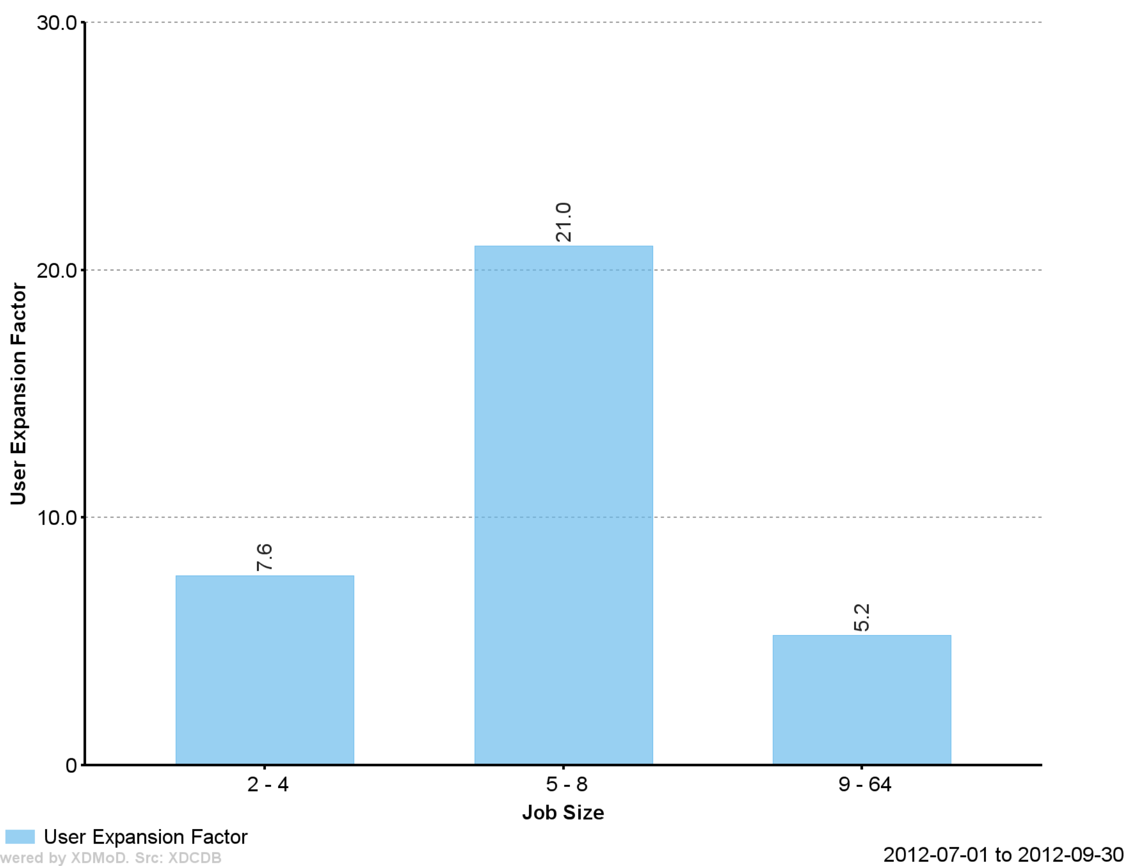
2012-07-01 to 2012-09-30



User Expansion Factor by Job Size

Resource = NCSA-FORGE

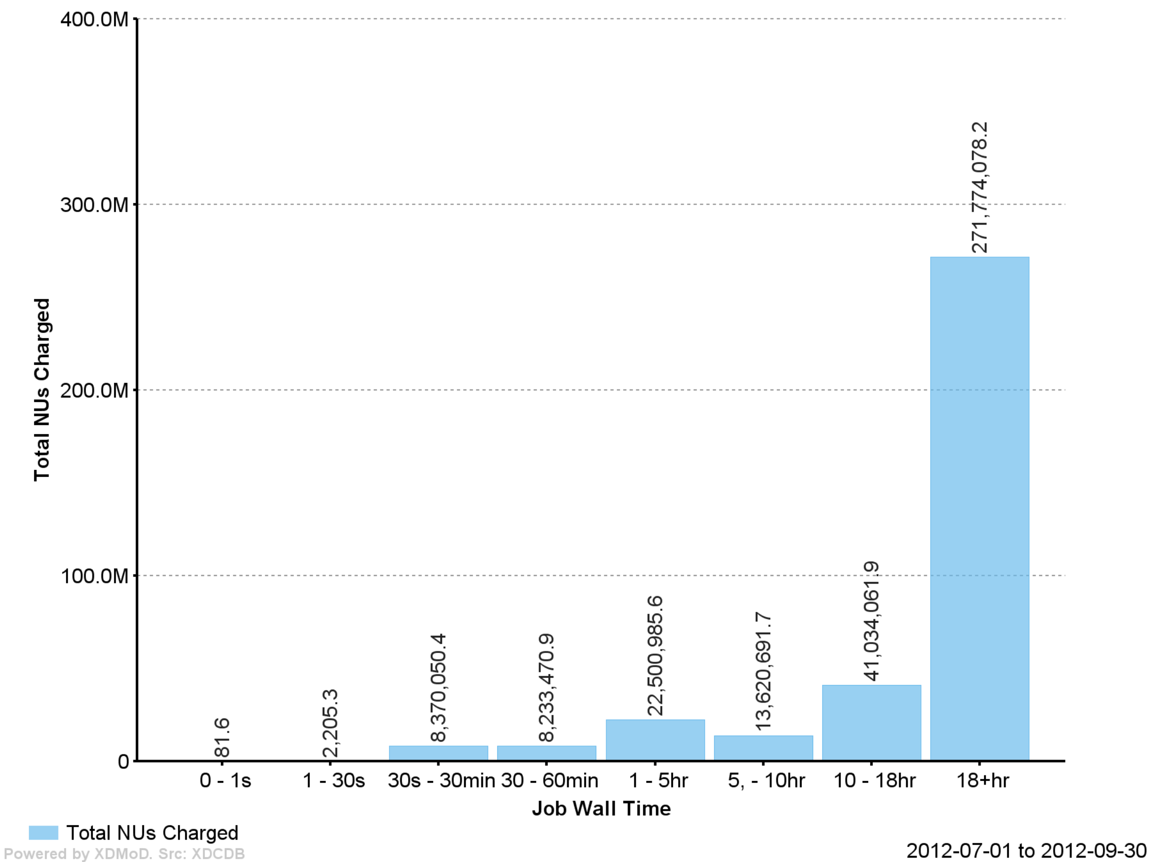
2012-07-01 to 2012-09-30



Total NUs Charged by Job Wall Time

Resource = NCSA-FORGE

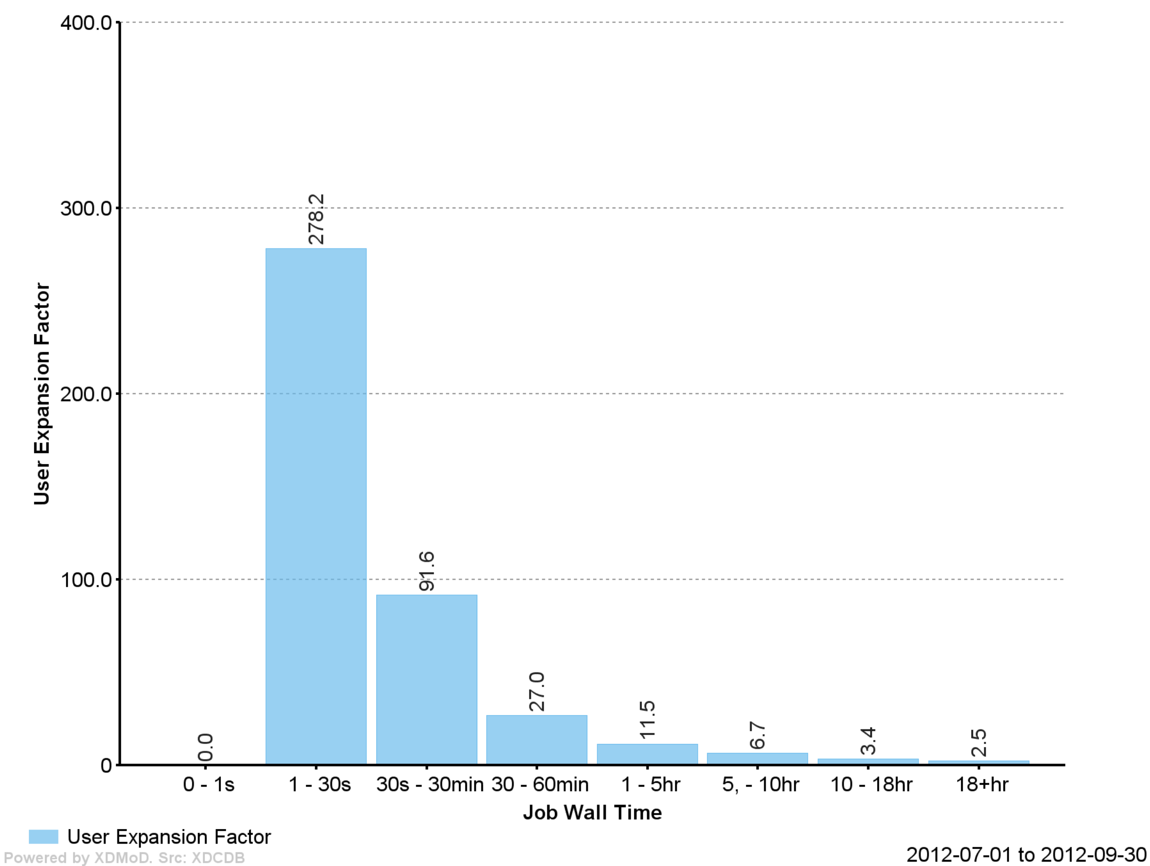
2012-07-01 to 2012-09-30



User Expansion Factor by Job Wall Time

Resource = NCSA-FORGE -- Service Provider = NCSA

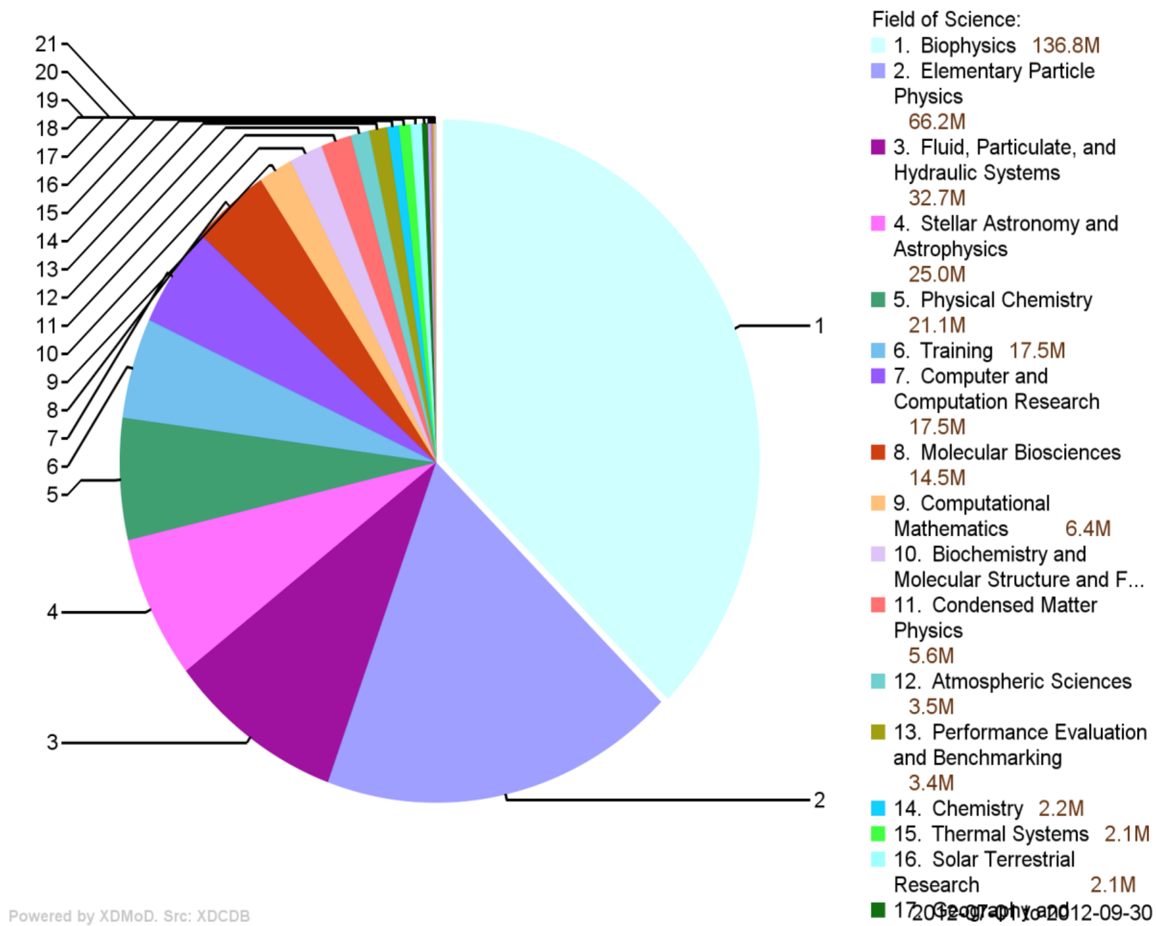
2012-07-01 to 2012-09-30



Total NUs Charged by Field of Science

Resource = NCSA-FORGE

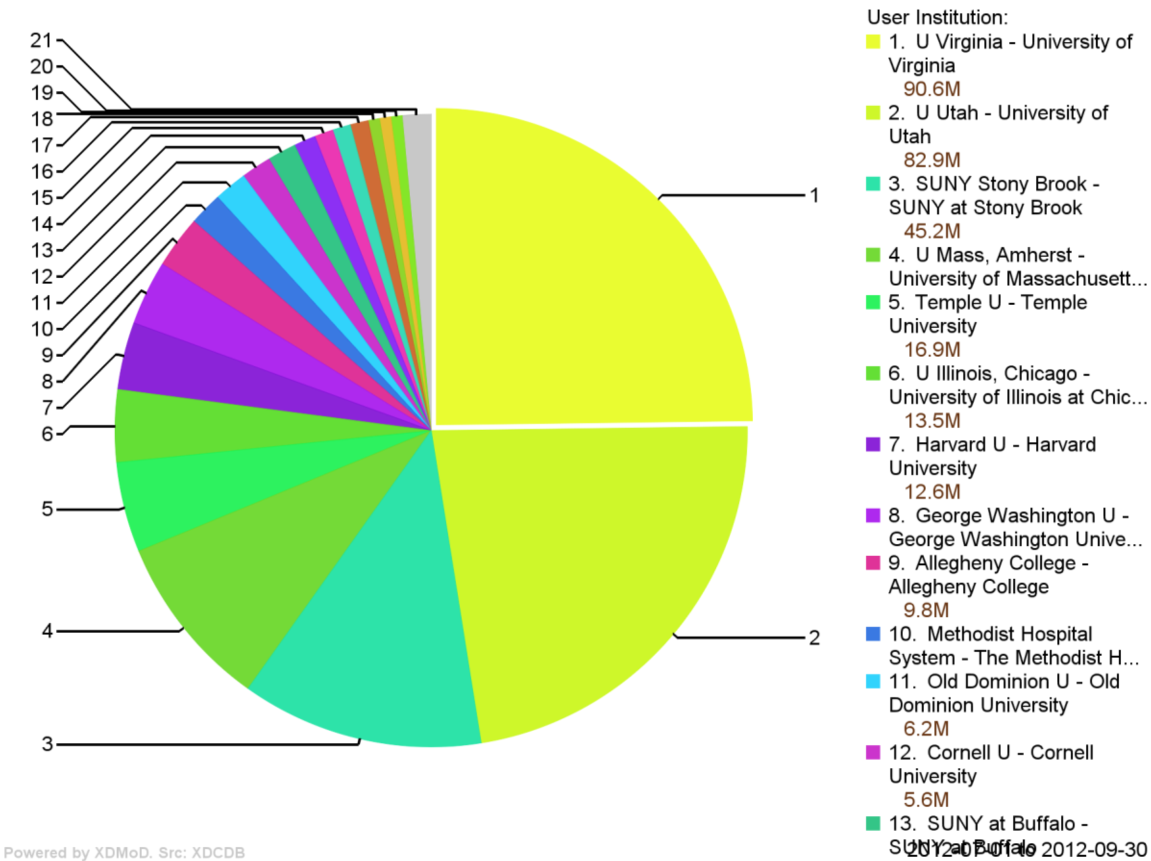
2012-07-01 to 2012-09-30



Total NUs Charged by User Institution

Resource = NCSA-FORGE

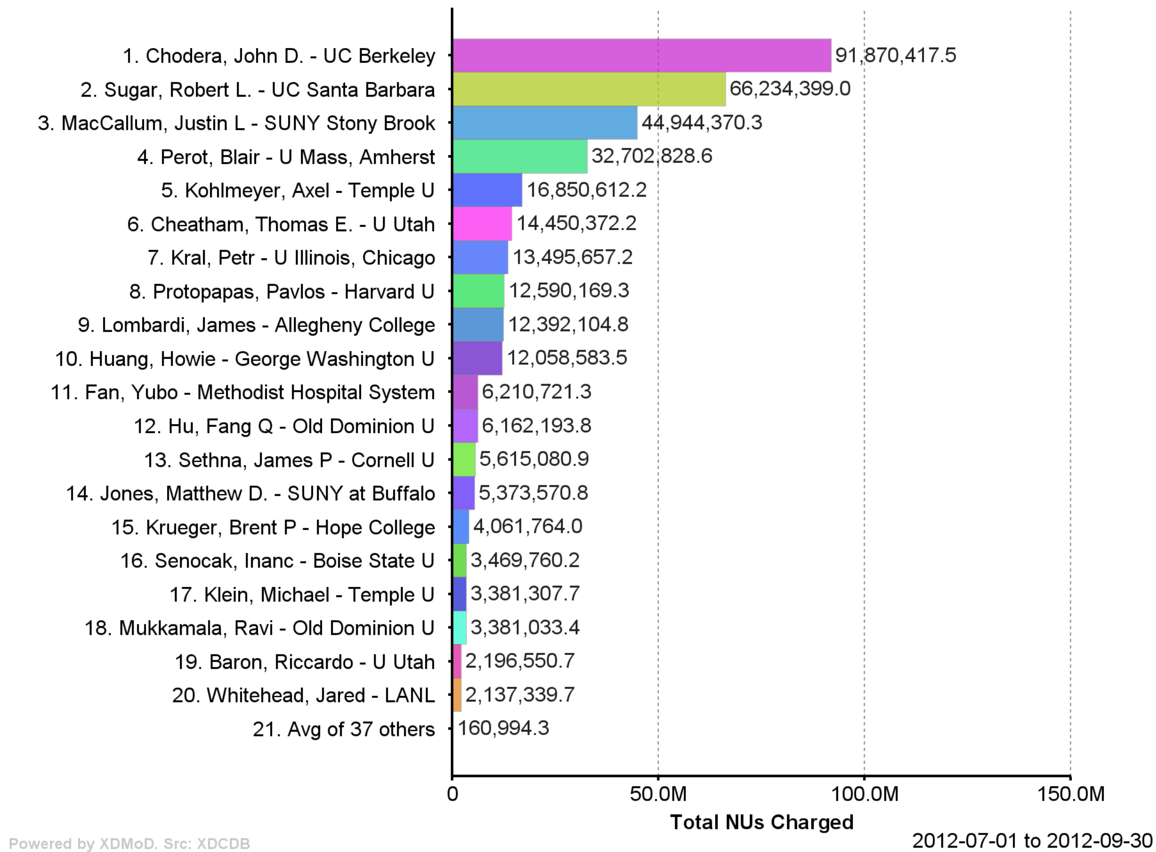
2012-07-01 to 2012-09-30



Total NUs Charged by PI

Resource = NCSA-FORGE

2012-07-01 to 2012-09-30



16 NICS - Service Provider Quarterly Report

16.1 Executive Summary

In 2009, the National Institute for Computational Sciences (NICS) delivered the first academic petaflop computer to the NSF community—a Cray XT5 called Kraken. By the end of 2010, systems at NICS were delivering more than 70% of all NSF compute cycles. This quarter, Kraken sustained a utilization of 96% and a 99% uptime while providing roughly 57% of the total CPU hours delivered by XSEDE resources (Figure 36).

The addition of the SGI Altix, called Nautilus, and the Remote Data and Visualization (RDAV) center serves to broaden the services provided by NICS to the NSF community and increases the potential for breakthrough science (Section 16.2). RDAV's purpose is to aid in the significant challenge of transforming large-scale data into knowledge and insight by providing scientists with well-engineered and well-supported remote visualization, analysis, and scientific workflow technologies. Nautilus provided a 98% uptime for the quarter and 36% utilization.

Support staff at NICS resolved 659 XSEDE tickets (Table 15) during the quarter with a median time to resolution of 16.3 hours.

16.1.1 *Resource Description*

NICS currently has two NSF funded computational resources: Kraken and Nautilus. These systems share a Network File System (NFS) that contains user directories, project directories and software directories. One-time password tokens provide secure access to both the computational and storage resources at NICS.

16.1.1.1 Kraken

Kraken is a Cray XT5 consisting of 9,408 compute nodes, each containing two 6-core AMD Istanbul Opteron processors and 16 GB of on-node memory. The result is 112,896 compute cores that deliver 1.17 PF at peak performance with 147 TB total memory. Communications take place over the Cray SeaStar2+ interconnect. A parallel Lustre file system provides 3.3 PB (raw) of short-term data storage.

16.1.1.2 Nautilus

Nautilus, an SGI Altix UV 1000 system, is the centerpiece of NICS Remote Data and Visualization (RDAV) Center that is also located at ORNL. It has 1024 cores (Intel Nehalem EX processors), 4 TB of global shared memory, and 8 GPUs in a single system image yielding 8.2 TF at peak performance. A parallel Lustre file system provides 427 TB (raw) of short-term data storage.

16.1.1.3 HPSS Archival Storage

The High Performance Storage System (HPSS), developed and operated by ORNL, is capable of archiving hundreds of petabytes of data and can be accessed by all major leadership computing platforms. Incoming data is written to disk and later migrated to tape for long term archiving. This hierarchical infrastructure provides high-performance data transfers while leveraging cost effective tape technologies. Robotic tape libraries provide tape storage. The center has four SL8500 tape libraries holding up to 10,000 cartridges each. The libraries house a total of 24 T10K-A tape drives (500 GB cartridges, uncompressed), 60 T-10K-B tape drives (1 terabyte cartridges, uncompressed), and 20 T10K-C tape drives (5 terabyte cartridges, uncompressed). Each T10K-A and T10K-B drive has a bandwidth of 120 MB/s. Each T10K-C tape drive has a bandwidth of 240 MB/s. Disk storage is provided by DDN storage arrays with nearly a petabyte of capacity and over 12 GB/s of bandwidth. This infrastructure has allowed the archival system to scale to meet increasingly demanding capacity and bandwidth requirements with more than 11 PB of NICS data stored as of October 2012.

16.2 Science Highlights

16.2.1.1 Planetary Science: Search for new life (Travis Metcalfe, Space Science Institute)

See main body of XSEDE quarterly report, 2.6.

16.2.1.2 Material Science: A Compound Problem (Stefano Curtarolo, Duke University)

Few things drive innovation more so than materials. From superconductors to more fuel-efficient cars to better batteries, materials are very often the bottleneck that makes or breaks progress.

In order for countless fields of technology to progress, new materials have to be developed and manufactured economically. It’s a difficult endeavor, one that encompasses the entire scientific cycle from theory to experiment. Luckily, materials researchers have a valuable ally in today’s most powerful computers.

Take Kraken for example. Capable of a peak performance of more than one petaflop (or a thousand trillion calculations per second) and managed by the University of Tennessee’s National Institute for Computational Sciences (NICS), Kraken is one of the integrated digital resources of the eXtreme Science and Engineering Discovery Environment (XSEDE), successor to the National Science Foundation’s TeraGrid project.

The Cray XT5, named after a mythical sea monster, is used by researchers whose interests span the scientific spectrum, from astrophysics to climate and weather prediction to, well, the modeling of chemical compounds for the development of novel materials, the same materials that promise to revolutionize technology.

Dr. Stefano Curtarolo of Duke University is a great example. He is part of a team harnessing the power of Kraken to model more than 400,000 chemical compounds, or combinations of elements that via chemical reactions can be separated back into their respective elements, in hopes of discovering new material systems or unknown properties that exist in currently used materials that have gone unnoticed.

“People know certain materials are great at certain things, but they might also be good at something else,” said Curtarolo.

The data for the compounds is derived from experiment and observation. However, only simulation can process and classify such a large number of compounds for a reasonable amount of money in a reasonable amount of time. Even if the compounds themselves are relatively cheap, said Curtarolo, experiments will likely still be expensive. And if the compounds are expensive, as they are likely to be, experiments will be even more expensive yet. With Kraken, the compounds are free, and better yet, the outcomes are fast.

However, all of the compounds are unique. “Some of the natural compounds are very, very big and are made up of many, many atoms,” said Curtarolo. “The more complex the compound, the more difficult the calculation.”

Getting Descriptive

Ultimately, Curtarolo’s team models a compound on Kraken to attain its wave function, or a mathematical probability of how a compound’s particles are behaving at different moments in time. “The wave function contains everything,” he said.

From there the wave function data is transferred to the team’s database at aflowlib.org, a consortium managed by Curtarolo and five other lead researchers, which contains descriptors—empirical quantities connecting the calculated microscopic parameters with the macroscopic properties—that look for novel properties in the modeled compounds.

“A database without descriptors is just a sterile set of calculations without any soul. The descriptor is what tells you good what’s good or bad. That’s what tells you about a particular material or phenomenon,” said Curtarolo.

Through the database, researchers can discover two things: novel materials or previously unknown phenomena exhibited by known materials. For example, it was well known for years that a more complex crystalline structure was necessary for superior thermoelectrics, or materials that convert changes in temperature to electricity. Thanks to Curtarolo’s group, researchers now know why and can quantify the effectiveness of a thermoelectric material based on its crystalline structure.

The team has also proposed some phenomena that should exist and actually found them. For instance, it was Curtarolo’s group that proposed the idea of lithium boron as a superconductor.

The team also solved the problem of nonproportiality for scintillators, or materials that can detect radioactivity. Some of these materials are better than others and Curtarolo’s team discovered the mechanism, research that was verified experimentally.

The list goes on and on, such as a group of cesium compounds that turned out to be topological insulators, or materials that behave as insulators on the interior while still allowing the movement of metallic charges at the surface. But Curtarolo admits that up until now the team has been better at describing phenomena than finding novel materials. “But it’s just a matter of time” until they catch up.”

All of these discoveries are the result of mega-database scanning. The team is currently creating the infrastructure for the database to be distributed, where anyone can download it and explore the entries. “In approximately one year it will be completely distributed . . . we share what we have,” he said.

The project is currently on its third year on Kraken. The runs are relatively small, from 64 to 128 cores, but that’s an asset when it comes to the database. “It’s better to have small jobs running longer than big jobs running shorter to maximize our throughput,” said Curtarolo.

The potential for the team’s research is difficult to quantify, but one thing is for sure: as more compounds are modeled the potential for transformational materials discoveries will be greatly accelerated, bringing tomorrow’s technology within reach.

16.2.1.3 Astrophysics: No Glasses Necessary (Adam Burrows, Princeton University)

3-D is all the rage these days. It makes everything seem more realistic, from Hollywood blockbusters to the Super Bowl. It is quickly emerging as an entertainment revolution.

Much like modern moviegoers, computational scientists also crave three-dimensions, not so much for the visual experience but for the accuracy it brings to simulations of various scientific phenomena.

Historically, even the world’s most powerful computers have lacked adequate muscle to accurately simulate numerous natural processes, relegating researchers to the realm of one or two dimensions, where phenomena could be investigated but in many cases at too elementary a level. Today, however, as supercomputers have entered the petascale (or reached peak speeds eclipsing a thousand trillion calculations per second), the third dimension is alive and well, much like the televisions in today’s department stores.

And few people are happier than Adam Burrows, an astrophysicist at Princeton University. Burrows and his team have been using supercomputers such as Kraken, a Cray XT5 capable of 1.17 petaflops (or more than a thousand trillion calculations per second) funded by National Science Foundation and managed by the University of Tennessee’s National Institute for Computational Sciences (NICS), to study the explosions of core-collapse supernovas (CCSNs).
Recent simulations by Burrows’ team suggest that perhaps neutrinos, those minute, neutral subatomic particles that seem omnipresent throughout the universe, may play a bigger role than previously thought in these extremely important and mysterious natural cataclysms.

Besides littering the interstellar medium with chemical elements necessary for life, CCSNs are also responsible for producing black holes, neutron stars, pulsars, and possibly gamma-ray bursts. The energy generated by these explosions is a major force behind star formation and galactic evolution. When they explode, CCSNs can be brighter than whole galaxies and their incredible luminosity is being investigated for use as standard candles against which to measure the size and shape of the universe. Understanding these events is “one of the most fundamental unsolved problems in astrophysics,” said Burrows.

With computers like Kraken, however, Burrows and others are getting closer to this understanding, simulating the entire evolution of these giant stellar explosions. While astrophysicists have been simulating these events for some time, it is only with the addition of the third dimension that they are becoming confident that that the truth is truly within reach.

While Burrows and his team would like to simulate the entire series of events in 3D, these calculations are extremely demanding and computationally expensive. Therefore, the team chooses to perform a variety of calculations with varying complexity for different phenomena, from the entire evolution of the explosion to individual phenomena such as the rotation or hydrodynamics of the star.

As the simulations ramp up, from 1D to 2D to 3D, more approximations have to be made to accommodate the limited horsepower that is inevitable even in machines such as Kraken. These approximations can negatively affect a simulation’s results as they compare with observation. In Burrows’ case, however, they are beginning to coincide with observation, precisely the reason the results are so exciting.

Explosions are a good thing

CCSNs begin as stellar masses eight times the size of our sun, or larger. For context, imagine a radius the length of Jupiter’s orbit, and a dense core roughly the size of the Earth.

Like all stars, however, their fusion-driven cores can only burn for so long. Eventually, they will become neutron stars or black holes, but not before spewing every element with a weight up to iron across the interstellar medium, providing the cold, dark universe with the raw materials for life itself.

As the progenitor stars of CCSNs evolve and the lighter elements fuse into heavier elements, the core becomes denser until it becomes iron and eventually hits the Chandrasekhar mass, or the point at which the repulsion of electrons can’t support the core’s mass. Then come the fireworks.

As the star explodes it sends a shockwave outward that eventually stalls due to the debilitating effects of the imploding matter through which it first passes. As the expanding shockwave driving the supernova explosion comes to a halt, matter outside the shockwave boundary enters the interior while there is massive neutrino loss from the core.

In nature, somehow the shock wave rebounds, and that’s where the surety of the simulations runs out. “With the best physics done in spherical symmetry in 1D, we don’t get generic explosions,” said Burrows. “The shock is just stuck there and accretes the outward material of the object and turns into a black hole." In other words, the star never explodes. It seems, said Burrows, that there is insufficient energy for an explosion, and that's where the neutrinos come in: it is thought that they might provide the missing energy that produces one of nature's most important cataclysms. On the upside, the 1D simulations reveal plenty of nonlinear, unstable turbulence and produced the idea that turbulence is indeed important to the final event.

When the same simulations are performed in 2D, however, explosions do occur, though not all the time, and still not with sufficient energy. Furthermore, added Burrows, it seems that the explosions nearly always were the result of a neutrino mechanism and turbulence within the neutrino context, lending credence to the neutrino-driven hypothesis.

But it's the third dimension that really makes things interesting. Most importantly, the simulations in 3D produce more explosions than both 1D and 2D, a sign that the simulations are moving towards reality. But that's not all: Burrows' team also sees pulsar kicks, a phenomenon indicative of an asymmetrical object, a property shared by CCSNs.

Ultimately, said Burrows, the latest 3D simulations reveal that the turbulence behind the shockwave acts differently in 3D than in 2D, a validation of their simulation approach, and that the revival of the shock is likely neutrino-driven.

"Finally, we have credible 3D simulations," said Burrows. "They are progressively more explosive as you add dimensions, which is good . . . we would like to be able to reproduce nature in 3D, but it's very computationally expensive, and therefore Kraken is very necessary."

Not to be confused with Fidel

Burrows' weapons of choice in his quest to unravel one of nature's greatest events is known as Compressible Astro (CASTRO), a state-of-the-art radiation/hydrodynamics code developed at Lawrence Berkeley National Laboratory with John Bell.

While Burrows' current runs on Kraken use only a few thousand cores, when the radiation and hydrodynamics are incorporated into the 3D simulations, CASTRO will easily begin to occupy cores in the tens of thousands. Eventually, said Burrows, it's realistic to believe that the team could require 150,000 or more cores as they continue to scale up the simulations, which would consume most or all of the world's most powerful computers.

Burrows' team has been using the code for approximately three years now, and it has been the platform for the team's most important discoveries. For instance, it has helped to downplay the role of magnetohydrodynamics, or the dynamics of magnetized fluids, and the rapid rotation of CCSNs in their eventual explosions, culminating in the latest idea of a neutrino-driven mechanism. "The neutrino mechanisms make sense," said Burrows, "but we need to be able to quantify it."

This year, the team was awarded 15 million hours on Kraken to continue exploring the mechanisms behind one of nature's most important events. But, said Burrows, even computers such as Kraken aren't yet powerful enough to paint the entire picture. "In the next few years, time will tell," he said. "As long as we get the resources, we'll be able to explain how these things explode."

Until then, however, the team will continue their work three dimensions, which, it turns out, isn't such a bad place to be, whether you're at the movies or Princeton.

16.3

16.4 User-facing Activities

16.4.1 System Activities

16.4.1.1 Kraken

Availability
Kraken had an overall system availability of 99% for this quarter with 15 total hours of downtime. Downtime for the quarter consisted of 7 hours of scheduled downtime and 8 hours of unscheduled downtime (Table 1).

Table 13: Summary of maintenance Stats for Kraken in Q1PY2.

Maintenance Stats – Kraken Cray XT5	
Number of planned reboots	2
Number of unplanned reboots	3
Total reboots	5
Number of job failures due to system faults	1083
Total time in period	2208 hours (100%)
Scheduled Downtime	7 hours (0%)
Unscheduled Downtime	8 hours (0%)
Total Downtime	15 hours (1%)
Total time available to users (total-downtime)	2193 hours (99%)
% System Utilization	96

16.4.1.2 Nautilus

Availability
Nautilus had an overall system availability of 98% for this quarter. Downtime for the quarter consisted of 11.5 hours of scheduled downtime and 23.13 hours of unscheduled downtime (Table 2).

Table 14: Summary of maintenance Stats for Nautilus in Q1PY2.

Maintenance Stats -- Nautilus SGI UV1000	
Number of planned reboots	3
Number of unplanned reboots	5
Total reboots	8
Total time in period	2208 hrs (100%)
Scheduled Downtime	11.5 hours (0%)
Unscheduled Downtime	23.13 hours (1%)
Total Downtime	34.63 hours (2%)
Total time available to users (total-downtime)	2173 hours (98%)

16.4.2 Services Activities

16.4.2.1 Kraken

Software Packages
NICS currently supports 374 unique application builds on Kraken that include pre-compiled binaries and builds with PGI, GNU, Cray, and Intel compilers. These builds include 191 unique versions and 126 unique applications and libraries.

Environment
During this quarter one software bug and one configuration issue were resolved that should improve user experiences. Since the upgrade to Cray Linux Environment (CLE 3.1) earlier this year, there have been occasional reports of jobs that hang without producing any output. After extensive debugging and working with Cray, this was discovered to be a bug in their Portals software. A patch has been installed on Kraken and no job failures of this variety have been reported since. The grid nodes on Kraken had also been experiencing a number of Out Of Memory (OOM) errors. Reducing the verbosity of logging by the GRAM software resolved this issue.

16.4.2.2 Nautilus

Software Packages
NICS' staff currently supports 387 unique application builds on Nautilus that include pre-compiled binaries and builds with PGI, GNU, and Intel compilers. These builds include 213 unique versions and 115 unique applications and libraries.

Environment
An update to version 3.0.3 of the TORQUE resource management software was deployed on Nautilus in December 2011 in the hopes that it would improve GPU scheduling. Unfortunately, this did not improve GPU scheduling, and NICS reverted to a known-working release early in 2012. Efforts to improve GPU scheduling on Nautilus are ongoing, and NICS and Adaptive Computing are working together to understand the unique requirements of GPU scheduling on the SGI UV platform. Progress has continued in this area, and NICS is currently evaluating new builds of TORQUE and Moab that will hopefully resolve these issues.

16.5 Security

No security incidents or enhancements occurred at NICS during the quarter.

16.6 Education, Outreach, and Training Activities

Title	Location	Date(s)	Hours	Number of Participants	Method
Petascale I/O: Challenges, Solutions, and Recommendations Crosby, L. D.; Mohr, R.	Extreme Scaling Workshop, Des Plaines, IL.	July 15, 2012	1.0		In-Person
Metrics and Measurement for Understanding usage of a Visualization and Analysis HPC System Szczepanski, Amy	Texas Advanced Computing Center, Austin TX	September 27, 2012	1.0	7	In-person
Extending Parallel Scalability of LAMMPS and Multiscale Reactive Molecular Simulations Peng, Y.; Knight, C.; Blood, P.; Crosby, L.; Voth G. A.	ECSS Symposium	September 18, 2012	1.5		Remote
JICS resources and centers	University of Tennessee Knoxville TN	September 12, 2012	1.5	8	In-person
Welcome to UT – Resources and Centers Yost, Christal	University of Tennessee Knoxville TN	August 21, 2012	2.0	20	In-person
Achieve Better Performance with PEAK on XSEDE Resources You, Haihang	XSEDE12, Chicago IL	July 18, 2012	0.5	30	In-person
TIPS: Toward Improved Performance Solutions on XSEDE Resources You, Haihang	XSEDE12, Chicago IL	July 16, 2012	8.0	5	In-person

16.7 SP Collaborations

EPSCOR

The Experimental Program to Stimulate Competitive Research, or EPSCoR, establishes partnerships with government, higher education and industry that are designed to effect lasting improvements in a state's or region's research infrastructure, R&D capacity and hence, its national R&D competitiveness. NICS participates along with researchers from twenty-seven other states and the Commonwealth of Puerto Rico. The partnership is based on existing and planned collaborations in the advanced materials and systems biology domains where computational science is driving new approaches and insights. The collaborative team has proposed to build cyberinfrastructure (CI) linked, community specific knowledge environments that embody the desktop to XSEDE ecosystem by using campus-based CI at a regional research institution as an essential bridge for connecting faculty investigators to national resources such as the XSEDE.

Keeneland

The Keeneland Project is a five-year, $12 million NSF Track 2D award that has enabled the Georgia Institute of Technology, NICS, and the Oak Ridge National Laboratory to deploy a small, experimental, high-performance computing system consisting of an HP system with NVIDIA Tesla accelerators attached. The project team has been using this initial system to develop scientific libraries and programming tools to facilitate the development of science and engineering research applications, while also providing consulting support to researchers who wish to develop applications for the system. NICS' staff provides administration and support for the Keeneland project.

In 2012, the project will upgrade the heterogeneous system to a larger and more powerful system based on a next-generation platform and NVIDIA accelerators. It is anticipated that the final system will have a peak performance of roughly 2 petaflops. The project will then operate the upgraded system as a XSEDE resource for two years.

NCSA Blue Waters Project

The National Institute for Computational Sciences (NICS) staff has begun collaboration with the National Center for Supercomputing Applications (NCSA) Blue Waters project to facilitate and assist with the configuration and deployment of the Cray XE/XK system. This effort is focused on application support and system management. The NICS team has contributed to the project by the sharing of experience and information via discussions and presentations. Additionally, NICS has assisted with system monitoring, resource management, and application porting and testing.

NICS staff visited NCSA on in January to begin the collaboration by sharing experiences, lessons-learned, and offering suggestions. These presentations were drawn from NICS experience of operating and supporting Kraken, a Cray XT system. Topics discussed included administrative and support topics such as system management, storage management, acceptance testing, library/application tracking, and third-party software management.

NICS staff has assisted with the management of the NCSA resource by assisting with system monitoring and providing configuration advice and materials for scheduling and resource management. Additionally, two scientific applications were ported and tested on the Blue Waters system. A majority of the resource was utilized in performance tests utilizing more than 98,000 processes.

NICS noted an influx of unexpected data over the XSEDE network in late May which sustained multi-gigabits per second with peaks that saturated a 10 gigabit connection. An analysis of the data showed that Kraken's file system was being used by users of the NCSA Blue Waters system to store large amounts of data. Due to upgrade plans, Blue Waters users were required to migrate data to other resources for storage. To aid users with both NICS and NCSA accounts and to keep from filling Kraken's scratch file system, an auxiliary, temporary 800 TB Lustre file system was quickly implemented at NICS.

Users, prior to the implementation of the auxiliary file system, initially moved data to Kraken's scratch file system. At the conclusion of the initial data transfer period, mid-June, over 269 TB of data was present on this auxiliary file system. Five users each stored more than 1 TB of data. However, data transferred from Blue Waters is currently being migrated from Kraken's scratch file system to this file system. At the time this report was prepared over 488 TB of data was present on this auxiliary file system.

16.8 SP-Specific Activities

AACE

In 2011 the Joint Institute for Computational Sciences (JICS) established the Application Acceleration Center of Excellence (AACE) in partnership with NICS, industry leading vendors, and academic institutions. The center's objectives are:

- Accelerate NSF projects toward exascale with state-of-the-art heterogeneous architectures
- Spur development of new algorithms and codes optimized for accelerator-based architectures
- Disseminate fundamental knowledge
- Facilitate effective exchange of expertise and cross-disciplinary collaboration

NICS is assisting NSF users with their transition to the Intel MIC architecture by researching parallelization techniques on the Intel MIC platform and by porting key NSF applications (already millions of lines of code) to the Intel MIC architecture in advance of its commercial release. NICS will also offer training on the Intel MIC architecture following its commercial debut.

"NICS has provided insight to Intel regarding the technology requirements of the scientific computing community," added Joe Curley, director of marketing for Intel's Technical Computing Group. "The impact of our partnership can be seen in the focus of our Intel MIC 'Knights Ferry' software development platform on extending well understood, high-level, standard programming languages and models."

NICS continues to engage a variety of technology providers to determine the role their technologies will play in the quest for exascale, while at the same time providing valued input for product development to meet the needs of the NSF research community.

Industrial Partnerships

NICS currently provides expertise and computational resources to three industrial partners. The goal of the partnerships is to speed innovations to market through application of leading edge simulation capabilities. The benefit to the industrial partners is a condensed design cycle and reduced prototyping and manufacturing costs.

16.9 Publications

16.9.1 User Publications

Submitted

1. Dodd M. & Ferrante A. "Direct numerical simulation of particle dispersion in a spatially developing turbulent boundary layer". International Conference on Multiphase Flow: Jeju, Korea, May 26- 31, 2013 (Submitted in August 2012).
2. Dodd M. & Ferrante A. "A coupled pressure- correction/volume of fluid method for DNS of droplet- laden isotropic turbulence". International Conference on Multiphase Flow: Jeju, Korea, May 26- 31, 2013 (Submitted in August 2012).
3. Bodo, G., Cattaneo, F., Mignone, A., Rossi, P., 2012, "Magnetorotational turbulence in stratified shearing boxes with perfect gas equation of state and finite thermal diffusivity", Astrophysical Journal, Submitted
4. E. J. Lentz, A. Mezzacappa, O. E. B. Messer, M. Liebendörfer, W. R. Hix, and S. W. Bruenn, "On the Interplay of Neutrino Opacities in Core-collapse Supernovae", Astrophys. J., submitted 2012.
5. Charlotte Christensen, Thomas Quinn, Fabio Governato, Adrienne Stilp, Sijing Shen, James Wadsley, "Implementing Molecular Hydrogen in Hydrodynamic Simulations of Galaxy Formation", Submitted to MNRAS, arXiv:1205.5567
6. Ji-hoon Kim, Mark R. Krumholz, John H. Wise, Matthew J. Turk, Nathan J. Goldbaum, Tom Abel, "Dwarf Galaxies with Ionizing Radiation Feedback. I: Escape of Ionizing Photons", Submitted to Astrophysical Journal

Accepted

7. Ferrante A. & Dodd M. "Direct numerical simulation of particle dispersion in a spatially developing turbulent boundary layer". American Geophysical Union, Fall Meeting: San Francisco, CA, December 3-7, 2012.
8. Dodd M., Webster K. & Ferrante A. "DNS of particle dispersion in a spatially developing turbulent boundary layer". American Physical Society, Division of Fluid Dynamics: San Diego, CA, November 18-21, 2012.
9. Ferrante A. & Dodd M. "A mass-conserving volume of fluid method for DNS of droplet-laden isotropic turbulence". American Physical Society, Division of Fluid Dynamics: San Diego, CA, November 18-21, 2012.
10. Shenoy, S., H. Nanda, and M. Lösche, "Membrane Association of the PTEN Tumor Suppressor: Electrostatic Interaction with Phosphatidylserine-Containing Bilayers and Regulatory Role of the C-Terminal Tail", J Struct Biol, 2012.
11. Perez, J.C., Mason, J., Boldyrev, S., Cattaneo, F., " On the energy spectrum of strong magnetohydrodynamic turbulence", Phys. Review 2012.
12. Tobias, S.M., Cattaneo,F., "On the measurement of the turbulent diffusivity of a large-scale magnetic field", J. Fluid Dynamics, 2012.

Published

1. Grinberg, L., Deng, M., Lei, H., Insley, J.A., and Karniadakis, G.E. "Multiscale simulations of blood-flow: from a platelet to an artery". In Proceedings of XSEDE 2012: Chicago, IL, July 16-20, 2012. Article Number 33. ACM, New York, 2012.
2. Jagannathan, S. and Donzis, D. "Massively Parallel Direct Numerical Simulations of Forced Compressible Turbulence: a Hybrid MPI/OpenMP approach". In Proceedings of XSEDE 2012: Chicago, IL, July 16-20, 2012. ACM, New York, 2012.
3. Baraldi A. & Ferrante A. "DNS of fully-resolved droplet-laden isotropic turbulence: a mass-conserving volume of fluid method". In Proceedings of 23rd International Conference of Theoretical and Applied Mechanics (ICTAM: Beijing, China, August 19-24, 2012.
4. Baraldi A. & Ferrante A. "A VoF method for DNS of droplet-laden incompressible turbulence". 7th International Conference on Computational Fluid Dynamics: Big Island, Hawaii, July 9-13, 2012.
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16.9.2 Staff Publications

Submitted

1. Qing Liu, Jeremy Logan, et al., "Hello ADIOS: The Challenges and Lessons of Developing Leadership Class I/O Frameworks," Submitted to Concurrency and Computation: Practice and Experience, September 28, 2012.
2. Betro, V., Godo, M., Wyman, N. "Meshing, Visualization, and Computational Environments Technical Committee Year In Review," AIAA Aerospace America, December 2012.
3. C.Y. Cardall, R. Budiardja, E. Endeve, and A. Mezzacappa 2012, "General Astrophysical Simulation System: I. Fundamentals", Astrophys. J. Suppl., submitted.
4. C.Y. Cardall, R. Budiardja, E. Endeve, and A. Mezzacappa 2012, "General Astrophysical Simulation System: II. Nonrelativistic Hydrodynamics", Astrophys. J. Suppl., submitted.

Accepted

1. Patel, P., et al., "OpenMP-style Parallelism in Data-Centered Multicore Computing with R, at the 17th ACM SIGPLAN 2012 Symposium on Principles and Practice of Parallel Programming (PPoPP)", New Orleans, LA, February 2012.
2. Scott Simmerman, James Osborne, Jian Huang, "Eden: Simplified Management of Atypical HPC Jobs", Computing in Science and Engineering (CISE), in press.
3. Crosby, L. D.; Mohr, R. "Petascale I/O: Challenges, Solutions, and Recommendations." In Proceedings of the Extreme Scaling Workshop, 2012.
4. Betro, V., Godo, M., Wyman, N. "Meshing, Visualization, and Computational Environments Technical Committee Year In Review," AIAA Aerospace America, December 2012.
5. C. Stewart, R. Knepper, J. Ferguson, F. Bachmann, I. Foster, A. Grimshaw, V. Hazlewood, D. Lifka, What is Campus Bridging and what is XSEDE doing about it?, XSEDE12, July 2012.
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1. Jeremy Logan, Scott Klasky, et al., “Understanding I/O Performance Using I/O Skeletal Applications”, In the proceedings of Euro-Par 2012, pp 77-88.
2. Scott Simmerman, Jingyuan Wang, James Osborne, Kimberly Shook, Jian Huang, William Godsoe, Theodore Simons, "Exploring Similarities Among Many Species Distributions", XSEDE12 Conference Proceedings, July 2012.
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11. David D. Jenkins*, Robert J. Hinde, and Gregory D. Peterson, “Quantum Mechanical Simulations of Crystalline Helium Using High Performance Architectures.” Supercomputing Conference. Salt Lake City, November 2012.
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13. Kiran Kasichayanula*, Dan Terpstra, Piotr Luszczek, Stan Tomov, Shirley Moore, and Gregory D. Peterson, “Power Aware Computing on GPUs.” Symposium on Application Accelerators for High Performance Computing. Chicago, July 2012. (Best paper award.)

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15. Rick Weber*, Gregory D. Peterson, and Robert Hettich, "For Three Easy Payments: Scoring Peptides With Portable Performance Using Specmaster." Symposium on Application Accelerators for High Performance Computing. Chicago, July 2012.
16. JunKyu Lee* and Gregory D. Peterson, "The Role of Precision for Iterative Refinement." Symposium on Application Accelerators for High Performance Computing. Chicago, July 2012.
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19. E. Endeve, C.Y. Cardall, R.D. Budiardja, A. Mezzacappa, and J.M. Blondin, "Turbulence and magnetic field amplification from spiral SASI modes in core-collapse supernovae", Physica Scripta, Proceedings of the International Conference: Turbulent Mixing and Beyond 2012.
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16.10 Metrics

16.10.1 Standard systems metrics

The following subsections contain system metrics for NICS' resources that are allocated through XSEDE: Kraken and Nautilus.

Note that job wait times and job expansion factors as reported by XDMoD are skewed by user specified job dependencies. NICS has implemented an "effective queue time" metric to eliminate the influence of job dependencies on these statistics. The effective queue time is a measure of the wait time incurred only once a job is eligible to run and is not a factor of individual workflows. In the future job wait times and expansion factors will be reported based on effective queue times.

Another issue with wait time and expansion factor by job size, as currently reported, is that the job size bins overlap multiple scheduling queues at NICS, and thereby, overlap multiple scheduling policies. This too will be corrected in future reporting. Also note that the error bars associated with the mean values in Figure 12, Figure 13, Figure 22 and Figure 23 represent the standard deviation of the sampled mean which is the standard deviation divided by the square root of N, where N is the sample size.

16.10.2 Kraken

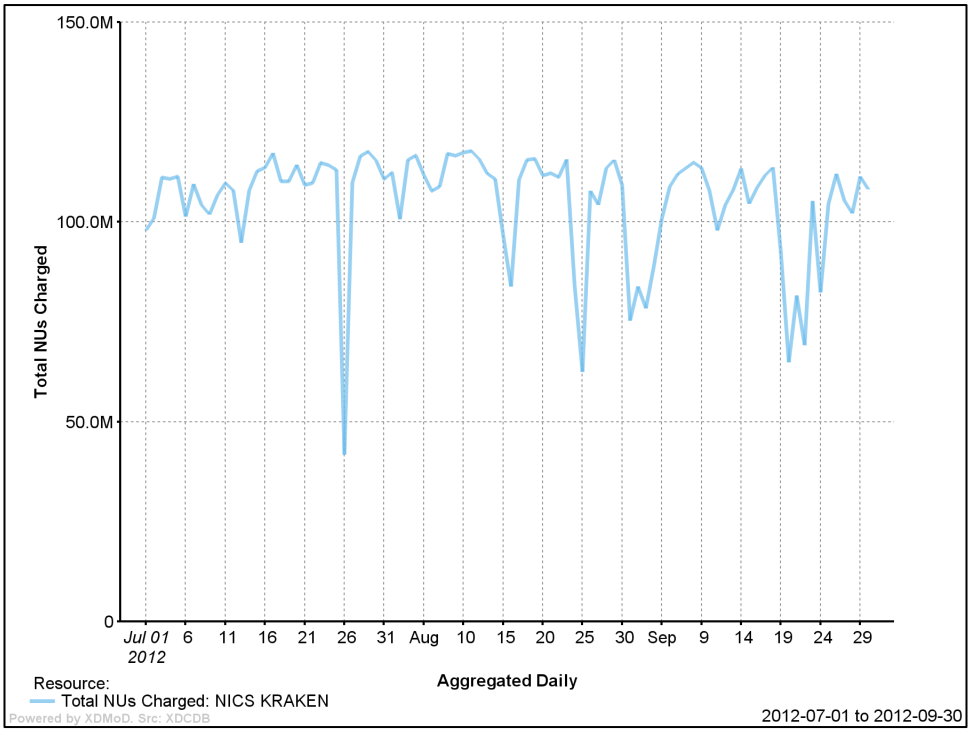

Figure 10: Daily resource consumption in Mega-normalized units ($1e^6$) charged on Kraken for Q1PY2.

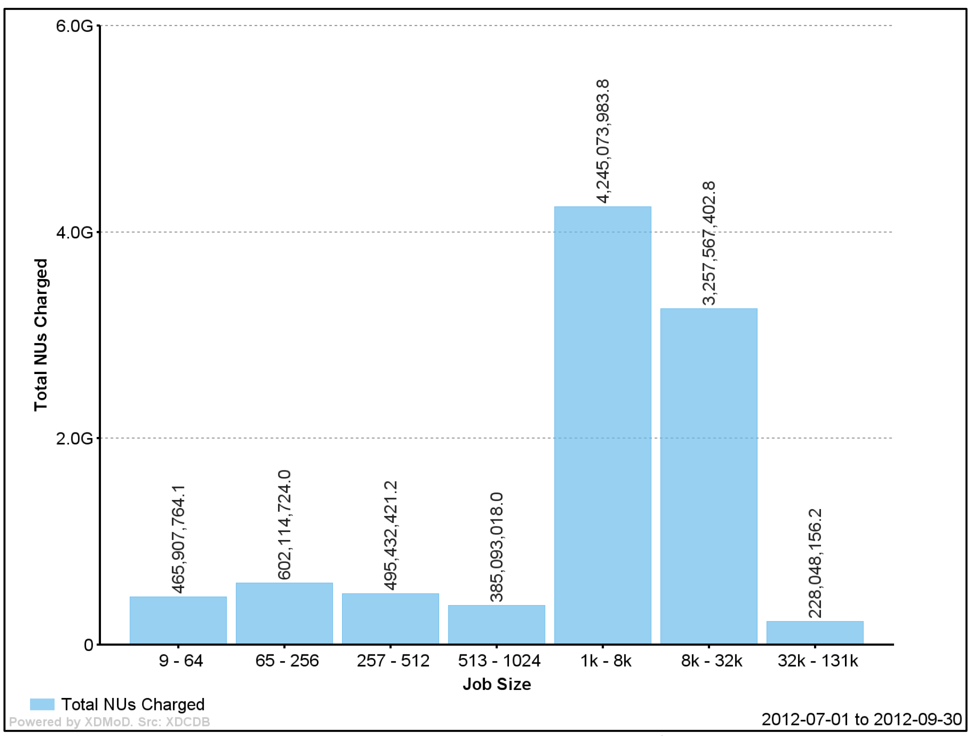

Figure 11: Total resource consumption in Giga-normalized units ($1e^9$) by job size for Kraken in Q1PY2.

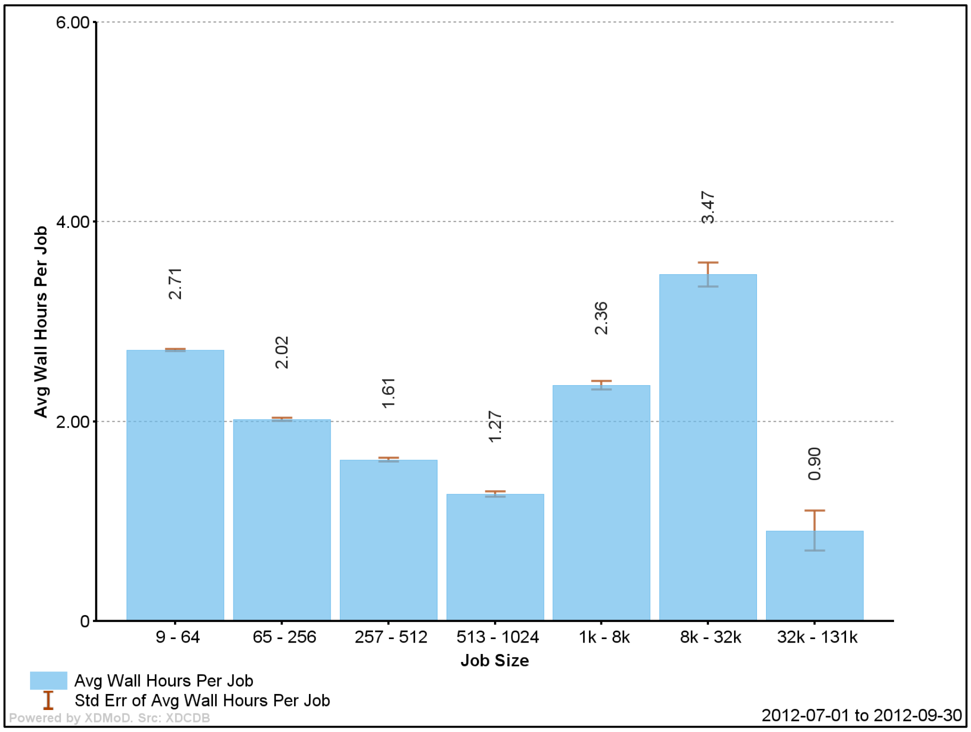

Figure 12: Average wall hours by job size on Kraken in Q1PY2.

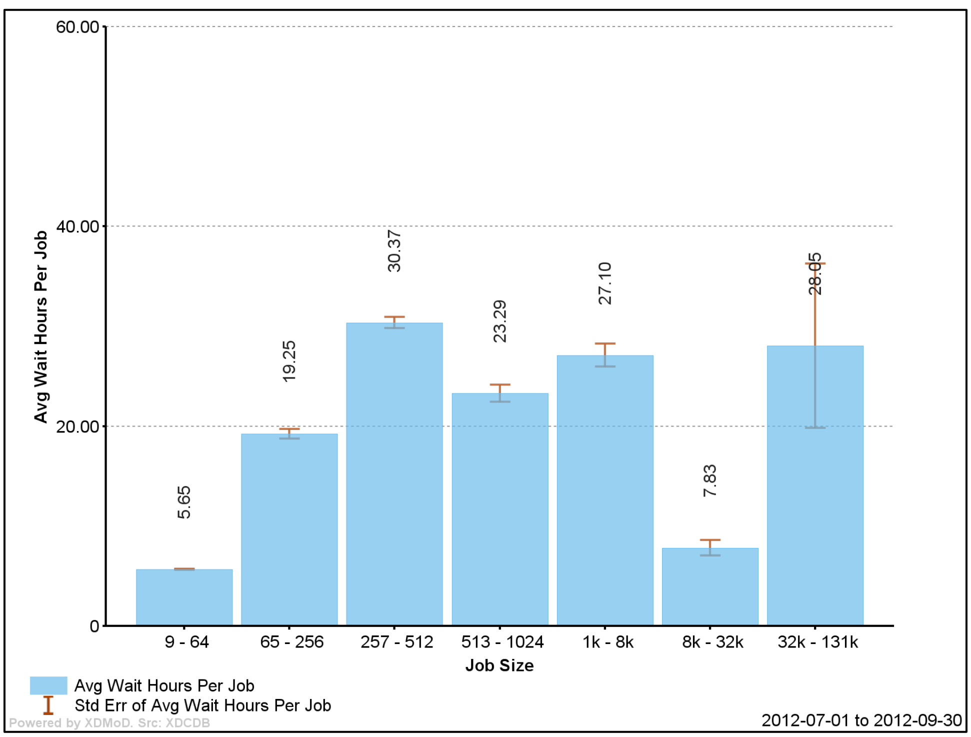

Figure 13: Average wait hours by job size on Kraken in Q1PY2.

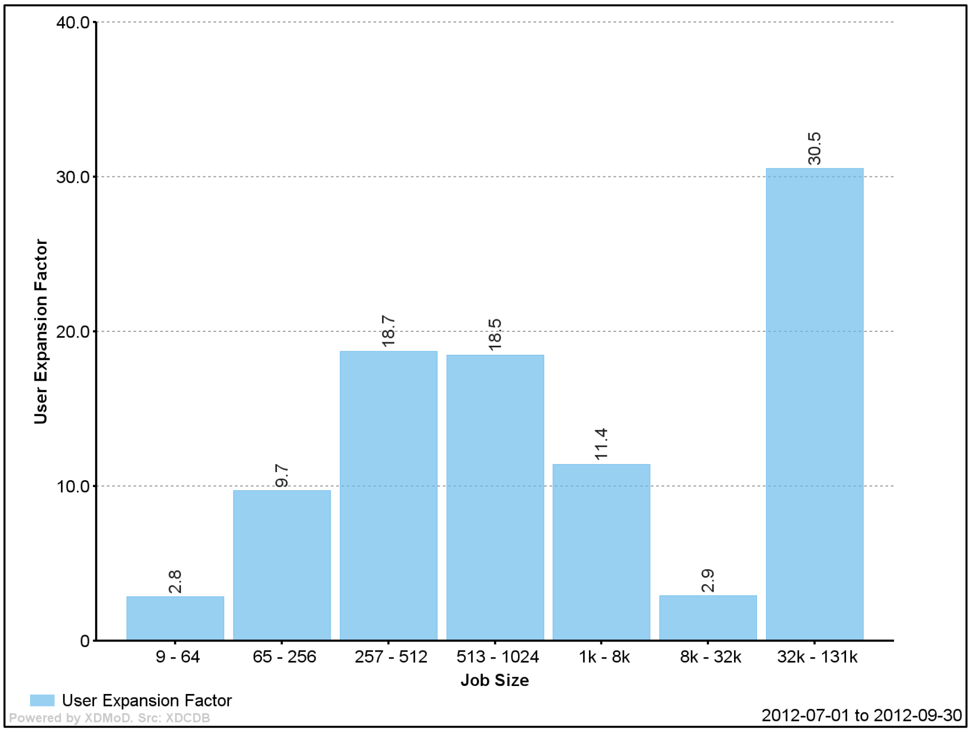

Figure 14: Expansion factor by job size for Kraken in Q1PY2.

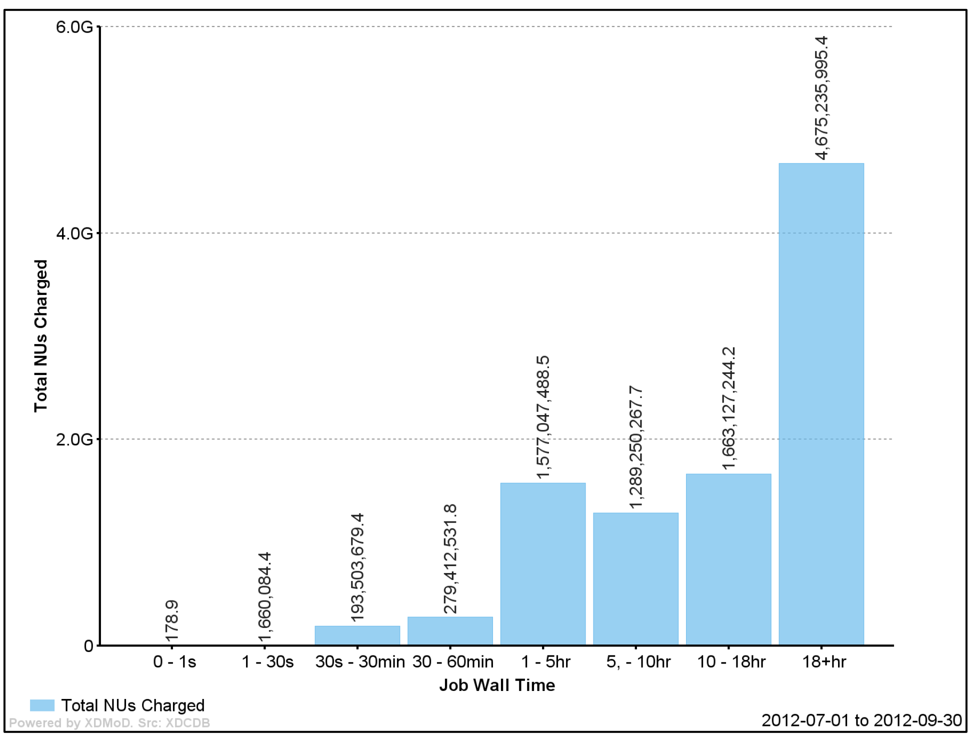

Figure 15: Total resource consumption in Giga-normalized units ($1e^9$) by wall time for Kraken in Q1PY2.

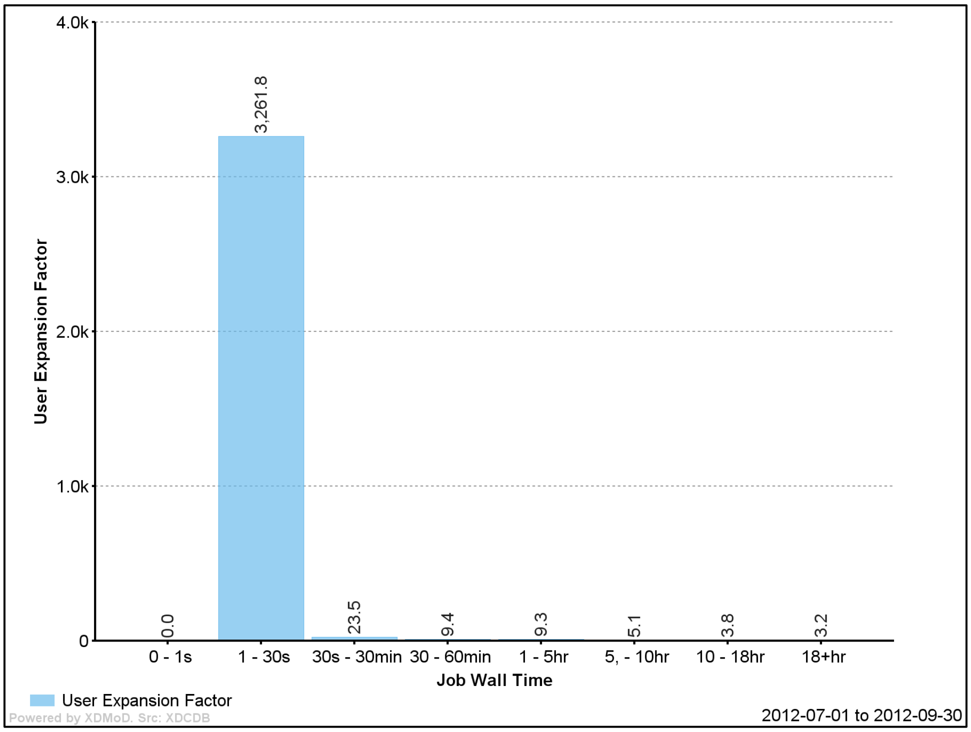

Figure 16: Expansion factor by wall time for Kraken in Q1PY2.

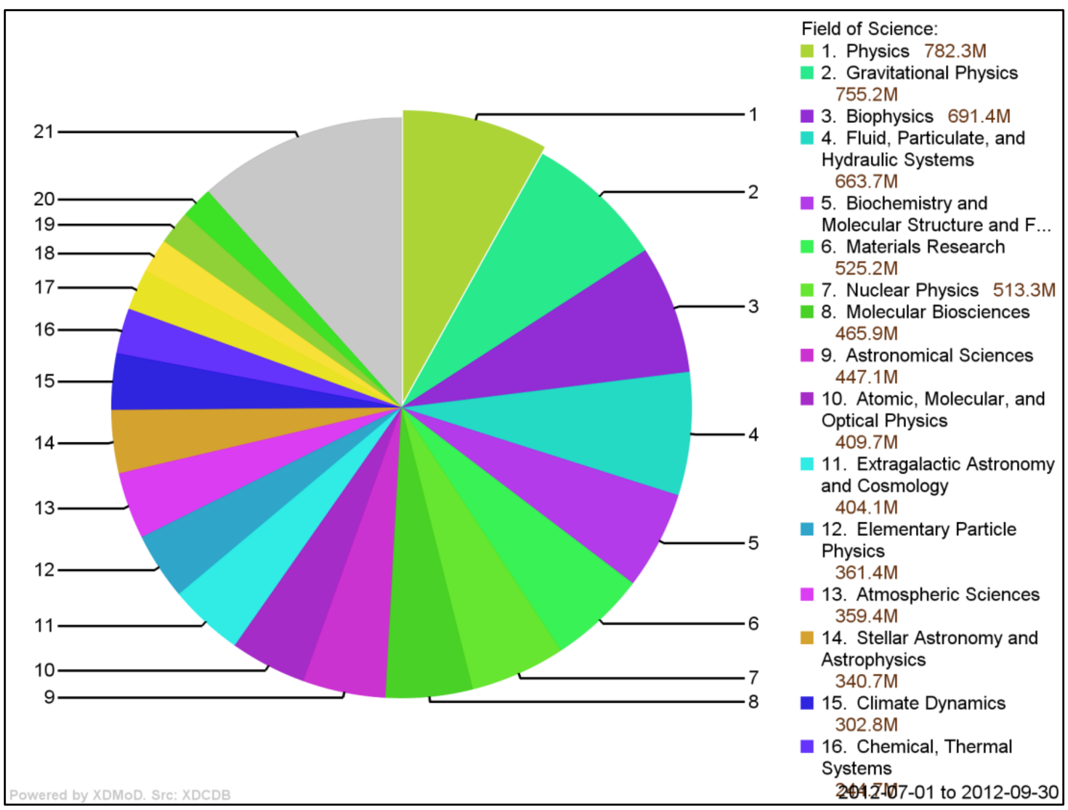

Figure 17: Resource consumption in mega-normalized units ($1e^6$) by field of science for Kraken in Q1PY

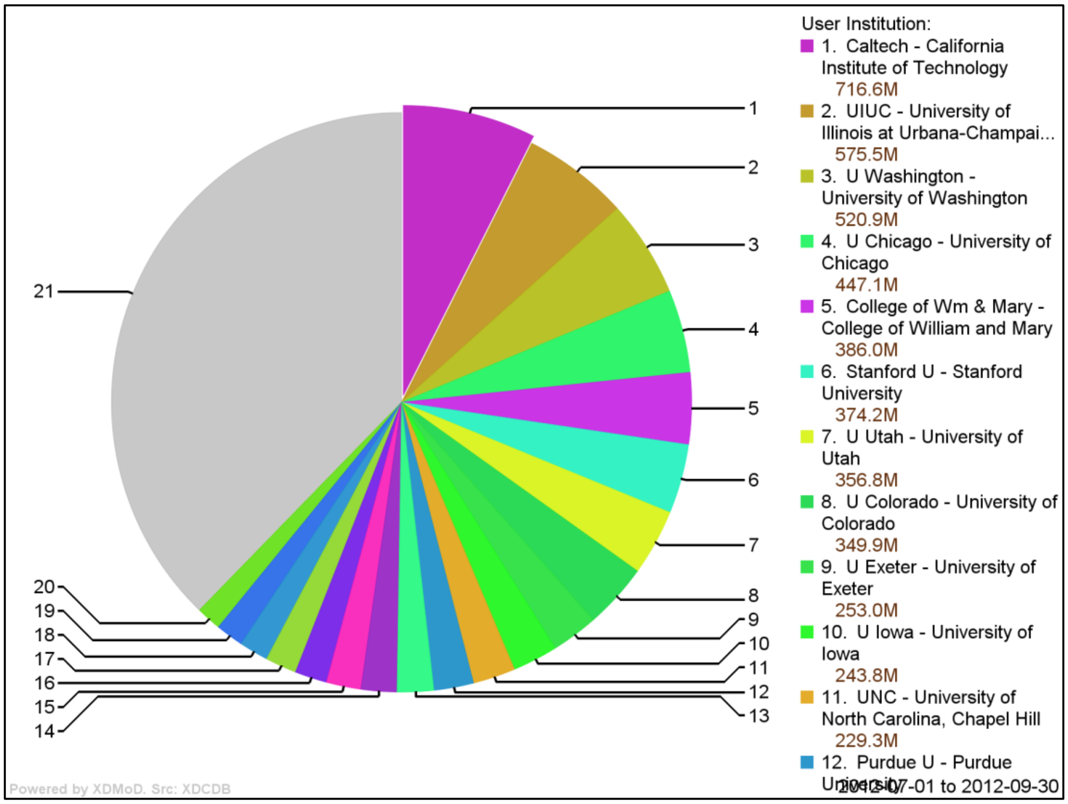

Figure 18: Resource consumption in mega-normalized units (1e^6) by institution in mega-normalized units for Kraken in Q1PY2.

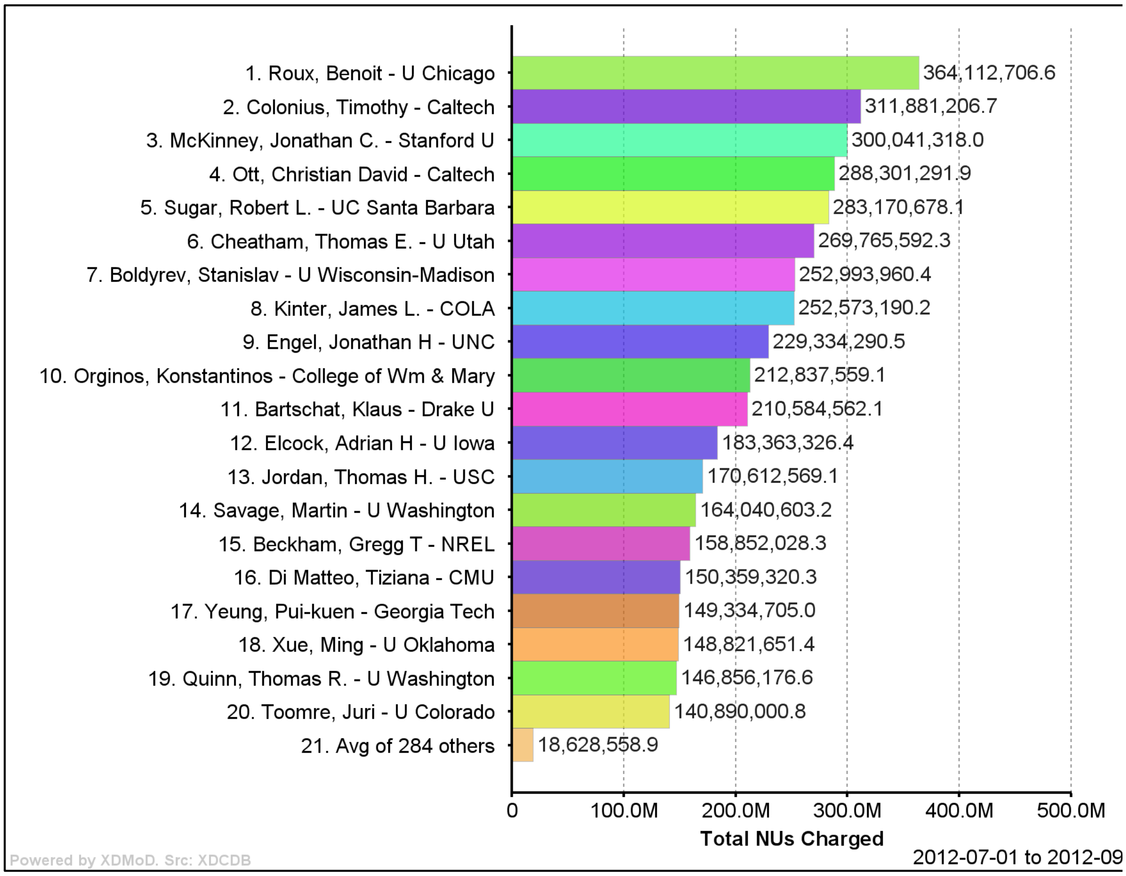

Figure 19: Resource consumption by PI in Mega-normalized units for Kraken in Q1PY2.

16.10.2.1 Nautilus

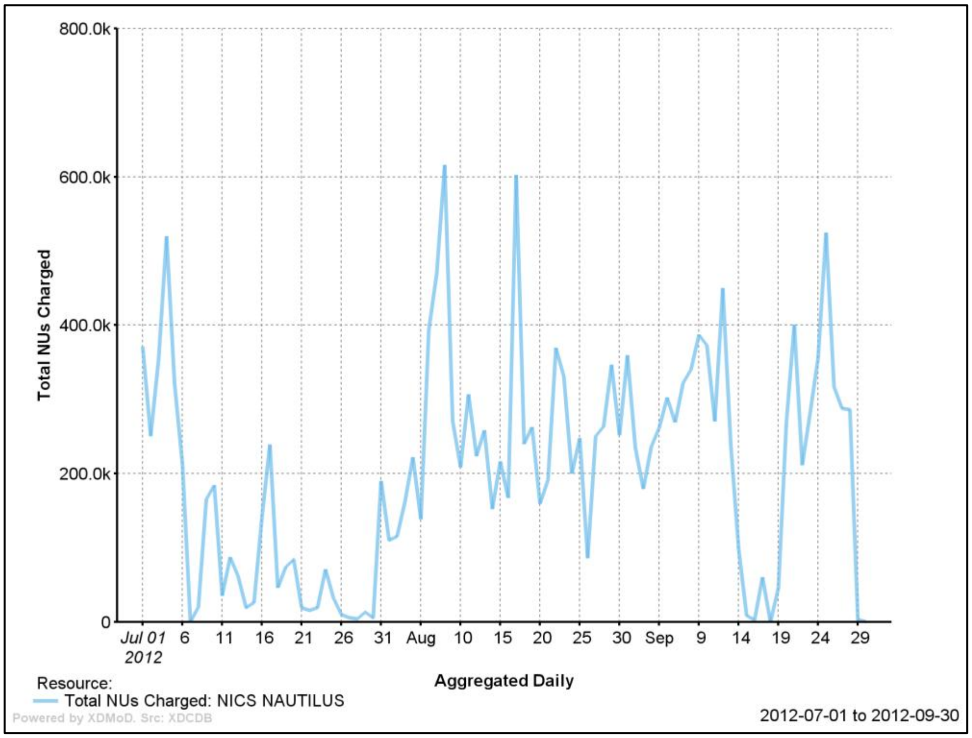

Figure 20: Daily resource consumption in kilo-normalized units ($1e^3$) charged on Nautilus in Q1PY2.

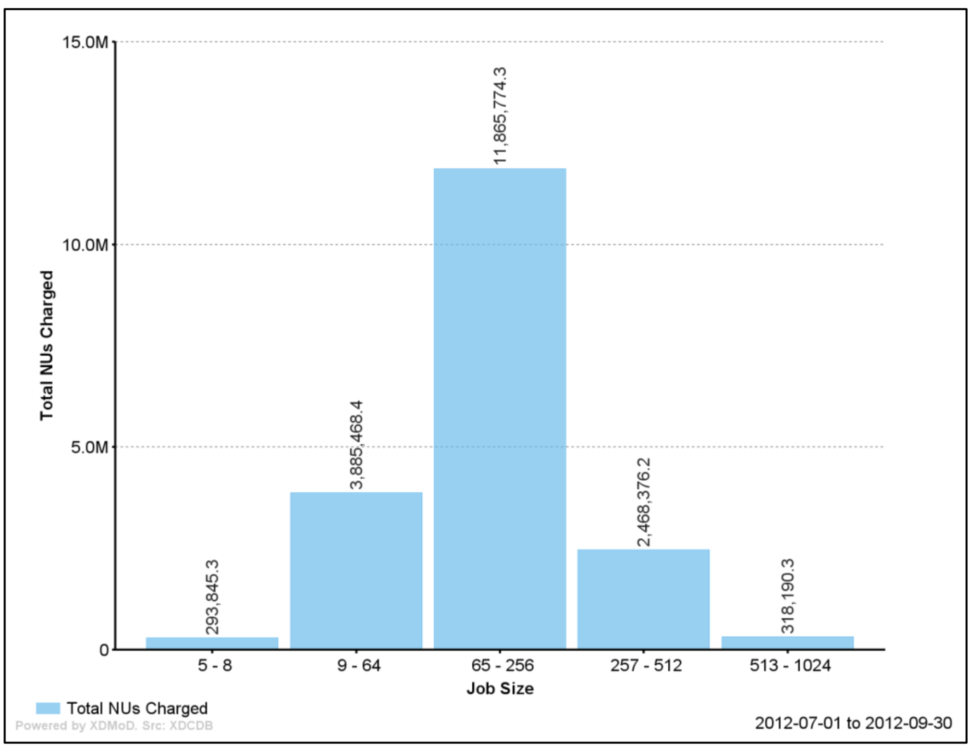

Figure 21: Total resource consumption in mega-normalized units ($1e^6$) by job size for Nautilus in Q1PY2.

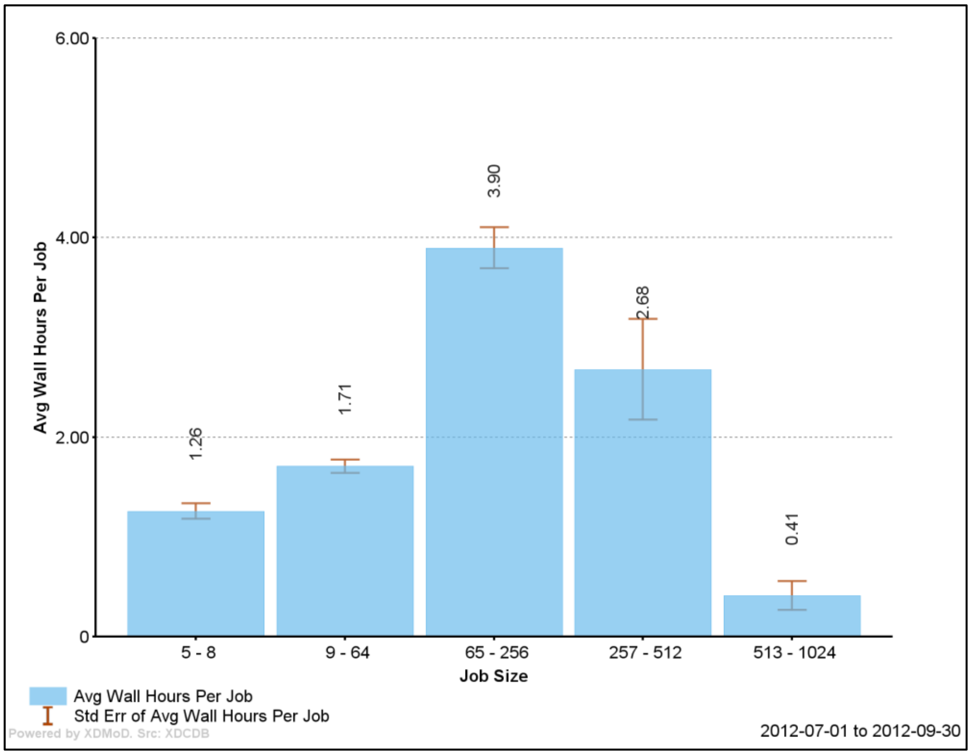

Figure 22: Average wall time in hours by job size on Nautilus in Q1PY2.

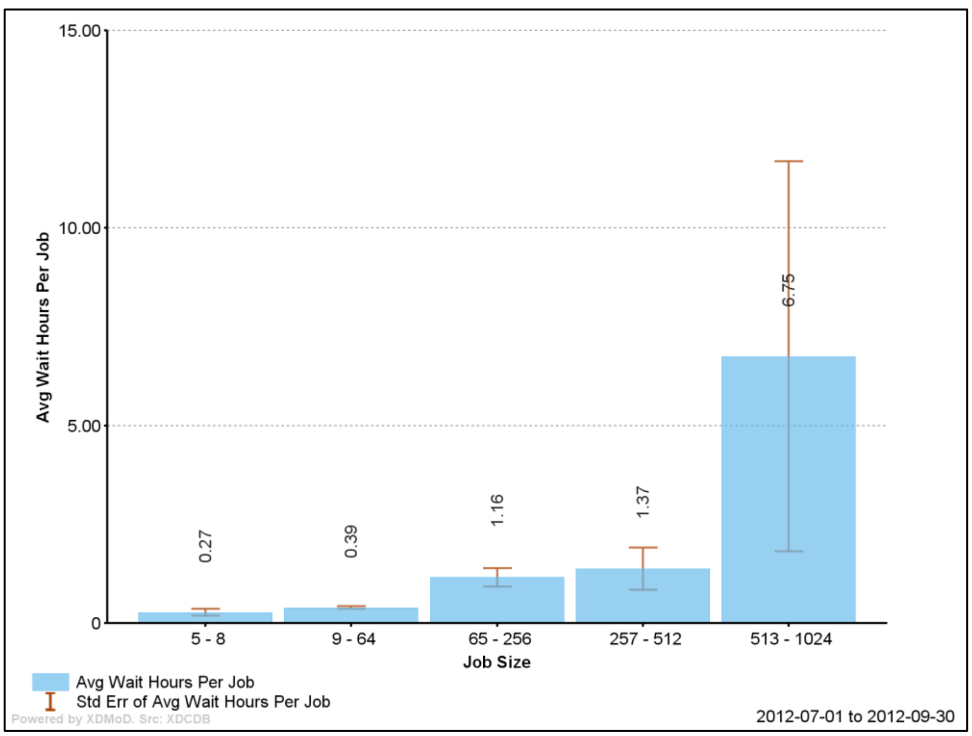

Figure 23: Average wait time in hours by job size for Nautilus in Q1PY2.

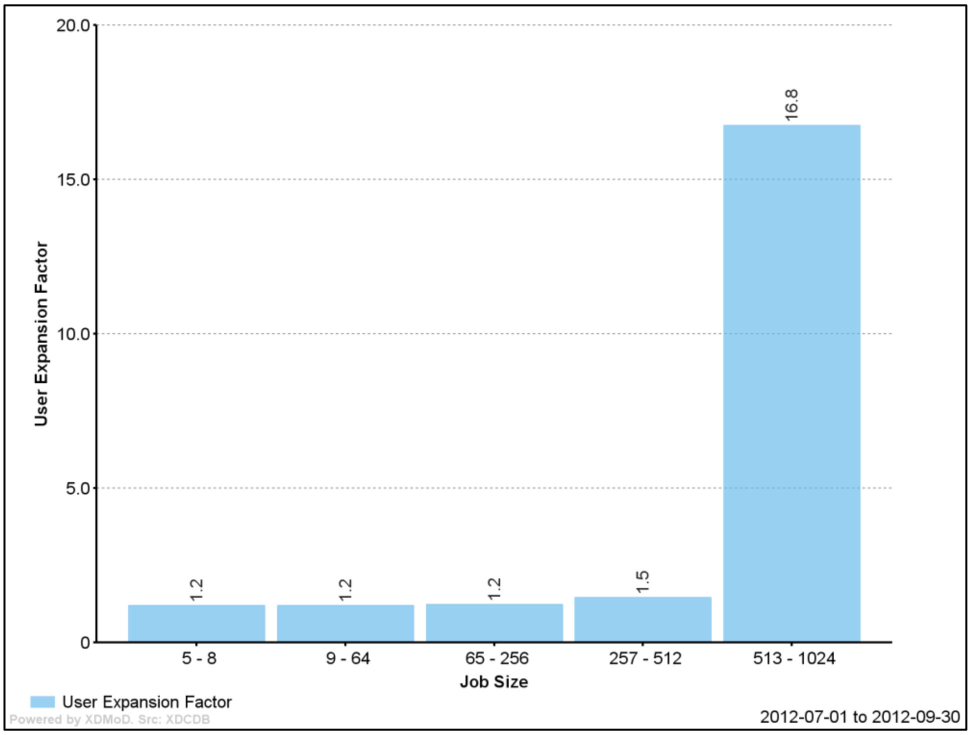

Figure 24: Expansion factor by job size for Nautilus in Q1PY2.

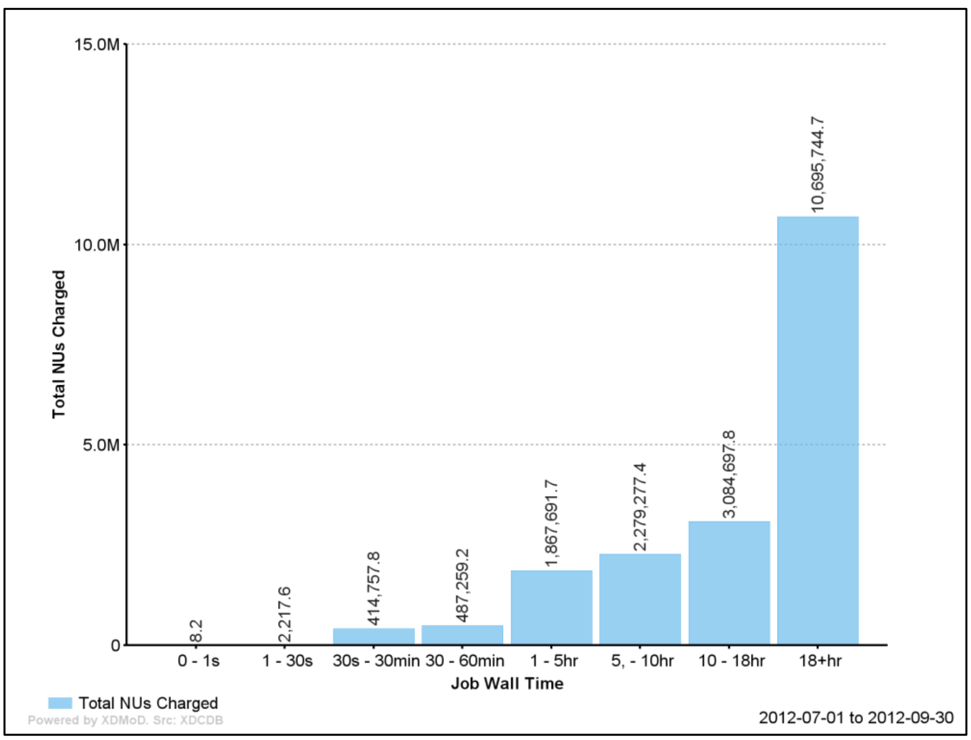

Figure 25: Total resource consumption in mega-normalized units (1e6) by wall time for Nautilus in Q1PY2.

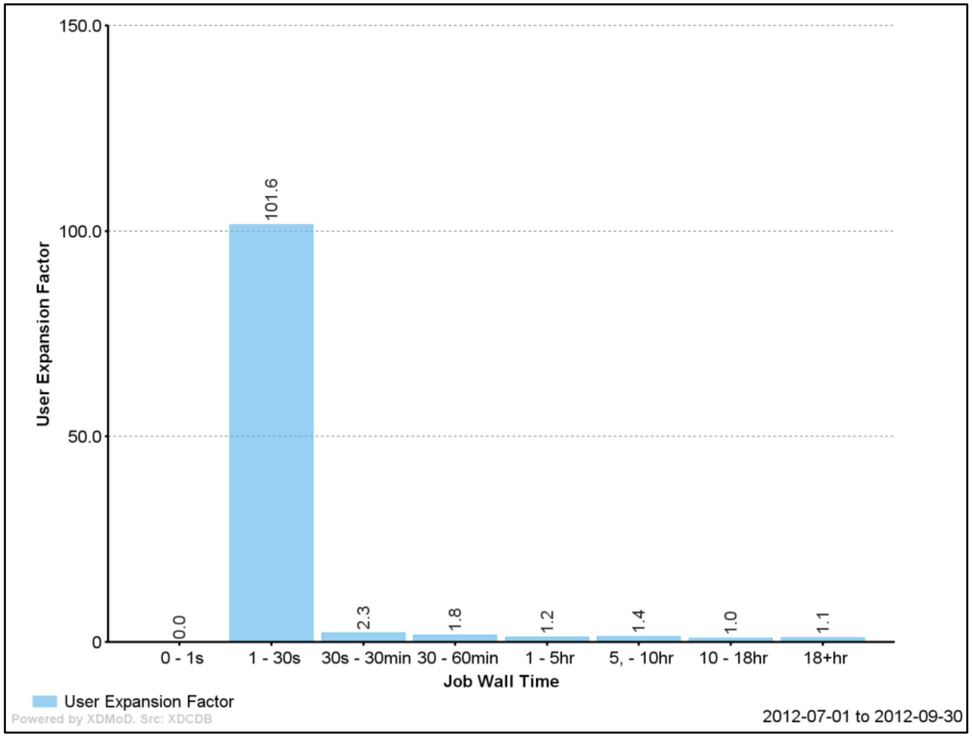

Figure 26: Expansion factor by wall time for Nautilus in Q1PY2.

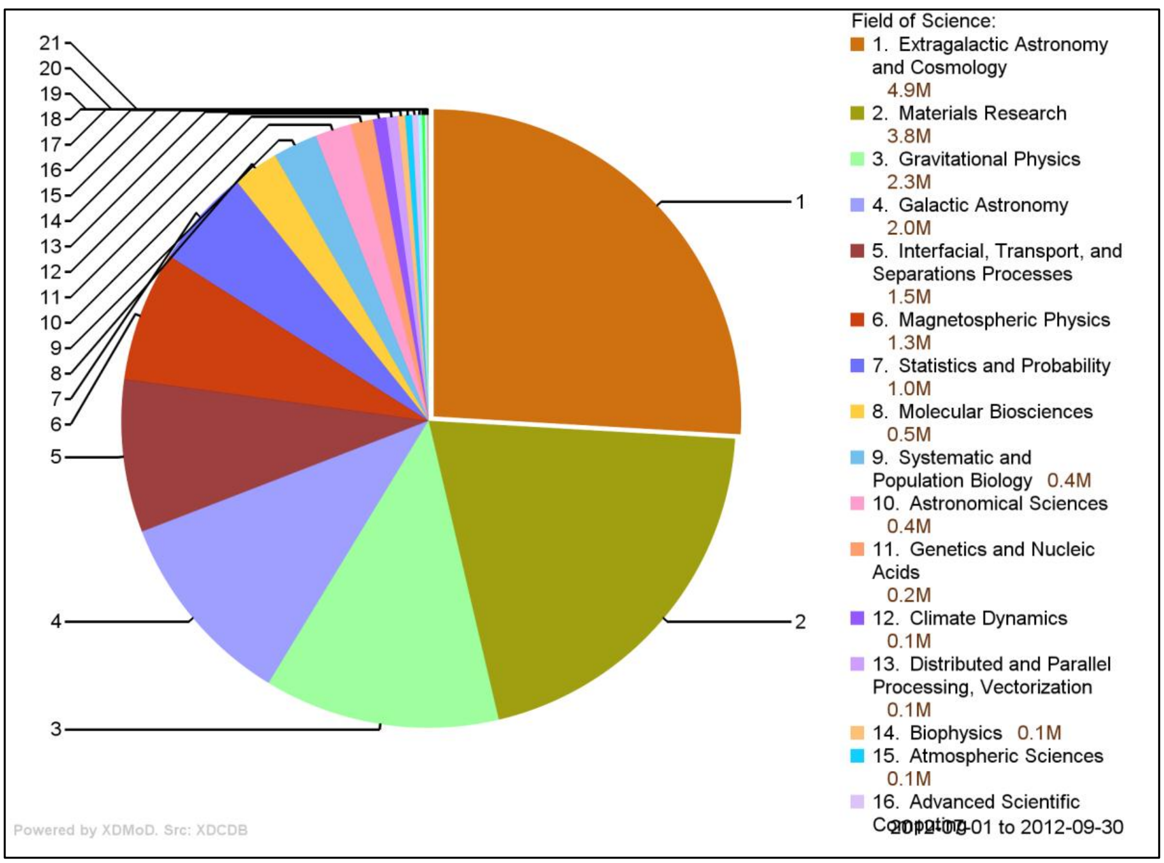

Figure 27: Resource consumption by scientific domain in mega-normalized units for Nautilus in Q1PY2.

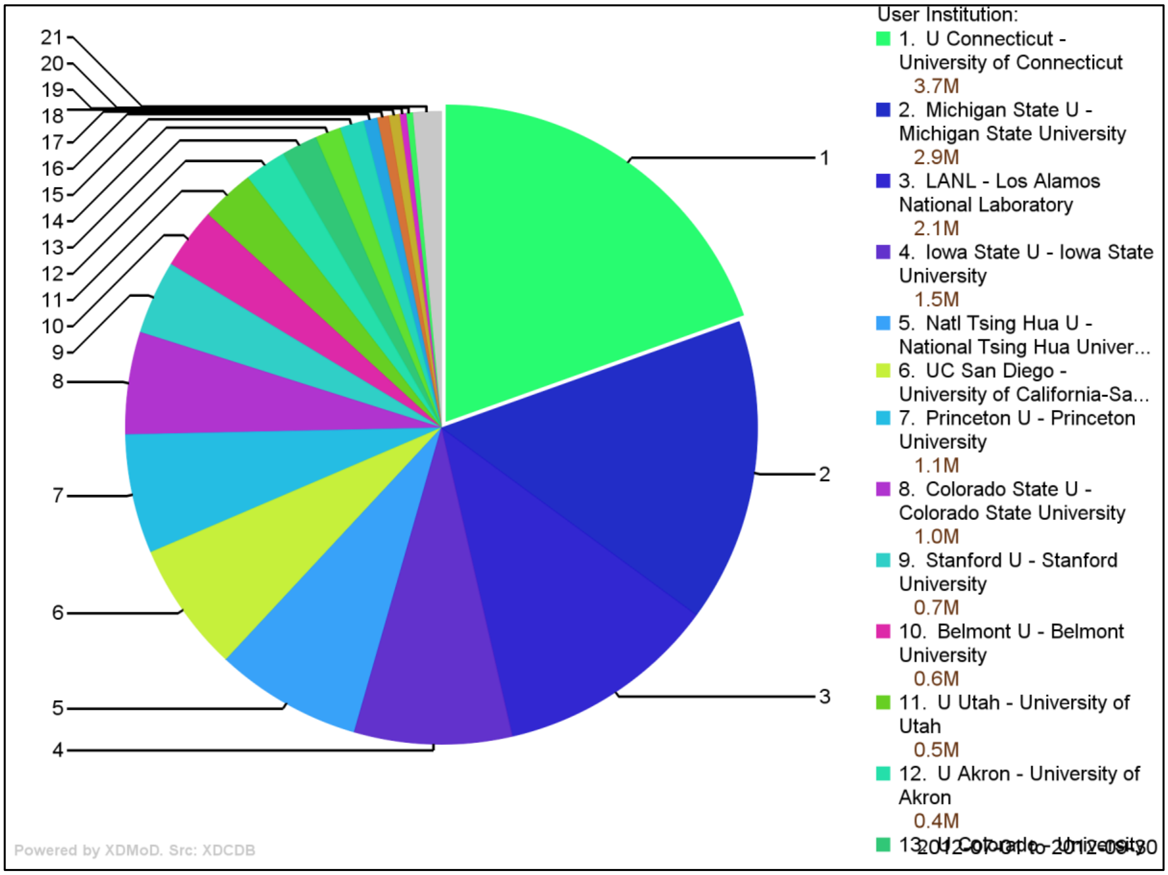

Figure 28: Resource consumption by institute in mega-normalized units for Nautilus in Q1PY2.

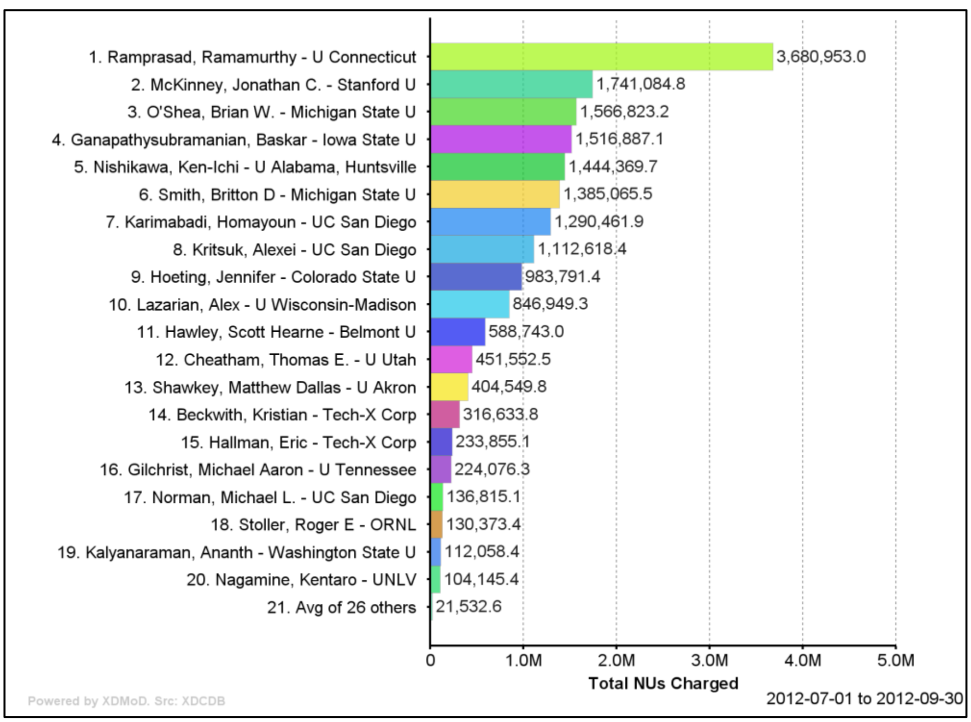

Figure 29: Resource consumption by PI in mega-normalized units for Nautilus in Q1PY2.

16.10.3 *Standard User Assistance Metrics*

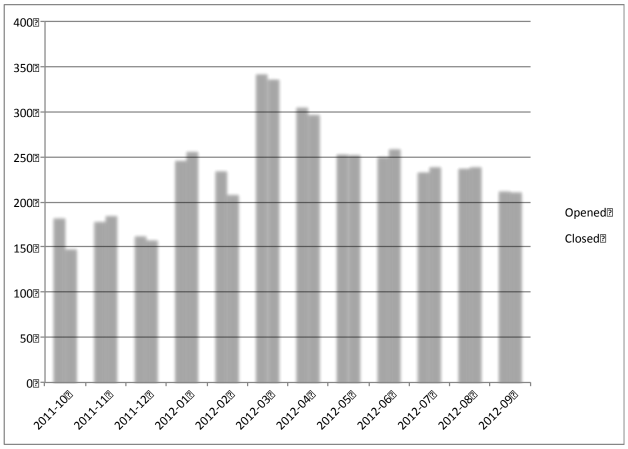

Figure 30: New XSEDE tickets opened by month.

NICS' front line user support resolved 659 XSEDE tickets in the quarter (Table 15). These tickets corresponded to a variety of issues with the majority falling into two groups: login/access issues and jobs/batch queues. Open tickets experienced a median time to resolution of 16.3 hours for the quarter with most tickets being resolved within 24 hours.

Table 15: Ticket resolution times by category for Q1PY2.

	account issues	file systems	grid software	inca messages	jobs / batch queues	login / access issues	mss / data issues	network issues	other	software / apps	system issues	Grand Total
0-1 hrs	7	3			18	75	8		6	10	2	**129**
1-24 hrs	25	13			59	121	8		4	25	6	**261**
1-7 days	15	6		3	32	37	7		9	25	6	**140**
1-2 weeks	2	1			18	18	5		2	9	5	**60**
> 2 weeks	4	2	1	1	21	6	2	3	1	24	4	**69**
Grand Total	**53**	**25**	**1**	**4**	**148**	**257**	**30**	**3**	**22**	**93**	**23**	**659**

16.10.4 *SP-specific Metrics*

NICS' resources provided roughly 57% of computational cycles that were delivered to the NSF community in this quarter (Figure 32), and NSF charges accounts for most of the total charges on these resources (Figure 31 and Figure 32).

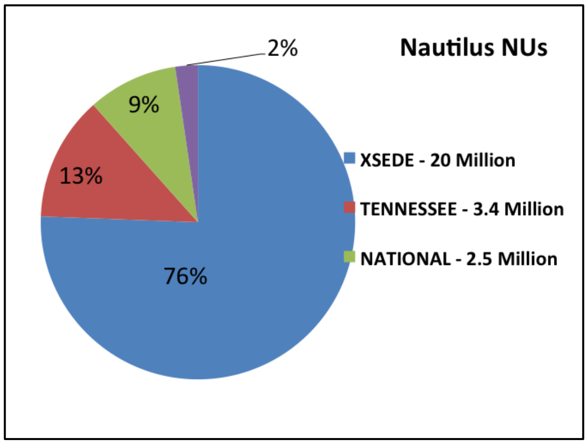

Figure 31: XSEDE charges as a percentage of total charges on Nautilus in Q1PY2.

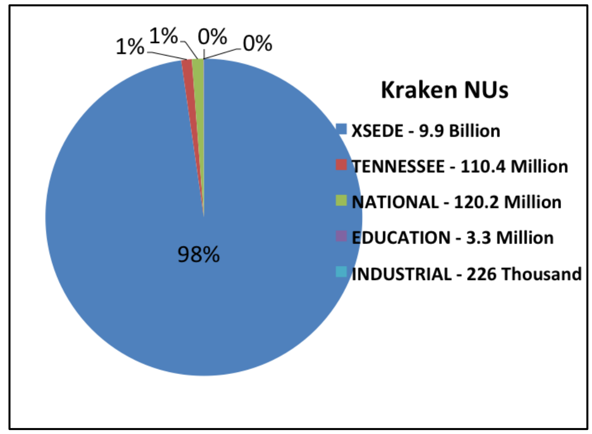

Figure 32: XSEDE charges as a percentage of total charges on Kraken in Q1PY2.

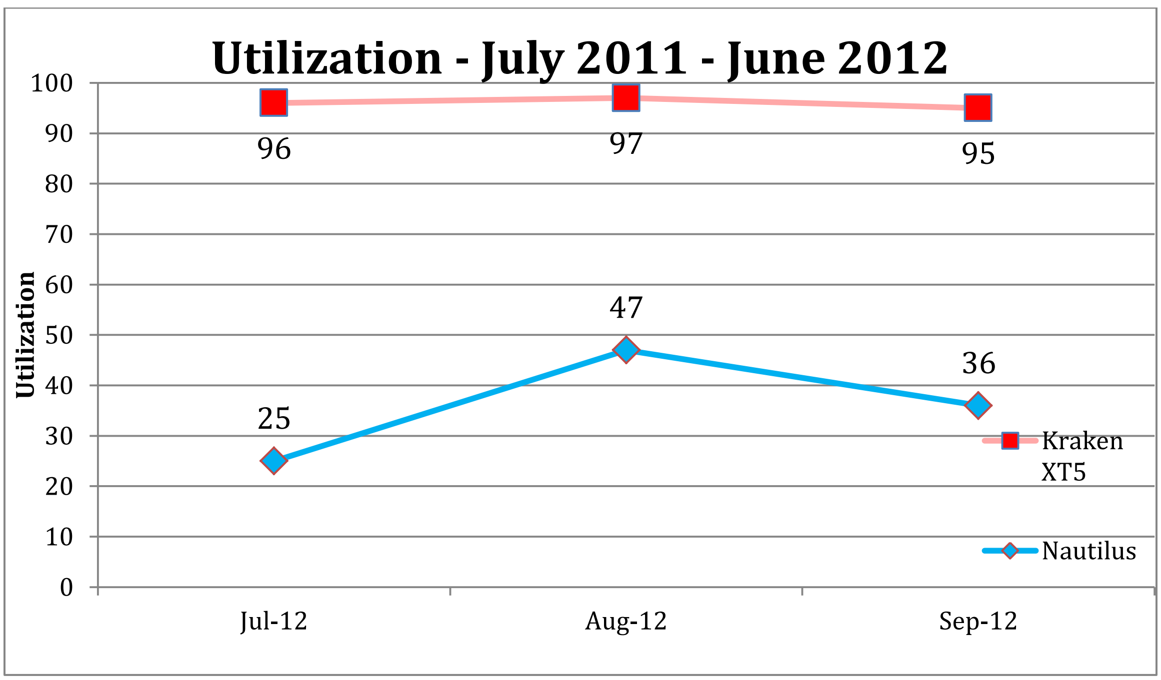

Figure 33: Monthly utilization for Kraken and Nautilus in Q1PY2.

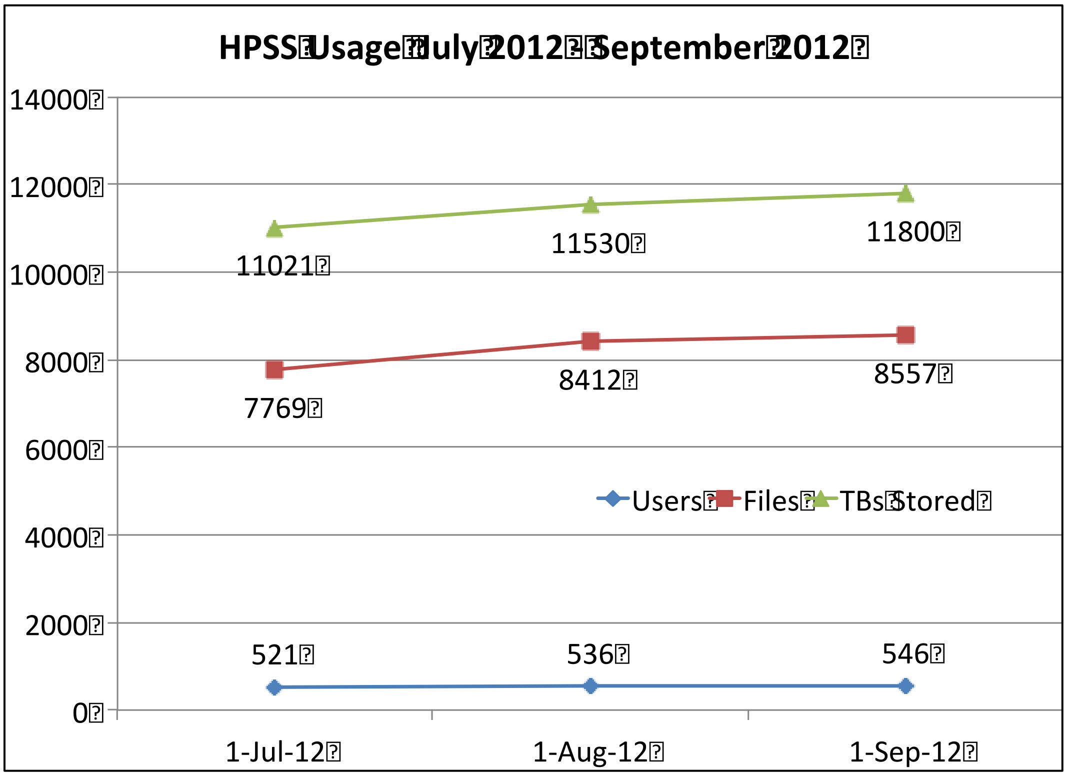

Figure 34: Archival storage usage on HPSS for Q1PY2.

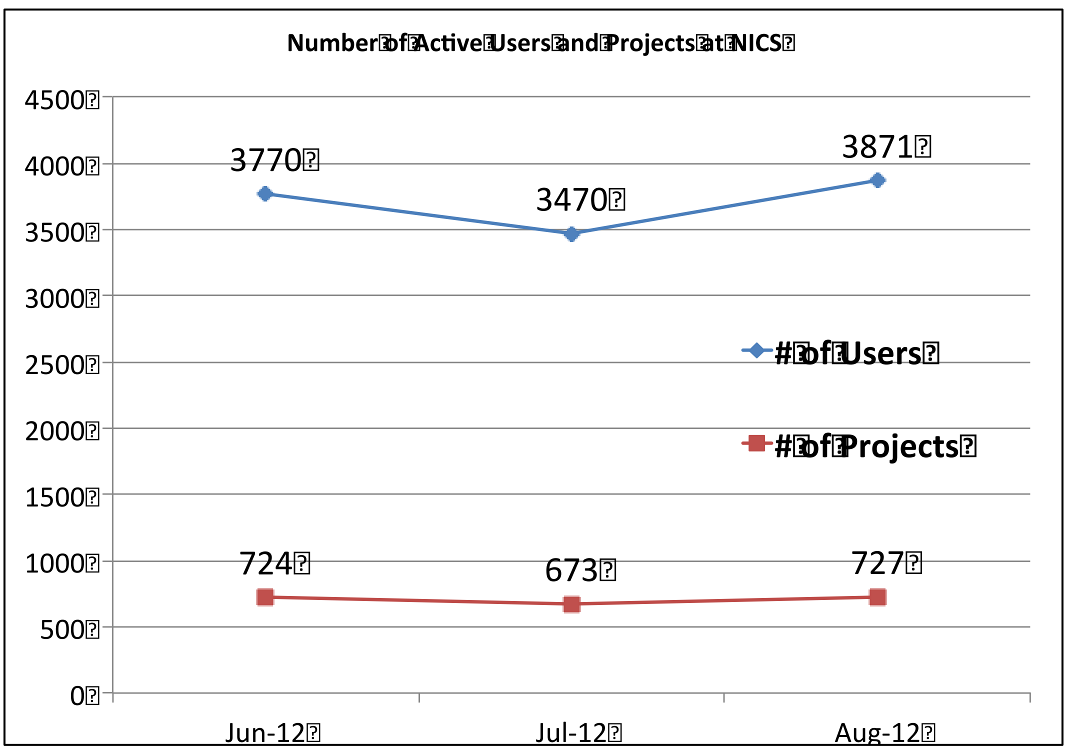

Figure 35: Number of active users and projects on NICS resources at the end of Q1PY2.

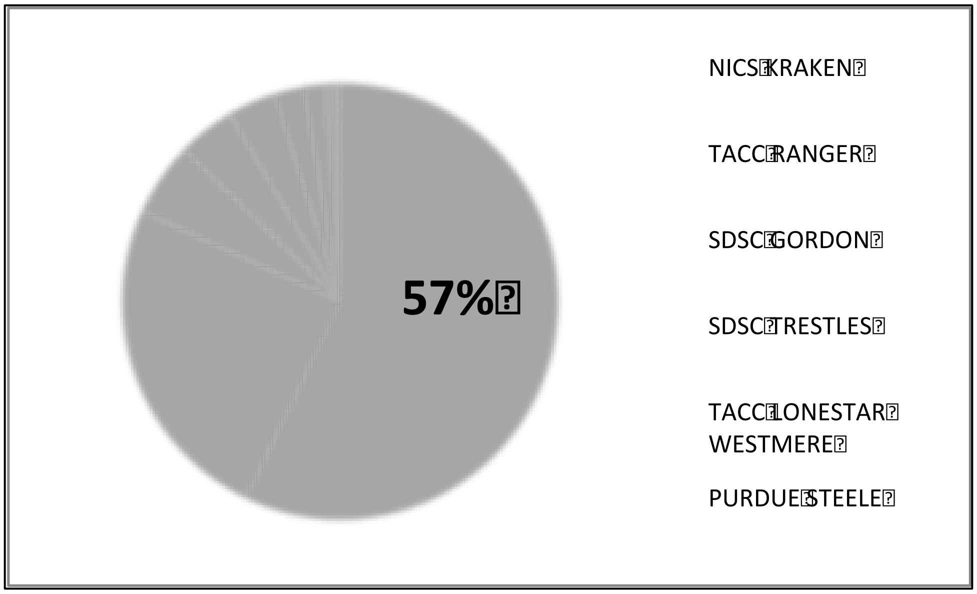

Figure 36: Kraken as a percentage of total CPU hours delivered by XSEDE resource in Q1PY2.

17 Pittsburgh Supercomputing Center - Service Provider Quarterly Report

17.1 Executive Summary

The Pittsburgh Supercomputing Center (PSC) operates and supports, *Blacklight*, a powerful and unique resource for the national research community. *Blacklight*, an SGI Altix UV 1000 acquired with the assistance of an NSF grant and operated as an XSEDE resource, is the world's largest shared-memory system, providing two partitions of 16TB each. *Blacklight*, as well as other PSC systems, is supported by a central file system, and extensive LAN, MAN and WAN infrastructure. For persistent storage such as archiving files, hosting data collections, etc., PSC operates Data SuperCell, a scalable, disk-only file repository that provides fast access to files. Its initial deployment has four petabytes. With operational funding from NIH, PSC also operates *Anton*, a special-purpose computer for molecular dynamics which is used by many NSF-supported researchers.

PSC resources enabled significant progress in many areas; e.g., genomics, molecular biology and game theory/artificial intelligence. Users are finding *Blacklight's* operating characteristics to be very valuable. For instance, Jeff Pummill (University of Arkansas) and his colleagues believe that when combined with PSC's user support staff "*Blacklight* is unique in its ability to handle [genome assembly problems]." Jobs that use more than 2 terabytes are now commonplace.

PSC user support people worked with many users on their applications and continue to earn high praise for their efforts. Similarly PSC's Three Rivers Optical Exchange (3ROX) is helping Internet users such as NOAA, Greenbank Observatory and Penn State with their connections to the Internet. For instance, PSC tuned the Galaxy-to-PSC application to achieve a sustained data rate of 5 Gbps (up to 45 TB in a single day) allowing the Galaxy project to successfully move their data from Penn State to a backup site at PSC.

Although users gave many compliments to PSC in the 2012 XSEDE User Satisfaction Survey, they also pointed out areas for improvement. In response, PSC has already begun to re-orient its user documentation toward less experienced HPC users as well as the more experienced ones and to provide more information on job scheduling practices and machine status. PSC will continue to study the user survey results and come up with further changes in its practices and procedures in the coming months.

PSC engaged in a range of Training, Education and Outreach activities, which included enlisting new communities into HPC, a major STEM education program, and HPC training workshops. PSC has a program of supporting undergraduate interns which has contributed to their career development.

In collaborative activities, the Buhl Foundation has funded PSC to work with the Pittsburgh Public Schools to advance computational skills and help to implement a "flipped" classroom concept that delivers instruction at home through interactive, teacher-created videos and moves homework to the classroom.

17.1.1 Resource Description

PSC provides a range of computing and storage platforms for the national science community.

For applications requiring very large shared memory, high-productivity programming models, and/or moderate parallelism with a high-performance system-wide interconnect, PSC operates *Blacklight*, an SGI UV 1000 cc-NUMA shared-memory system comprising 256 blades. Each blade shares 128GB of local memory, and holds two Intel Xeon X7560 (Nehalem) eight-core processors, for a total of 4,096 cores and 32 TB across the whole system. Each core has a clock rate of 2.27 GHz, supports two hardware threads and can perform 9 Gflop/s for a total system floating point capability of 37 Tflop/s. *Up to 16 TB of this memory is accessible as a single memory space to a shared-memory program.* Message-passing and PGAS programs can access all 32 TB on the system. *Blacklight* is part of the National Science Foundation XSEDE integrated national system of cyberinfrastructure.

Additionally, PSC has an SGI Altix 4700 system called *Salk*, smaller than *Blacklight*, which is also targeted at applications requiring large shared memory, high-productivity programming models, or moderate parallelism with a high-performance, system-wide interconnect. *Salk* is administered for the NIH-funded National Resource for Biomedical Supercomputing (NRBSC) and offers 144 Montvale processors providing a peak aggregate speed of 0.96 Tflop/s with 288 GB shared memory. This system supports advanced programming languages and models including UPC and Star-P.

PSC operates an *Anton* special-purpose supercomputer for molecular dynamics (MD) simulation that performs up to 100 times faster than conventional supercomputers. Designed by D. E. Shaw Research (DESRES) and provided to PSC without cost by DESRES, it is available for non-commercial research use by universities and other non-profit institutions. This machine, the only *Anton* computer operated outside DESRES, is hosted by PSC and is available to the national biomedical community with funding from NIH's National Institute of General Medical Sciences. Computing time on *Anton* is allocated by a peer-review committee convened by the National Research Council. A large number of *Anton* users are NSF supported investigators. The *Anton* computer is supplemented by a high performance file storage system for simulation trajectories and an analysis cluster (*Kollman*). Each of the four nodes in the analysis cluster consists of two Intel Westmere six-core processors and 96 GB of memory. The high-performance file storage system consists of a 500-TB Lustre file system. The file system and the analysis cluster nodes are interconnected over Quad Data Rate (QDR) InfiniBand. Availability of the *Anton* system has been extended until September 2014.

PSC operates several Linux clusters for scientific research as well as several high-end servers and powerful workstations for development, analysis, and visualization tasks.

The production workload on all of the PSC computing platforms is managed by PBS/Torque. Several scheduler policy modules used include a locally-developed module, *Simon*, and the Maui scheduler.

All of the PSC computing platforms have access to *Brashear,* PSC's shared, central file system using the Lustre file system architecture. It comprises eight storage nodes and 350 TB of direct-attached disks, forming a large I/O cluster globally accessible within the PSC site. Access to the file system is provided by InfiniBand, 10-Gigabit Ethernet and 1-Gigabit Ethernet. Each node in the I/O cluster is a Lustre Object Storage Server (OSS) hosting multiple Object Storage Targets (OSTs).

PSC has been a partner in the Lustre *Albedo* Wide Area File System project that is being decommissioned and had taken the lead by managing the metadata service for it in addition to providing a portion of its bulk object storage.

PSC's archive file repository is a disk-only system that is less costly than a disk-tape system and provides much faster file access. Each building block in the repository has one petabyte of useable disk storage, which is managed by the ZFS file system and the PSC-developed SLASH2 replicating distributed file system. ZFS and SLASH2 provide multiple layers of robust data integrity checking to protect user data against data corruption. This building-block architecture will enable the repository to scale well beyond its initial deployment of four petabytes.

Users can access the repository from within PSC using the familiar PSC file archiving utility, *far*. From outside PSC, users can employ a variety of well-known file transfer methods such as SCP and gridftp. These transfers are handled by a series of dedicated data transfer servers.

PSC network facilities consist of production and research Local Area Network (LAN), Metropolitan Area Network (MAN), and Wide Area Network (WAN) infrastructures.

Local Area Network Infrastructure: The LAN infrastructure consists of switched Ethernet with speeds up to 10 Gb/s. The LAN architecture was constructed to overcome issues of buffer contention in data center Ethernet switches on the Science DMZ[1]. This allows for higher bandwidth data transfers to the data transfer nodes.

3 Rivers Optical Exchange: PSC operates and manages the 3 Rivers Optical Exchange (3ROX) a regional network aggregation point that provides high-speed commodity and research network access, primarily to sites in Western and Central Pennsylvania and West Virginia. While the primary focus of 3ROX is to provide cost-effective, high-capacity, state-of-the-art network connectivity to the university community, this infrastructure also provides well-defined network services to both community (K-12, government) and commercial entities in Western Pennsylvania. University member sites currently include Carnegie Mellon University, the Pennsylvania State University, the Pittsburgh Supercomputing Center, the University of Pittsburgh, WVnet, and West Virginia University.

3ROX Metropolitan Area Network Infrastructure: 3ROX MAN infrastructure is DWDM-based and supports multiple 10-Gigabit Ethernet waves. It is capable of supporting 40 and 100-Gigabit waves as the need arises. This DWDM network connects four different locations around the city that include long haul service providers, a co-location hotel, a campus based co-location facility, and the Northern Pike machine room.

3ROX Wide Area Network Infrastructure: 3ROX WAN infrastructure has both Commodity Internet and Research and Education components. Explicit routing is used to maintain the acceptable use policies associated with the various production and research network infrastructures.

The 3ROX Commodity Internet component consists of multiple high-performance WAN connections to major Internet service providers, including a Gigabit Ethernet connection to Cogent and a 10-Gigabit Ethernet connection to Level 3. In addition, 3ROX provides connectivity to both regional and national Internet2 and content peering infrastructures, in particular access to the Internet2 based TR/CPS content peering services; regional peering with Southern Cross Roads (SOX), OARnet and Comcast; along with a recent direct peering connection with Google.

The 3ROX Research and Education component includes a 10-Gigabit Ethernet connection, with 5 Gb/s of bandwidth, to the Internet2 network. In addition to the Internet2 connection, 3ROX also has a 10-Gigabit Ethernet connection to National LambdaRail; a 10-Gigabit Ethernet connection to the XSEDE backbone network; a 10-Gigabit Ethernet connection between PSC's offices and its remote supercomputing machine room at 4350 Northern Pike; and a 10-Gigabit Ethernet connection to Penn State University (PSU) to provide XSEDE connectivity to PSU.

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[1] From http://fasterdata.es.net/science-dmz/: The Science DMZ is a portion of the network, built at or near the campus or laboratory's local network perimeter that is designed such that the equipment, configuration, and security policies are optimized for high-performance scientific applications rather than for general-purpose business systems or "enterprise" computing.

17.2 Science Highlights

In addition to major science accomplishments that are highlighted in the XSEDE report, we present selected others specific to PSC.

17.2.1 Genetics and Nucleic Acids: Whole Genome Sequencing of the Timber Rattlesnake, Crotalus horridus (Douglas Rhoads, Steve Beaupre and Jeff Pummill, University of Arkansas; Michael Berumen, King Abdullah University of Science and Technology)

Douglas Rhoads (PI), Steve Beaupre, and Jeff Pummill of the University of Arkansas along with Michael Berumen of KAUST in Saudi Arabia have made the following progress on whole genome sequencing of the Timber Rattlesnake:

The Timber Rattlesnake (*Crotalus horridus*) common to the central, eastern and southeastern regions of the United States is now threatened with extinction in about half of the states in its original distribution. The species has become a model organism for behavior and physiology. In particular, it is representative of extreme low-energy adaptation that is common to advanced snakes, but particularly pronounced in rattlesnakes and their close kin. These snakes are capable of surviving up to two years of starvation and in nature they undergo muscular hypertrophy without exercise. Understanding these capabilities has implications for human health (long-term bed-care) and possibly even spaceflight (maintenance of muscle mass in zero G environments). Genomic sequencing should provide valuable tools for understanding low-energy adaptation.

The Timber Rattlesnake (*Crotalus horridus*): Its survival capabilities may have implications for human health and possibly spaceflight.
Photo credit: Steve Beaupre

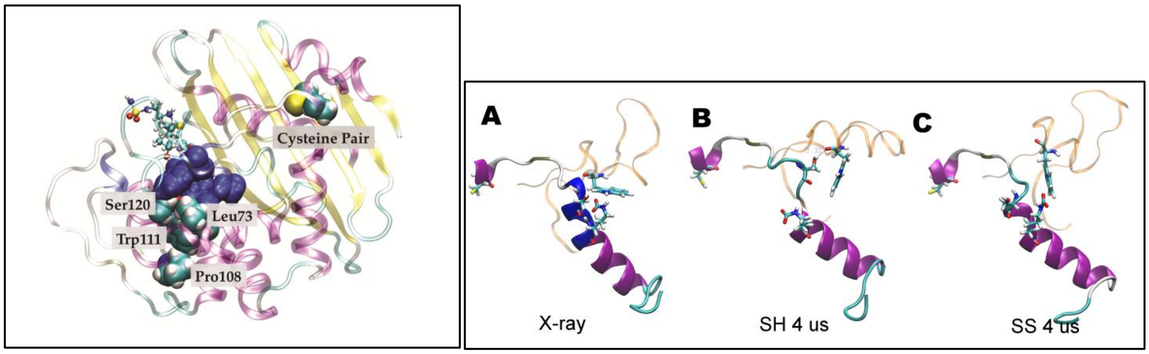
A single blood sample was drawn from a healthy adult female Timber Rattlesnake from a long-term study population in northwest Arkansas. As no reference genome existed, the project required *de novo* assembly. The team chose to use the software package Velvet for the assembly and worked with PSC consultant Phil Blood and Oklahoma State researcher Brian Couger to run Velvet on *Blacklight*. Resource demands were rather steep as each run required approximately 400GB of memory and a maximum amount of wall time on the system. In a reasonably short time, the team completed a draft genome—a milestone that they attribute largely to the *Blacklight* system. The research team is now refining the genome assembly through tweaks in the assembly parameters and will soon add transcriptomic data (from multiple tissue samples from an unrelated individual) to the model using the Trinity application.

Rhoads, et al selected *Blacklight* for this work because the problem has steep memory requirements and Velvet has been parallelized only for SMP architectures such as *Blacklight*. Additionally, *Blacklight* has an in-memory scratch file system which provides a virtual directory in RAM, thus taking advantage of faster I/O which is important when dealing with very large data sets. Furthermore, the Trinity transcriptome assembly code has also been shown to favor *Blacklight's* architecture, taking advantage of the ability to set processor affinity combined with the large memory footprint. Considering *Blacklight's* capabilities and the guidance and help they received from PSC's scientific support staff, they believe that PSC is unique in its ability to support their work.

Current sequence data has been produced using the Illumina platform for short reads and mate-pair reads, and Roche454 for longer reads. Co-assembly using multiple data types is the preferred methodology for more complex assemblies.

Once an assembly has been produced, it will be shared among the members of the Mid-South Computational Biology and Bioinformatics Society (www.mcbios.org), which has taken on assembly and annotation of the rattlesnake genome as a collaborative project. The assembly and annotated genome will then be the subject of a publication and posting on genome browsers.

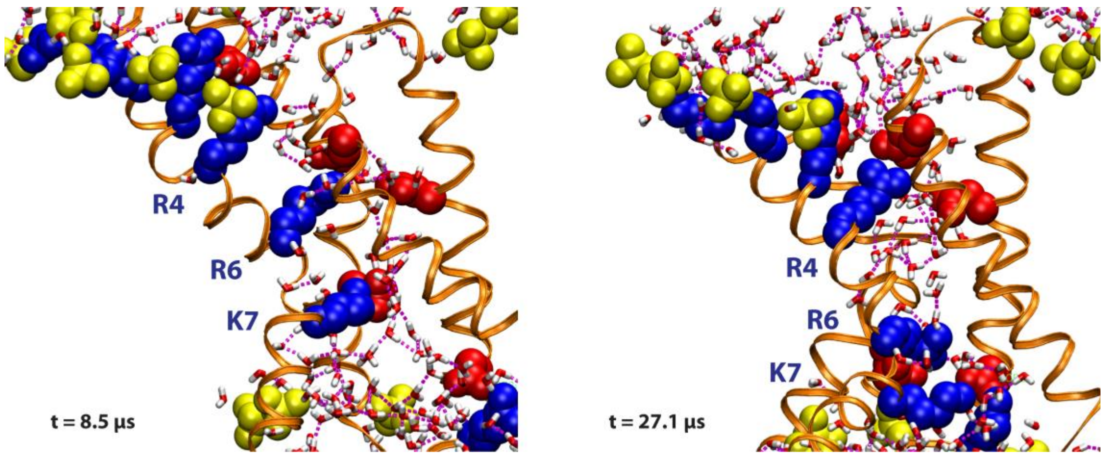
17.2.2 Biochemistry and Molecular Structure and Function: Force-Field Parameterization Toolkit, Exploration of Long Timescale Simulations of Beta-Lactamase (Troy Wymore, Pittsburgh Supercomputing Center)



(Left) The OXA-1 structure with labels attached to residues conserved within the clade but not within the family. Residues in blue make up the active site. **(Right)** Comparison between active site structure (part of large helix) based on x-ray electron density maps and 4 microseconds of MD simulation with cysteine pair (on left end of representation) in reduced (B) and oxidized (C) form. In the reduced form, the active site structure is significantly degraded.

Nikolay A. Simakov and Troy Wymore of Pittsburgh Supercomputing Center (PSC) have developed several tools to aid in the molecular mechanical (MM) force-field parameterization of small molecules using the CHARMM General Force Field (CGenFF) approach of Vanommeslaeghe, Hatcher, et al. The accuracy of the force field is critical for computational studies of intermolecular interactions between small organic molecules and biological macromolecules which underlie many important biological processes. Accuracy of the force field is important, furthermore, for long timescale molecular dynamics (MD) simulations enabled by the capabilities of today's supercomputing platforms, such as PSC's *Anton*. Given the massive variety of organic compounds, quite often the parameters for the small organic molecules of interest are not present in existing molecular force fields, or at least not well developed and thus need to be derived through extensive quantum-chemistry calculations. Although, the CGenFF protocol is sufficiently detailed, the parameterization remains a labor-intensive task. Simakov and Wymore developed tools that decrease the labor effort, lower manual input errors and reduce the time needed for accurate MM parameterization. With this toolset Wymore and colleagues developed parameters for a carboxylated lysine residue that is critical for the function of class D beta-lactamase enzymes. The ability of beta-lactamases to inactivate beta-lactam antibiotics underlies the major mechanism of antibiotic resistance. Beta-lactamases adapt quickly to new therapeutics, which is of grave clinical concern. To overcome this resistance requires deeper understanding of both the structure of the biomolecular system and its history. To this end, the team of A. Szarecka, K.R. Lesnock, C. A. Ramirez-Mondragon, H.B. Nicholas, Jr. and Wymore conducted a large-scale, high-resolution phylogenetic analysis of beta-lactamases and subsequent long timescale (microseconds) atomistic MD simulations on PSC's *Anton*, with results reported in *Protein Engineering Design and Selection* **10**, 801-09 (Oct 2011). The researchers found accessible, functionally-relevant conformations and the surrounding conformational landscape. Most significant was the discovery of a likely disulfide bond in a large group composed of alpha, beta and gamma proteobacteria that would contribute to enzyme stability and hence bacterial viability under antibiotic assault. The results of the MD simulations (see figure) begin to validate the phylogenetic analysis and suggest new target areas for allosteric inhibition that leads to core disruption. Further understanding of these sequence-structure-function relationships would benefit efforts to design a new generation of antibiotics as well as to predict evolutionary mechanisms in response to such therapies.

17.2.3 Molecular Biophysics: Microscopic Origin of Gating Fluctuations in a Potassium Channel Voltage Sensor (Alfredo Freites and Douglas J. Tobias, University of California, Irvine)



Snapshots from simulation of the voltage sensing domain (orange) with associated lipid bilayer phosphate groups (yellow) before (left) and after a sudden change in the electrical potential at nine microseconds. The displacement of three highly-conserved, positively charged amino-acid residues (blue — R4, R6 & K7) gives rise to a gating-current event. As these charges move through the water molecules (white and red) in the VSD interior, they exchange interactions with negatively charged amino-acid residues (red).

Every communication in the central nervous system is possible because ions flow across the cell membrane. Voltage-gated ion channels open in nerve cells, and ions —usually sodium and potassium — flow through the opened gates, creating electrical currents that cause muscle fibers to contract. The ions flow through what's essentially a hole in the membrane formed by proteins, called voltage-gated ion channels. These channels open and close based on the ability of part of the protein, called the "voltage sensing domain" (VSD), to respond to changes in electrical potential. Laboratory studies over many years have shown that currents — called "gating currents" — in the VSDs are associated with motions that trigger opening of the channel. Until the availability of the *Anton* system, however, it hadn't been possible to track what structural changes happen in the VSD during the gating event. With *Anton*, Alfredo Freites and his colleagues Eric Schow, Stephen White and Douglas Tobias were able to run MD simulations over a timescale that corresponds to a VSD gating-current event. They simulated the VSD embedded in a lipid bilayer, representing the cellular membrane, along with surrounding water with an applied electric field for a period of 30 microseconds. At this timescale, the researchers were able to make direct comparisons between MD simulations and laboratory data. "With any other high-performance computing resource," says Freites, "it would be impractical to do this." Their findings — reported in *The Biophysical Journal* (June 2012) — were, in general, consistent with the data from laboratory studies. The detail of the MD results suggests, nevertheless, that gating-charge measurements from electro-physiological lab studies "may not represent a single charge displacement but may instead be the superposition of many events occurring faster than the instrument response." Their findings also go beyond prior studies in showing that the presence of water molecules within the VSD is necessary for the gating current to flow and pull the channel open.

17.3 User-facing Activities

17.3.1 System Activities

XCDB: During his Operations presentation at the recent XSEDE Quarterly Meeting, Stephen McNally of NICS (XSEDE Level3 Manager) singled out PSC's Ed Hanna and Rob Light for the good work that they did in a particularly involved effort to provide failover for the XCDB.

Galaxy: PSC successfully tuned the Galaxy-to-PSC application to achieve a sustained data rate of 5 Gbps and transferred up to 45 TB in a single day. As a result, the Galaxy project was able to successfully move their data from Penn State to PSC. The bottleneck had been enforcement of bandwidth limits within the Penn State campus infrastructure. PSC is continuing discussions with Penn State on mechanisms for increasing the bandwidth for applications such as Galaxy without negatively impacting other production network traffic on their backbone.

Network Connections: Penn State's dedicated and redundant 10-GE lambda, connecting Penn State to their new machine room space at PSC's Allegheny Center Mall point-of-presence, has been tested and was placed into operation the week of September 17.

NOAA has renewed their contract with PSC's Three Rivers Optical Exchange (3ROX) for their 10-GE link from Pittsburgh to Fairmont, WV. In Addition, PSC is working with NOAA to implement a 10-GE path from their Fairmont, WV facility to Cleveland, OH. This 10-GE link will be a redundant path to their existing 10-GE link to Pittsburgh. We are collaborating with both WVnet and OARnet on segments of the link in order to ensure the link is both cost effective and fully redundant.

PSC's new 10-GE based connection to Level3 was placed into production in early September, replacing the 1-GE based connection to Global Crossing. We have purchased a committed data rate of 2 Gbps on the new link, up from 400 Mbps on the old link.

A 10-GE peering connection to Google was placed into production in mid-September, with peak inbound traffic loads of roughly 3.4 Gbps during the week. With the addition of this peering connection, along with some changes to our TR/CPS link, we are seeing daily peaks in our commodity peering connectivity of over 6 Gbps.

17.3.2 Services Activities

Appreciation of PSC Staff: Among the many words of praise we receive about PSC staff members' services activities, here are two that came in recently.

> **Alex Hall, UCLA Dept. of Atmospheric & Ocean Sciences**: In an oral interview about his research use of *Blacklight*, Alex Hall gave high praise for PSC's Dave O'Neal. Because Hall was speaking off the cuff, it's not possible to extract an exact quote that is simultaneously pithy, comprehensive and coherent, but Hall said that O'Neal is "[one of] the most knowledgeable and helpful and professional [people] that we've dealt with in these various computing centers … he's definitely a good guy. And very helpful." Hall added, "I'll probably never meet him, but he takes his job pretty seriously, even though he doesn't know anyone he's dealing with, really. So … that's worthy of some kind of recognition. And it really is important—you know, we have a lot of problems on these machines sometimes, and we just don't know what to do. So having someone to help out—that's actually really nice."

Patti Redd, NICS (XSEDE User Support): John Towns forwarded an email that he received about Ken Hackworth from Patti Redd. Redd said, "I just wanted to take a minute to let you know what a fantastic job Ken Hackworth is doing as the allocation manager. He is clearly cares about the users and their work but is equally concerned with the resource providers. He is excellent at negotiating between the two, has been creative with solutions, and yet he is capable of setting limits when needed. His positive personality makes dealing with difficult situations much easier. I appreciate his leadership and just wanted to let you know."

Documentation and Status Information: In response to the 2012 XSEDE User Satisfaction Survey, PSC is reviewing its practices and procedures. To date we have determined that we will do the following:

- Re-orient PSC user documentation to account for less experienced HPC users as well as the more experienced ones
- Provide more specific information on our job scheduling practices
- Provide tools for users to get more information on the scheduling status of their jobs
- Provide more information to users on *Blacklight's* operational status and make it readily accessible

We expect to come up with more ideas for changing our practices and procedures in the coming months, and we will provide status updates in future reports as the work progresses.

17.4 Security

PSC had no security incidents.

17.5 Education, Outreach, and Training Activities

Type	Title	Location	Date(s)	Hours	Number of Participants	Number of Under-represented people	Method
Tutorial	Web10G	Palo Alto, CA	15 JUL 2012	2	30		Live
Work shop	Accelerator Programming with OpenACC and CUDA	Chicago, IL	16 JUL 2012	4	30		Live
Tutorial	XSEDE New User Training	Chicago, IL	16 JUL 2012	1.5	35		Live
Tutorial	XSEDE New User Training	Online	27 JUL 2012	1.5	10		Webcast
Work shop	CAST Summer Institute	Pittsburgh PA	6-9 AUG 2012	28	9	8	Live

Type	Title	Location	Date(s)	Hours	Number of Participants	Number of Under-represen ted people	Method
Confer-ence talk	An Introduction to The Americas Grid Policy Management Authority (TAGPMA) and the International Grid Trust Federation (IGTF)Performance Computing	Latin American Conference on High Performance Computing, Panama City, Panama	29 AUG 2012	1	100		Live

Web10G: PSC networking staff members with collaborators at the National Center for Supercomputing Applications are developing Web10G, a tool that will enable enable ordinary users to effectively use advanced networks. Regarding the tutorial on Web10G given by Chris Rapier, Andy Adams and John Estabrook (NCSA) on July 15, over 30 people attended the tutorial with 10 people participating in the hands on portion. In the ensuing discussion, there was significant enthusiasm for what the community can do with Web10G. Most of the proposed applications focused on improving the ability to report on TCP/IP functions within a host as well as modifying performance monitoring tools for use on diagnosing end-to-end networking problems. Chris Rapier also gave an update during the regular Joint Techs session. We are currently looking for an appropriate venue for a developers' workshop.

The team's request for a Web10G BoF was accepted by Internet2 for their Fall Member Meeting in Philadelphia. The BoF will be a follow-on to the Web10G workshop and presentation at the Summer Joint Techs meeting and will include a demonstration of simple diagnostic tools that utilize the Web10G kernel.

17.6 SP Collaborations

Pittsburgh Public Schools: We received confirmation from the Buhl Foundation that they will fund PSC for a total of $45,000 over three years for a program to work with the Pittsburgh Public Schools to advance computational skills and help to implement a "flipped" classroom concept. A flipped classroom is "a reversed teaching model that delivers instruction at home through interactive, teacher-created videos and moves 'homework' to the classroom. Moving lectures outside of the classroom allows teachers to spend more 1:1 time with each student. Students have the opportunity to ask questions and work through problems with the guidance of their teachers and the support of their peers - creating a collaborative learning environment." (See http://www.techsmith.com/flipped-classroom.html.)

17.7 SP-Specific Activities

Tuomas Sandholm, Carnegie Mellon University Computer Science: The Sandholm group's poker-playing agent submitted for the two-player no-limit Texas Hold'em division did well in the Annual Computer Poker Competition at the AAAI meeting held in Toronto on July 22–26, 2012. The agent finished in 2nd place using the instant runoff scoring rule (which favors equilibrium agents) and in 3rd place using the total bankroll scoring rule (which favors exploitative agents). The algorithm used was a gradient-based algorithm, using an improved version of Nesterov's excessive gap technique specialized for poker (Hoda, et al. 2010). The computation was run using *Blacklight* at the Pittsburgh Supercomputing Center.

More detail about the rules and results can be found at http://www.computerpokercompetition.org/, and a detailed description of the agent can be found at http://www.cs.cmu.edu/~sganzfri/AAAI2012.pdf.

Bettis Briefing: PSC hosted 23 scientists/engineers from Bettis Atomic Power Laboratory for the 12th annual Bettis Technology Briefing September 25-26. Each year PSC tailors the agenda to topics of particular interest to Bettis. This year, topics included both system technology updates (interconnects, file systems, Data SuperCell) and trends in applications development (OpenACC, collaboration tools, NoSQL/Hadoop/Graph databases). Participants' evaluations of the briefings continue to be very good.

17.8 Publications

Simmel, D., Rae, S., and Stolk, A. An Introduction to The Americas Grid Policy Management Authority (TAGPMA) and the International Grid Trust Federation (IGTF). Latin-American Conference on High Performance Computing (CLCAR), in Panama City, Panama, August 27-31, 2012.

17.9 Metrics

17.9.1 Standard User Assistance Metrics

Numbers in Table 1 refer to all tickets handled by the PSC help desk in PSC's local ticket system.

Table 1: Distribution of times to resolution for the 428 tickets that were created as well as resolved between 7/1/2012 and 9/30/2012.

Ticket Type	Account issues	File systems	Jobs/batch issues	Login/access issues	Software /apps	System issues	Other
0-1 hr	4	3	14	1	1	6	0
1-24 hr	16	13	96	3	23	35	10
1-7 day	24	17	37	0	33	27	13
1-2 weeks	0	2	2	0	20	2	0
>2 weeks	3	5	1	0	17	0	0

Numbers in Table 2 refer to tickets relating to PSC that were handled in the central XSEDE Ticket System.

Table 2: Distribution of times to resolution

Time to Resolution	account issues	file systems	grid software	jobs/batch queues	login/access issues	mss/data issues	network issues	software/apps	system issues	other
0-1 hr				1						
1-24 hr	1					1		2		1
1-7 d	1	3		7	7			3		2
1-2 wk	1	1		4		1		3		2

Time to Resolution	account issues	file systems	grid software	jobs/batch queues	login/access issues	mss/data issues	network issues	software/apps	system issues	other
> 2 wk	1		1	6	1	2		11		1
Still Open	1			3	2			5		

17.9.2 SP-specific Metrics

Key system statistics for *Blacklight* for 7/1 to 9/30/2012 are shown in Table 3.

Table 3: Operational Statistics - *Blacklight*		
Number of unplanned outages	20	
Number of planned outages	2	
Total outages	22	
Number of job failures due to system faults	376	
Total time* in period (hours)	4,416.00	100.00%
Scheduled Downtime (hours)	122.75	2.78%
Unscheduled Downtime (hours)	11.00	.25%
Total Downtime (hours)	133.75	3.03%
Total time available to users (total-downtime)	4,282.25	96.97%
% System Utilization	77.24%	

* On *Blacklight* a node is half the machine. Time values listed are expressed in node hours.

17.9.3 Standard systems metrics

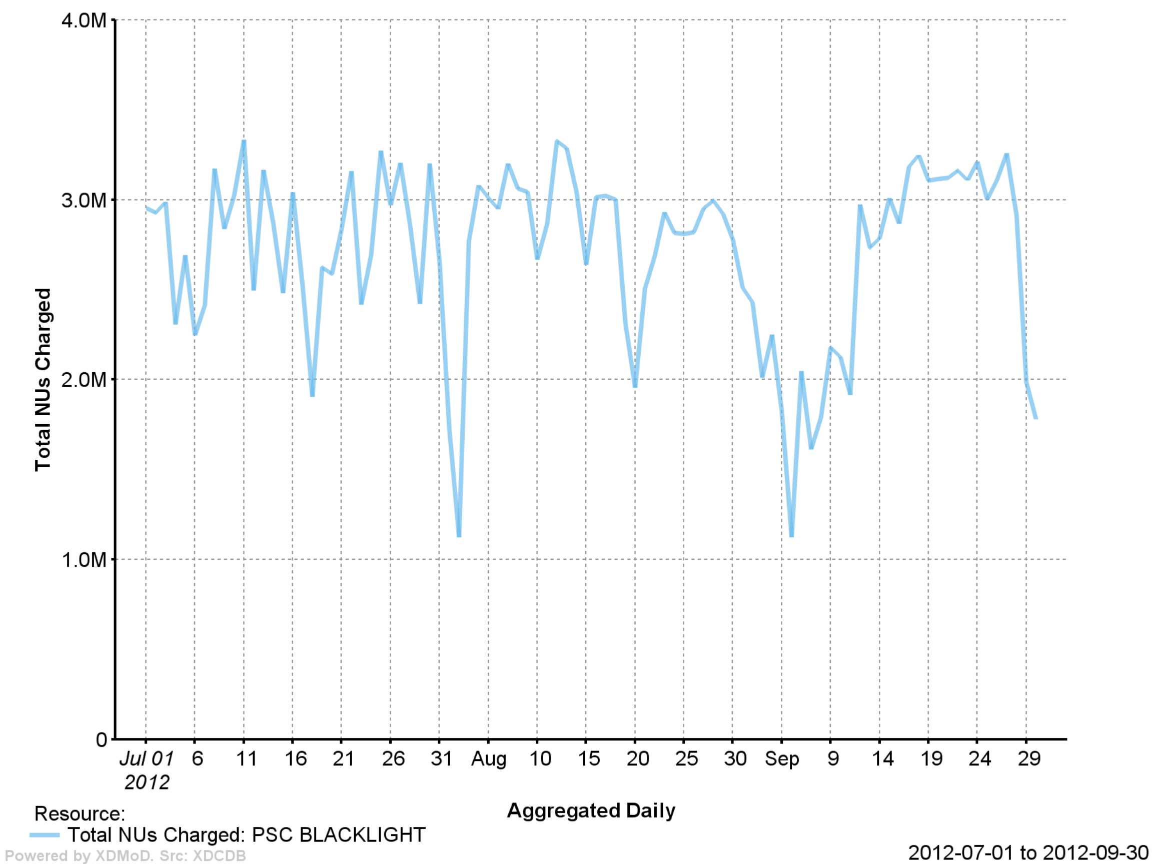
The following ten charts of standard system metrics for *Blacklight* were provided by the XDMoD service of the Technology Audit Services team.

PSC-BLACKLIGHT Quarterly Report

Total NUs Charged by Resource

Service Provider = PSC

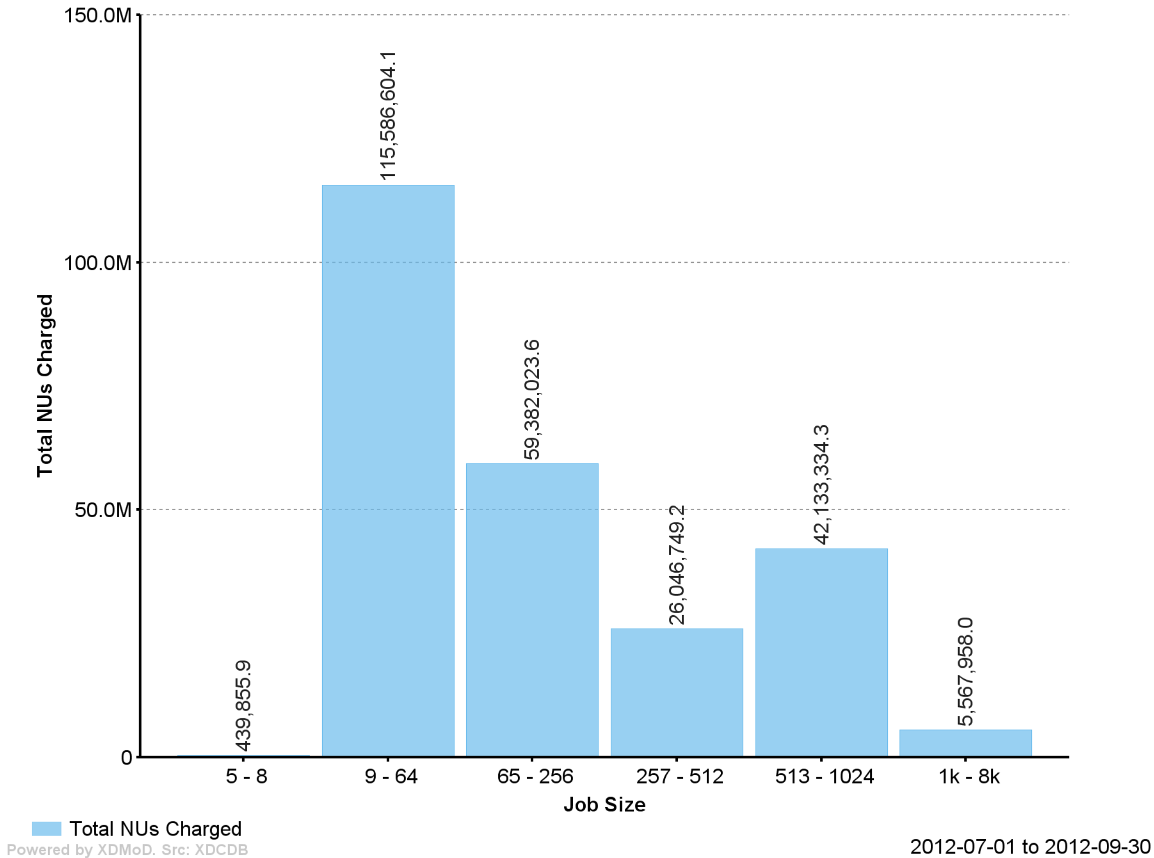
2012-07-01 to 2012-09-30



Total NUs Charged by Job Size

Resource = PSC-BLACKLIGHT

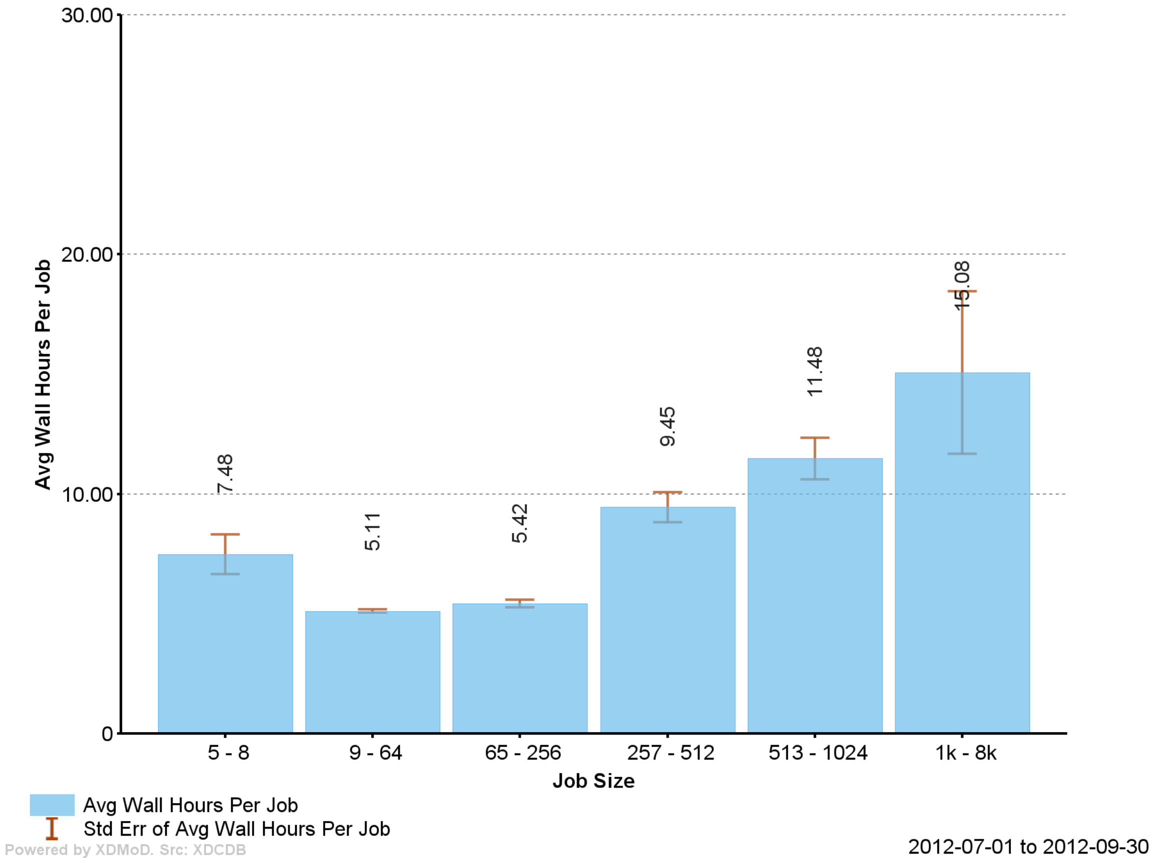
2012-07-01 to 2012-09-30



Avg Wall Hours Per Job by Job Size

Resource = PSC-BLACKLIGHT

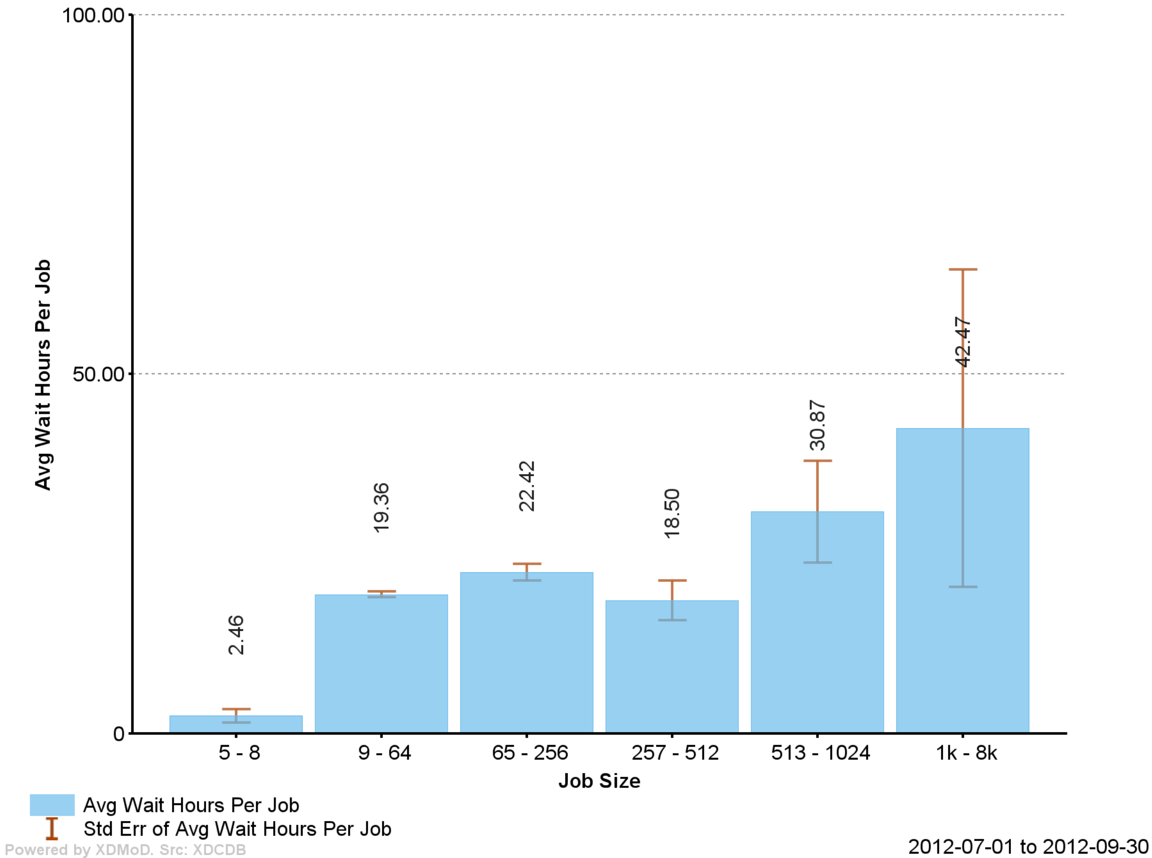
2012-07-01 to 2012-09-30



Avg Wait Hours Per Job by Job Size

Resource = PSC-BLACKLIGHT

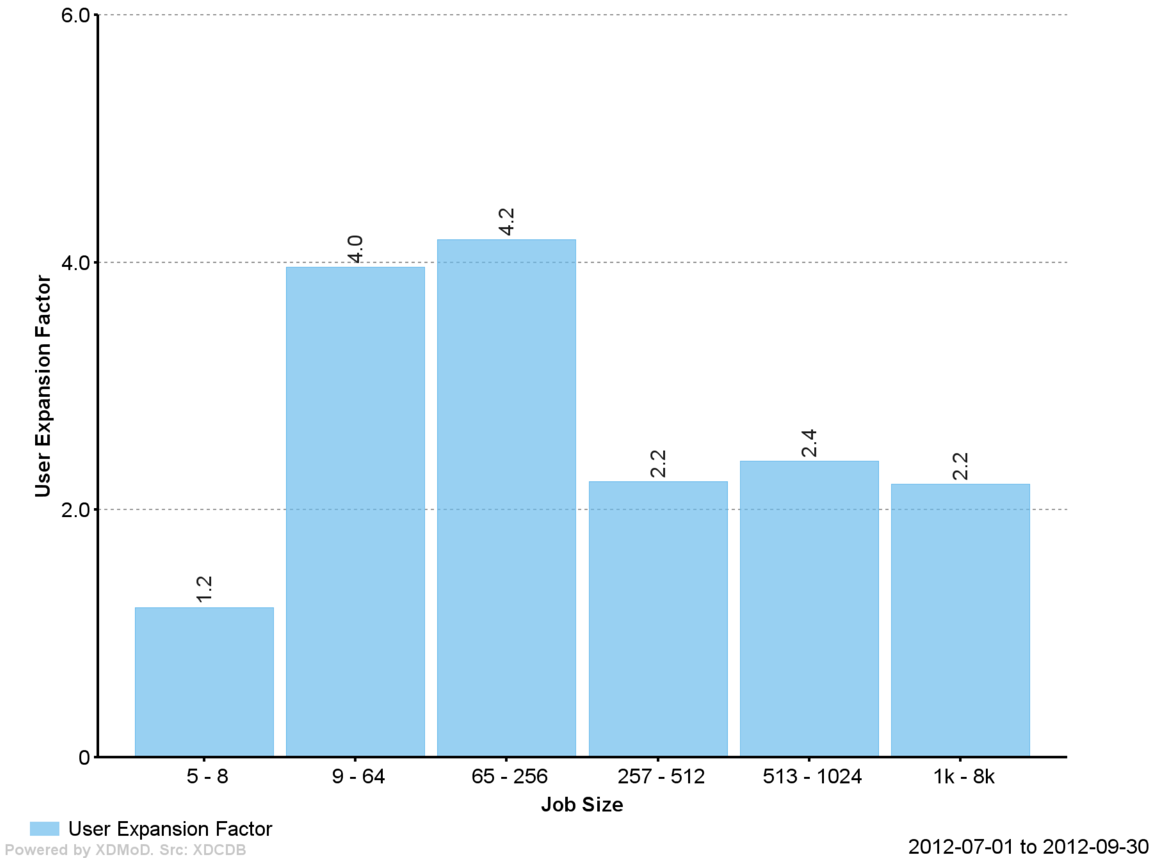
2012-07-01 to 2012-09-30



User Expansion Factor by Job Size

Resource = PSC-BLACKLIGHT

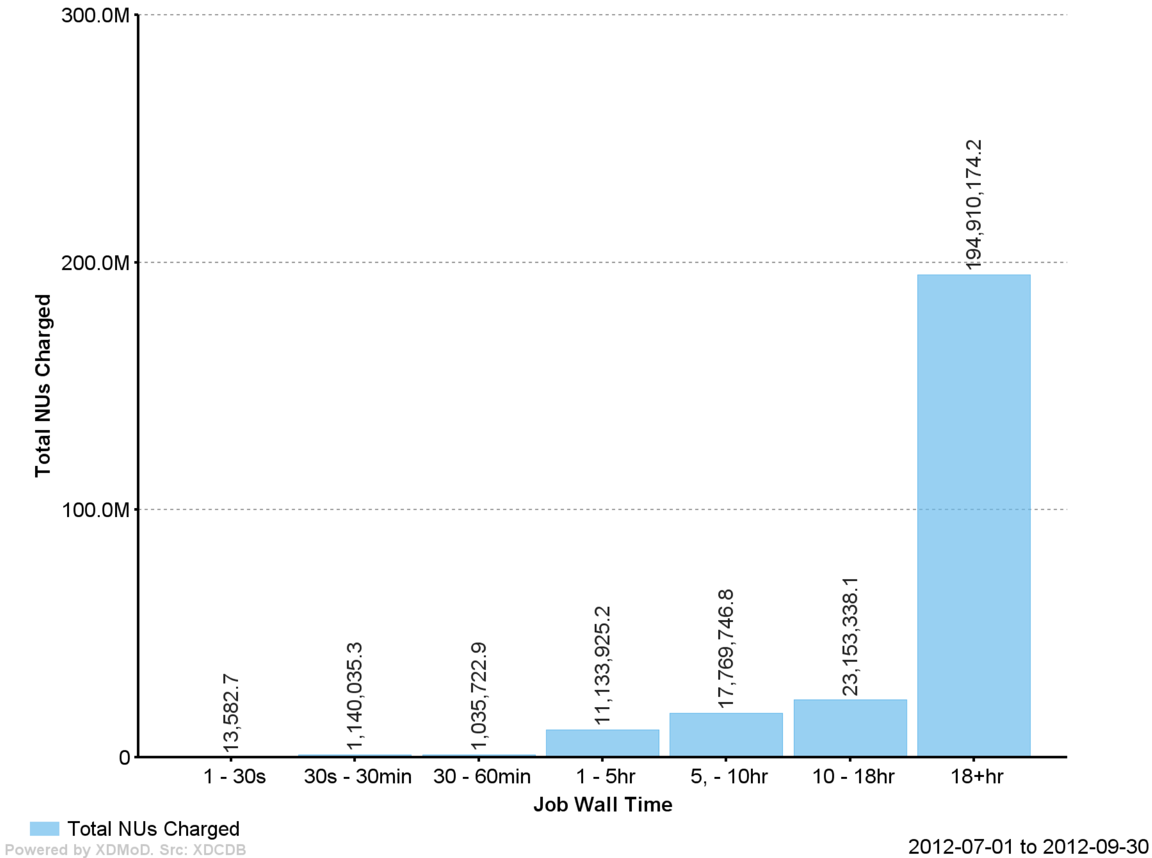
2012-07-01 to 2012-09-30



Total NUs Charged by Job Wall Time

Resource = PSC-BLACKLIGHT

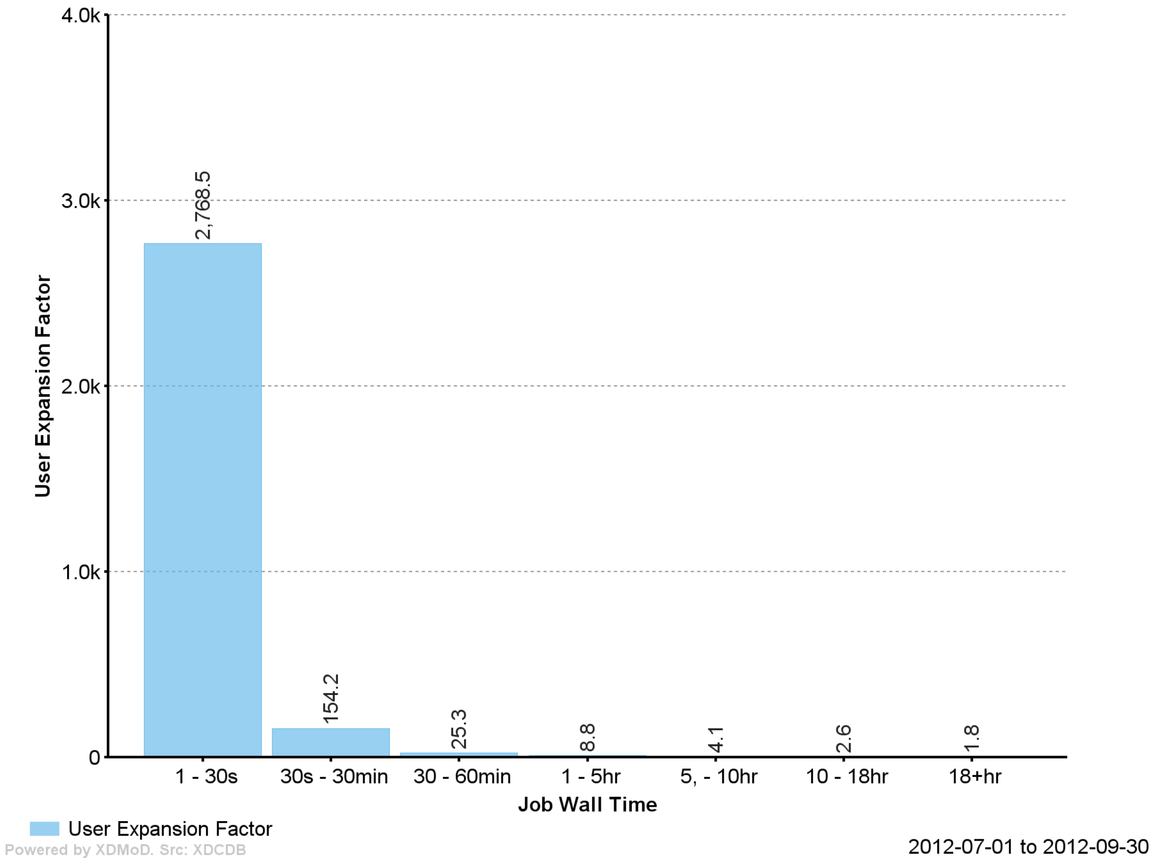
2012-07-01 to 2012-09-30



User Expansion Factor by Job Wall Time

Resource = PSC-BLACKLIGHT -- Service Provider = PSC

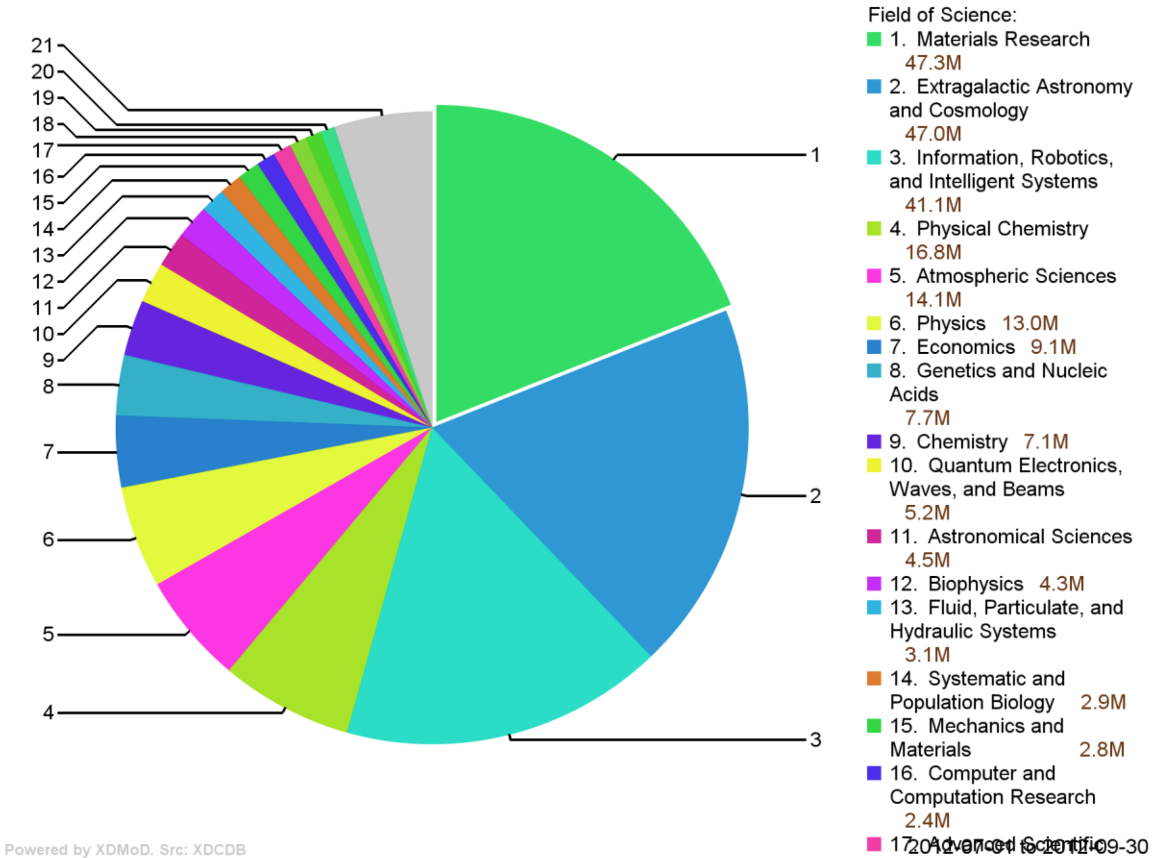
2012-07-01 to 2012-09-30



Total NUs Charged by Field of Science

Resource = PSC-BLACKLIGHT

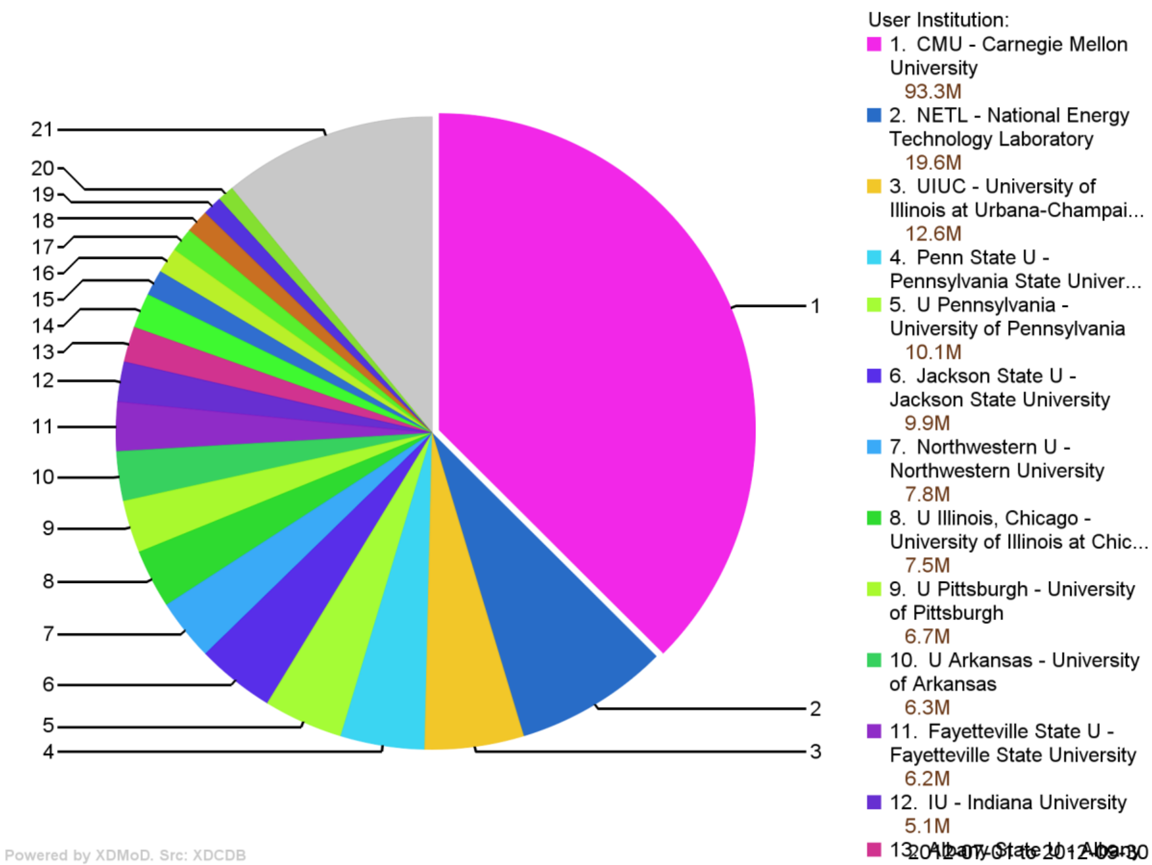
2012-07-01 to 2012-09-30



Total NUs Charged by User Institution

Resource = PSC-BLACKLIGHT

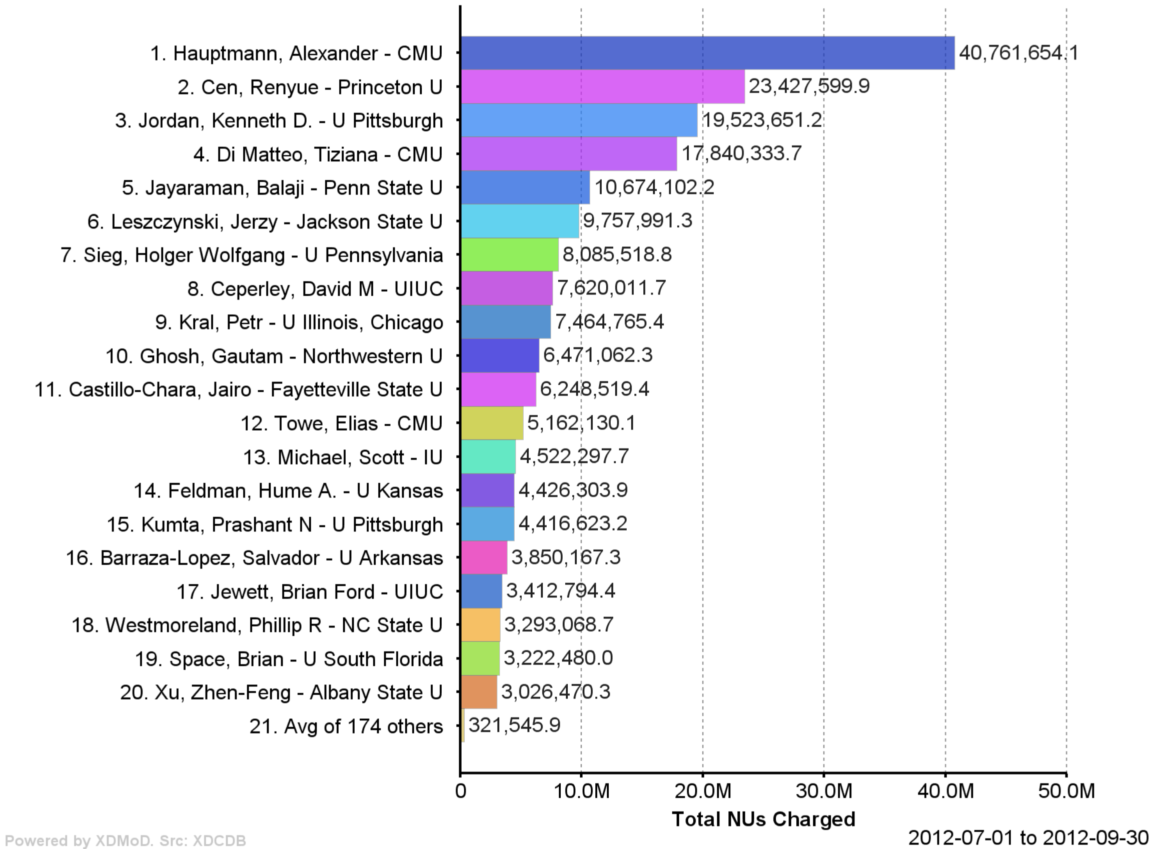
2012-07-01 to 2012-09-30



Total NUs Charged by PI

Resource = PSC-BLACKLIGHT

2012-07-01 to 2012-09-30



18 Purdue University - Service Provider Quarterly Report

18.1 Executive Summary

The Purdue SP provides an HPC cluster (Steele), a high-throughput computing resource (the Purdue Condor pool), and a cloud resource (Wispy) to XSEDE community XSEDE's resource allocation process. The SP operates the systems and provides helpdesk and user support, as well as participate in XSEDE-wide operations, security, software, training and outreach activities. Purdue contributes its expertise in HPC, high-throughput computing, virtualization and science gateway development to assist XSEDE users through training events, tutorials and demonstrations, as well as to the XSEDE ECSS staff on its conference calls and at conferences. These activities are funded by the NSF awards #0503992, #0932251. Purdue XSEDE resources have supported 152 users (95 projects) from 70 institutions during the reporting quarter. More 600K science gateway jobs were completed on the Purdue SP resources during this quarter.

As a service provider, Purdue continues to support a number of science gateways which provide XSEDE resource-powered scientific simulation and modeling tools, to bridge OSG computation high-throughput HPC (HTHPC) jobs to XSEDE resource, and to develop, deploy virtualization tools to support scientific users of cloud resources as part of the joint TeraGrid-OSG project ExTENCI. Purdue SP staff also supports and contributes to various XSEDE EOT activities and campus information technology community.

Purdue continues to contribute to the XSEDE project by leading the Campus Champions program, providing OSG liaison to help users utilize OSG resources and leverage OSG user support and training activities, and providing extended collaborative support to help XSEDE users who need in-depth assistance. A total of 16 new campus champions from 14 institutions have joined XSEDE in this quarter. A survey of campus champions was conducted at XSEDE12 with more than 60 champions attended. Purdue staff provided technical support to 14 campus champions during the quarter. More details of these XSEDE activities are being reported in the overall XSEDE report.

18.1.1 *Resource Description*

Steele

The Steele cluster consists of 893 dual quad-core Dell 1950 compute nodes, running Red Hat Enterprise Linux, version 4. Each node thus has 8 64-bit Intel 2.33 GHz E5410 CPUs and either 16 GB or 32 GB of RAM. They are interconnected with either Gigabit Ethernet or InfiniBand. The machine offers access to the 120 TB scratch space. Steele's peak performance is rated at 66.59 TFLOPS. Steele cluster is well suited for a wide range of both serial and parallel jobs. Steele replaced the Purdue Lear cluster and was made available to TG users in May 2008. Its projected useful lifetime is through July 2013. In October 2009, Purdue RP has increased the TG *dedicated* portion of Steele from 22 nodes to nearly 200 nodes (1600 cores). Steele has no effective runtime limit on XSEDE jobs. Additionally, XSEDE users may leverage the larger Steele cluster by utilizing the standby queues with no node limit but subject to 4 or 8 hour runtime limits.

Condor Pool

The Purdue Condor pool is a shared resource among the resource owners (academic users at Purdue) and XSEDE/OSG users. Consisting of approximately 50,000 processor cores, the Condor pool is an opportunistic resource which allows Condor jobs access to machines that are not being used by their owners. The Purdue Condor pool is designed for high-throughput computing, and is excellent for parameter sweeps, Monte Carlo simulation, or most any serial application. In addition, some classes of parallel jobs (master-worker) may be run effectively in Condor. 30% of all Condor-usable cycles are available to XSEDE users at a minimum level of service. On average the Purdue Condor pool is able to provide up to 10 million CPU hours to XSEDE users per year.

The Purdue Condor resource, recently named *DiaGrid*, has expanded tremendously from a total of 7700 CPUs at the end of 2007 to its current size of about 50,000 cores (system information shown in Table 1). The Purdue Condor pool consists of nodes from 10 institutions, including Purdue's West Lafayette campus, University of Wisconsin-Madison, University of Nebraska-Lincoln, Indiana University, University of Notre Dame, and a number of Purdue's regional campuses. Memory on most of the compute nodes is 1 GB, 2 GB and 4 GB per core, while a small number of nodes have larger memory (e.g., 10GB per core). With a total of approximately 390 TFLOPS available, the Purdue Condor pool can provide large numbers of cycles in a short amount of time. All shared areas and software packages available on Steele are available on Condor. Available to TeraGrid/XSEDE users since 2006, the Condor pool is self-renewing as old machines in the pool are retired and new ones, e.g., from Purdue's community clusters, added over time.

Table 1: Purdue Condor pool information as of July 31, 2012

System Information	Cores	Total Memory	Local Interconnect	Processor Speed
X86_64 LINUX	49,100	129 TB	IB, 10 Gb or 1 Gb Ethernet	Various (2.1, 2.33, 2.5, 3.2 GHz)
INTEL & X86_64 WINDOWS	409	1.09 TB	1 Gb or 100Mb Ethernet	Various (2.13, 2,66, 3.6GHz)
INTEL LINUX	44	66 GB	1 Gb or 100Mb Ethernet	various
Total	**49,553**	**130 TB**		

Wispy

Purdue's *Wispy* is a special XSEDE resource, a cloud computing platform for research and education use. Wispy consists of 8 64bit, 16-core HP SL230 connected via 1 Gigabit Ethernet network with the capacity of supporting 128 VMs. Wispy runs KVM and the Nimbus cloud software. It provides users with the capability of packaging their applications and operating systems completely inside the Virtual Machine (VM) images, submitting these VMs to run in Wispy with up to 14 CPUs and 32GB of memory each, and have full control over the execution environment. Current usage includes small, instant, on-demand clusters for various tasks and running complicated or prepackaged applications on additional hardware resources.

18.2 Science Highlights

Extragalactic Astronomy: An Ultraviolet-to-Infrared Census of Dust in the Local Universe
PI: Karl Gordon, Space Telescope Science Institute.

Karl Gordon, whose motto is "Have Dust-Will Study," isn't looking to sweep that dust under the rug. It would take a mighty big rug to do so in any event because what Gordon, an astronomer at the Space Telescope Science Institute, focuses on in his research is dust of interstellar variety in the Milky Way and in other, nearby galaxies. His main interest is in understanding the nature of interstellar dust grains (size, shape and composition) and how they change from region to region in our Galaxy and other galaxies. He uses data from instruments observing from the ultraviolet through submillimeter frequency ranges and models galaxies using dusty radiative transfer, dust emission and stellar evolutionary synthesis codes. He employs Monte Carlo methods in his modeling and the parameter sweeps involved make the large computational resources XSEDE is able to provide essential. This type of computation is best suited for high-throughput computing systems such as the Purdue Condor pool. In the past 12 months, the group's work has consumed more than 2 million processor hours, completing more than 203K jobs on the Purdue Condor pool. The densest regions of the interstellar medium, the matter that exists in space between the star systems of galaxies, are the incubators for new stars and dust plays a central role in star formation and galaxy evolution. Among other things, dust helps shape the interstellar medium and so directly influences the process of star formation. It is a crucial component of molecular clouds, often referred to as stellar nurseries, and is the main formation site for molecular hydrogen, a key ingredient for forming new stars. Some of the research findings have been published in the Astrophysical Journal: "Young, Ultraviolet-bright Stars Dominate Dust Heating in Star-forming Galaxies" Law, K.-H., Gordon, K. D., & Misselt, K. A. 2011, ApJ, 738, 124 (doi:10.1088/0004-637X/738/2/124).

18.3 User-facing Activities

18.3.1 System Activities

The Steele cluster continues to be busy and highly utilized by the XSEDE users during the reporting period. Steele continues to see higher allocation requests than its available cycles each quarter, and the trend is even higher demand in the September allocation cycle (as high as 62M SUs while only 8M SUs are available). XSEDE users access Steele through the XSEDE queues, and in addition to the NSF funded portion of the cluster, XSEDE users have access to the entire cluster through its standby queues with a wall clock limit of 4 hours for the jobs. In this manner, XSEDE users typically consumes as high as three times of the cycles allocated for XSEDE on a monthly basis. Figure 1 illustrates the total usage on Steele by XSEDE users since July 2011. The trend line shows that the actual usage has doubled in the past year.

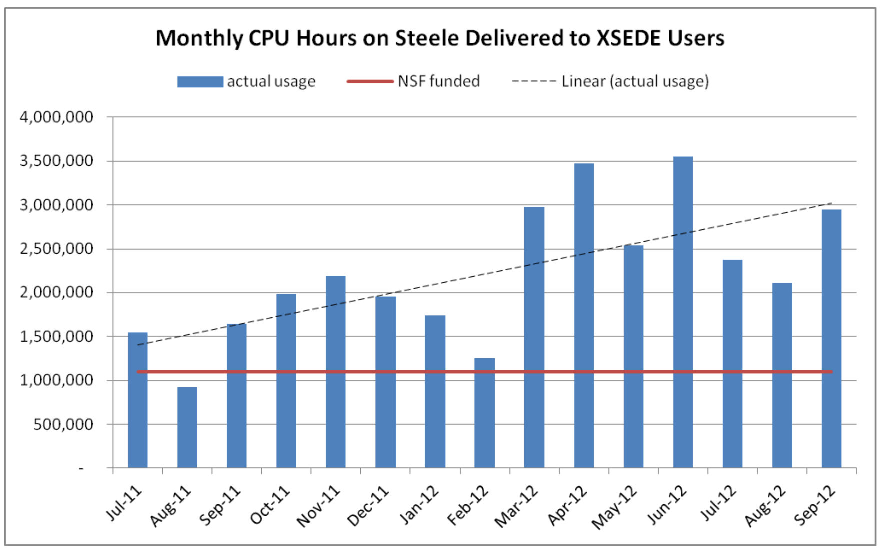


Figure 1. Usage of Steele delivered to XSEDE users, July 2011 – Sept. 2012

The SP strives to provide the highest level of system availability to its cluster users (see table of uptime percentages at right). There was an unscheduled downtime on Steele in August. The SP staff discovered a software bug and worked with the vendor to resolve a problem with the scheduler. Access to the Lustre filesystem was interrupted due to a power outage and was restored promptly.

	%Uptime (monthly)		
2012	Condor	Steele	Wispy
July	100%	100%	100%
Aug	100%	97%	100%
Sep	100%	100%	100%

Usage on the Wispy cloud resource includes those from the joint TeraGrid/OSG ExTENCI project in the development, testing of virtualization technologies for science users. Wispy was upgraded in July 2012 to new hardware based on Intel's Sandy Bridge series of processors. The SP staff resolved a few configuration issues after the update and kept it running since. The SP staff has revamped the authentication on Wispy, simplifying the process for XSEDE users and providing clear documentation for Wispy access (https://www.xsede.org/web/guest/purdue-wispy). Currently, Wispy is available to XSEDE users. Non-XSEDE users can request access directly from Purdue SP.

18.3.2 Services Activities

Purdue SP provides both helpdesk support and consulting support to XSEDE users. The SP user support staff worked with many XSEDE users during the quarter. Most of the support requests were related to troubleshoot issues. Categories of user issues and requests are summarized in the table in Section 1.9.2.

18.4 Security

During this quarter, Purdue SP disabled two XSEDE accounts due to compromises at other SP sites.

18.5 Education, Outreach, and Training Activities

18.5.1 EOT Events

Type	Title	Location	Date(s)	Hours	Number of Participants	Number of Under-represented people	Method
Conference talk	"WaterHUB: Enabling hydrological exploration, modeling and collaboration", HUBbub 2012 conference	Indianapolis, IN	9/25/2012	0.33	40-50	n/a	live
Demonstration	"Simulating land use change at a national scale with fine resolutions" presented at the Visualization Showcase, *XSEDE 2012 Conference*	Chicago, IL	7/18/2012	2	Approx. 150?	n/a	Live demo
Conference presentation	"WaterHUB – A Resource for Students and Educators for Learning Hydrology", EOT track presentation at XSEDE12 conference	Chicago, IL	7/17-20, 2012	.5	25-30	n/a	Live
Tutorial	"Selecting and Using XSEDE Resources for Maximum Productivity" by Kim Dillman at the XSEDE12 conference	Chicago, IL	7/16/2012	4	Approx. 20	n/a	Classroom, hands-on

Tutorial	"High-Throughput Computing With XSEDE", Kim Dillman contributing with other co-authors at XSEDE12 conference	Chicago, IL	7/16/2012	4	Approx. 10	n/a	Classroom, hands-on
Tutorial	"DiaGrid and Blast", tutorial of running BLAST app on DiaGrid	West Lafayette, IN	9/19/2012	2	20	n/a	Live

18.5.2 Education

Purdue SP continues to recruit and involve students to work on the SP staff team and train them in advanced system administration, software maintenance, and scientific application support. The SP is currently funding one undergraduate student, Wesley Weber, to assist with system administration tasks. Wesley is a second year computer engineering student. He handles hardware fixes and front line support for the SP staff. We have added two graduate students to the staff to provide application support to improve services and capabilities. They are assisting with online modeling tools (CESM, soil water assessment model (SWAT) and land data assimilation model (HRLDAS) on XSEDE resources and integrating data movement tools into these gateways to support large datasets.

18.6 SP Collaborations

The SP staff has worked with an USDA funded project (USDA-NIFA no. 2011-68002-30220), an integrated research and extension project working to improve farm resilience and profitability in the North Central Region by transforming existing climate information into usable knowledge for the agricultural community. The researchers in this project are conducting modeling and data synthesis which often require long runs on resources such as those available on XSEDE and high performance data storage. The SP staff is assisting the research group to investigate how to make the large number of simulation runs manageable by designing workflows, identifying appropriate resources, as well as assisting with data processing tasks.

The SP collaborates with an NSF funded SI2 project, HydroShare, to develop interoperable tools and an online collaborative environment for scientists to easily discover and access hydrologic and related data and models, retrieve them to their desktop, and perform analyses in a high performance computing environment. This project aims at leveraging national cyberinfrastructure such as the XSEDE resources and services to accomplish the comprehensive set of goals of the project. The Purdue team will contribute its expertise in HPC and HTC, knowledge of XSEDE resources, and the experience with science gateway development to the hydrologic CI project.

18.7 SP-Specific Activities

The Purdue SP continues to support science gateways that utilize advanced cyberinfrastructure including XSEDE, OSG, campus clusters, and HUBzero collaboration platforms. One of the highlights – we are preparing for an official release of the Community Earth System Model (CESM) science gateway in late 2012. Growing out of an TeraGrid science gateway project where Purdue SP collaborated with NCAR and NOAA teams, this portal now integrates online modeling using the latest CESM codes, comprehensive metadata generation, data publishing (to Earth System Grid at NCAR), post processing, and NOAA-PMEL's Live Access Server to visualize, subset and access in different ways of geo-referenced scientific data.

In support of the WaterHUB project (funded by NSF CI-TEAM program), the SP staff ported the latest version of the watershed simulation model SWAT (Soil Water Assessment Tool) to Linux and enabled it on XSEDE (Steele). This science gateway has been used by hydrologic engineering students. WaterHUB will be released to production in the fall.

18.8 Publications

V. Merwade, L. Zhao, C. X. Song. WaterHUB – A resource for students and educators for learning hydrology. XSEDE 2012 Conference, Chicago, IL, July 16-19, 2012.

18.9 Metrics

18.9.1 Standard User Assistance Metrics

Purdue SP ticket resolution times by category from XSEDE ticket system:

Time to Resolution	account issues	file systems	grid software	jobs/batch queues	login/access issues	mss/data issues	network issues	software/apps	system issues	other
0-1 hr										
1-24 hr					1					
1-7 d	1	1		12	3	2			6	6
1-2 wk	1			7	2			1	6	
> 2 wk				12	4	1		5	4	7
Still Open										

18.9.2

18.9.3 SP-specific Metrics

Purdue SP ticket summary:

Category	**Tickets Received**	**Tickets Closed**	**Activities**
account issues	7	7	custom group creation, training accounts, shell change
csa requests	0	0	
filesystems	4	4	quota increases, group change
gateways	0	0	
gpfs-wan	0	0	
grid software	1	1	measure energy consumption
inca test reports	9	9	MDS stale providers and failures
jobs / batch queues	32	31	
login / access issues	19	19	shell change, unable to login, .modules not working, GSI-SSH help, account not enabled, password questions, direct ssh
mss / data issues	1	1	disk quota exceeded
network issues	0	0	
other	5	4	Usage update, MDS providers, quota increase, shell

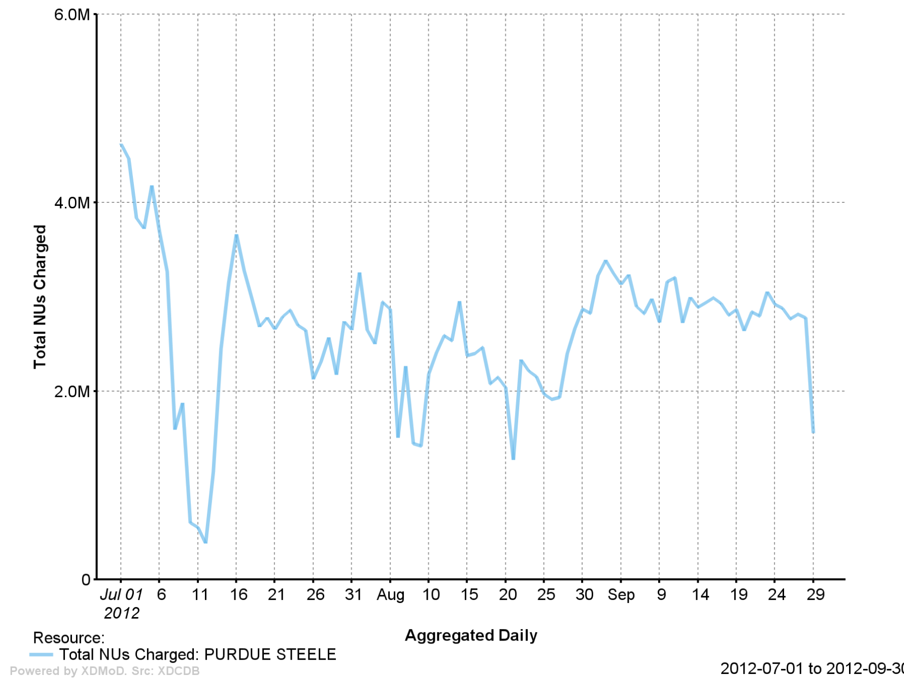
			change
refund request	0	0	
reservation request	0	0	
security	0	0	
software / apps	8	7	CPAN, NCO, MATLAB on Condor, condor questions, remaining SUs, iperf, NAMD
system issues	19	18	stale MDS providers, expired authentication certificates, SU conversion, extra storage
workshops	0	0	
TOTAL	105	101	

18.9.4 Standard systems metrics

PURDUE-STEELE Quarterly Report

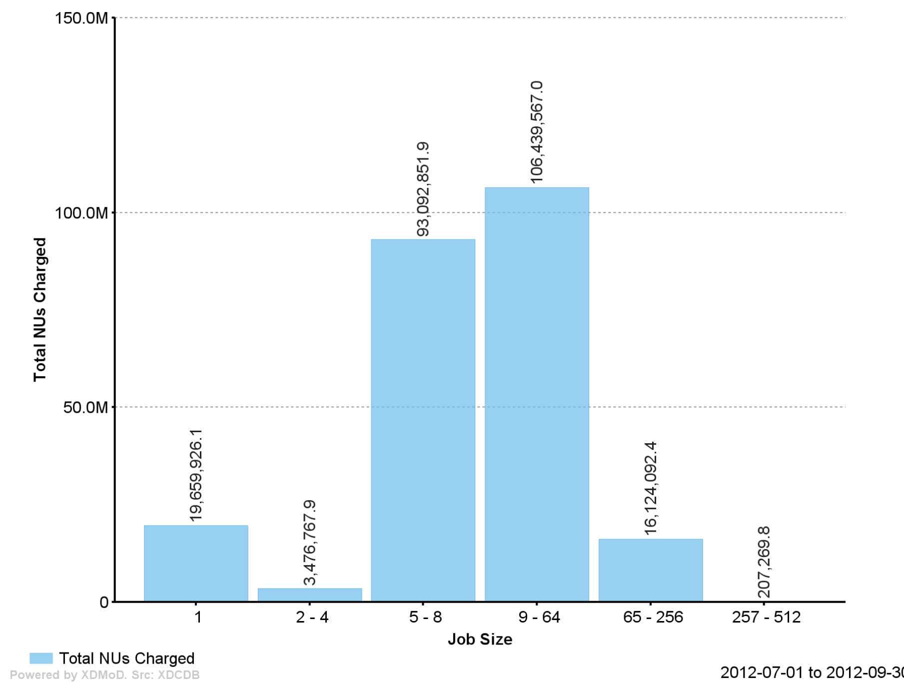
Total NUs Charged by Resource

Service Provider = PURDUE



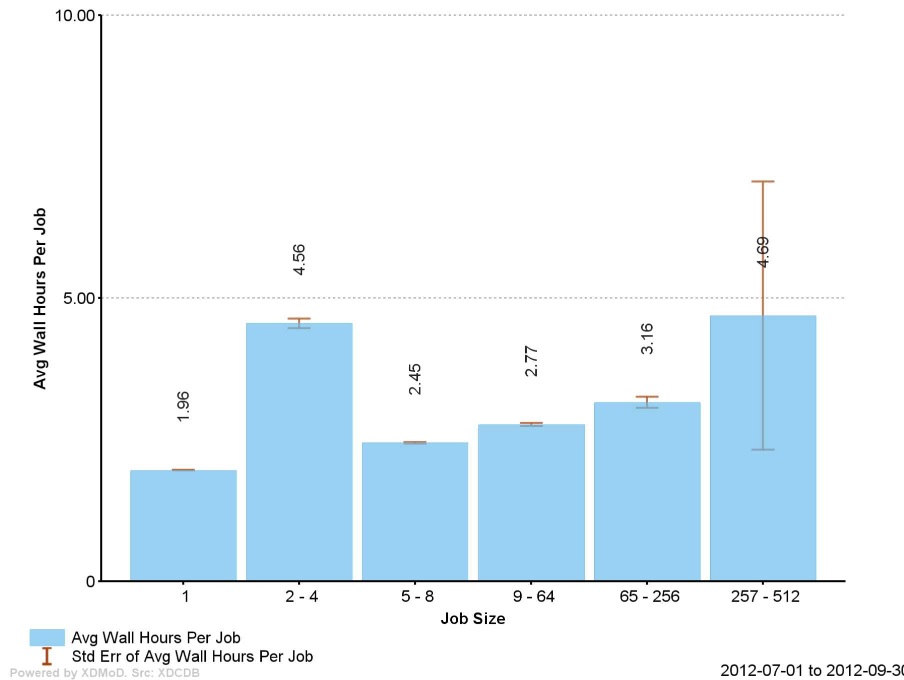
Total NUs Charged by Job Size

Resource = PURDUE-STEELE



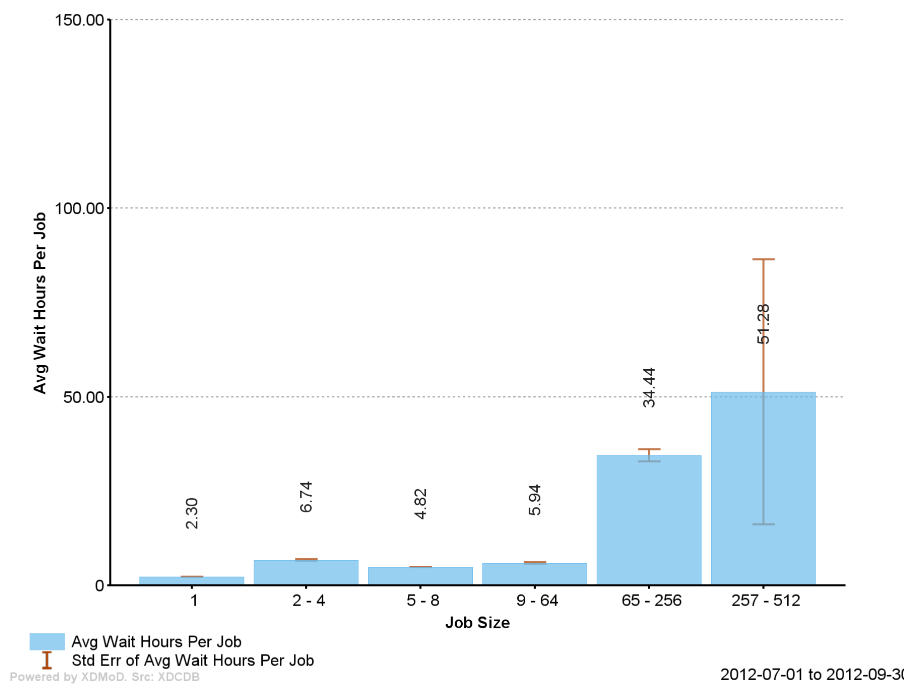
Avg Wall Hours Per Job by Job Size

Resource = PURDUE-STEELE



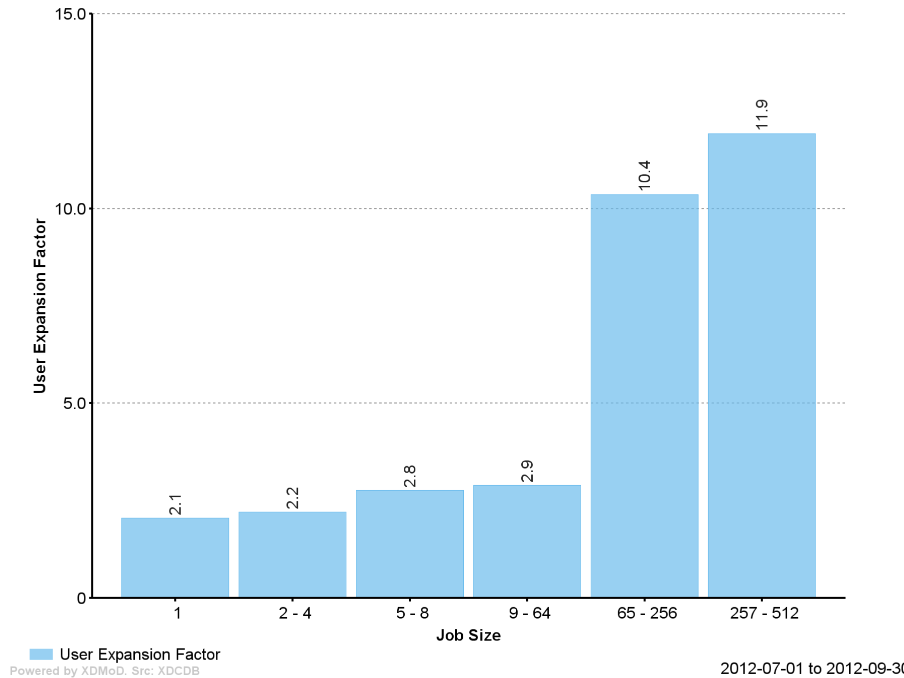
Avg Wait Hours Per Job by Job Size

Resource = PURDUE-STEELE



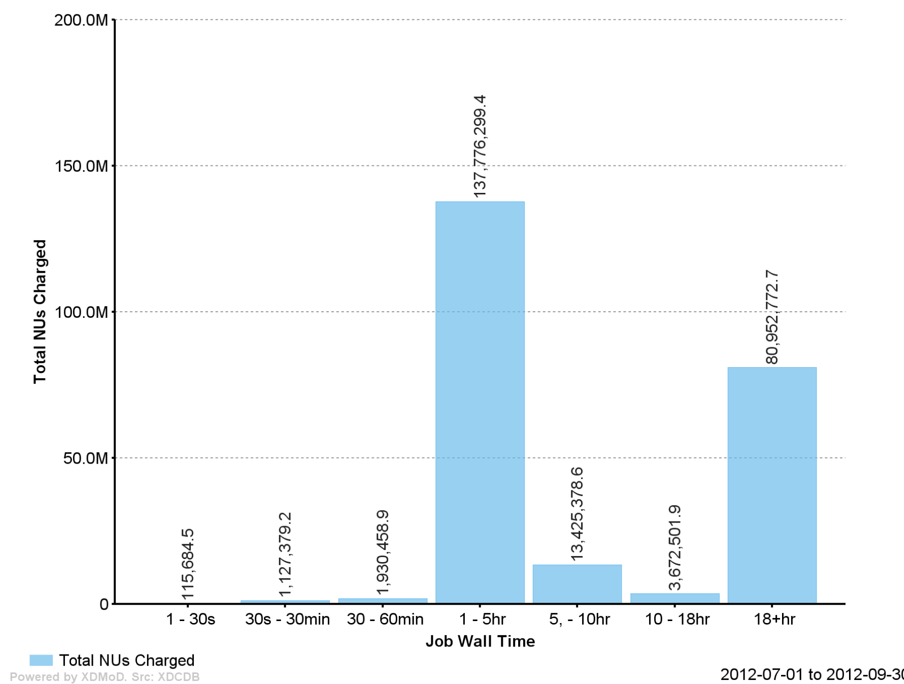
User Expansion Factor by Job Size

Resource = PURDUE-STEELE



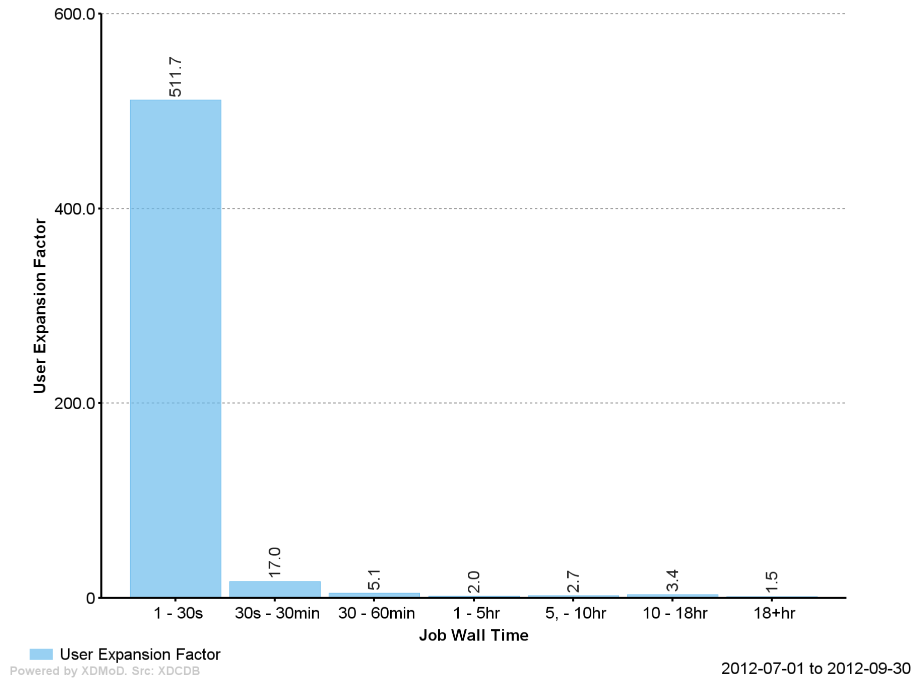
Total NUs Charged by Job Wall Time

Resource = PURDUE-STEELE



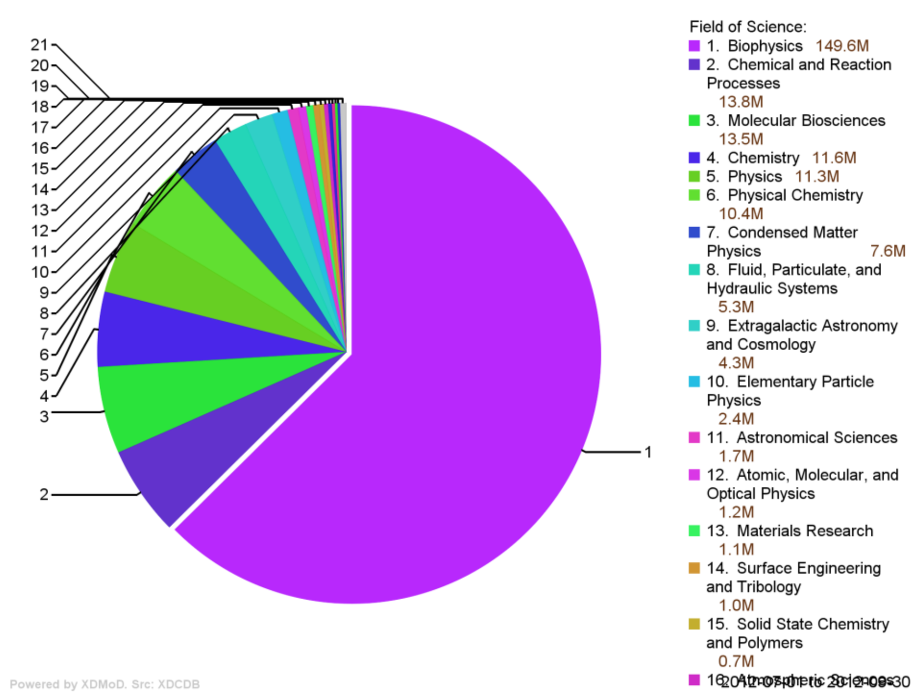
User Expansion Factor by Job Wall Time

Resource = PURDUE-STEELE -- Service Provider = PURDUE



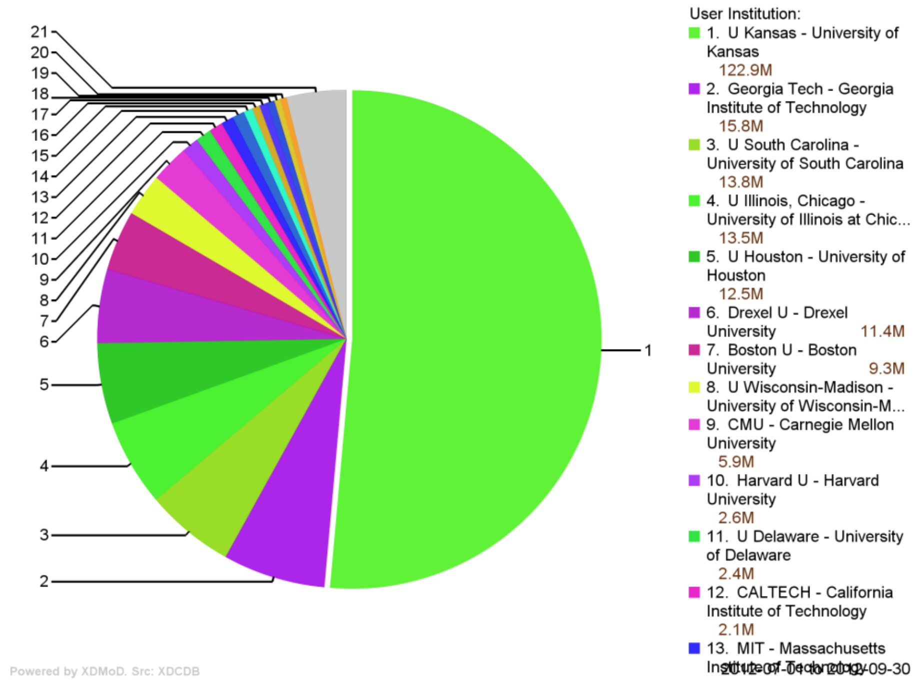
Total NUs Charged by Field of Science

Resource = PURDUE-STEELE



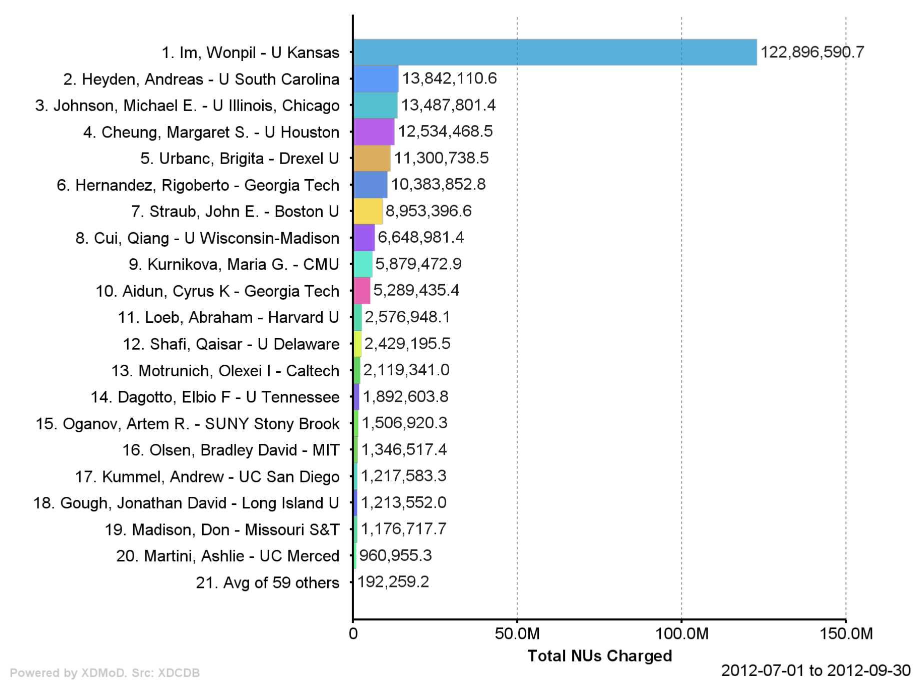
Total NUs Charged by User Institution

Resource = PURDUE-STEELE



Total NUs Charged by PI

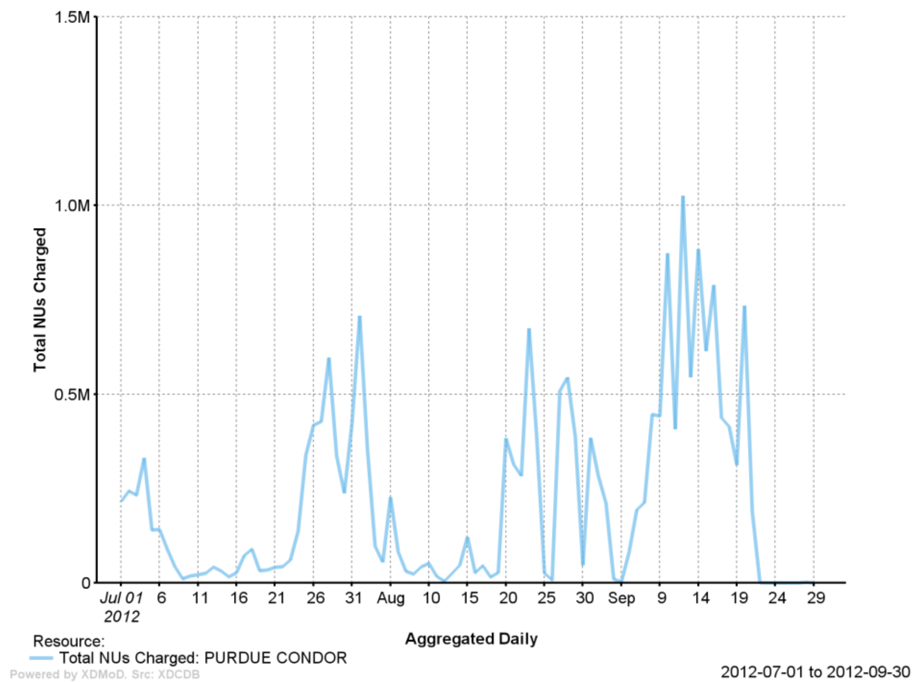
Resource = PURDUE-STEELE



PURDUE-CONDOR Quarterly Report

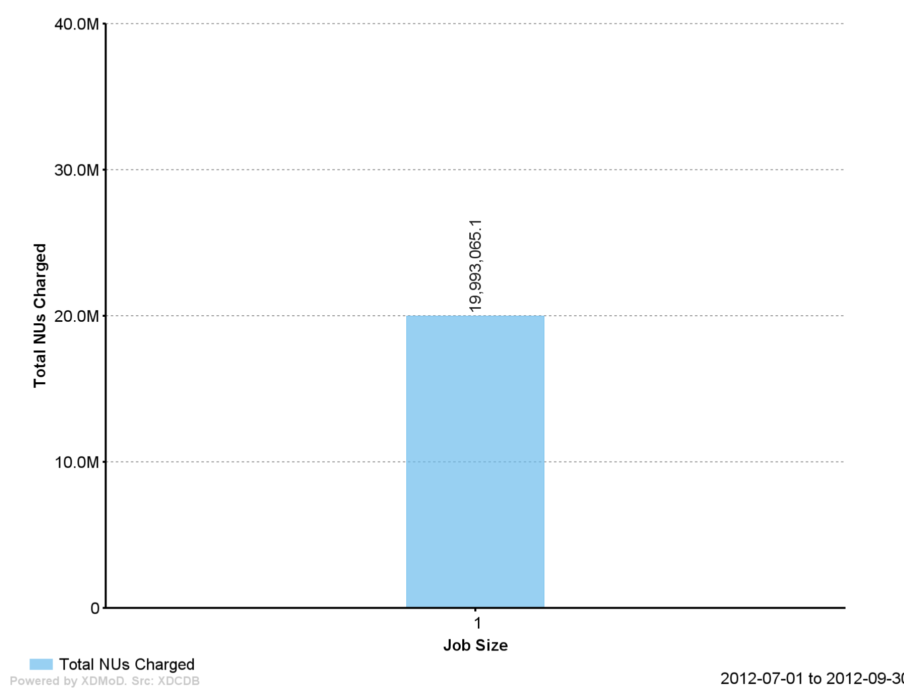
Total NUs Charged by Resource

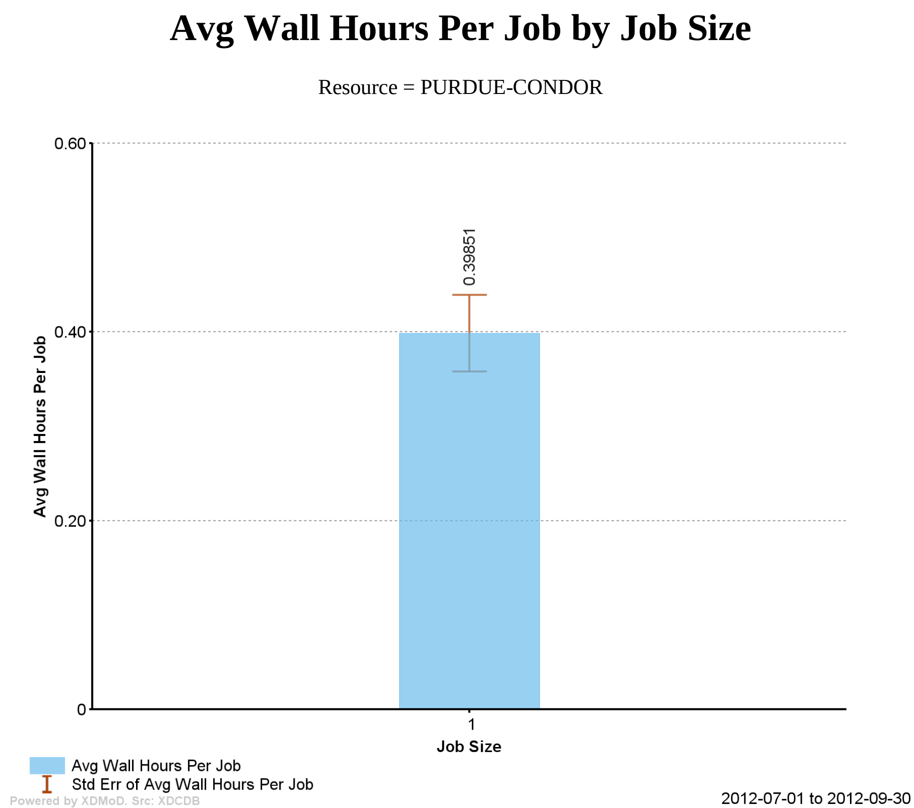
Service Provider = PURDUE



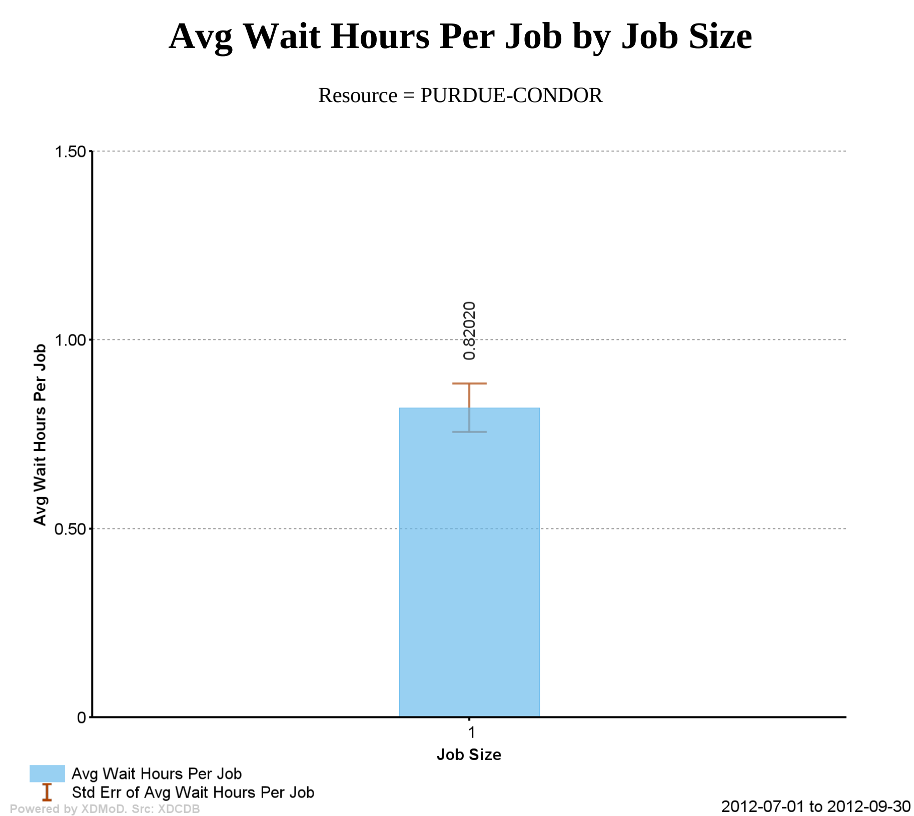
Total NUs Charged by Job Size

Resource = PURDUE-CONDOR





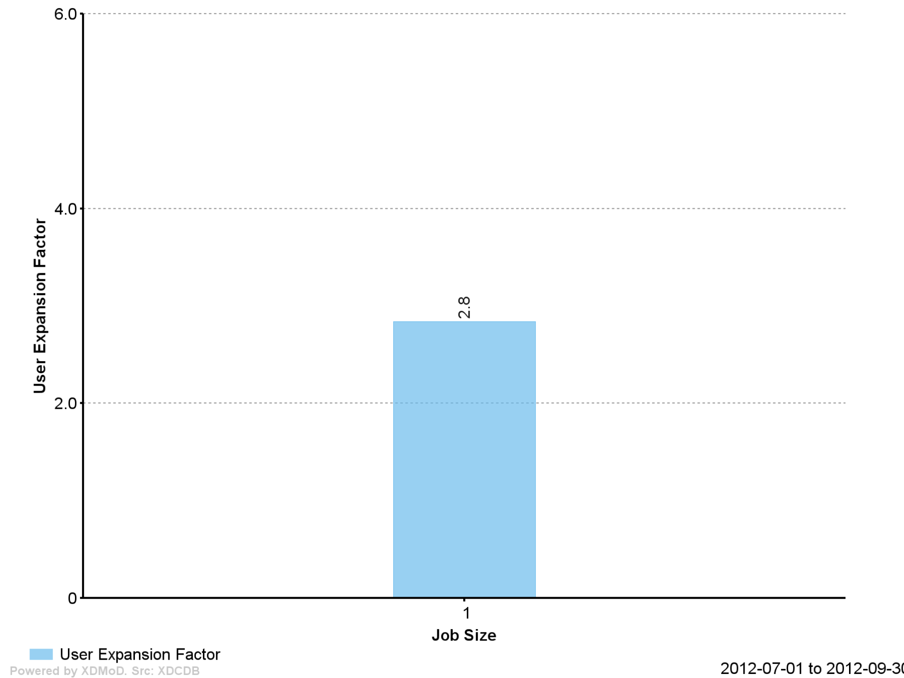
Avg Wall Hours Per Job by Job Size
Resource = PURDUE-CONDOR
0.60
0.40
0.20
0
0.39851
Avg Wall Hours Per Job
1
Job Size
Avg Wall Hours Per Job
Std Err of Avg Wall Hours Per Job
Powered by XDMoD. Src: XDCDB
2012-07-01 to 2012-09-30



Avg Wait Hours Per Job by Job Size
Resource = PURDUE-CONDOR
1.50
1.00
0.50
0
0.82020
Avg Wait Hours Per Job
1
Job Size
Avg Wait Hours Per Job
Std Err of Avg Wait Hours Per Job
Powered by XDMoD. Src: XDCDB
2012-07-01 to 2012-09-30

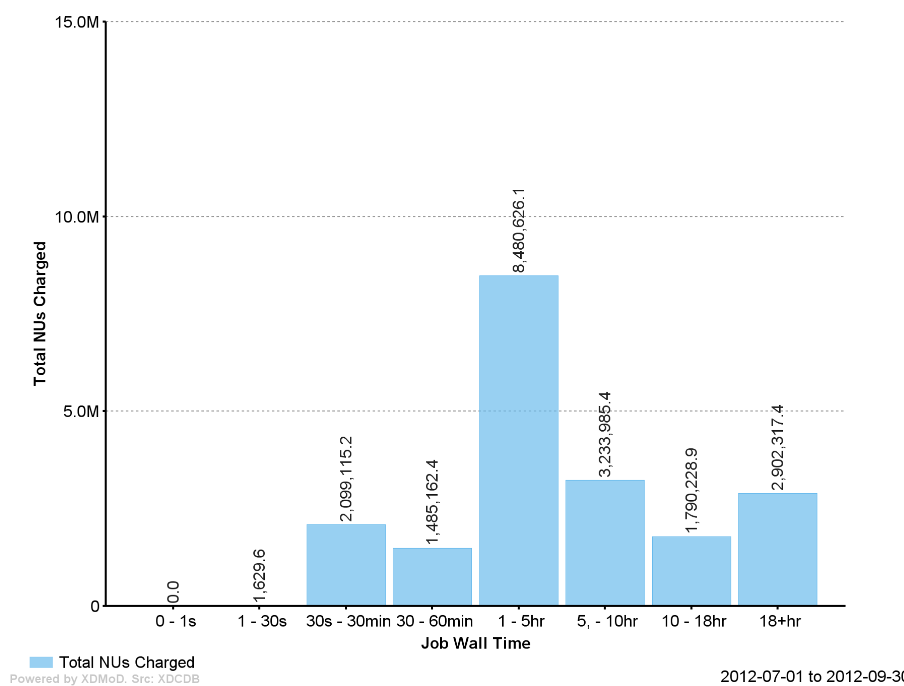
User Expansion Factor by Job Size

Resource = PURDUE-CONDOR



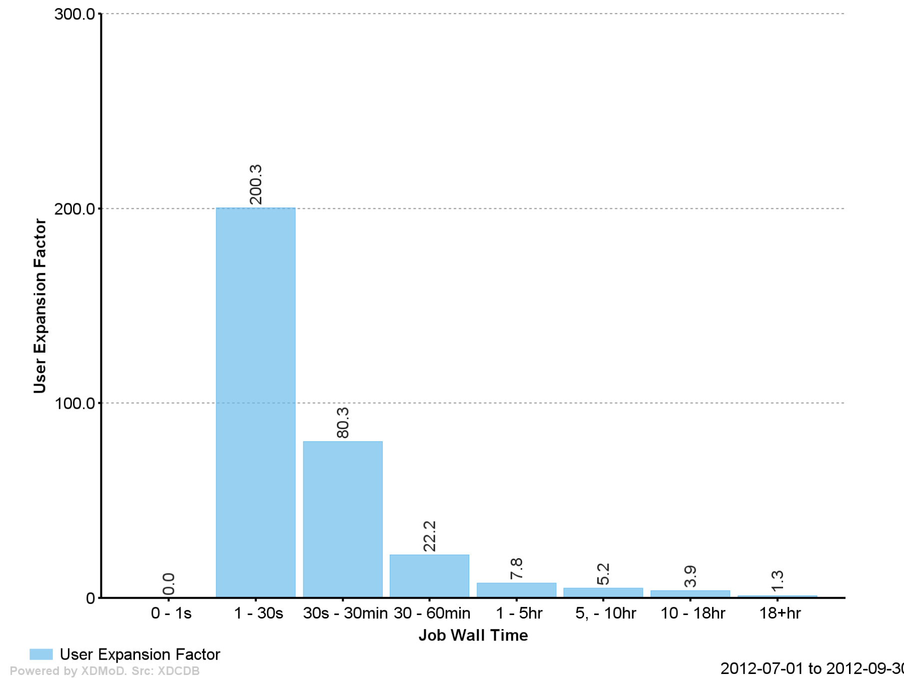
Total NUs Charged by Job Wall Time

Resource = PURDUE-CONDOR



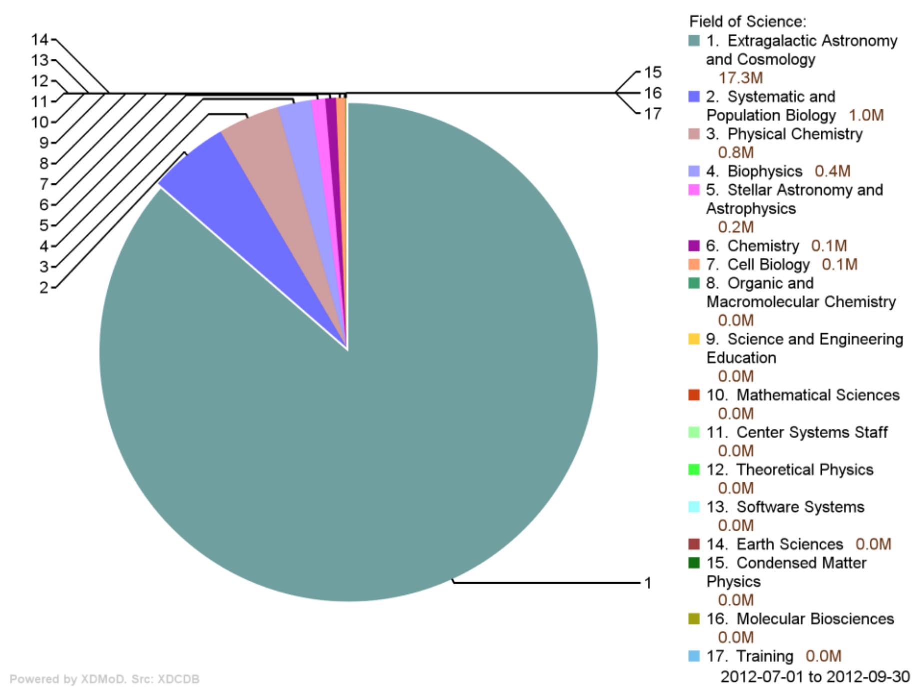
User Expansion Factor by Job Wall Time

Resource = PURDUE-CONDOR -- Service Provider = PURDUE



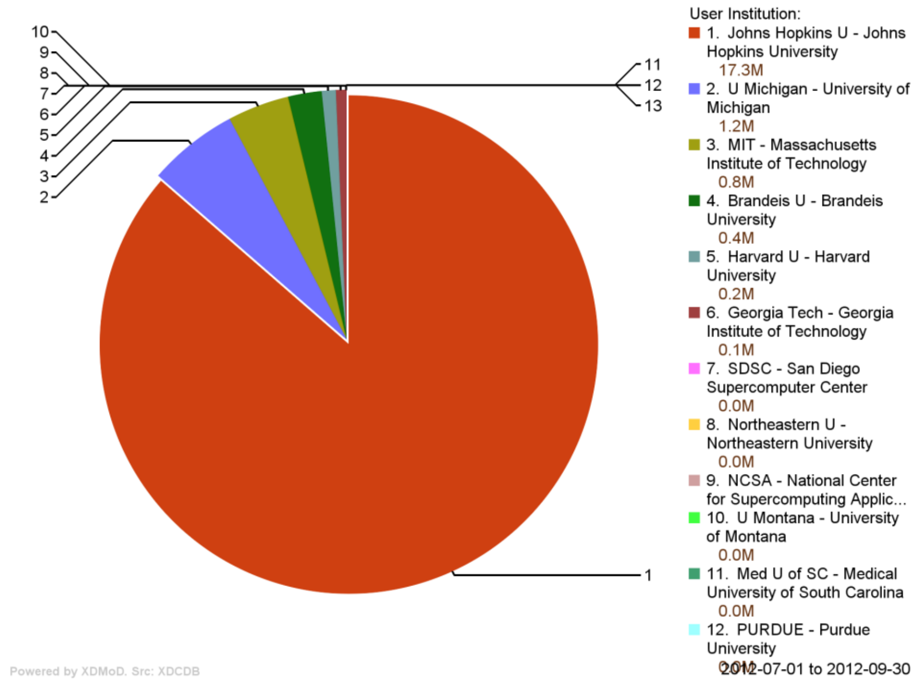
Total NUs Charged by Field of Science

Resource = PURDUE-CONDOR



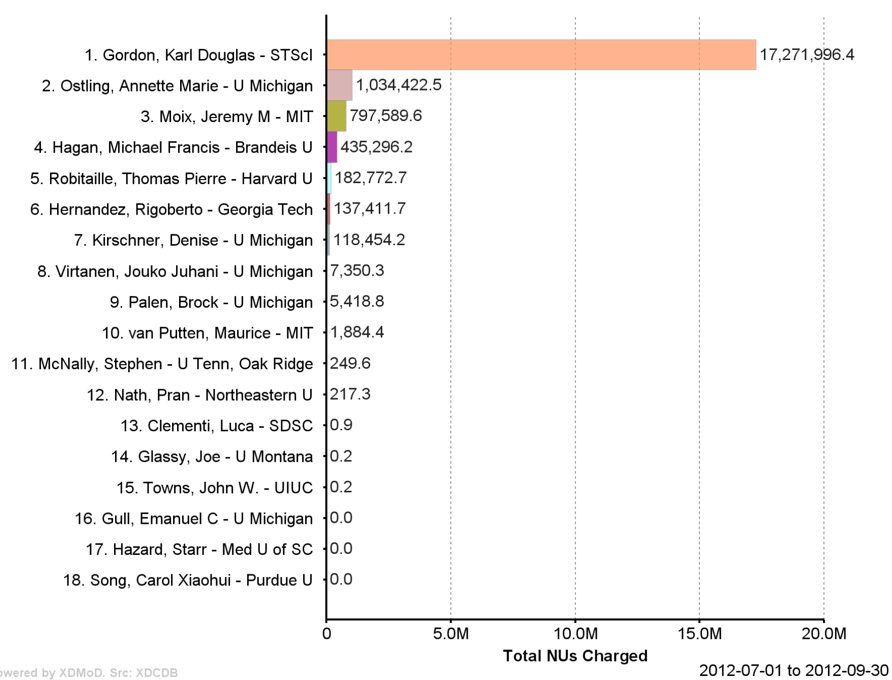
Total NUs Charged by User Institution

Resource = PURDUE-CONDOR



Total NUs Charged by PI

Resource = PURDUE-CONDOR



19 San Diego Supercomputer Center (SDSC) Service Provider Quarterly Report

19.1 Executive Summary

Gordon, which entered production XSEDE operations in Q1, 2012, completed its third quarter of operations during the reporting period. Gordon was conceived and deployed as the first XSEDE system to address challenges of data intensive computing. The use of massive amounts of flash memory, large memory nodes, and a high performance parallel file system are proving useful to researchers in a wide range of domains. Startup requests by users who are interested in exploring these features are increasing as are full XRAC requests. 25M SU's were awarded for a July 1, 2012 start date and the growth in requests makes it clear that Gordon will be fully allocated at its one year production anniversary.

Trestles is now in its seventh quarter of production and is successfully supporting the modest-scale/gateway user community, with a focus on user productivity and fast turnaround. The system is well over-requested in the allocation process. The system utilization and associated queue wait times have generally moderated from the high levels in 2012Q2 closer to the desired levels that are consistent with our allocations. Based on financial projections, we are committing to extend the operational life of Trestles at least through June 2014 (was December 2013).

SDSC continued with the project storage pilot project, having allocating roughly half of the 400TB of initial project storage. As noted previously, this resource will grow by another 2 PB in the coming months as part of the *Gordon* delivery by Appro.

After successfully migrating all data requested for retention by XSEDE and legacy users, SDSC decommissioned GPFS-WAN in June 2012 and its SAM-QFS tape archive in August 2012.

SDSC conducted a large number of effective education, outreach and training activities that engaged users, students and new user communities with conferences, summer workshops and education programs. Most notably, SDSC had a major presence at the XSEDE '12 meeting, contributing papers, invited talks, tutorials, and BOF's for both Trestles and Gordon. The paper, *Analyzing Throughput and Utilization on Trestles*, won best paper in the technical track.

SDSC conducted its annual summer institute which attracted 35 students from 20 different institutions. There were sections on using Gordon and Trestles, as well as tutorials on science gateways, OpenMP, TAU, shared memory programming, and visualization. Students were also given much free time in order to work on their projects and seek support from SDSC staff and other attendees.

SDSC hosted a 2-week summer school in astroinformatics, in conjunction with the University of California's High-Performance AstroComputing Center (UC-HiPACC) July 9-20. The summer school was designed to help the next generation of astronomers manage the ever-increasing amount of data generated by new instruments, digital sky surveys, and simulations.

19.1.1 Resource Descriptions

Gordon

Gordon is a dedicated XSEDE cluster designed by Appro and SDSC consisting of 1024 compute nodes and 64 I/O nodes. Each compute node contains two 8-core 2.6 GHz Intel EM64T Xeon E5 (Sandy Bridge) processors and 64 GB of DDR3-1333 memory. The I/O nodes each contain two 6-core 2.67 GHz Intel X5650 (Westmere) processors, 48 GB of DDR3-1333 memory, and sixteen 300 GB Intel 710 solid state drives. The network topology is a 4x4x4 3D torus with adjacent switches connected by three 4x QDR InfiniBand links (120 Gbit/s). Compute nodes (16 per switch) and I/O nodes (1 per switch) are connected to the switches by 4x QDR (40 Gbit/s). The theoretical peak performance of Gordon is 341 TFlop/s.

Trestles

Trestles is a dedicated XSEDE cluster designed by Appro and SDSC consisting of 324 compute nodes. Each compute node contains four sockets, each with a 8-core 2.4 GHz AMD Magny-Cours processor, for a total of 32 cores per node and 10,368 total cores for the system. Each node has 64 GB of DDR3 RAM, with a theoretical memory bandwidth of 171 GB/s. The compute nodes are connected via QDR InfiniBand interconnect, fat tree topology, with each link capable of 8 GB/s (bidirectional). Trestles has a theoretical peak performance of 100 TFlop/s.

19.2 Science Highlights

SDSC's *Gordon* Supercomputer Used in 61-Million-Person Facebook Experiment
A recently published study led by UC San Diego in collaboration with Facebook and done in part using large-scale simulations on the SDSC's data-intensive *Gordon* supercomputer, confirms that peer pressure helps get out the vote while demonstrating that online social networks can affect important real-world behavior. The study, published last month in the science journal *Nature*, found that about one-third of a million more people showed up at the ballot box in the United States on November 2, 2010 because of a single Facebook message posted on that Election Day.
Please see http://www.sdsc.edu/News%20Items/PR092012_fb_vote.html for the full story.

Researchers Reveal Behaviors of the Tiniest Water Droplets
A new study by researchers at UC San Diego and Emory University has uncovered fundamental details about the hexamer structures that make up the tiniest droplets of water, the key component of life – and one that scientists still don't fully understand. The research, recently published in *The Journal of the American Chemical Society (JACS)*, provides a new interpretation for experimental measurements as well as a vital test for future studies of our most precious resource. Moreover, understanding the properties of water at the molecular level can ultimately have an impact on many areas of science, including the development of new drugs or advances in climate change research. Researchers used SDSC's new data-intensive *Gordon* supercomputer, among other SDSC resources, to conduct the data-intensive simulations.
Please see http://www.sdsc.edu/News%20Items/PR081512_water_behavior.html for the full story.

19.3 User-facing Activities

19.3.1 System Activities

Key systems activities during the last quarter included:

- Supporting the UC-HiPACC International Summer School on Astro-Computation and SDSC Summer Institute
- Deploying "big flash" nodes on Gordon
- Testing parallel and network file systems for Gordon
- Lustre usage accounting

Beyond routine maintenance, much of the systems effort at the start of the quarter focused on customization and application installation in preparation for the UC-HiPACC International Summer School on Astro-Computation and SDSC Summer Institute. As detailed in the next section, several new applications were installed ahead of the HiPACC School and our Institute, including visualization, analysis, and performance tools. The topic of the third HiPACC Summer School was AstroInformatics, and Gordon supported the school in part through the use of a dedicated IO node providing a high-performance database accessible within the cluster over the 40Gb/s InfiniBand network, and publicly via a standardized HTTP protocol. This allowed students to upload data to the database from analysis jobs on Gordon, and easily query their results remotely. This pattern is being reused for other dedicated IO node projects.

Trestles's production configuration underwent little change, with most of the work on that system, other than application installation, aimed at maintaining a consistently low expansion factor. For Gordon, we continue to innovate with ways to access Gordon's flash storage for a variety of usage models. In September, one rack of Gordon was configured to have 4 "big flash" nodes. While each compute node in the rack retains its local SSD, the flash drives from each of the four associated IO nodes are aggregated to a single compute node, providing a 4.8TB SSD-backed file system accessed over a single hop on the InfiniBand fabric. These "big flash" nodes are intended for use by jobs accessing large datasets with a random IO pattern, while the remaining compute nodes in the rack suit jobs where the local SSD is sufficient. We recently began gathering statistics on per-job flash usage, and will report the observed patterns in the future. Looking forward, we have begun reassessing various parallel and network file system including Red Hat's GFS2, OrangeFS, and NFS/RDMA as tools to access flash storage across compute nodes in a single namespace.

Lustre quota accounting was implemented on all of the Data Oasis file systems, including Trestles' and Gordon's scratch areas, and our locally-allocated NSF project space. The Lustre quota system is primarily used for usage monitoring across all our Lustre file system, and for quota enforcement on the project space. We are incorporating our storage usage monitoring into Graphite, the same tool used for SDSC's recharge-funded storage services, such as the SDSC Cloud. Graphite allows for flexible data ingestion and querying, and our intention is to use it as our local usage database for allocated and non-allocated storage systems. Other work related to Data Oasis included design discussion for the 2PB expansion coming as a Gordon milestone.

Hardware and other outages on both Trestles and Gordon were minimal this quarter. At the end of August Gordon's primary management node suffered a motherboard failure, necessitating its migration to a spare chassis. This was invisible to the users, largely because of key services like batch and scheduling residing on a separate server and failover for the InfiniBand subnet manager working as expected.

19.3.2 Services Activities

Between the two tickets systems used to support Trestles and Gordon (the XSEDE ticket system and SDSC's local ticket system) a total of 483 tickets were created between July 1 and September 30, 2012. These tickets included account questions, file system issues, software requests, Globus support, code support, password resets, code optimizations and debugging, allocation refunds/problems, project space requests, software support, licensing queries, and resource availability. 414 of those tickets were closed, leaving 69 tickets that we are still working to resolve. The average time to close the tickets across the two systems was 8.9 days, with a median time of 3 days.

Gordon is now in its third quarter of operation and supporting users from 3 XRAC allocation cycles. Typical *Gordon* support included fielding questions and providing information on Gordon's system architecture, updating documentation, and software install requests. Testing of performance tools (PAPI, TAU, IPM) was completed and they were put into production. Network configuration was modified to allow for use of Hadoop via the IPoIB interfaces. Testing was completed, with networking monitoring to verify that the Hadoop traffic was going over the Infiniband interfaces. The Hadoop installation has now been opened for friendly users and will be put into production shortly.

In support of *Trestles* users, SDSC user services staff fielded questions on gridftp usage, allocations/accounts, new software installs, filesystem use/troubleshooting, and projects space requests. New software installs/support included parallel WIEN2K, bowtie2 (newest version), and tophat/2.0.4. New example scripts illustrating the use of SSD local scratch for multi-node runs were installed on the login nodes and provided to users who requested them. Additionally, a new version of VisIt software was installed and tested on both machines.

19.4 Security

We had two minor security incidents involving compromised user accounts this quarter. Three affected user accounts were disabled as a result of these incidents.

This quarter, we made improvements to the *gx-map* program suite to support several new certificate authorities recognized by XSEDE. Additionally, we began the process for the security assessment of the *Trestles* upgrade, though the vast majority of the work remains for next quarter.

In the coming quarter, we expect to continue with the above security assessment as well as continue to modify *gx-map* as needed to support the needs of the XSEDE community.

19.5 Education, Outreach, and Training Activities

Type	Audiences	Title	Location	Date(s)	Hrs	# Participants	# Under-rep.	Method *
		TRAINING						
Tutorial	F. D. G. U.	Harnessing the Power of Visualization: Concept to Execution	XSEDE 12 Chicago	Jul 16	4	15-20	5	S, live
Tutorial	F. D. G. U	Using *Gordon*, a data-intensive supercomputer (1)	XSEDE 12 Chicago	July 16	4	15-20	5	S, live
Tutorial	F. D. G. U	Using *Gordon*, a data-intensive supercomputer (2)	XSEDE 12 Chicago	July 16	4	15-20	5	S, live
Tutorial	F. D. G. U	Hands-on Tutorial for Building Science Gateway Applications	XSEDE 12 Chicago	July 16	4	15-20	5	S, live
Workshop	F.D. G.U	HIPACC International Summer School on AstroComputing	UCSD/SDSC	July 9 - 20	60	30	5	S, live
Workshop	F. D. G.	Building an OptIPortal for Collaborative Research and Education	UCSD	August 1-3	16	18	15	S, live
Workshop	F. D. G. U	SDSC 2012 Big Data Summer Institute	UCSD/ SDSC	August 6-10	35	34	5	S, live
Tutorial	F. D. G. U.	Introduction to visualization using Visit	SDSC	Aug 8	3	30	6	S, live
		EDUCATION						
Workshop	S	Intro to Securing Computer Systems	SDSC	July 2-6	24	18	3	S, class
Workshop	S	Alice™ -Beginning Computer Programming in a 3D Environment	SDSC	July 9-13	30	17	6	S, class
Workshop	S	Intro to App Creation for iPads and iPhones	SDSC	July 9-13	30	14	2	S, class
Workshop	S	Creating Your Own Animated Films with Adobe Flash	SDSC	July 16-20	30	14	6	S, class
Workshop	S	Introduction to Object Oriented Programming using	SDSC	July 16-20	30	19	2	S, class

		Java						
Work shop	S	Modeling and Animation with Maya	SDSC	July 23-27	30	16	4	S, class
Work shop	S	Prep for CS 1: Alice(tm) for High School Students	SDSC	July 30-August 3	30	16	3	S, class
Work shop	S	Intermediate Securing Computer Systems: Secure Your Computer Like a Pro!	SDSC	August 6-10	30	17	2	S, class
Work shop	S	Design and Program Your Very Own Video Game: Make Your Ideas a Reality!	SDSC	August 6-10	30	22	2	S, class
Work shop	S	App Inventor: Learn to Program Android Phone Applications!	SDSC	August 13-15	18	16	4	S, class
Work shop	S	Basics of Computer Programming to Create Images, Animations and Interactions	SDSC	August 16-17	12	17	4	S, class
Work shop	S	Introduction to Digital Art and Media	SDSC	August 20-24	30	12	7	S, class
		OUTREACH						
Conf. Talk/ Paper	F. D. G. U.	*Gordon: Design, Performance, and Experiences Deploying and Supporting a Data Intensive Supercomputer (Strande, Moore, Tatineni, Sinkovits)*	XSEDE 2012 Chicago, IL	July 17	.5	200	10	S, Live
Conf. Talk/ Paper	F. D. G. U.	*General Session Opening Remarks (Wilkins-Diehr)*	XSEDE 2012 Chicago, IL	July 18	.5	200	10	S, Live
Conf. Talk/ Paper	F. D. G. U.	*Building Collaborations for Computing Principles Education (Baxter and Simon)*	XSEDE 2012 Chicago, IL	July 18	.5	60	30	S, Live
Conf. Panel	F. D. G. U.	*XSEDE Outreach to MSIs – Lessons Learned from Case Studies (Baxter co-facilitator w/Akli)*	XSEDE 2012 Chicago, IL	July 19	2	20	18	S, Live
Conf. Talk/	F. D. G. U.	*Analyzing Throughput and*	XSEDE 2012 Chicago, IL	July 16-20	.5			Sync

Paper		*Utilization on* ***Trestles*** *(Moore, Carson, Ghadersohl, Jundt, Yoshimoto, Young)*						
Conf. Talk/ Paper	F. D. G. U.	*The CIPRES Science Gateway: Enabling High-Impact Science for Phylogenetics Researchers w/Limited Resources (Miller, Pfeiffer, Shwartz)*	XSEDE 2012 Chicago, IL	July 16-20	.5			Sync
Conf. Talk/ Paper	F. D. G. U.	*XSEDE and Science Gateways (Wilkins-Diehr)*	XSEDE 2012 Chicago, IL	July 16-20	.5			Sync
Conf. Poste r	F. D. G. U.	*Memory Layout Experiments for Common Visualization Tasks (Chourasia)*	XSEDE 2012 Chicago,IL	July16-20	1	100		S, Live
Conf. VisS howc ase	F. D. G. U.	*Snapshots of a Volcano Eruption Simulation (Chourasia)*	XSEDE 2012 Chicago,IL	July16-20	2	100		S, Live
Conf. VisS howc ase	F. D. G. U.	*Role of visualization in porting a seismic simulation from CPU to GPU architecture (Chourasia)*	XSEDE 2012 Chicago,IL	July16-20	2	100		S, Live
Conf. Boot h	F. D. G. U. S. P.	XSEDE Booth Participation (Chourasia)	SIGGRAPH 2012 Los Angeles, CA	Aug 5-9	30	20,000		S, Live
Sem	F, I, D	*Scheduling requirements and strategies for Gordon, Trestles and the Future (Yoshimoto)*	Appro	Aug 29	1	30		S, Live
Sem	F. D. G. U.	*Gordon: A novel high performance computing system for data and memory intensive applications* (Sinkovits)	MURPA: Monash Undergraduat e Research Projects Abroad (Australia, virtual)	Aug 31	1	20		S/ A, Live/ Webca st
Conf.	F. D. G. U.	*Gordon - A Flash-based Supercomputer for Data Intensive Computing*, @ BIO-IT Cloud Summit (Sinkovits)	San Francisco, CA	September 11	.5	100		S, Live

Conf.	F. D. G. U. I.	*Early Experiences with Gordon – A Flash-based Cluster for Data-Intensive Applications* (Norman)	Lyon, France	Sept 11-14	1	200		S, Live
Conf.	F. D. G. U.	*The Challenge of Big Data in Science-Keynote* (Sinkovits)	Karlsruhe, Germany	September 25	1	200		S, Live

* *S=synchronous, A=asynchronous*

19.5.1 Training

The third quarter of 2012 training reflected growing community interest in SDSC's newest XSEDE resources, exemplified by SDSC's 2012 *Big Data Supercomputing* Summer Institute. This 1-week summer institute August 6-10, 2012 provided a unique opportunity for participants to focus on specific challenges in their research. Whether it was optimizing a computationally intensive piece of code, improving I/O, or beginning the process of refactoring software to make best use of SDSC's HPC resources, participants experienced hands-on lessons to complement the lectures and opportunities to work on their applications together with SDSC staff.

Topics covered included:

- Overview of the Gordon and Trestles architectures
- Data intensive computing
- Developing shared memory applications
- Improving I/O performance with flash storage
- Using vSMP for large shared memory
- Visualization using Gordon
- Developing Science Gateways
- Overview of software, libraries, tools, and compiler options for achieving optimal performance
- XSEDE allocations process and writing a strong proposal

SDSC led three short tutorials (two at XSEDE 12) and hosted three major workshops at SDSC (see table above). Most notable among these workshops were the UC High Performance Astro-Computing Center (HiPACC) summer school July 9-20, and the annual SDSC Big Data Summer Institute August 6-10. Both of these focused on training the next generation of researchers to deal with the big data challenge, and more generally how to exploit the power of supercomputers to make sense of the data deluge. On August 1-3, UCSD hosted a three-day hands-on tutorial for building an OptIPortal display wall to support collaborative research and education, with participants from several minority-serving institutions. This workshop was a follow-up to a series of SDSC-led workshops on CI for Research and Education at Minority-Serving Institutions.

19.5.2 Education

SDSC's NSF-funded Computing Education for a 21st Century Workforce (CE 21) project, entitled "Computing Principles for ALL Students' Success" (ComPASS) supports teacher professional development to implement a new computer science principles course at the college and pre-college levels. The course paves the way for a new AP (Advanced Placement) test in computer science; one that will focus on the foundation principles of computational thinking. SDSC/UCSD-led professional development seminars and workshops for secondary school teachers led to eight new schools offering this course starting in September 2012. This brings the total local high schools offering Computer Science Principles to 12 as a result of SDSC professional development for secondary school teachers. Of these schools, ten serve a high proportion of students on free and reduced-price lunches, with very high numbers of Hispanic and African-American students.

Late in June, SDSC received notice of an REU award supplement for *Gordon*. One student started working with Bob Sinkovits in September 2012, and recruitment for the second position will re-open shortly for work to be done in spring and summer 2013.

SDSC hosted two major national-scope HPC-related workshops during July and August of 2012, which have been listed under "Training" in the table above. But in addition, 14 courses and workshops for secondary school students were offered during the same period that focused on building computational skills.

SDSC's popular Research Experiences for High School Students (REHS) internships drew a very large group of talented participants. Their poster session for UCSD students, faculty, SDSC researchers, and their families was held on Friday, August 10, 2012, including two students whose research posters and presentations were included at XSEDE 12.

19.5.3 Outreach

XSEDE TEOS Blog: SDSC's Ange Mason posted 44 articles to the XSEDE TEOS blog, a combination of single news posts and the XSEDE weekly Newsroom posts. The weekly Newsroom name has now changed to HPC Research and Education News for the Week of – – – sponsored by XSEDE, to reflect its joint presence on the XSEDE and HPCU sites.

SDSC's Ange Mason continued participation in the HPCU website redesign committee to revise and update the HPC University site. She is adding content on a more frequent basis, continuing to update the calendar and submitting new items to make this a valuable resource for HPC users.

The SDSC Research Experience for High School Students (REHS) program wrapped up the summer with 39 interns at SDSC. Two 2012 REHS students presented posters at XSEDE 12.

SDSC staff extended outreach to national and international colleagues through professional conference presentations and tutorials related to XSEDE Data-Intensive computational services, included in the table above.

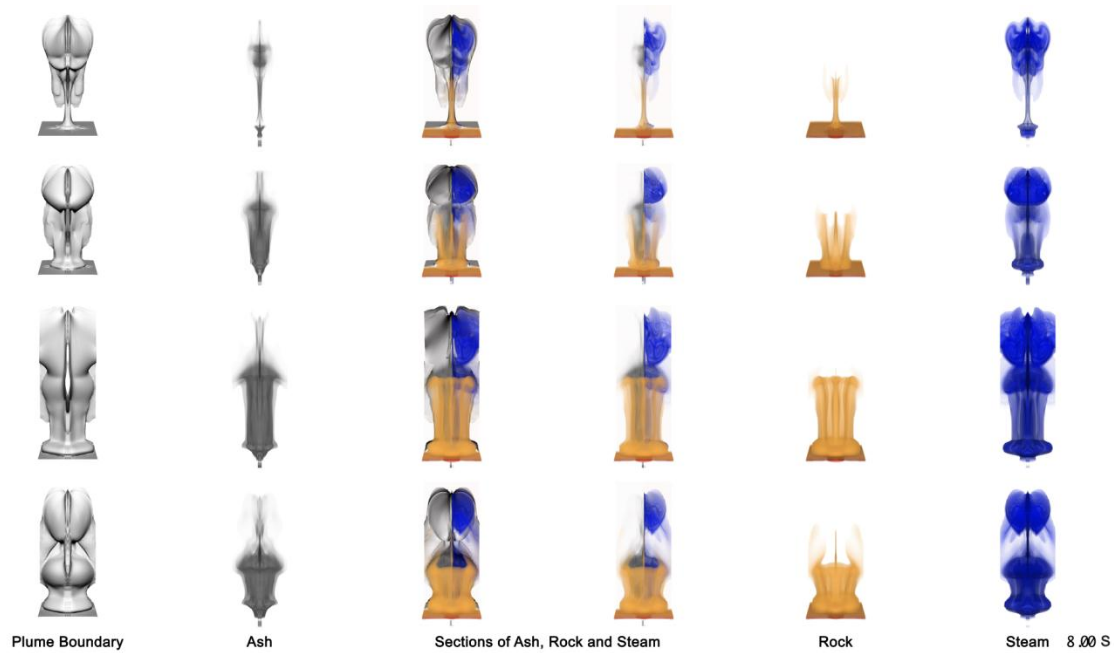
19.6 SP Collaborations

1.1.1 Collaborations with SP XSEDE Users

- Pietro Cicotti worked with Yoav Freund (UCSD) to deploy Hadoop on Gordon for a large data analytics class.
- Robert Sinkovits collaborated with Ramon Huerta (UCSD) to obtain a further 2x speedup of a previously optimized autoregressive kernel application. Relative to original version of code, total speedup is now approximately 170x.
- Pietro Cicotti worked with members of the Protein Data Bank (PDB) to port a distributed structure comparison application to Gordon. Using a dedicated I/O node on Gordon together with 16 compute nodes enables the work to be done approximately four times faster than on the Open Science Grid. Note that this project is bandwidth rather than compute limited and takes full advantage of Gordon's flash drives.
- Robert Sinkovits began collaborating with Doug White, a computational social scientist from UC Irvine. A key algorithm used for maximum clique detection (largest fully connected sub-graph) in large graphs has been optimized to run at least six times faster for large, sparse graphs.
- Robert Sinkovits worked with Richard Scheuermann (J. Craig Venter Institute) to port flow cytometry application to Gordon. Addressed portability issues and obtained 4.5x

speedup for realistically sized data sets. The CIPRES team (Wayne Pfeiffer, Mark Miller, Terri Schwartz) and Robert Sinkovits are both pursuing future collaborations with JCVI.

- Paul Rodriguez, Nicole Wolter, and Jerry Greenberg worked with Prof. Jim Folwer and Chris Fariss from the UCSD Political Science Department to set up and run social network simulations that gather statistics over various interaction parameters. The work was used in a *Nature* publication (Fowler, et al., 2012).
- Paul Rodriguez has started working with Prof. Anders Dale from UCSD Departments of Neuroscience and Radiology on Genomic and Neuroimaging analysis.
- Amit Majumdar, Subhashini Sivagnanam & Kenneth Yoshimoto began collaborating with Ted Carnevale & Michael Hines from Yale School of Medicine and MaryAnn Martone, Anita Bandrowski & Vadmin Astakhov from NIF, UCSD in porting NEURON, a neuronal simulation software, to Trestles machine. This is a part of NSF funded project to build NeuroScience Gateway (NSG) which will allow neuroscientists to access and use neuronal software on XSEDE resources
- Wayne Pfeiffer provided support to a number of CIPRES gateway users who were unable to independently complete their runs
    - Made an expedited run on Gordon of MrBayes 3.2.1, the newest version of that phylogenetics code, for Natalie Jameson of Wayne State University. The run took 155 hours to complete 100 million generations on 8 cores of a single node. Jameson previously analyzed the same data set with an older version of the code for 20 million generations on a computer at Wayne State. She reported that "the analysis took a few months and did not come close to convergence."
    - Jessica Grant from Smith College reported that one of her RAxML phylogenetics analyses consistently failed when run on Trestles via the CIPRES gateway. Upon investigation, Pfeiffer determined that the problem only occurs for the hybrid parallel version of the code built with MVAPICH2. However, he was unable to determine whether the apparent bug is in RAxML or MVAPICH2. As a temporary work-around, the version of RAxML used by the gateway was switched from that built with MVAPICH2 to that built with OpenMPI. The latter is typically a few percent slower, but is evidently more reliable. Pfeiffer successfully ran Grant's analysis with the newly built version of the code in 10 hours on Trestles and sent the results to her.
    - Made an expedited run of the production, 3.1.2h version of MrBayes on Gordon for Haiwei Luo of the University of Georgia. Luo's original attempt via the CIPRES gateway failed to converge, but Pfeiffer's rerun converged and completed in 194 hours.
    - Made expedited runs of RAxML 7.3.1 on Trestles for Dimitar Dimitrov of the University of Copenhagen and The George Washington University and Alexandre Pedro Selvatti Ferreira Nunes of the Universidade Federal do Rio de Janeiro in Brazil. Their original submissions via the CIPRES gateway failed because of unknown system problems. Also, Nunes tried to run RAxML-Light when regular RAxML works better and runs faster. The rerun for Dimitrov took 119 hours, while that for Nunes took 29 hours.
- Amit Chourasia continued work with PI Darcy Ogden on Visualization of new data from nine simulations of volcanic eruption. http://visservices.sdsc.edu/projects/volcano



- Amit Chourasia continued collaboration with SCEC on visualization of w2w1hz80SN earthquake simulation as well as created visualization for diagnosis and validation of results for porting of AWP simulation from CPU to GPU architecture.

1.1.2 Collaborations with External Partners

Amit Chourasia continued collaboration with Prof. Tannishtha Reya at School of Medicine at UCSD on visualization of stem cells in bone marrow. The visualization results are available at http://visservices.sdsc.edu/projects/stemcells/

Rick Wagner's work with Joseph Insley from Argonne National Laboratory was presented during the XSEDE12 Visualization Showcase, and has been accepted for the SC'12 Visualization Showcase. Rick is also the Vice-Chair for the Theory Interest Group of the International Virtual Observatory Alliance, and led the technical coordination effort for the UC-HiPACC AstroInformatics Summer School.

19.7 SP-Specific Activities

CIPRES Gateway

Two new versions of the BEAST phylogenetics code were installed and benchmarked on Trestles by Wayne Pfeiffer. Initially Version 1.7.3 was installed, but because of a serious bug, that was superseded shortly afterward by Version 1.7.4. Pfeiffer then helped Mark Miller and Terri Schwartz upgrade the version available via the CIPRES gateway from 1.7.2 to 1.7.4.

Most of the benchmarks had run times similar to those for previous versions of BEAST, but two benchmarks had run times that were 2x to 8x longer than before! This was evidently because the default value of the beagle_scaling option was changed from dynamic to delayed "to help discrete trait models run" according to the BEAST Web site. Nonetheless, it was decided to continue using dynamic as the beagle_scaling option for gateway runs.

Pfeiffer installed Version 1.0.9 of the RAxML-Light phylogenetics code on Trestles, upgraded the bash script to execute RAxML-Light along with regular RAxML and Parsimonator, and ran some tests. After all checked out, Pfeiffer helped Miller and Schwartz upgrade the version available via the CIPRES gateway from 1.0.5g to 1.0.9.

Scheduling and Resource Optimization

To accommodate gateway use of the GRAM service on Trestles, two approaches were used to support alternate MPI environments through GRAM. The first was use of jobtype=single to specify an alternate path to mpirun and use of RSL environment variables and command line arguments to define the MPI environment. The second was development and deployment of an alternate jobmanager for use in test mode by the gateway requesting an alternate MPI environment.

A bug in the topology-aware scheduling code for Catalina Scheduler was fixed, to allow efficient node allocation of noflash/flash/bigflash nodes on Gordon.

SDSC to support the XSCDB and AMIE central instance in Q3. In collaboration with NCSA, both the XSCDB and AMIE protocol were enhanced to support the seamless resolution of duplicate user names. All sites are expected to be compliant early in Q4.

19.8 Publications

Baxter, Diane and Simon, Beth, (2012). "Building Collaborations for Computing Principles Education" Presented at XSEDE 12 Conference, Chicago, July 2012

Chourasia, Amit (2012). "Memory Layout Experiments for Common Visualization Tasks" Presented at XSEDE 12 Conference, Chicago, Jul 2012.

Chourasia, Amit; Ogden, D.; Choi, D. J.; and Wohletz, K. (2012) "Snapshots of a Volcano Eruption Simulation". Presented at Visualization Showcase at XSEDE 12 conference, Chicago, July 2012.

Chourasia,Amit, Zhou, J. ; Cui, Y.; Choi, D.J. ; Olsen, K. B. ; (2012)"Role of visualization in porting a seismic simulation from CPU to GPU architecture". Presented at Visualization Showcase at XSEDE 12 conference, Chicago, July 2012.

Dickson, C.J.; Rosso, L.; Betz, R.M.; Walker, R.C.; Gould, I.R., "GAFFlipid: a General Amber Force Field for the accurate molecular dynamics simulation of phospholipid.", Soft Matter,2012, 8, 9617-9627, DOI: 10.1039/C2SM26007G

Isborn, Christine; Goetz, Andreas W.; Walker, Ross C.; Martinez, Todd - "Ab Initio QM/MM Molecular Dynamics with TeraChem and AMBER: Exploring Environmental Effects on the Absorption Spectrun of Photoactive Yellow Protein", Gordon Research Conference in Computational Chemistry, Mount Snow, VT., July 2012. (Poster).

Moore, R. L.; Carson, L.; Ghadersohi, A. ; Jundt, A.; Yoshimoto, K.; Young, W.; "Optimization of Throughput and Utilization on Trestles." XSEDE'12, July 2012, Chicago, IL, USA. ACM TBD.

Pierce, L.C.T.; Salomon-Ferrer, R.; de Oliveira, C.A.F.; McCammon, J.A.; Walker, R.C., "Routine access to millisecond timescale events with accelerated molecular dynamics.", Journal of Chemical Theory and Computation, 2012, 8(9), 2997-3002, DOI: 10.1021/ct300284c

Salomon-Ferrer, R.; Case, D.A.; Walker, R.C.; "An overview of the Amber biomolecular simulation package", WIREs Comput. Mol. Sci., 2012, in press, DOI: 10.1002/wcms.1121

Strande, S.M; Cicotti, P.; Sinkovits, R.S.; Young, W.S.; Wagner, R.P.; Tatineni, M.; Hocks, E.; Snavely, A.; Norman, M.; "Gordon: Design, Performance, and Experiences Deploying and Supporting a Data Intensive Supercomputer.", Presented at XSEDE 12 Conference, Chicago, July 2012.

Skjevik, A.A,; Madej. B.D.; Walker, R.C.; Teigen, K.; "LIPID11: A Modular Framework for Lipid Simulations Using Amber", Journal of Physical Chemistry B, 2012, 116 (36), pp 11124-11136, DOI: 10.1021/jp3059992

Walker, R. C., "Extreme acceleration of AMBER molecular dynamics: Sampling for the 99%", Gordon Research Conference in Computational Chemistry, Mount Snow, VT, Invited Speaker. July 2012.

Walker, R. C., "Transforming Molecular Biology through Extreme Acceleration of Molecular Dynamics", XSEDE 12 Conference, Chicago, Il, July 2012.

Walker, R. C.; "Extreme acceleration of AMBER molecular dynamics." Joint Charmm/Amber meeting, NIH, MD. July 2012, Invited Speaker.

19.9 Metrics

Appendices 1.9A-C includes the following metrics:

- 1.9-A XSEDE-generated user ticket statistics
- 1.9-B *Trestles* and *Gordon* Quarterly stats from XDMoD (July – September 2012)
- 1.9-C Local *Trestles* stats related to achieving user productivity objectives

19.9.1 Appendix 1.9A Standard User Assistance Metrics

Time to Resolution	***account issues***	***file systems***	***grid software***	***jobs/batch queues***	***login/access issues***	***mss/data issues***	***network issues***	***software/ apps***	***system issues***	***other***
0-1 hr				**1**	**1**			**1**	**0**	**0**
1-24 hr	**5**	**6**		**32**	**6**	**1**		**14**	**3**	**1**
1-7 d	**9**	**11**	**2**	**46**	**8**	**6**		**11**	**5**	**2**
1-2 wk	**1**	**6**	**1**	**11**	**3**	**2**		**4**	**0**	**1**
> 2 wk	**0**	**4**		**27**	**5**	**3**		**12**	**2**	**0**
Still Open	**2**	**3**	**2**	**19**	**3**	**2**		**16**		**3**

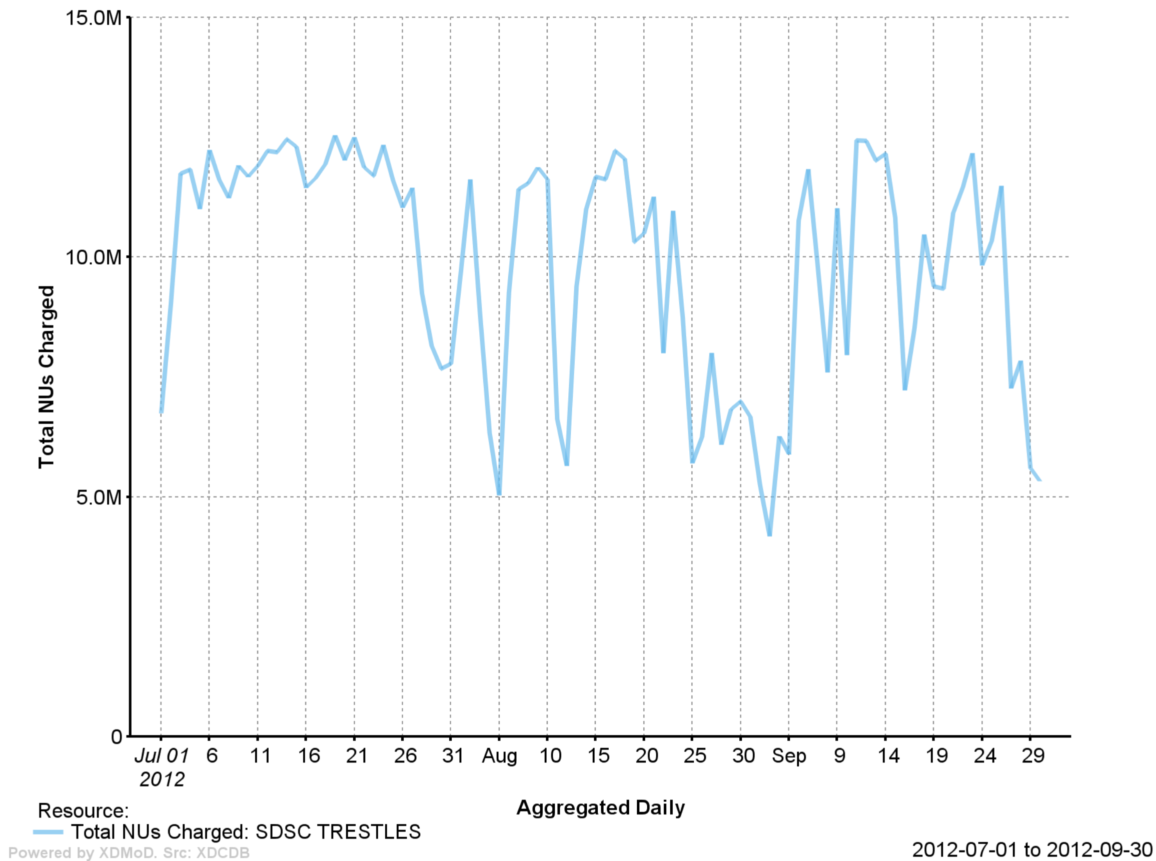
Appendix 1.9B Trestles and Gordon Quarterly Usage Statistics

SDSC-TRESTLES Quarterly Report

Total NUs Charged by Resource

Service Provider = SDSC

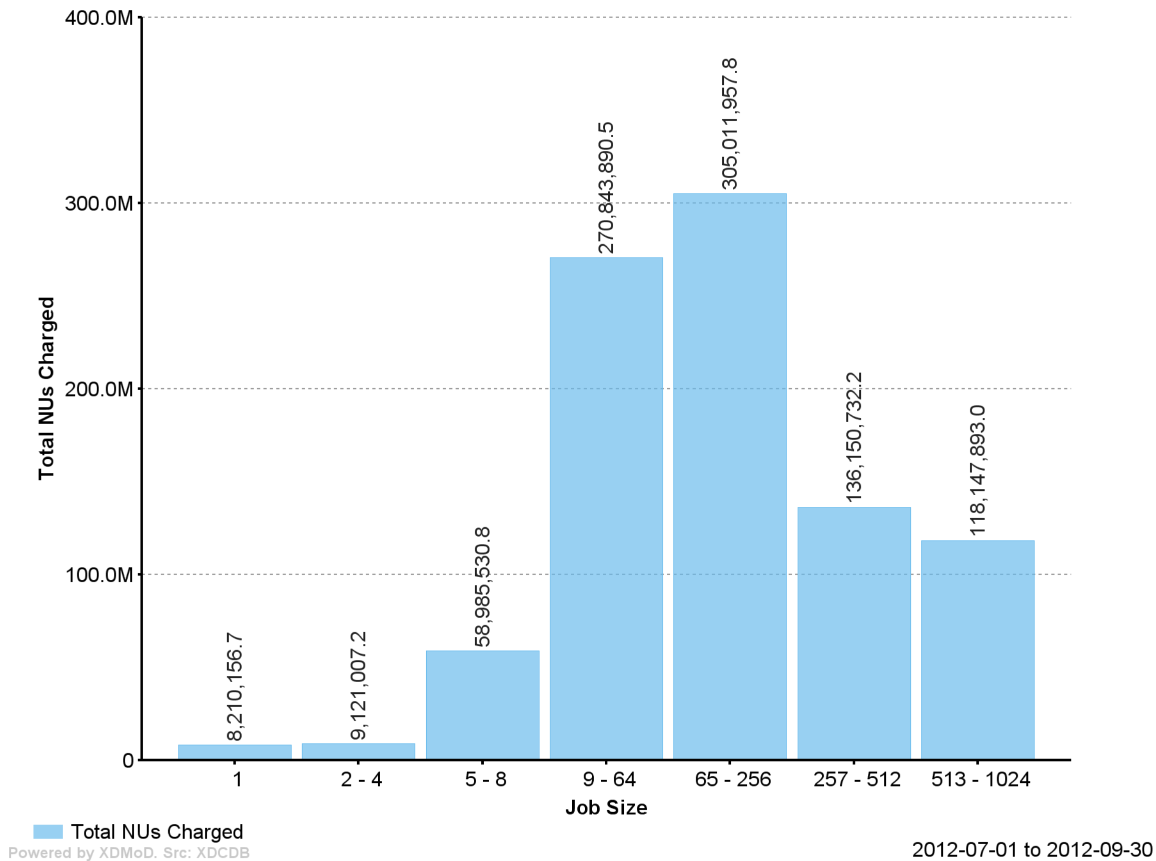
2012-07-01 to 2012-09-30



Total NUs Charged by Job Size

Resource = SDSC-TRESTLES

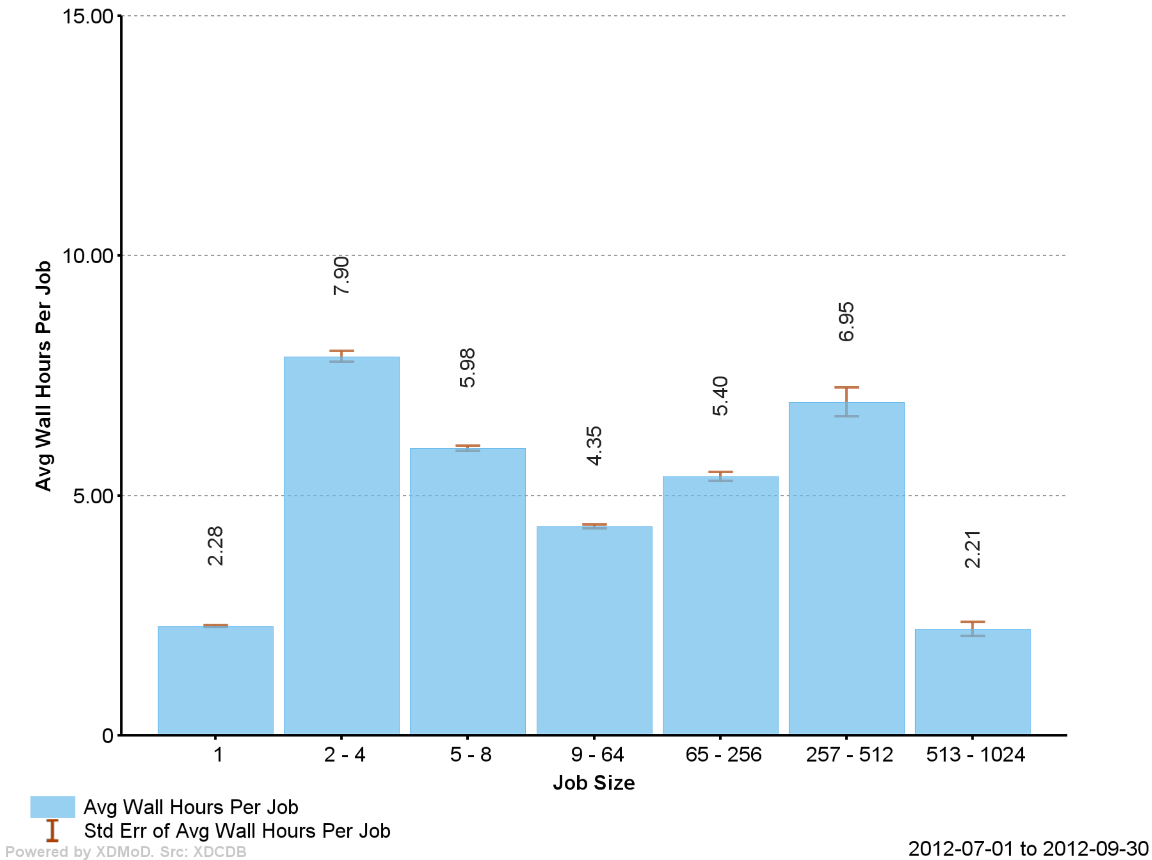
2012-07-01 to 2012-09-30



Avg Wall Hours Per Job by Job Size

Resource = SDSC-TRESTLES

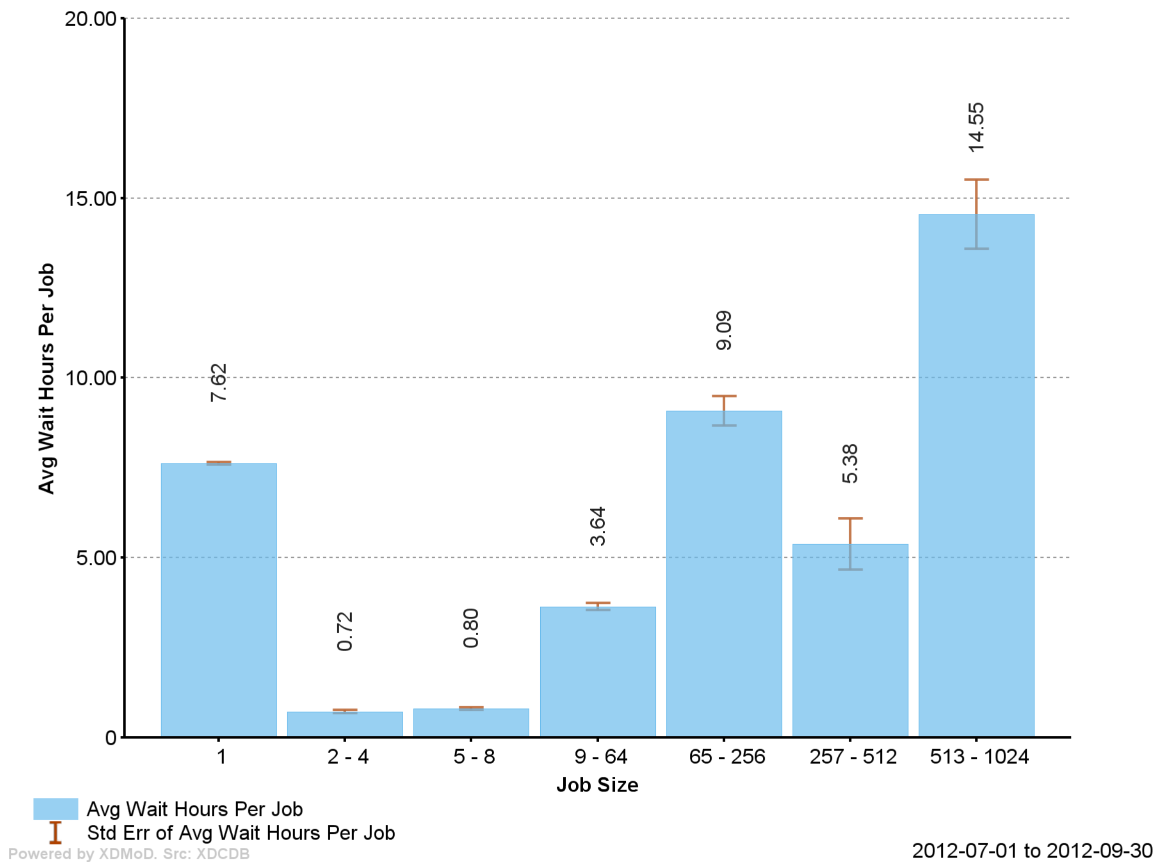
2012-07-01 to 2012-09-30



Avg Wait Hours Per Job by Job Size

Resource = SDSC-TRESTLES

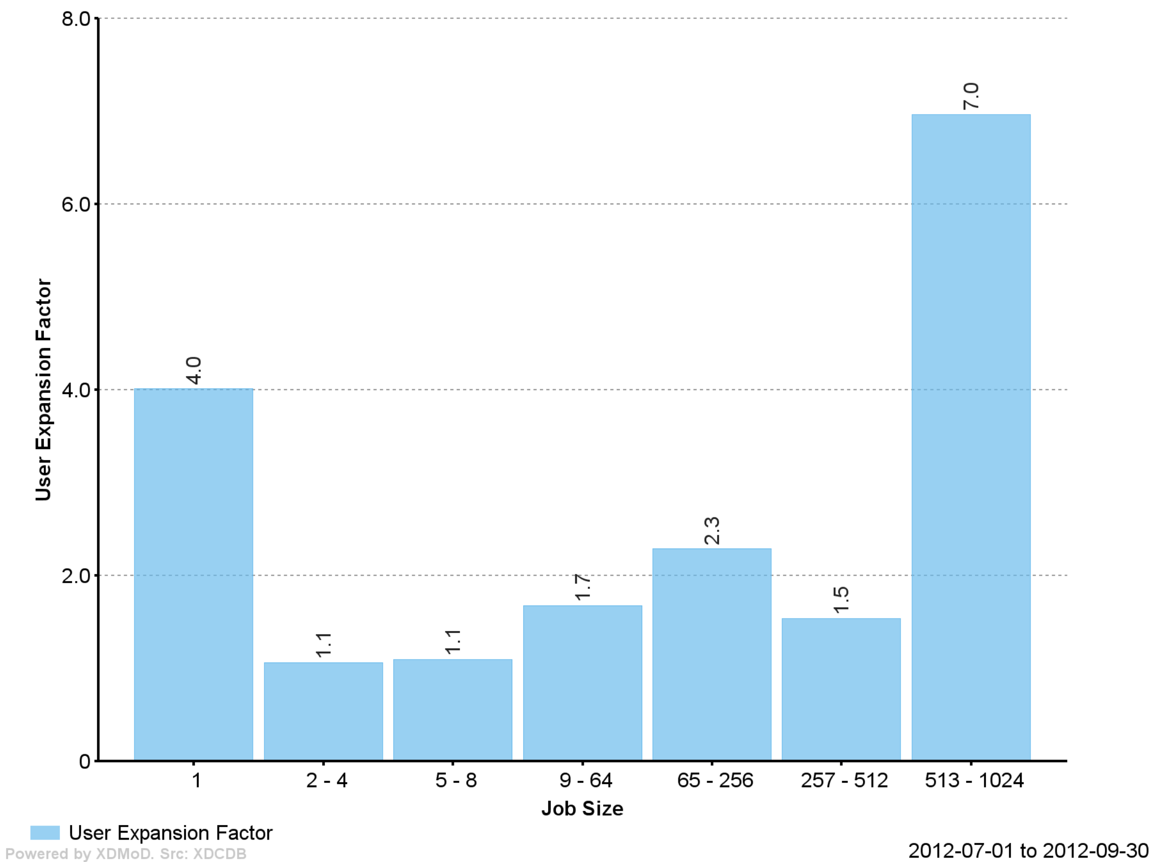
2012-07-01 to 2012-09-30



User Expansion Factor by Job Size

Resource = SDSC-TRESTLES

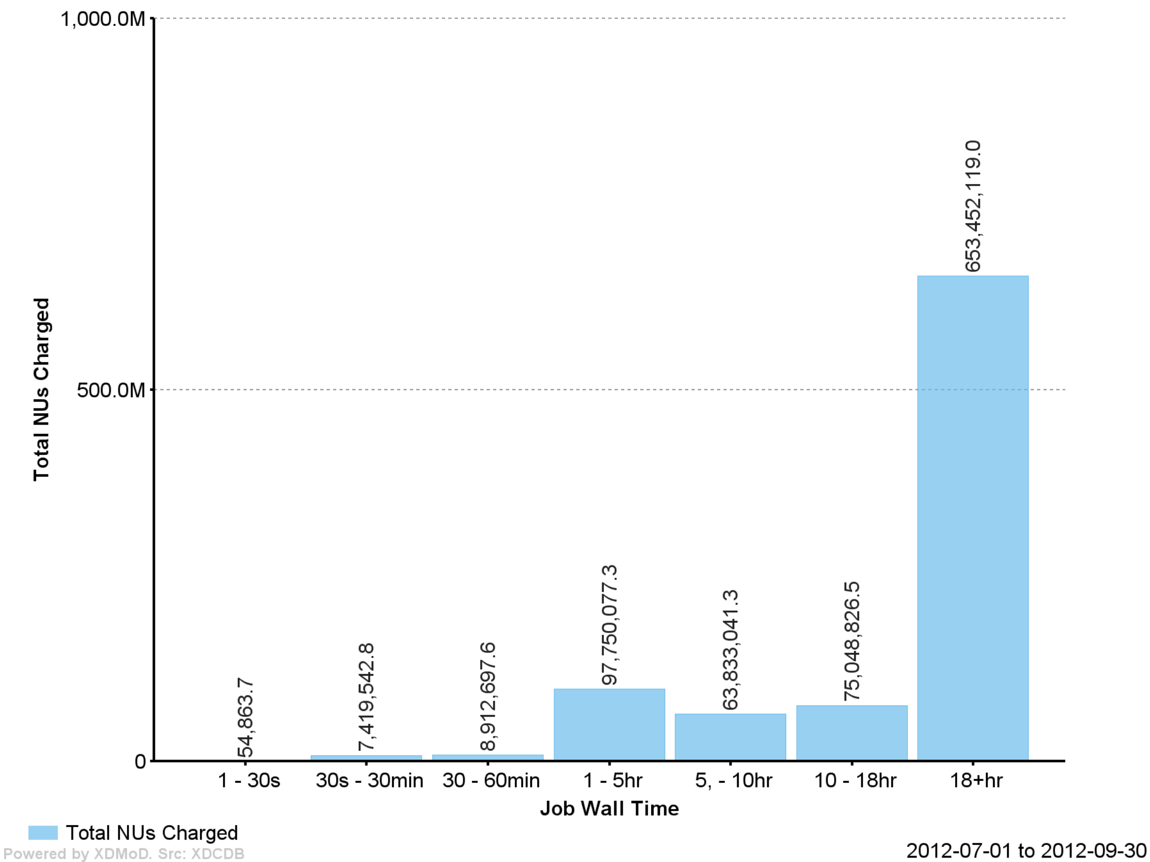
2012-07-01 to 2012-09-30



Total NUs Charged by Job Wall Time

Resource = SDSC-TRESTLES

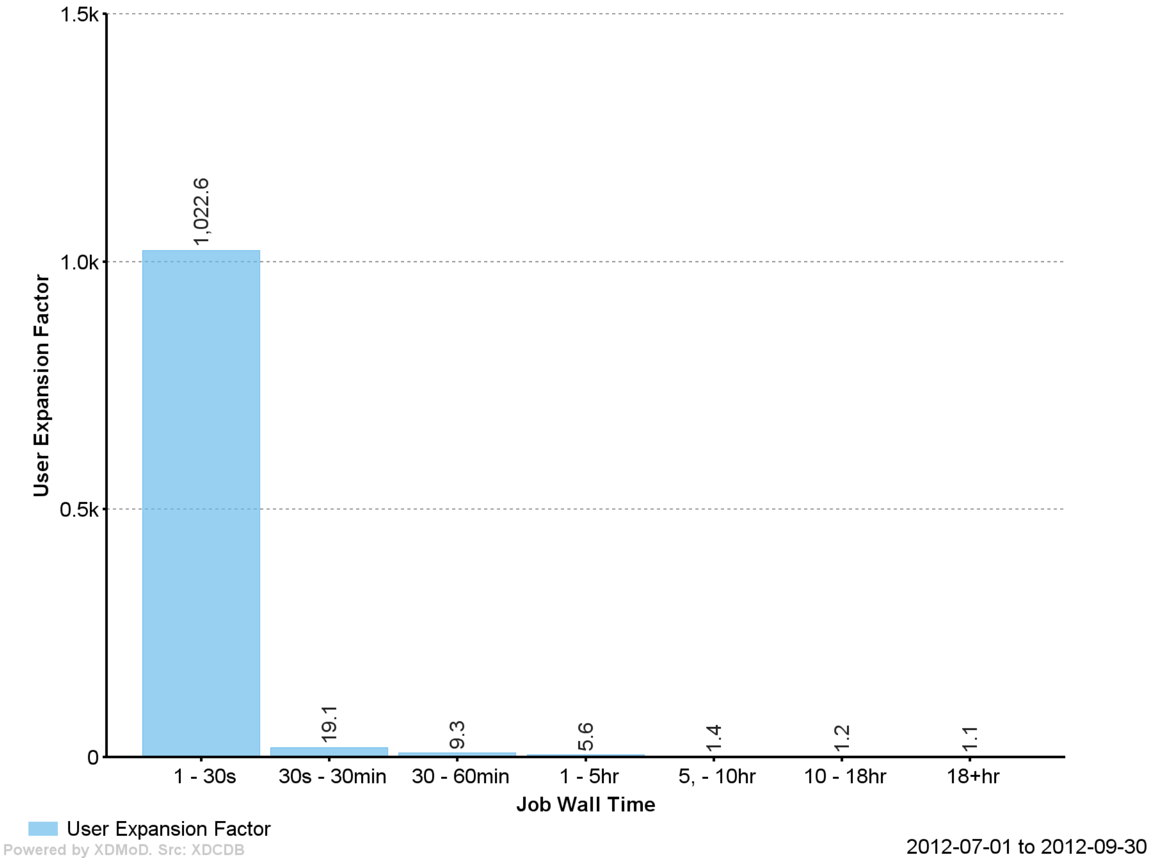
2012-07-01 to 2012-09-30



User Expansion Factor by Job Wall Time

Resource = SDSC-TRESTLES -- Service Provider = SDSC

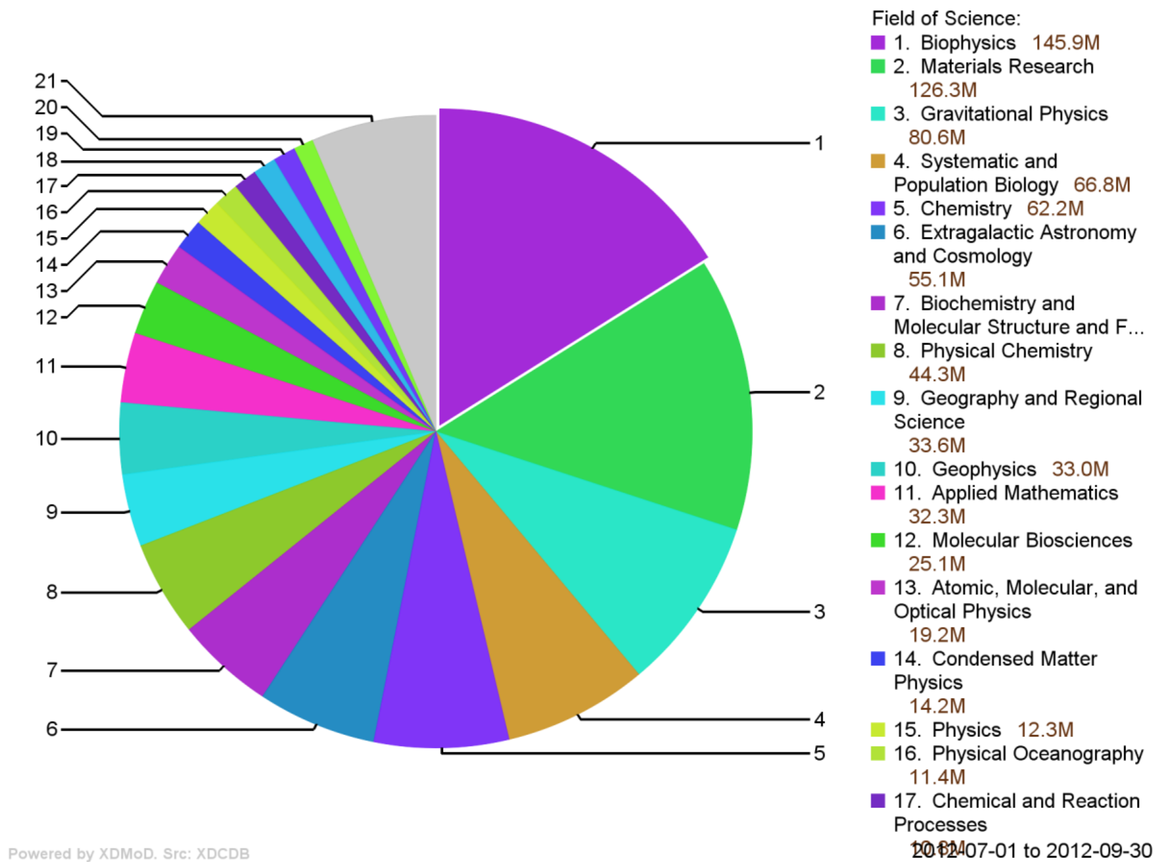
2012-07-01 to 2012-09-30



Total NUs Charged by Field of Science

Resource = SDSC-TRESTLES

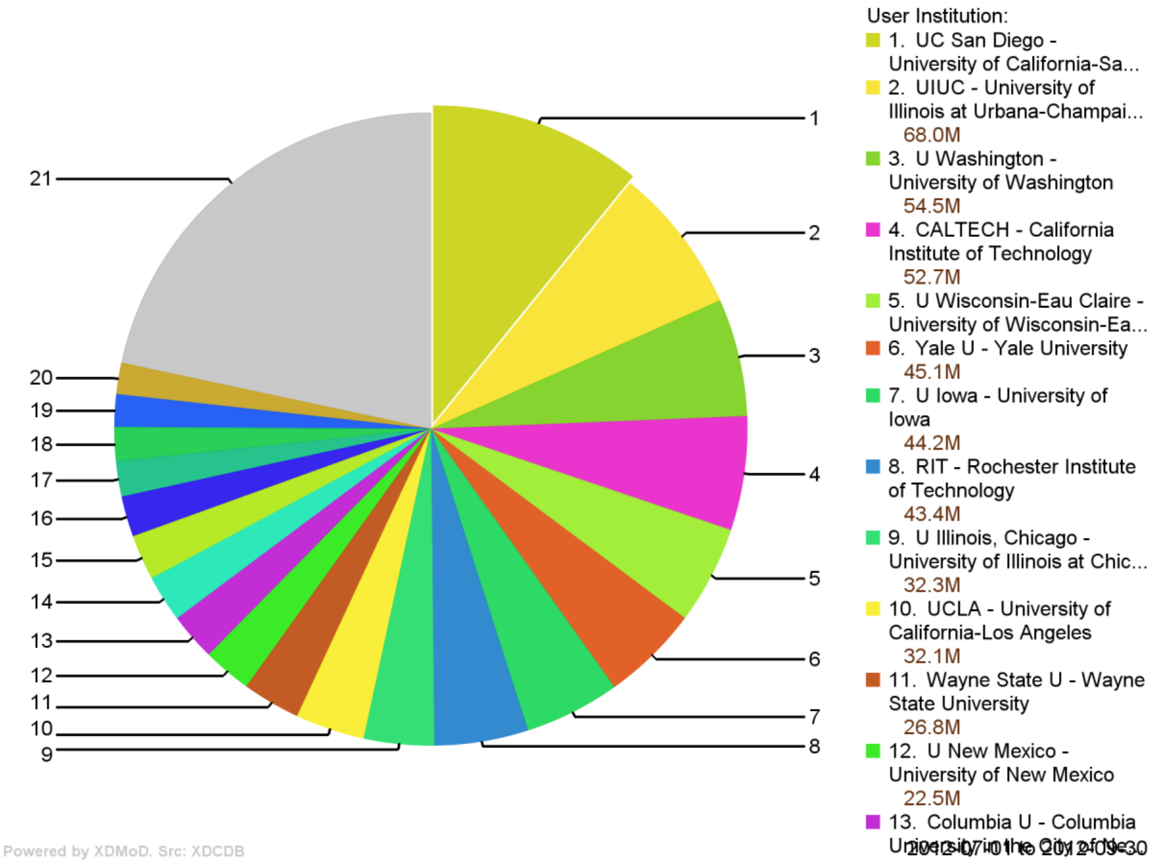
2012-07-01 to 2012-09-30



Total NUs Charged by User Institution

Resource = SDSC-TRESTLES

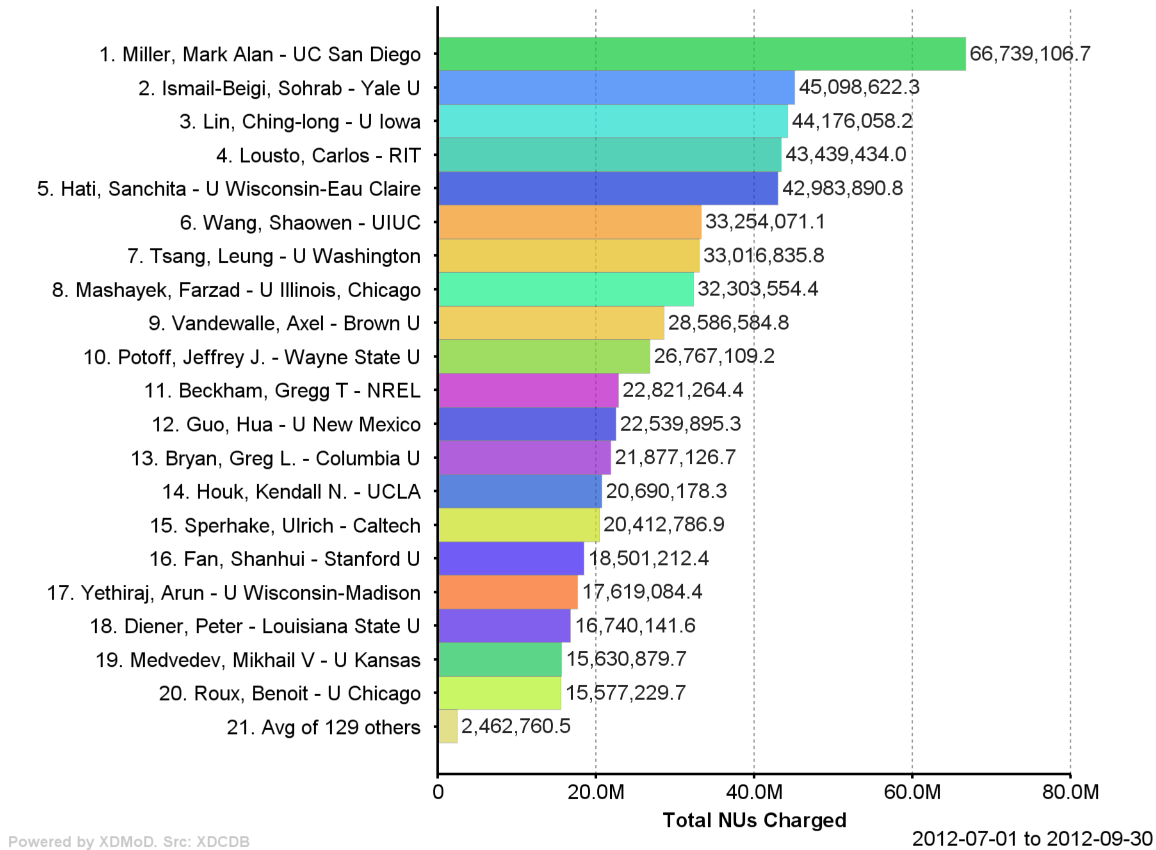
2012-07-01 to 2012-09-30



Total NUs Charged by PI

Resource = SDSC-TRESTLES

2012-07-01 to 2012-09-30

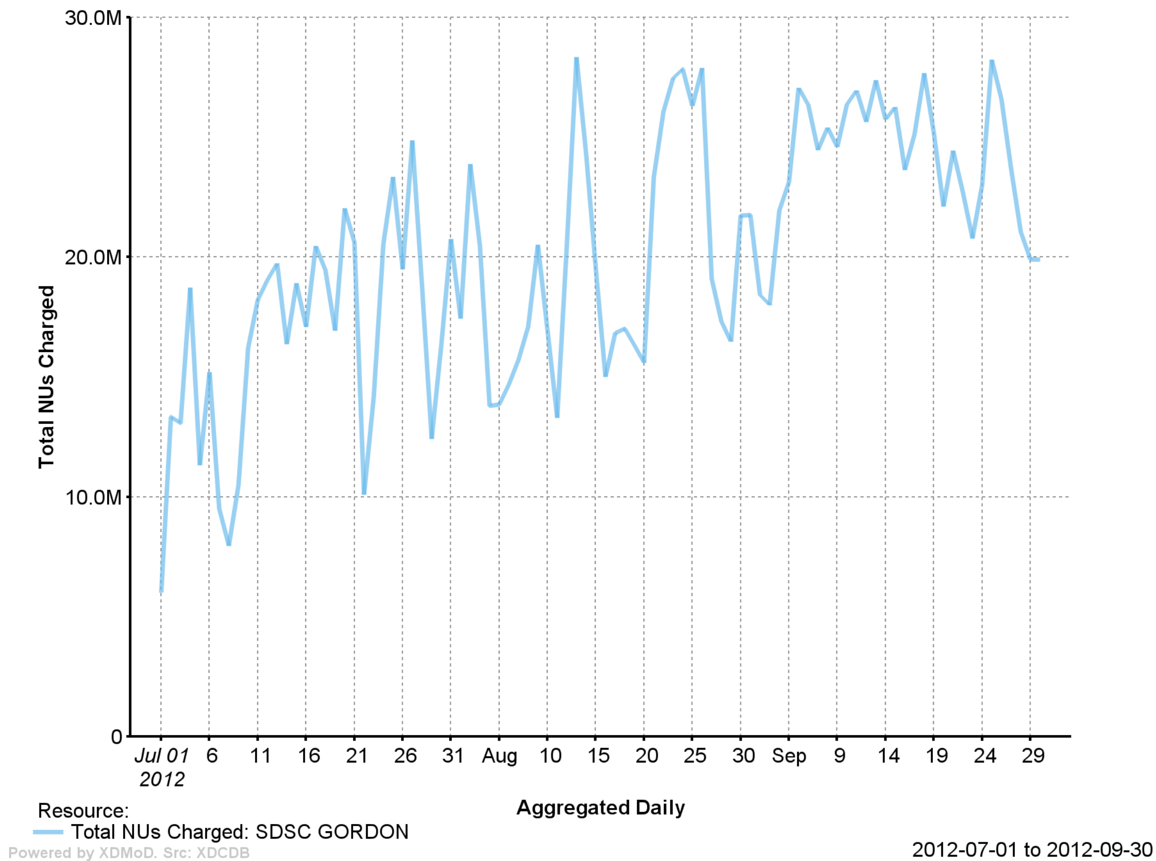


SDSC-GORDON Quarterly Report

Total NUs Charged by Resource

Service Provider = SDSC

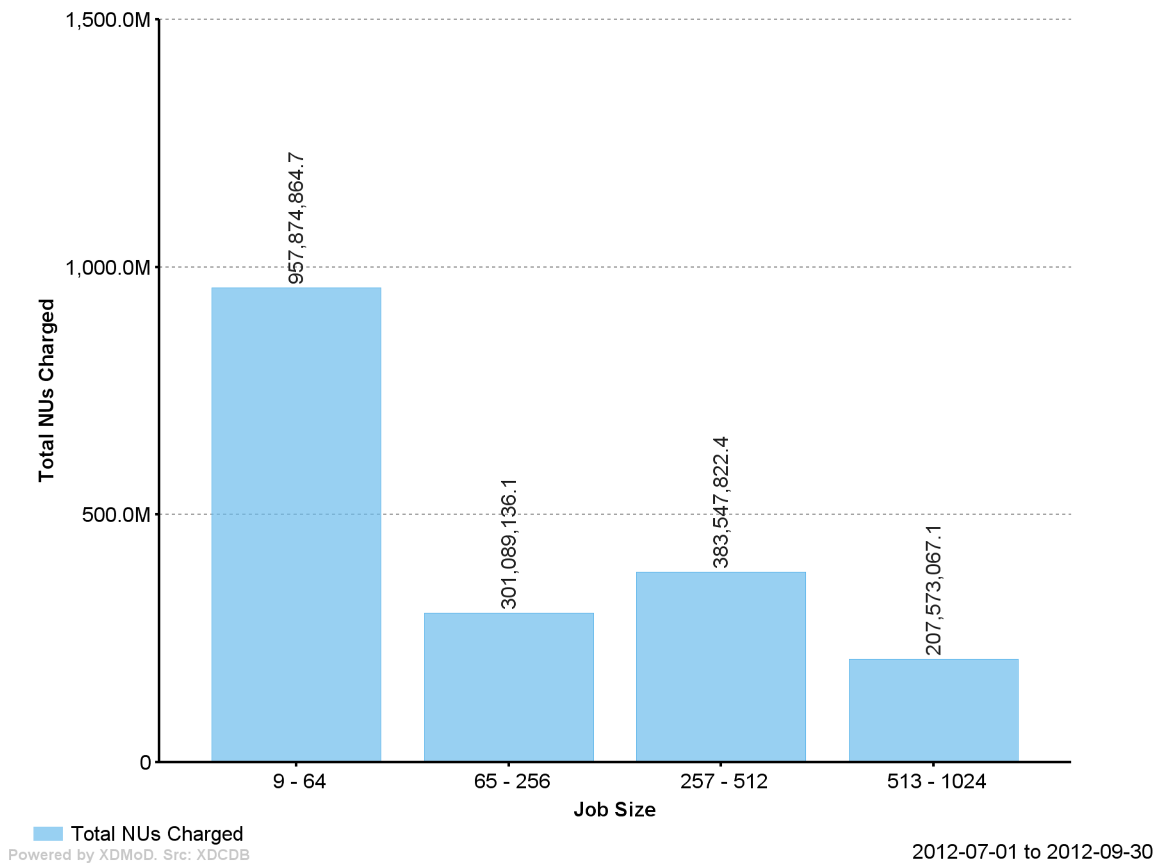
2012-07-01 to 2012-09-30



Total NUs Charged by Job Size

Resource = SDSC-GORDON

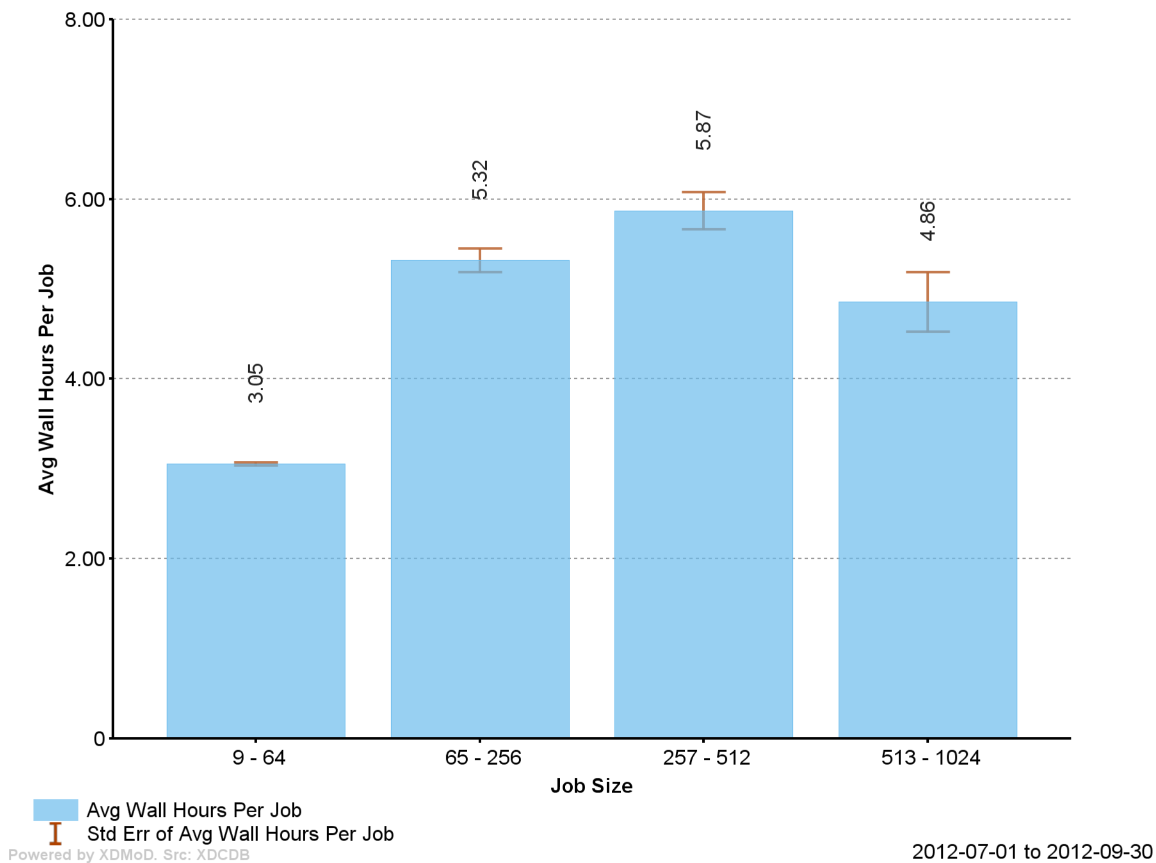
2012-07-01 to 2012-09-30



Avg Wall Hours Per Job by Job Size

Resource = SDSC-GORDON

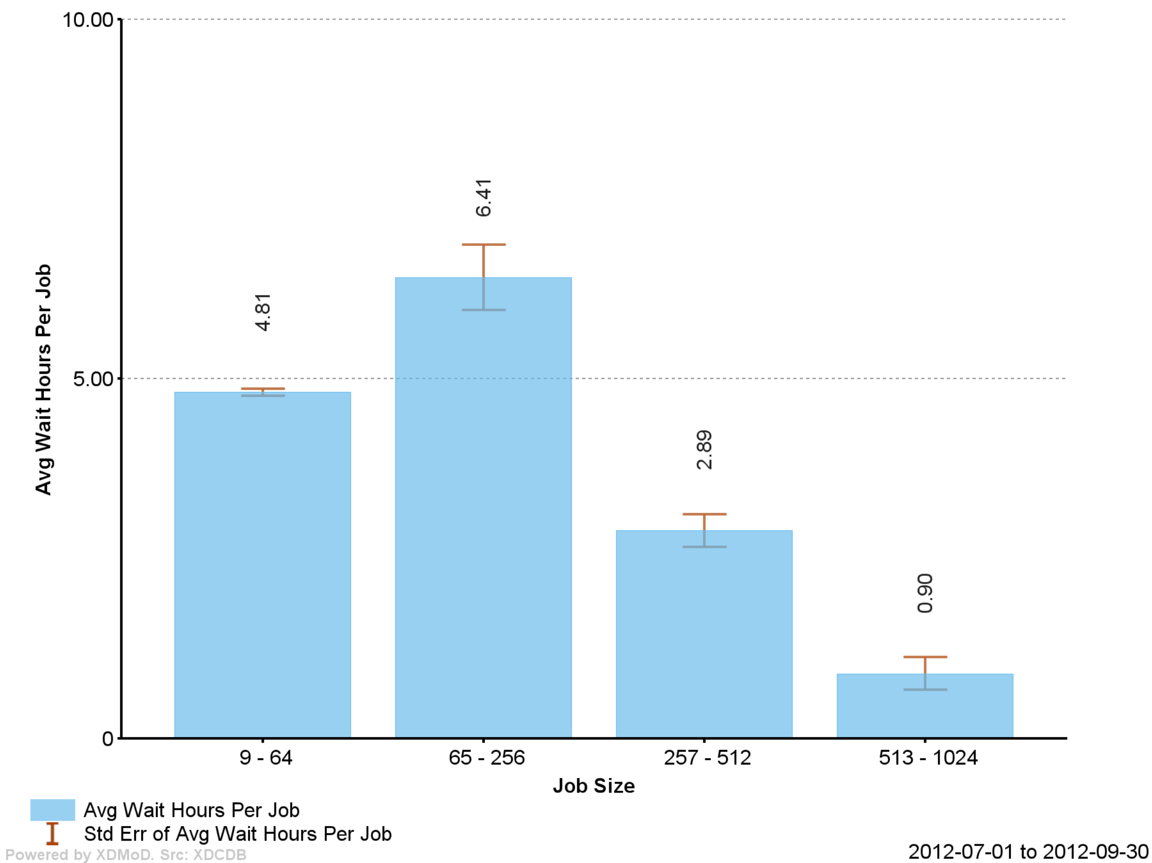
2012-07-01 to 2012-09-30



Avg Wait Hours Per Job by Job Size

Resource = SDSC-GORDON

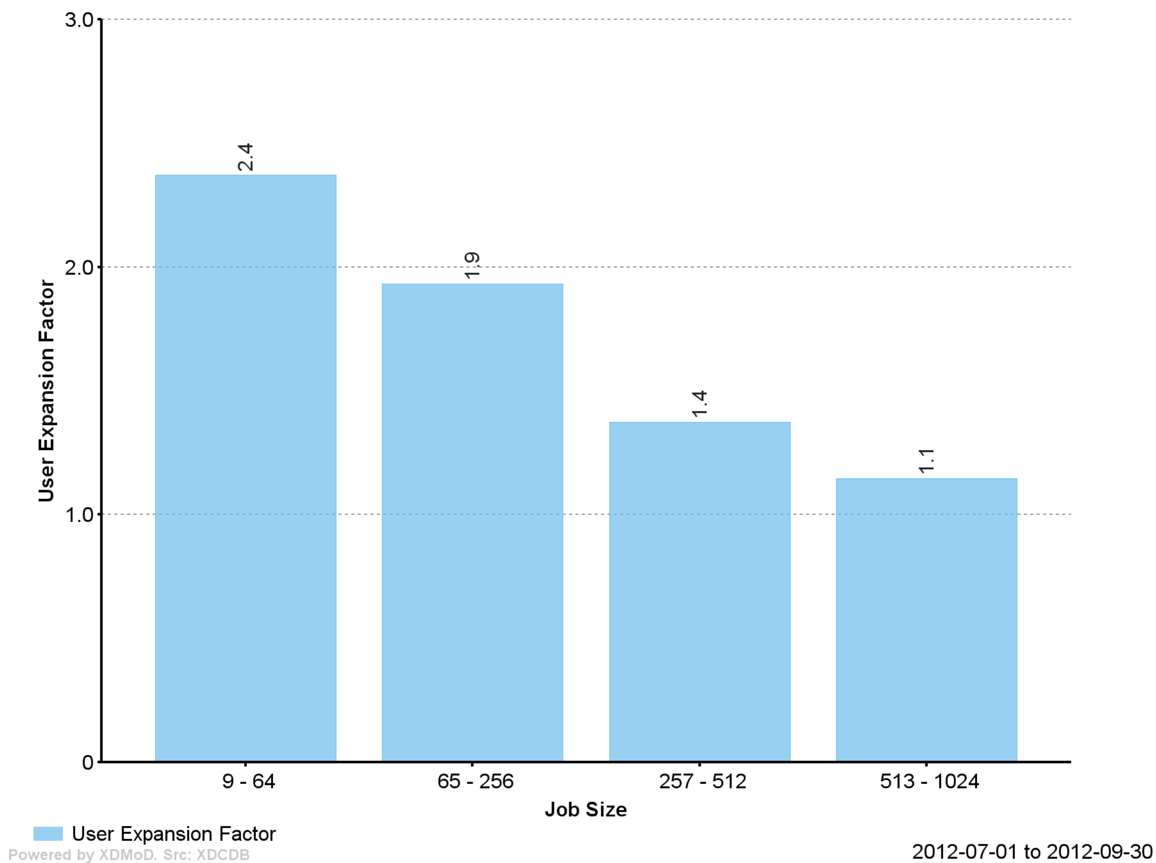
2012-07-01 to 2012-09-30



User Expansion Factor by Job Size

Resource = SDSC-GORDON

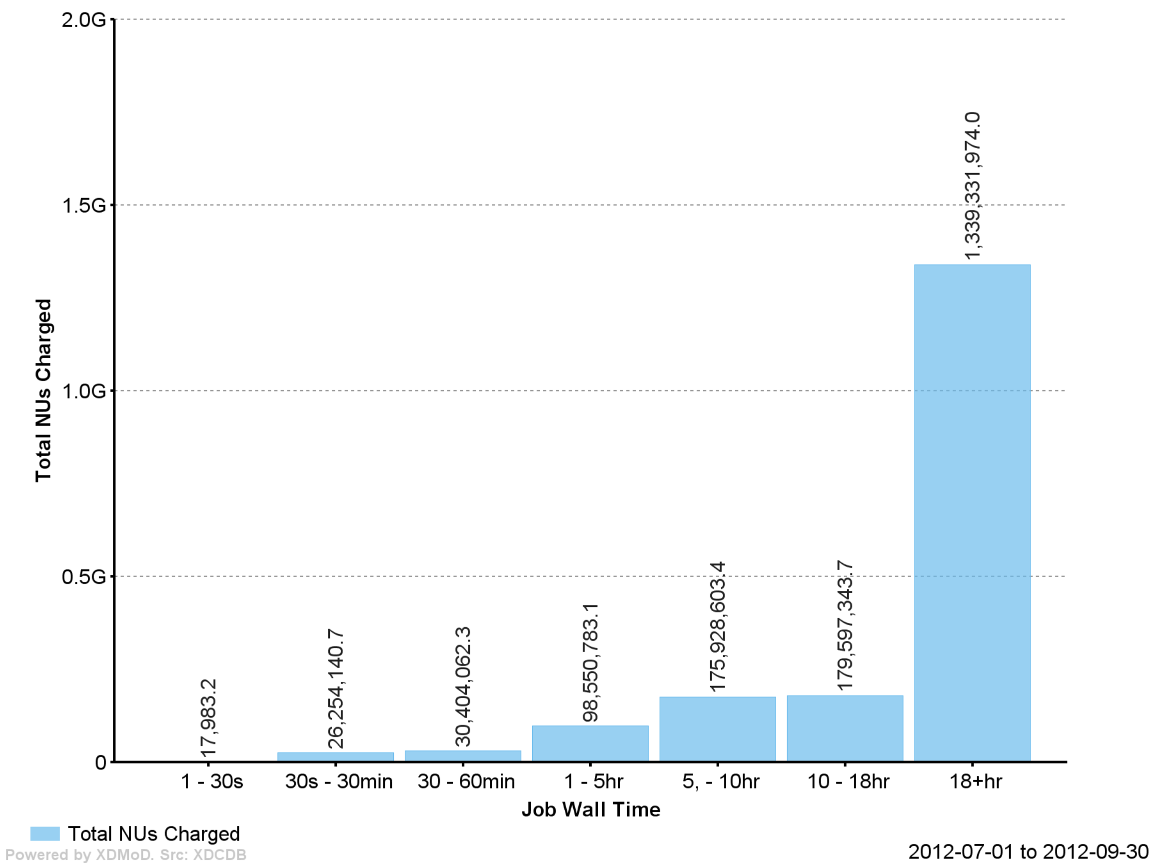
2012-07-01 to 2012-09-30



Total NUs Charged by Job Wall Time

Resource = SDSC-GORDON

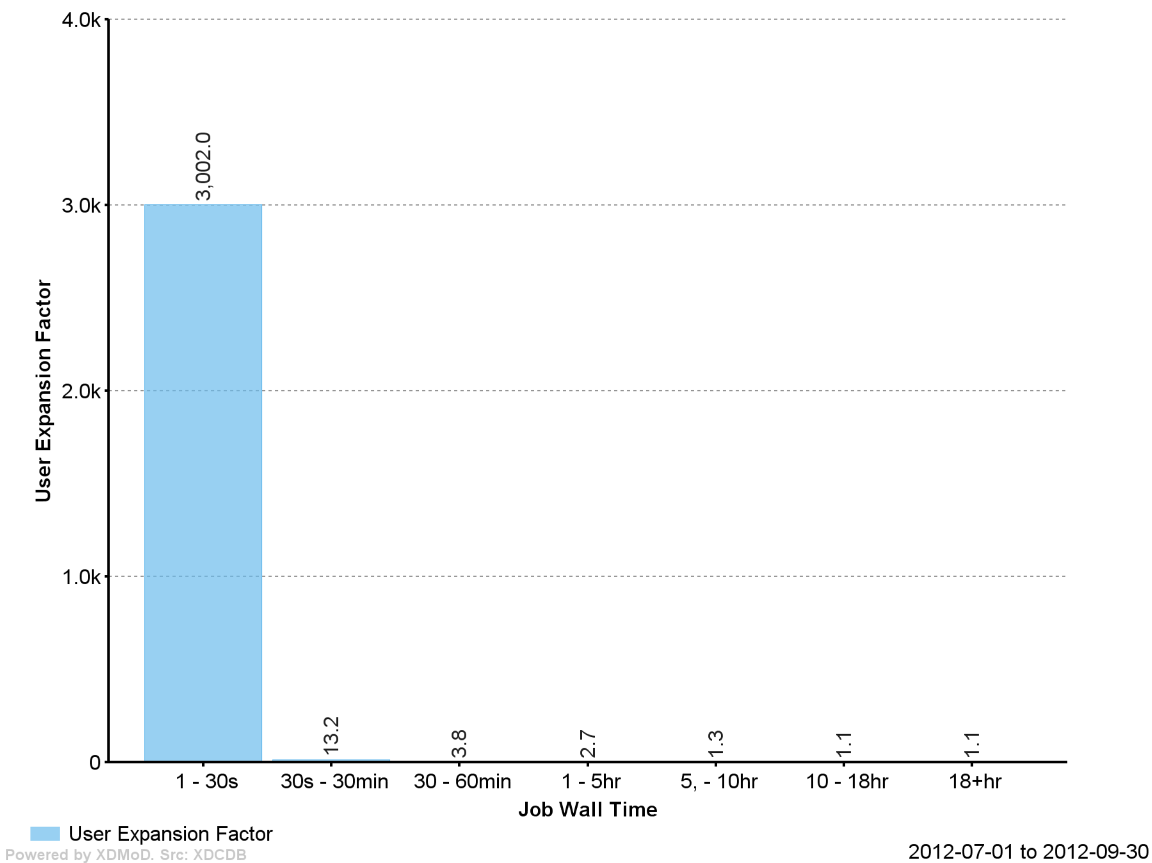
2012-07-01 to 2012-09-30



User Expansion Factor by Job Wall Time

Resource = SDSC-GORDON -- Service Provider = SDSC

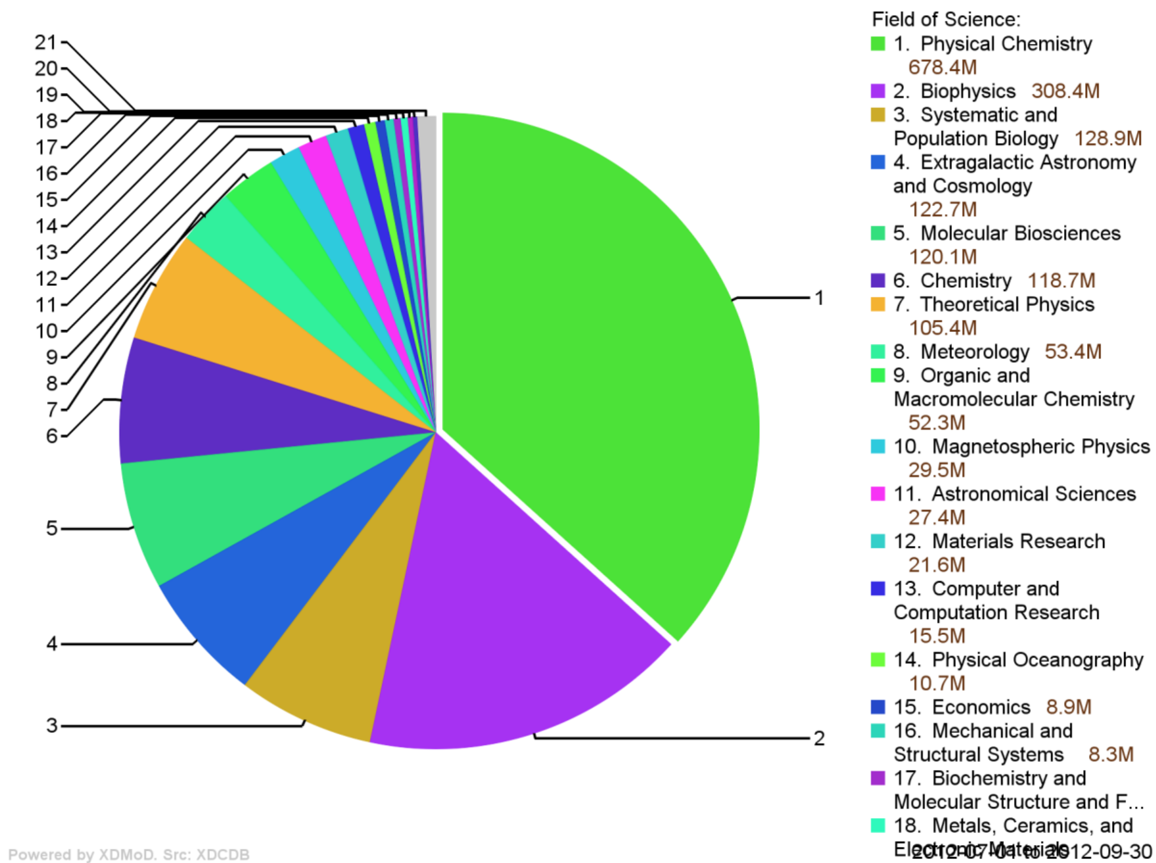
2012-07-01 to 2012-09-30



Total NUs Charged by Field of Science

Resource = SDSC-GORDON

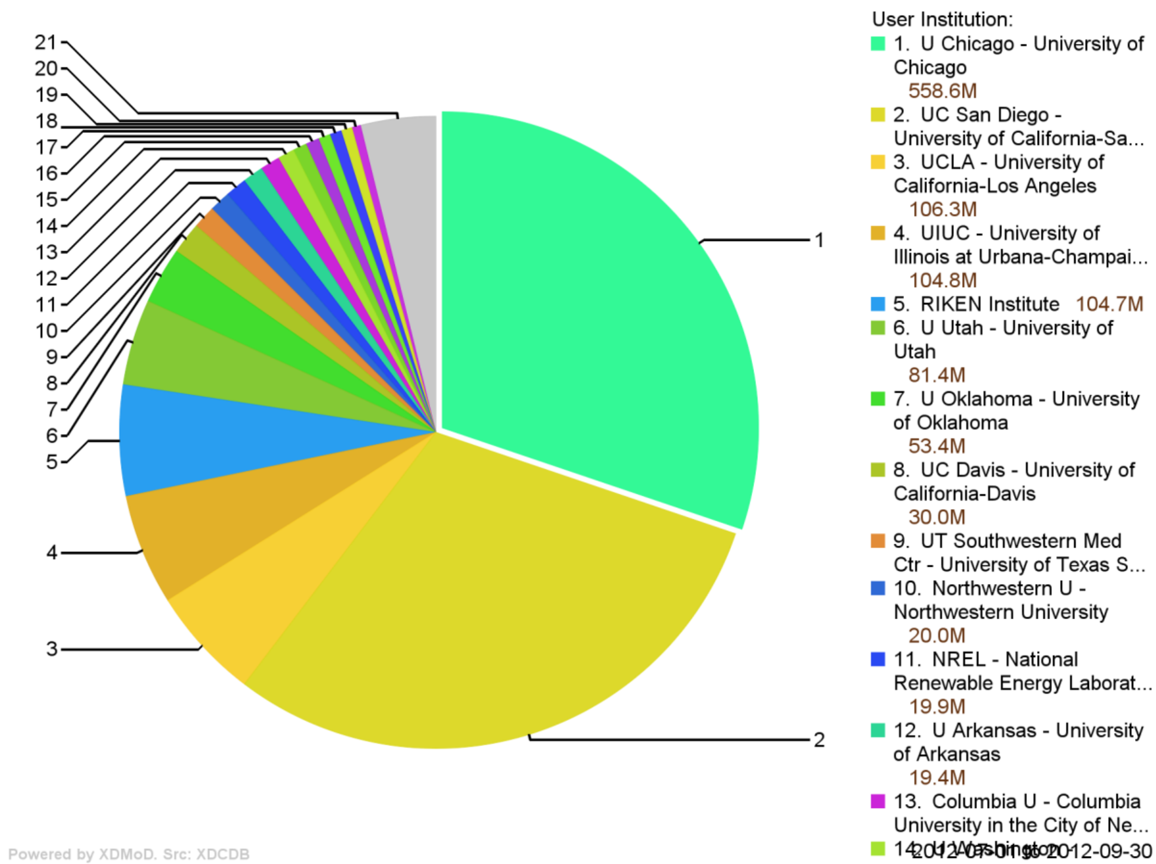
2012-07-01 to 2012-09-30



Total NUs Charged by User Institution

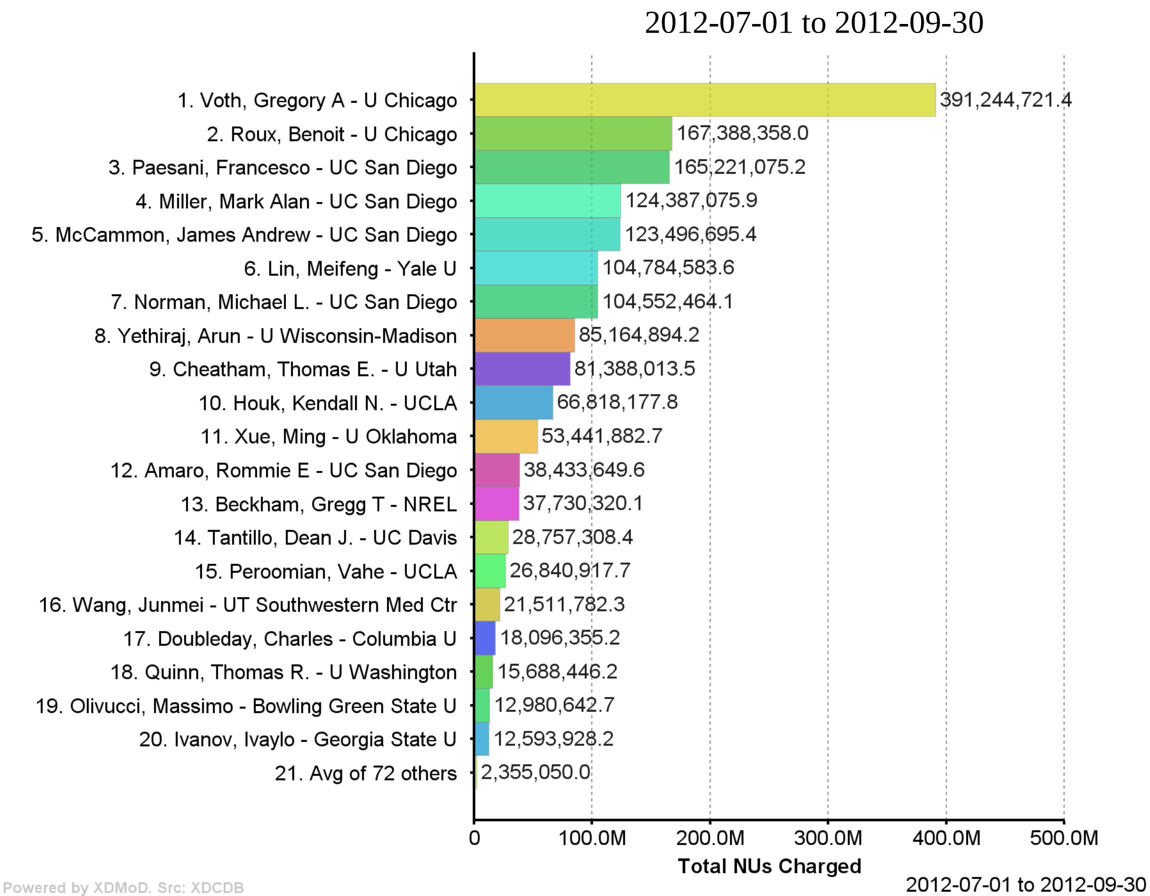
Resource = SDSC-GORDON

2012-07-01 to 2012-09-30



Total NUs Charged by PI

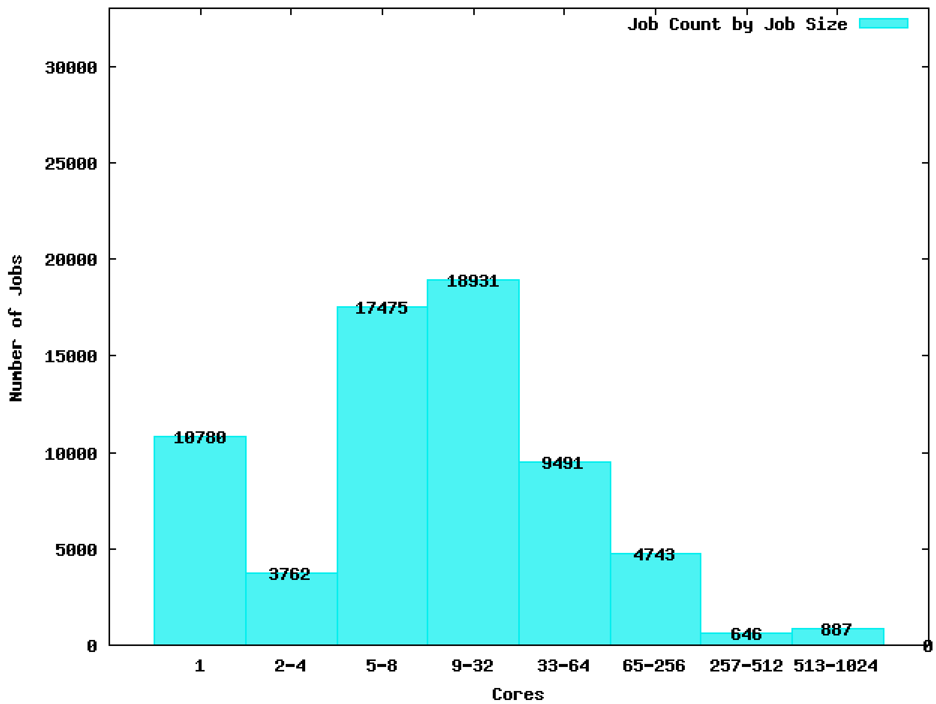
Resource = SDSC-GORDON



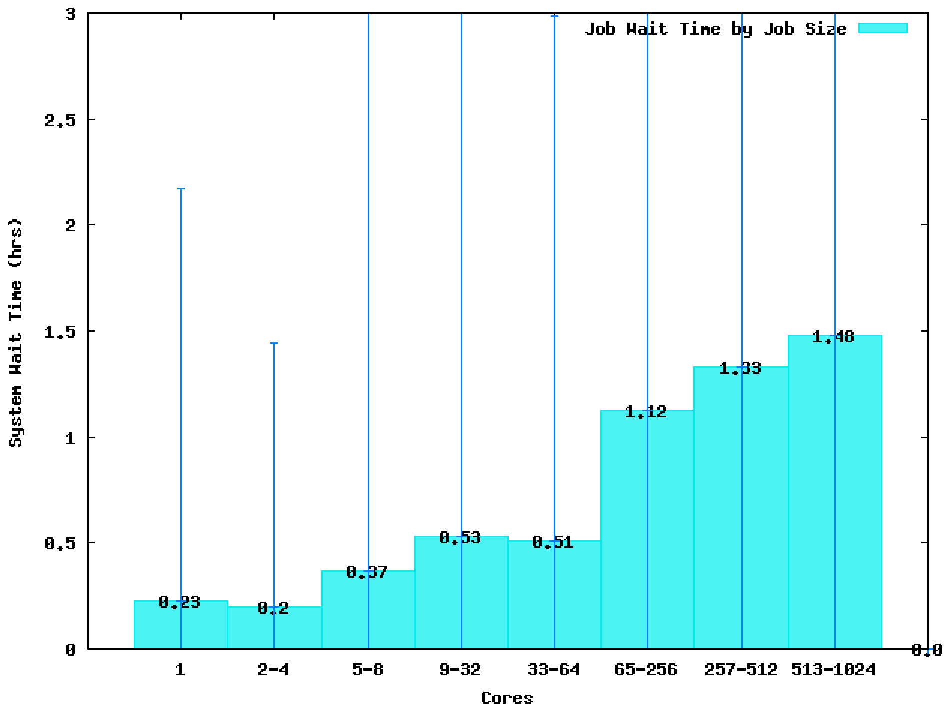
19.9.3 *Appendix 1.9C Trestles SP-specific Metrics*

2012-07-01 to 2012-09-30

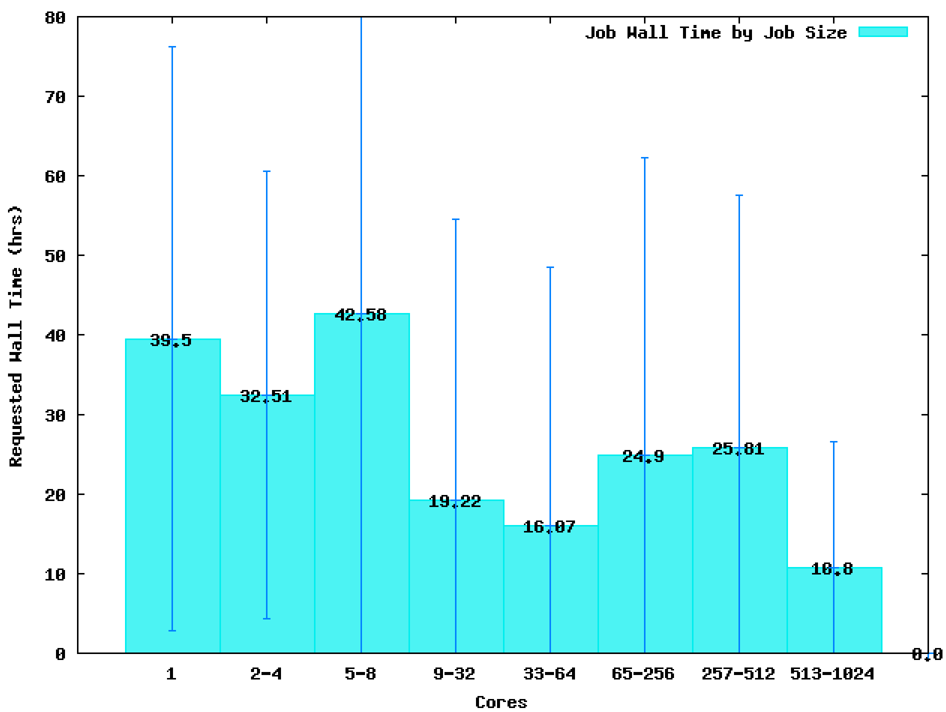
Number of Jobs run by Job Size (Cores)



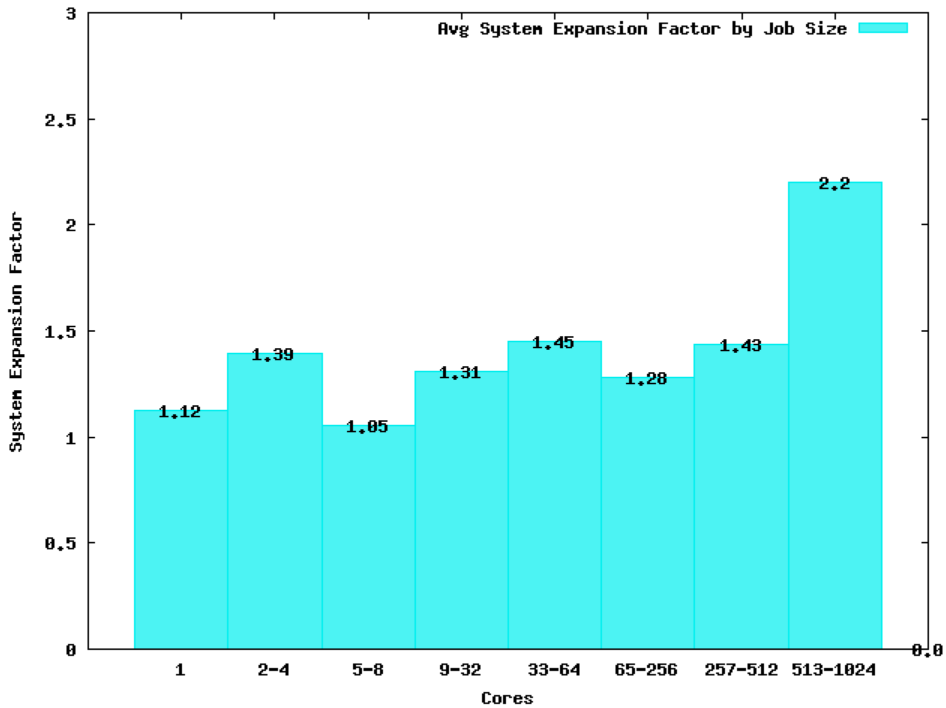
Average System Wait Time (Hours) by Job Size (Cores)



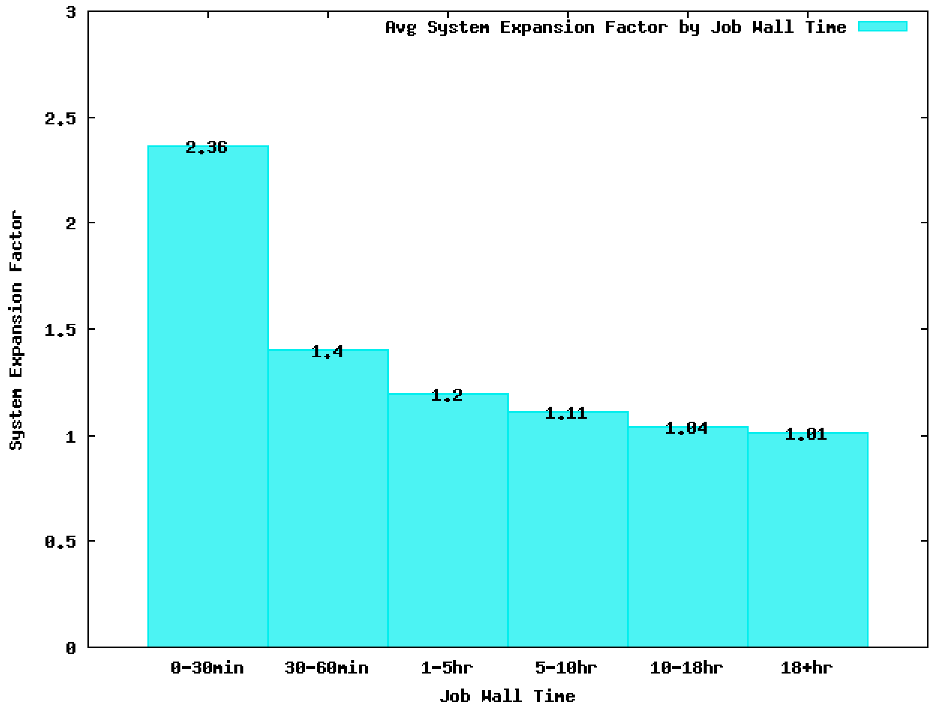
Average Requested Wall Time (Hours) by Job Size (Cores)



Average “Scheduler” Expansion Factor by Job Size (Cores)
(Requested Wall Time + System Wait Time)/Requested Wall Time


Avg System Expansion Factor by Job Size
System Expansion Factor
Cores
1
2-4
5-8
9-32
33-64
65-256
257-512
513-1024
1.12
1.39
1.05
1.31
1.45
1.28
1.43
2.2
0
0.5
1
1.5
2
2.5
3
0.0

Average Scheduler Expansion Factor by Requested Wall Time (Hours)



20 TACC - Service Provider Quarterly Report

20.1 Executive Summary

The Texas Advanced Computing Center (TACC) at The University of Texas at Austin (UT Austin) develops and deploys an integrated infrastructure of advanced computing resources to enhance the research and education activities of the faculty, staff, and students at UT Austin, and in Texas and across the US through its involvement in various state and national programs, including the NSF funded eXtreme Digital Resources for Science and Engineering (XD) project. This infrastructure includes high performance computing (HPC) systems, advanced scientific visualization (SciVis) systems, data servers and storage/archival systems, grid computing servers, IT systems, high-bandwidth networks, and a comprehensive software environment comprising applications, tools, libraries, databases, and grid software. TACC services include technical documentation, consulting, and training in HPC, SciVis, and grid computing.

TACC staff continued to contribute to the success of the XSEDE project to date. Significant effort was expended in the User Services User Engagement, User Interaction & Interfaces, and Training activities, XSEDE web site, and the Extended Collaborative Support Services area.

TACC continues to take a leadership role in XSEDE training efforts by offering 6 training workshops attended by 211 students during the reporting period, including the annual TACC Summer Supercomputing Institute that attracted 35 attendees from around the world. The Cornell University team continued to add training modules to and improve the Ranger virtual workshop.

Expansion of the TACC computing center to accommodate the new Stampede cluster was completed on August 14, 2012. Construction of the system is in progress with production scheduled for early January 2013.

20.1.1 Resource Descriptions

Ranger

The TACC Sun Constellation Cluster contains 62,976 cores (2.3 GHz) within 3,936 Sun Constellation blades (nodes), an X4600 Rocks master node, 4 X4600 user login nodes, 4 X4600 user gridftp nodes, 4 X4600 data movers, 2 X4600 nodes dedicated to supporting the SGE batch system, 2 X4600 external management service nodes, 2 X4600 InfiniBand subnet management nodes, an X4100 software build node, and 6 X4600 metadata server nodes to support the Lustre parallel file systems. Multiple work and home file systems are configured from 1.7 PB of storage managed by the Lustre parallel file system management software. Two Sun Data Center 3456 switches are the core of an InfiniBand fabric through which all components are connected. The basic configuration is as follows:

- 3936 Sun Constellation Blade Servers, each with
  - four quad-core 2.0 GHz processors
  - 32 GB of Memory
  - 8 GB flash drive
- 1.7 PB of storage managed by the Lustre Parallel File System software
- InfiniBand Interconnect

Lonestar

The TACC Dell Westmere Cluster contains 22,656 compute cores (3.33 GHz) within 1,888 Dell PowerEdge M610 compute blades (nodes), 15 PowerEdge R610 compute-I/O server-nodes, and 2 PowerEdge M160 login/management nodes. Each compute node has 24 GB of memory, and the login/development nodes each have 24 GB. 14 large memory (1TB) nodes are available for high-throughput computing and applications that require access to a shared-memory architecture and 8 GPU nodes are configured for visualization and applications that can take advantage of the computational speed of the GPUs. The system storage includes a 421 TB parallel WORK Lustre file system, a 841 TB parallel SCRATCH Lustre file system, and 275 TB of local compute-node disk space (146GB/node). A QDR InfiniBand switch fabric interconnects the nodes (I/O and compute) via a fat-tree topology, with a point-to-point bandwidth of 40Gb/sec. The basic configuration is as follows.

- 1888 Dell PowerEdge M610 Blade Servers, each with
    - Dual Intel Westmere 6-core, 3.33 GHz processors
    - 24 GB of Memory
    - 146 GB of Local Disk
- 14 Dell PowerEdge R910 servers, each with
    - Four 6-core, 2.0 GHz Intel Xeon processors
    - 1 TB of Memory
    - 292 GB of Local Disk
- 8 Dell PowerEdge C6100 servers, each with
    - Two NVIDIA M2070 GPUs
    - Two 6-core, Intel Xeon X5670 2.93 GHz processors
    - 24 GB of Memory
    - 146 GB of Local Disk
    - 16-lane PCI Express to Dell C410x PCI expansion box housing the NVIDIA GPUs
- 421 TB Lustre Parallel File System (WORK)
- 841 TB Lustre Parallel File System (SCRATCH)
- QDR InfiniBand Interconnect

<u>Longhorn</u>

The TACC DELL/NVIDIA Visualization & Data Analysis Cluster, Longhorn, is a hybrid CPU/GPU system designed for remote, interactive visualization and data analysis. In addition, Longhorn supports production, compute-intensive calculations on both the CPUs and GPUs via off-hour queues. The large, per-node memory is intended to support serial and parallel visualization and analysis applications that take advantage of large memories, multiple computing cores, and multiple graphics processors. Longhorn is an ideal companion resource for working with large data sets created on Ranger, since Longhorn can directly access Ranger's Lustre parallel file system through a 10 GigE network link.

The system consists of 256 dual-socket nodes, each with significant computing and graphics capability. Total system resources include 2048 compute cores (Nehalem quad-core), 512 GPUs (128 NVIDIA Quadro Plex S4s, each containing 4 NVIDIA FX 5800s), 13.5 TB of distributed memory and a 210 TB global file system. Longhorn configuration details can be found below.

128 NVIDIA Quadro Plex S4s, each with

- 4 NVIDIA FX 5800 GPUs
- 16GB Graphics Memory (4GB per GPU)
- 2 independent graphics busses, one per GPU pair

240 Dell R610 Compute Nodes, each with

- 2 Intel Nehalem quad-core processors (8 cores) @ 2.53 GHz
- 48GB RAM
- 73GB local disk
- connected to 2 dedicated NVIDIA FX 5800 GPUs via Quadro Plex graphics bus

16 Dell R710 Compute Nodes, each with

- 2 Intel Nehalem quad-core processors (8 cores) @ 2.53 GHz
- 144GB RAM
- 73GB local disk
- connected to 2 dedicated NVIDIA FX 5800 GPUs via Quadro Plex graphics bus

Mellanox QDR InfiniBand Interconnect

14 Dell PowerVault MD1000 Direct Attached Storage Arrays (210TB global file system, managed by the Lustre Parallel File System)

Spur

TACC's Terascale Sun Visualization Cluster contains 128 compute cores, 1 TB aggregate memory and 32 GPUs. Spur acts not only as a powerful stand-alone visualization system: it also enables researchers to perform visualization tasks on Ranger-produced data without migrating to another file system and to integrate simulations and rendering tasks on a single network fabric. The cluster consists of the following hardware:

- 1 Sun Fire X4600 server with 2 NVIDIA Quadro Plex model 4. The X4600 contains 8 dual-core CPUs (16 cores total) and 256GB of RAM. Each Quadro Plex model 4 contains 2 NVIDIA Quadro FX5600 GPUs;
- 1 Sun X4400 servers, with 4 quad-core CPUs (16 cores total) and 128GB of RAM, connected to 2 NVIDIA Quadro Plex model 4. Each Quadro Plex model 4 contains 2 NVIDIA Quadro FX 5600 GPUs;
- 6 Sun X4400 servers, each with 4 quad-core CPUs (16 cores total) and 128GB of RAM, and each connected to an NVIDIA Quadro Plex S4. Each Quadro Plex S4 contains 4 NVIDIA Quadro FX 5600 GPUs; and
- Total system capability: 128 cores, 1TB aggregate memory, 32 GPUs.

Because Spur shares Ranger's interconnect fabric and file systems, researchers will be able to easily transition between HPC runs to generate and visualize data. Furthermore, visualization software is able to harness both the rendering power of the graphics hardware and the compute power of Ranger to enable the analysis of terascale and larger data sets.

20.2 Science Highlights

2012 Q3 Highlights - TACC

Environmental Biology: Advancing Evolutionary Insights through Next-Generation Sequencing (PIs: Eileen Lacey and Matthew MacManes, University of California-Berkeley)

Aaron Dubrow (aarondubrow@tacc.utexas.edu)

In the foothills of the Santa Cruz Mountains two closely related species of mice share a habitat and a genetic lineage, but have very different social lives. The California mouse (Peromyscus californicus) is characterized by a lifetime of monogamy; the deer mouse (Peromyscus maniculatus) is sexually promiscuous. Researchers from UC Berkeley examined the differences between these two species of mice on a microscopic and molecular level. They discovered that the lifestyles of the two mice had a direct impact on the bacterial communities that reside within the female reproductive tract of the species. These differences correlate with enhanced diversifying selection on genes related to immunity against bacterial diseases. The results were published in the May 2012 edition of *PLoS One*. To reach these conclusions, post-doctoral researchers Matthew MacManes performed a genetic analysis on the variety of DNA present in each species, revealing hundreds of different types of bacteria. He found that the promiscuous deer mouse had twice the bacterial diversity as the monogamous California mouse. Since many bacteria cause sexually transmitted infections (like chlamydia or gonorrhea), he used the diversity of bacteria as a proxy for risk of disease.

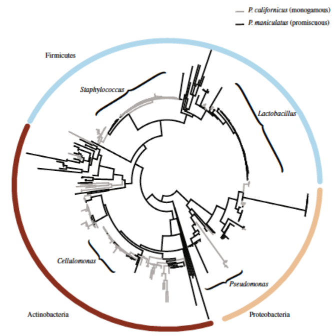


Figure n. Phylogeny of the 16S rRNA sequences used in this study. Gray branches correspond to the bacterial sequences recovered from the monogamous P. californicus, while the black branches related to the promiscuous P. maniculatus.

The researchers next studied how the bacterial diversity in the promiscuous mice might translate into changes to the genes involved in immune function. MacManes hypothesized that selective pressures caused by generations of bacterial warfare had fortified the genomes of the promiscuous deer mouse against the array of bacteria it hosts. Based on a comparison of the two species' genotypes he confirmed that the promiscuous mice had much more diversity in the genes related to their immune system. The results match findings in humans and other species with differential mating habits. They show that differences in social behavior can lead to changes in the selection pressures and gene-level evolutionary changes in a species. The researchers used NSF supercomputers allocated through the Extreme Science and Engineering Discovery Environment (XSEDE) to analyze datasets too big for their university laboratory clusters.

The alignment and analysis that MacManes accomplished on Ranger in a few weeks would have taken years with his local resources, allowing him to rapidly find insights about the relationship between genes and behavior.

Molecular Biosciences: Simulations of Protein Folding and Aggregation (PI: Joan-Emma Shea, University of California-Santa Barbara)

Aaron Dubrow (aarondubrow@tacc.utexas.edu)

Alzheimer’s disease is one of the most dreaded and debilitating illnesses. Currently, the disease afflicts 6.5 million Americans and the Alzheimer’s Association projects it to increase to between 11 and 16 million by 2050. Long knotty fibrils, formed from misfolded protein fragments, are almost always found in the brains of diseased patients. These accumulations, known as amyloid plaques, were

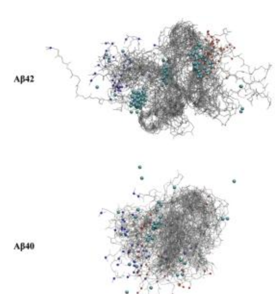


Figure n. Binding of Aβ(39−42) to Aβ42 and to Aβ40. The positively charged N-termini and negatively charged C-termini are indicated by small blue and red balls, respectively. The C-terminal fragments are noted by the larger cyan balls.

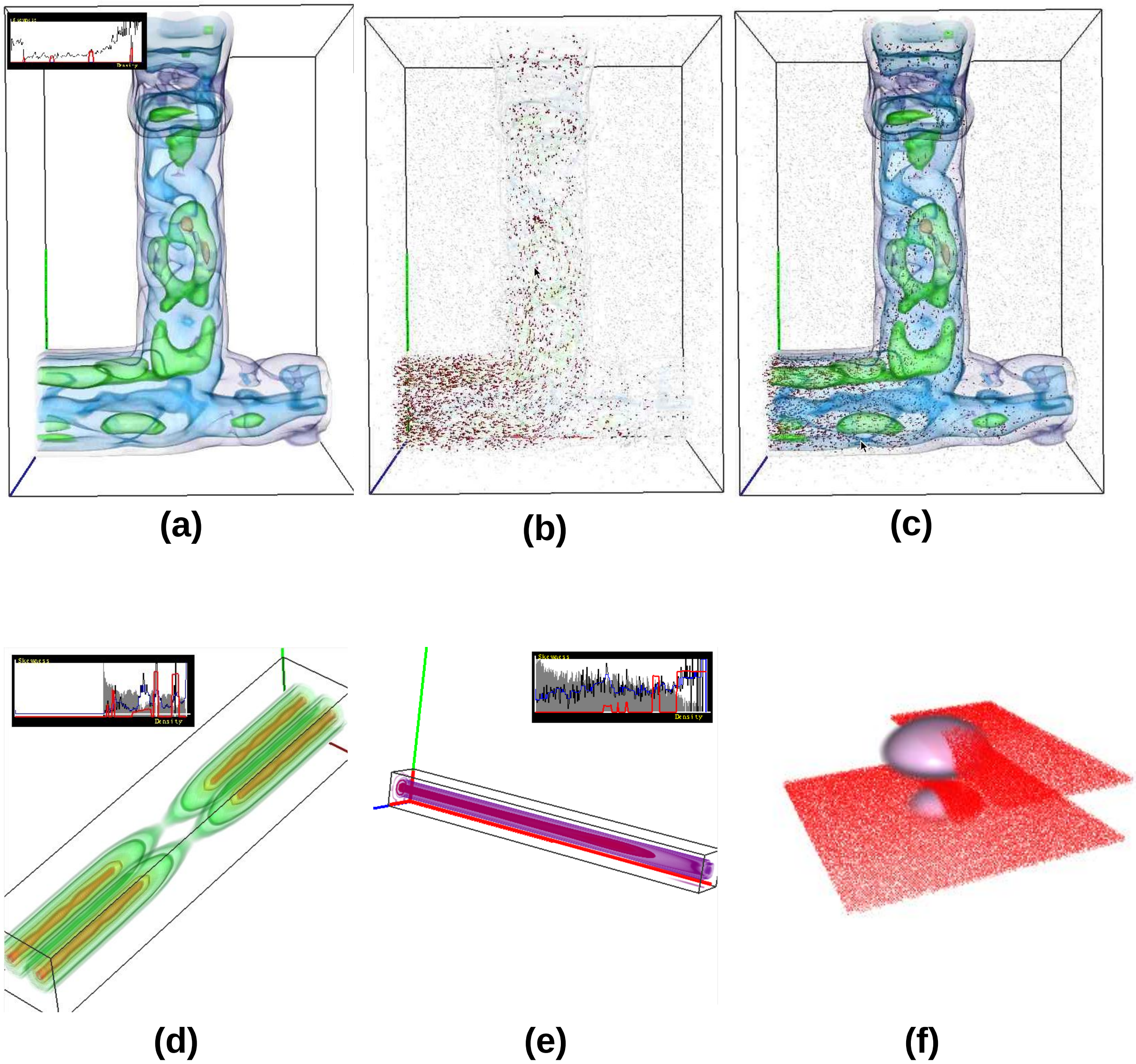
presumed to be the cause of the disease. However, new findings support a hypothesis that the amyloid plaques are a by-product of the disease rather than the toxic agent. This paradigm shift changes the research focus to smaller, intermediate molecules that form and dissipate quickly, and are difficult to perceive in brain tissue.

In 2007, Shea and Michael Bowers, professor of chemistry and biochemistry at UCSB received a grant from the National Institutes of Health to investigate small peptide-based inhibitors that would prevent these oligomers from forming. To understand the structure, formation and behavior of amyloid accumulations in the brain. the Shea group at University of California-Santa Barbara relies upon computer simulations. Since 2007, Shea has run thousands of simulations of amyloid peptides using the Ranger supercomputer at the Texas Advanced Computing Center (TACC). The simulations helped to identify the important structures that are adopted by these peptides at a resolution that exceeds what can be examined experimentally. In a recent paper in *Biophysical Journal*, Shea and postdoctoral researcher Luca Larini studied the conformations adopted by small oligomers of peptide amyloids encountered within the cell. They found that hairpin-shaped forms of the peptide initiated the aggregation of oligomers that ultimately led to the formation of a fibril.

The supercomputer simulations have not only helped uncover the role of oligomers in the onset of Alzheimer's, but they are aiding in research that is trying to stop oligomer formation altogether. A paper in the November 2011 edition of *Biochemistry* described how a class of small molecules known as c-terminal inhibitors stopped the formation of oligomers, possibly halting disease progression. Since 2009, the project has used more than 13 million hours of compute time on TACC's Ranger and Lonestar supercomputers. The simulations are helping researchers identify where the inhibitors bind and are leading to new ideas about how inhibition can be improved.

Longhorn Science Highlights

Gerhard Klimeck, Purdue University: This group does research on nanoelectronic modeling and simulation, and has interest in Purdue's visualization tools to visualize simulation data generated by NEMO5 (the fifth edition of the nanoelectronics modeling tools) developed in his group. The Longhorn Purdue project partners have worked with the Nanoelectronic Modeling Group at Purdue University. The current users of the simulation tool are Dr. Klimeck's group, Intel, and Samsung Electronics, but more users in academia and industry are expected. Simulation data is stored in VTK, OpenDX, Silo, and their own data format (nanoHUB.org). These data formats are supported now. Shown below are examples of the NEMO5 simulation tool and other simulation tools on the nanoHUB with respective.



(a), (b), and (c) shows an electron distribution density and current flow from the NEMO5 simulation. (d) Quantum transport simulation of silicon nanowire transistor using nanoHUB Nanowire tool. (e) Electronic structure of the nanowire represented in an atomistic tight binding basis (diamond structure). (f) Quantum dot molecule (two vertically stacked quantum dots) obtained from NEMO 3D.

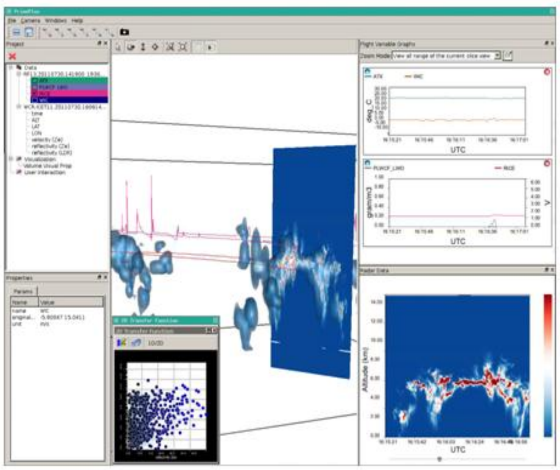
Chris Sims (Institute for Computational Engineering and Sciences, The University of Texas at Austin):

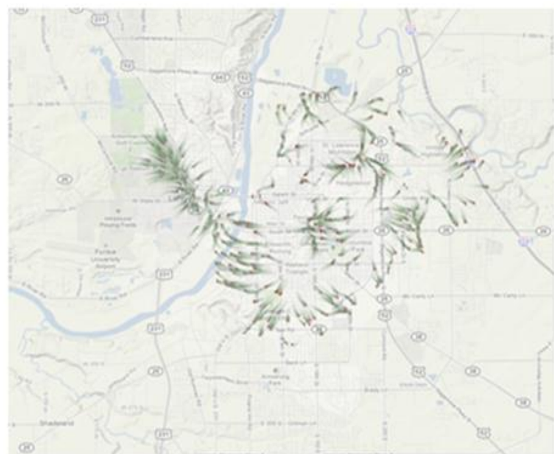
While Longhorn is used primarily for interactive visualization and data processing, the fast CPUs coupled with larger-than-typical memory and the QDR interconnect have also been used to advance the level of accuracy routinely accessible to vibronically-coupled hamiltonians. Certain classes of wavefunction-based ab-initio methods have been relegated to out-of-core algorithms to tackle problems on the cutting edge. One such problem is the quantitative parameterization of the quasi-diabatic hamiltonian of the nitrate radical (NO3), which is the dominant oxidant in Earth's atmosphere at night.

While parameterizing the quasi-diabatic hamiltonian based on numerical fits to the fixed-nuclei potential energy surfaces is an embarrassingly parallel problem, the number of simultaneous calculations that can be done on a single system is usually limited to 4-16, depending on the I/O bandwidth of the global file system. This is due to the fact that on most systems, an out-of-core method must be used due to the large memory requirements of a single point at the level of theory / basis set size needed to accurately characterize the vibronically coupled states. Because of the large memory of each node and the QDR interconnect on Longhorn, we were able to develop a new, MPI-based "out of core" algorithm to solve the scalability issues. Instead of writing out contents of memory to disk for each calculation, jobs used remote node memory as if it were its own. This decreased turn around time for the entire calculation from 300 days on a typical HPC system to just over 30 days on Longhorn.

Department of Earth & Atmospheric Science, Purdue University:

We have been focusing on information-assisted visualization methods for cloud radar data and trends of discrete events (e.g, crimes and healthcare). Our research consists of two parts: 1) visual analytics application for cloud radar datasets and 2) flow analysis for spatiotemporal datasets. We have been working with experts in the Department of Earth & Atmospheric Science at Purdue University to effectively visualize their cloud radar data.





(Left) The user interfaces for cloud radar data analysis. (Right) The temporal trend analysis for spatiotemporal data on the map.

More than 50% of the earth's precipitation originates in the ice phase. Ice nucleation, therefore, is one of the most basic processes that lead to precipitation. The poorly understood processes of ice initiation and secondary ice multiplication in clouds result in large uncertainties in the ability to model precipitation production and to predict climate changes. (http://www.eol.ucar.edu/projects/ice-t/). The goal of the Ice in Clouds Experiment - Tropical (ICE-T) is to show that direct ice nucleation measurement(s) or other specific measurable characteristics of the aerosol can be used to predict the number of ice particles formed by nucleation mechanisms in selected clouds, under given conditions. We have been developing a visual analytics tool to support ICE-T data analysis. The figure shown above (Left) shows the user interfaces of the tool. This work includes reflectivity and velocity volume rendering and slice views, and linked view with flight variables and radar data variables.

20.3 User-facing Activities

20.3.1 *System Activities*

Plans are in place to replace the underlying infrastructure of the Ranch archive facility. An upgrade, tentatively scheduled for Q4CY2012, will result in a replacement of the current cache and the server that supports the cache and the two robotic mechanisms. Approximately 1PB of high-performance cache will support the user community following the upgrade.

20.3.2 *Services Activities*

The TACC Life Sciences group continued to increase the number of software packages available on Ranger and Lonestar in support of the computational biology community.

The TACC HPC group provided extensive support to Dr. David Soto, visiting professor in the Russell Poldrack neurobiology Imaging Center at UT at Austin. Staff facilitated Dr. Soto's custom experiments that made it possible for him to predict the duration of planned MRI analysis jobs.

TACC staff worked with a student of XSEDE PI Margaret Cheung (University of Houston) to enable implementation of a replica exchange simulation using the research group's modified version of Amber (project that started at the TACC Summer Supercomputing Institute). Integration with the Grid Engine scheduler was necessary to achieve a successful simulation on both Ranger and Lonestar. During the project a race condition was identified and TACC staff implemented a new file locking approach to eliminate it.

Longhorn several users were given queue exceptions to run at large core counts or longer durations. Ronald Cohen (tg458678) of the Carnegie Institute for Science, PI for project EAR080016N was given extended runtime for his computational study of planetary materials.

20.4 Security

There have been no changes in TACC security procedures or security incidents/responses within the reporting period.

20.5 Education, Outreach, and Training Activities

TACC Outreach Activities

XSEDE activity in Q3 2012 continued with participation in monthly All-TEOS meetings led by Scott Lathrop (NCSA), bi-weekly Outreach meetings led by Laura McGinnis (PSC), and bi-weekly Underrepresented Outreach meetings led by Linda Akli (SURA). Year two outreach events were finalized in the Q3 Outreach meetings. The TEOS all calls continued to provide an opportunity for information and clarification of activities across TEOS and a chance to identify opportunities for collaboration within the existing planned year two activities.

The first cohort of the XSEDE Student Engagement Program completed their appointments the first two weeks of August, as determined by when they started their assignments. The cohort had 16 participants. PSC sponsored 6 students with 4 working remotely. NICS sponsored 4 students, with 3 working remotely. TACC sponsored 6 students with 1 working at SDSC, 3 working at TACC and 2 working remotely. TACC based participants included graduate students from the University of Texas, Clemson University, and University of Colorado. The students presented their works-in-progress at XSEDE 12 in Chicago. Each student gave a PowerPoint presentation and poster presentation.

Underrepresented outreach conducted a successful invitation only 3-hour workshop at XSEDE 12 to discuss scaling up outreach to Minority Serving Institutions. Representatives were in attendance from University of Arkansas Pine Bluff, Clark Atlanta University, Florida A&M University, Florida International University, Howard University, New Mexico State University, Norfolk State University, North Carolina Central University, Sinte Gleska University, Southern University, and Texas Southern University, University of Texas El Paso. John Townsend and Steve Gordon also joined the meeting. Several attendees were Campus Champions. Current MSI XSEDE users presented their experience to their peer MSIs. They discussed the XSEDE services they currently use, the challenges they face, and the process they followed to achieve buy-in from their administration. The attendees walked away with a matrix of nearly all of XSEDE's cyberinfrastructure services and tentative consultations set on first time or additional services they desired.

Several follow-ups to the workshop began in Q3, including a regional training workshop scheduled for February 2013 to be hosted by the University of Texas at El Paso, a consultation with Florida International University and their administration about XSEDE services, a curriculum consultation with Sinte Gleska University in South Dakota (the only 4-year Tribal College), a faculty development consultation with Howard University, and a faculty development consultation with New Mexico State University.

Follow ups also continued in Q3 with contacts from the highly productive assortment of networking activities at the National Science Foundation Joint Administrative Meeting (JAM), in Q2 in Washington, D.C. for Principal Investigators in the EHR Directorate.

The Campus Champion discussion with Austin Community College (ACC), a two-year college in Austin, Texas continued in Q3. The awarding of a $4.5 million Department of Labor grant to ACC for innovate learning, including computer programming course development, represents an opportunity for a defined role for a Campus Champion liaison to XSEDE.

The Austin Forum on Science, Technology & Society

In Q3, TACC hosted a total of 3 monthly Austin Forum events with invited speakers from areas of interest focusing on science and technology. The goal of The Austin Forum on Science, Technology & Society is to engage and educate the local community about the numerous ways in which science and technology enhance the quality of their everyday lives, as well as the health, prosperity and security of the nation. One hour is devoted to a presentation and Q&A discussion between the speaker and guests. Ample time for networking is offered, both preceding and following the speaker presentation. The speaker series has become increasingly popular in the community, attracting a total of 781 people this quarter. Average attendance nearly doubled since the last quarter.

TACC Facility Tours and Presentations

From K-12 and higher education groups, and special populations including seniors, TACC conducted facility tours and outreach presentations impacting 444 people in Q3 2012, 30% of who were under-represented. An overview of XSEDE and TACC were given at each event.

This quarter, TACC presented to two large groups (120+ people): 1) the Sun City Texas Computer Club, which serves retired citizens in the community of Sun City, and 2) Breakthrough Austin, a non profit organization that creates first-generation college students, presented in collaboration with the department of Petroleum and Geoscience Engineering (PGE) at the Cockrell School of Engineering, The University of Texas at Austin.

Type	Title	Location	Date(s)	Number of Participants	Number of Under-represented people

The Austin Forum on Science, Technology and Society	"Securing Texas' Water Future" w/Dr. Danny Reible	AT&T Conference Center	7/3/12	139	Not tracked.
Vislab Tour	TX MBA + Leadership Program, UT McCombs	Vislab	7/10/12	4	Not tracked.
Vislab Tour	UT CNS: FRI	Vislab	7/11/12	8	Not tracked.
Vislab Tour	VIP: Union Pacific	Vislab	7/17/12	6	1
Vislab Tour	Breakthrough Austin (middle school students, ages 12-15)	Vislab	7/19/12	121	108
Vislab Tour	UTPREP- UTeach Outreach	Vislab	7/25/12	23	23
Machine Room Tour	NASA	PRC	8/2/12	10	1
The Austin Forum on Science, Technology and Society	"From Sous Vide to Social Search: How Technology is Changing How We Cook and Eat" w/Addie Broyles and Michael Chu	AT&T Conference Center	8/7/12	257	Not tracked.
Presentation	Presentation: Camp Texas, new UT students	Vislab	8/10/12	50	Not tracked.
Presentation	Presentation: Camp Texas, new UT students	Vislab	8/12/12	50	Not tracked.
Machine Room Tour	VIP Tour: Tulane/ Dell	PRC	8/14/12	4	1
Machine Room Tour	VIP: State Farm Insurance	PRC	8/15/12	8	2
Presentation	Sun City Computer Club	Sun City	8/20/12	150	Not tracked.
Machine Room Tour	VIP: Tour	PRC	8/16/12	7	Not tracked.
Machine Room Tour	VIP: Melyssa	PRC	8/30/12		Not tracked.
The Austin Forum on Science, Technology and Society	"TEDxAustin: A Million Decisions Behind One Big Idea" w/Shawna Butler and Nancy Giordano	AT&T Conference Center	9/4/12	385	Not tracked.
Tour of Lonestar	TexSOAR group at Applied Research Labs	PRC	9/27/12	3	Not tracked.

XSEDE12 Activities

Several TACC staff members attended and contributed to activities at the XSEDE12 conference. Contributions by TACC staff to tutorial and presentation events are listed in section 1.8. TACC staff also contributed to planning and organization conference activities.

TACC Education Activities

Scientific Computing Curriculum and Courses

TACC's Fall 2012 courses started near the end of Q3. Waitlists for classes continue to grow and students in the academic courses continued expressing interest in additional training courses offered at TACC. In addition, the GPU Programming class was offered in the long summer session overlapping Q2 and Q3, with an enrollment of 16 students. The class is being revamped for the future to account for the advancements in GPUs and GPU programming. The Q3 class included content on GPGPU programming. Fall enrollment scientific computing course totals were 27 graduate students and 49 undergraduates. Courses being taught by TACC staff include: Introduction to Scientific Programming (9 graduate students and 20 undergraduates), Scientific and Technical Computing (12 graduates and 16 undergraduates), and Visualization and Data Analysis (6 graduate students and 13 undergraduates). Students in the introduction to Scientific Programming and Scientific and Technical Computing classes were assigned accounts on

Ranger. Students in the Visualization and Data Analysis class were assigned accounts on *Longhorn*.

The courses are offered in the Flawn Academic Center located on the main UT Austin campus in a customized classroom housing both lecture space and a computer instruction laboratory. The classroom customization was made possible through a partnership with Chevron to increase instruction in scientific computing.

The partnership with the UT Austin Division of Statistics and Scientific Computation (DSSC) continues with DSSC being the home of the Scientific Computation courses. DSSC offers an Undergraduate Certificate and a Graduate Portfolio Program in Scientific Computation, both commonly being referenced as the certificate program. Four of the scientific computing classes taught by TACC fulfill requirements for the certificate and portfolio. Documentation of students completing the certificate program appears on their transcript as a notation. As of Q3, 11 students have completed the program since its inception. For Q3 2012, 50 students are enrolled in the program. Enrollment in the certificate program includes 48% from the College of Natural Science (which is home to mathematics, statistics, and computer science), 28% from the Cockrell School of Engineering, 16% from the College of Liberal Arts, and 8% from the McCombs School of Business. DSSC's scientific computing course descriptions are online at:

http://www.tacc.utexas.edu/education/academic-courses

Training

TACC staff conducted 6 training workshops within the reporting period. A total of 211 attended the workshops either in person or via webcast. Most workshops were recorded and a link to the recorded provided to attendees for later viewing or to pass on to colleagues. The following table lists the date, title, location, and attendance for each workshop.

Type	Title	Location	Date(s)	Hours	Number of Participants	Number of Under-represented people	Method
Wrkshp	TACC Summer Supercomputing Institute 2012	TACC	7/30-8/3	40	35	13	S
Wrkshp	Structured Data, Metadata and Provenance in the context of Scientific Data Management Projects	TACC	8/23	2	35	9	S
Wrkshp	Intro to Scientific Visualization on Longhorn	TACC	9/6	8	16	4	S
Wrkshp	XSEDE Resources Overview for EPSCOR	TACC	9/13	1.5	NA	NA	S
Wrkshp	Linux/Unix Basics for Life Scientists	UT Austin	9/18	3	24	NA	S
Wrkshp	Linux/Unix Basics for HPC	TACC	9/20	3	101	18	S

The Virtual Workshop provides users access to twenty-four training modules with new modules under development and existing modules being reviewed for updates. Users who are logged in to the XSEDE portal can pass-through to the Virtual Workshop, or they can use guest registration.

<u>Available Modules</u>

<u>Programming Languages</u>
An Introduction to Linux
An Introduction to C Programming
An Introduction to Fortran Programming
Python for High Performance
Balancing Scripts and Compiled Code in Scientific Applications
MATLAB Programming

<u>Parallel Computing</u>
Parallel Programming Concepts and High-Performance Computing
Ranger Environment
Message Passing Interface (MPI)
MPI Point-to-Point Communication
MPI Collective Communications
MPI One-Sided Communication
MPI Advanced Topics
Parallel I/O New
OpenMP
Hybrid Programming with OpenMP and MPI

<u>Code Improvement</u>
Profiling and Debugging
Optimization and Scalability Series Part 1: Planning for Parallel
Computational Steering

<u>Data Analysis</u>
Large Data Visualization
Paraview
VisIt
Using Databases
MapReduce New

Modules Currently in Development
Allocations
Data Transfers
PerfExpert
R
Transition to Stampede
Intro to Python (we already have Python for HPC)
MATLAB
Optimization and Scalability, parts 2 & 3
Advanced Batch

Virtual Workshop Usage

	Page Loads	Unique Visitors	First Time Visitors	Returning Visitors
Q1 ‘11	4,456	920	730	190
Q2 ‘11	16,281	2,988	2,509	479
July – Sept 2011	9,208	2,905	2,457	448
Oct – Dec 2011	10,068	3,615	3,019	596
Jan – Mar 2012	16,800	5,318	4,249	1069
Apr – Jun 2012	17,875	5,860	4,795	1,065
July – Sept 2012	23,888	5,611	4,442	1,169

Note: the Q2 ’11 numbers were a result of high activity after an online news release on the Virtual Workshop was sent out.

20.6 SP Collaborations

The Longhorn visualization team collaborated with the Intel software group to demonstrate new software capabilities with the goal of supplying the software to TACC users across XSEDE systems.

20.7 SP-Specific Activities

Ranger continued to be a resource in high demand this quarter, with full utilization on a variety of large and small jobs (more than 167,000 jobs and 120M SUs delivered). A single outage this quarter on Ranger was due to an area-wide power outage at an Austin Energy substation. The system recovered fully from this unscheduled outage with no loss of data. Large projects on Ranger this quarter include hurricane analysis, simulations of proteins involved in DNA mismatch recognition, biological membrane proteins, and modeling of diffusive convection. Ranger continues to operate on an extension year and is scheduled to be decommissioned in four more months, on February 4th, 2013. Operations will continue unchanged, and security upgrades/patches and application upgrades will continue, but no major upgrades to the software environment will happen for the remainder of the system life.

The Longhorn project continued to recruit new users, developing effective visualizations, developing tools to respond to evolving user needs, and training current and next generation scientists and engineers. Efforts have focused on increasing visualization and data analysis usage on Longhorn. Additionally, the visualization team concentrated on the enhancement and improvement of the user experience by improving the remote visualization capabilities, particularly through the Longhorn Visualization Portal. Longhorn usage has continued to increase with a diverse portfolio of users wanting interactive Visualization and Data Analysis.

The Longhorn software team collaborated with the Intel graphics group to prepare software to demonstrate large-scale rendering and image streaming capabilities from TACC systems to the SC12 conference.

20.8 Publications

Rane A., Browne J., Koesterke L. “A Systematic Process for Efficient Execution on Intel’s Heterogeneous Computation Nodes” *Presentation at XSEDE12 Conference*

Schulz K. “A Distributed Memory Out-of-Core Method on HPC Clusters and its Application to Quantum Chemistry Applications” *Presentation at XSEDE12 Conference*

Hanning C., Zhu X. “Electrostatic Screening Effects on a Model System for Molecular Electronics” *Presentation at XSEDE12 Conference*

Willmore F. “Tools for the Visualization and Analysis of Free Volume in Materials” *Presentation at XSEDE12 Conference*

Chourasia A., Gaither K., Ahern S. “Harnessing the Power of Visualization: Concept to Execution” *Tutorial at XSEDE12 Conference*

Stanzione D., Koesterke L., Barth B., Milfeld K. “Preparing for Stampede: Programming Heterogeneous Many-Core Supercomputers, OpenMP and Offloading” *Tutorial at XSEDE12 Conference*

Stanzione D., Koesterke L., Barth B., Milfeld K. “Preparing for Stampede: Programming Heterogeneous Many-Core Supercomputers, Vectorization” *Tutorial at XSEDE12 Conference*

20.9 Metrics

20.9.1 Standard User Assistance Metrics

TACC staff members continue to provide trouble ticket support via the XSEDE ticket system and the TACC Consulting System. 348 tickets, submitted via the XSEDE ticket system, were handled by TACC staff during the report period with 315 being closed. Both trouble ticket systems are monitored 7x24x365 and approximately 25 TACC staff members are engaged in this front-line support activity. The following table indicates the number of tickets opened, closed, and a breakdown of the ticket category.

Issue Category	Number of tickets opened	Number of tickets closed
Jobs/Batch Queues	90	78
Software/Applications	63	52
Login/Access Issues	80	79
System Issues	25	24
Account Issues	28	26
Filesystem Issues	15	12
Other	47	46

XSEDE users also may submit requests for assistance via the TACC User Portal (TUP). During the reporting period 247 tickets were submitted through the TUP; 213 have been resolved, 27 are pending user response, and 7 are in progress.

20.9.2 SP-specific Metrics

Allocation usage in section 1.9.3 reflects utilization of TACC resources by the XSEDE user community. There are allocation pools on TACC resources for the non-XSEDE community; the following table indicates the breakdown of available allocation and usage during the reporting period for both major communities. Allocation and usage information is reported in system units (SUs) with an SU being a core hour.

XSEDE/UT Quarter Usage

System	SUs Available	TG SUs Delivered	TG Usage (%)	UT SUs Delivered	UT Usage (%)	Total SUs Delivered
Ranger	136,059,648	103,785,278	86.19	16,631,075	13.81	120,416,353
Lonestar	50,118,380	16,388,358	35	30,737,937	65	47,126,295
Longhorn	4,467,712	1,140,347	52	1,040,383	48	2,180,730
Spur	276,544	20,329	72	8,082	28	28,411

The following table contains system availability statistics for the reporting period for TACC compute, visualization, and storage resources.

TACC Resource Availability Statistics

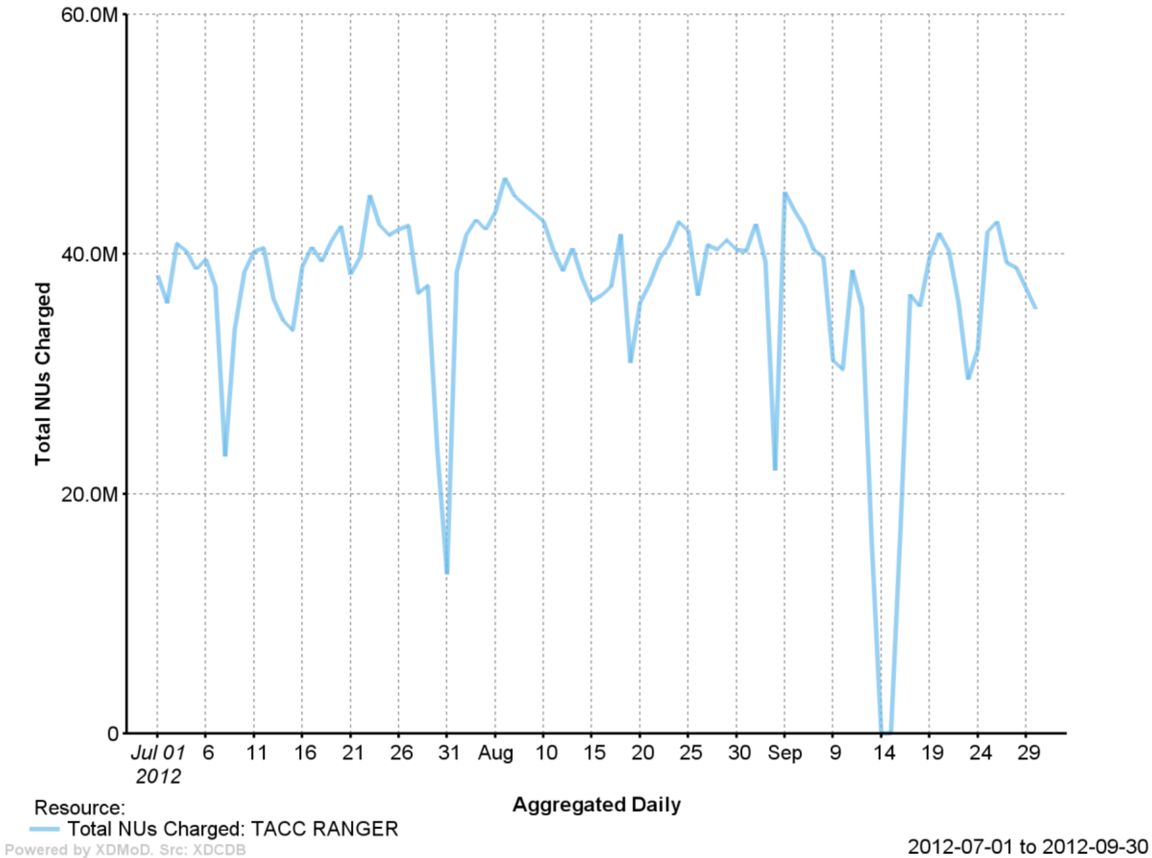
	Lonestar					Spur				
	Uptime					Uptime				
	PM		Outage			PM		Outage		
Month	#	Hrs	#	Hrs	%Up	#	Hrs	#	Hrs	%Up
2012-7	1	12.75	0	0.00	98.3	1	12.50	0	0.00	98.3
2012-8	1	9.50	0	0.00	98.7	0	0.00	0	0.00	100.0
2012-9	0	0.00	1	18.00	97.5	0	0.00	1	35.00	95.1
	Ranger					Ranch				
	Uptime					Uptime				
	PM		Outage			PM		Outage		
Month	#	Hrs	#	Hrs	%Up	#	Hrs	#	Hrs	%Up
2012-7	1	12.50	0	0.00	98.3	1	3.00	1	0.50	99.5
2012-8	0	0.00	0	0.00	100.0	0	0.00	0	0.00	100.0
2012-9	0	0.00	1	35.00	95.1	0	0.00	3	28.25	96.1
	Longhorn									
	Uptime									
	PM		Outage							
Month	#	Hrs	#	Hrs	%Up					
2012-7	1	10.50	0	0.00	98.6					
2012-8	0	0.00	0	0.00	100.0					
2012-9	0	0.00	1	16.00	97.8					

20.9.3 Standard systems metrics

TACC-RANGER Quarterly Report

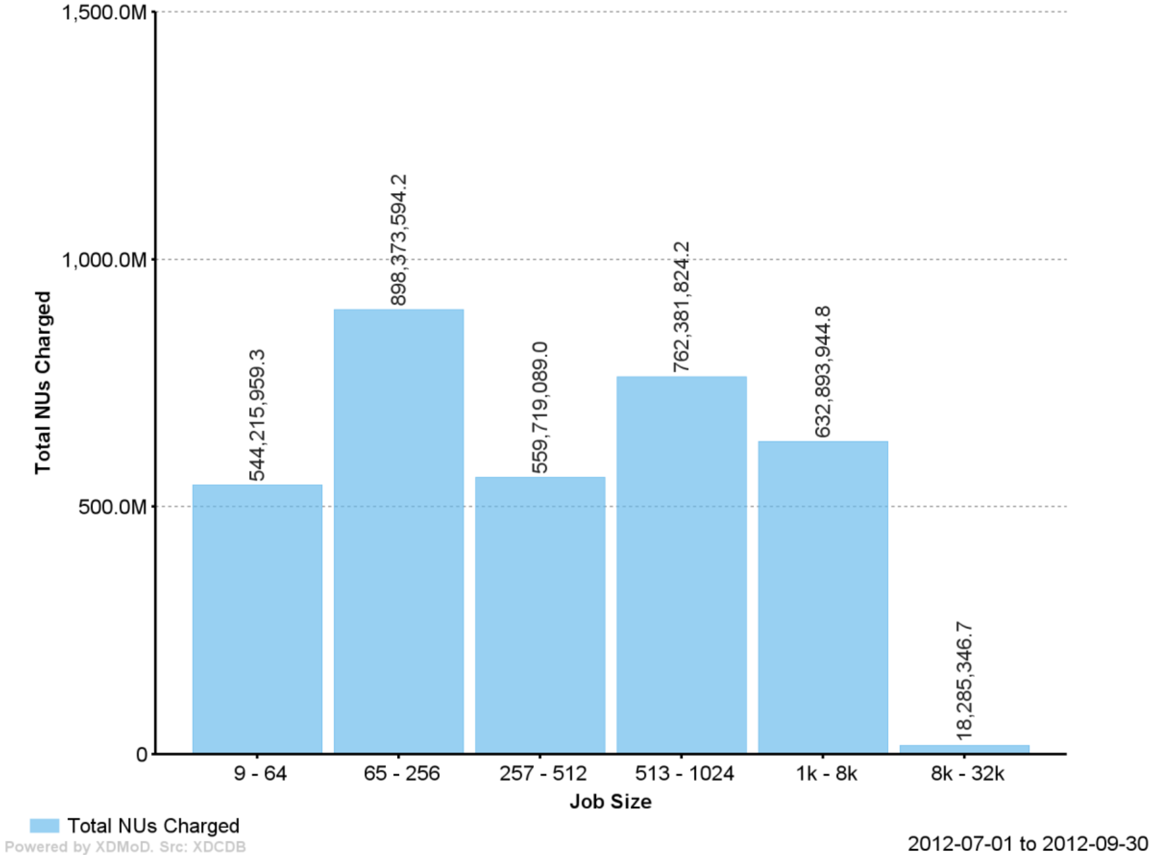
Total NUs Charged by Resource

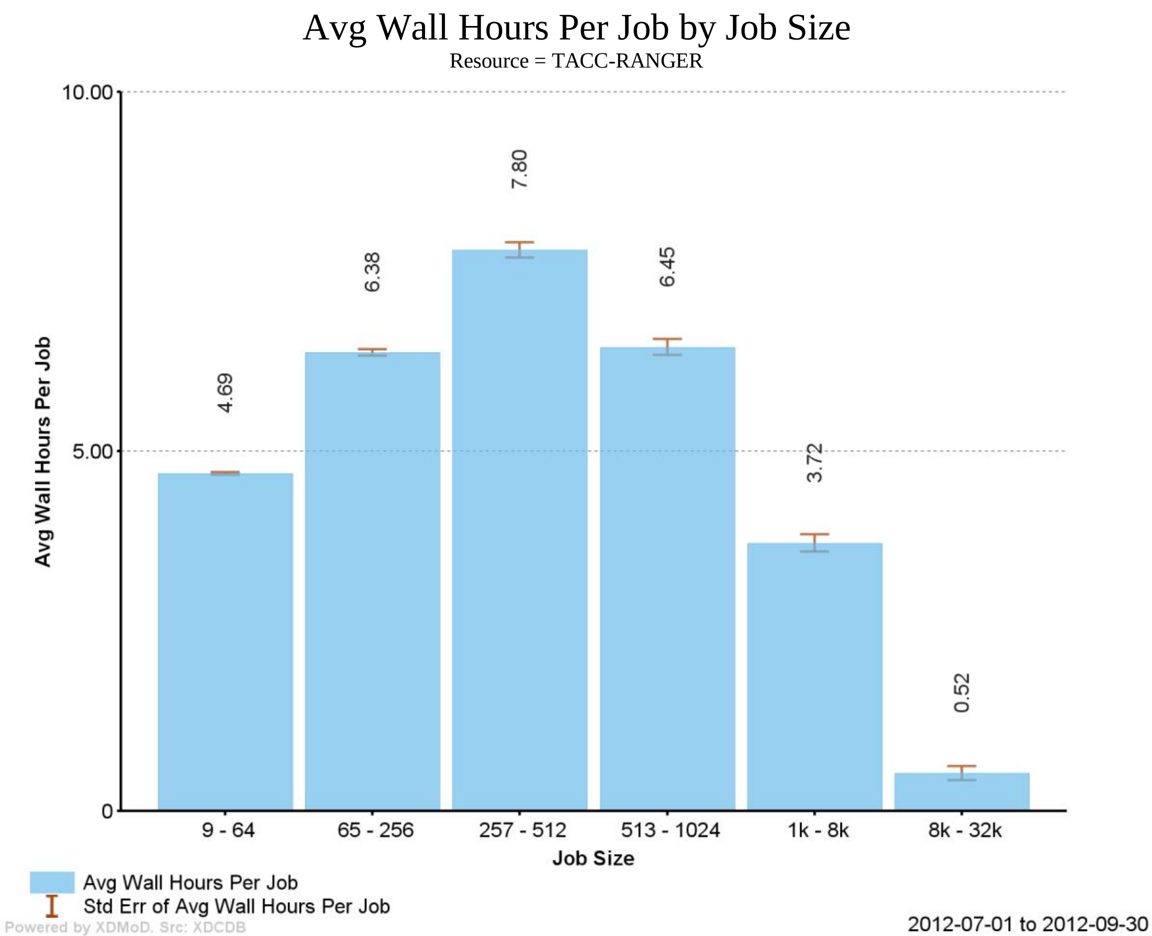
Service Provider = TACC



Total NUs Charged by Job Size

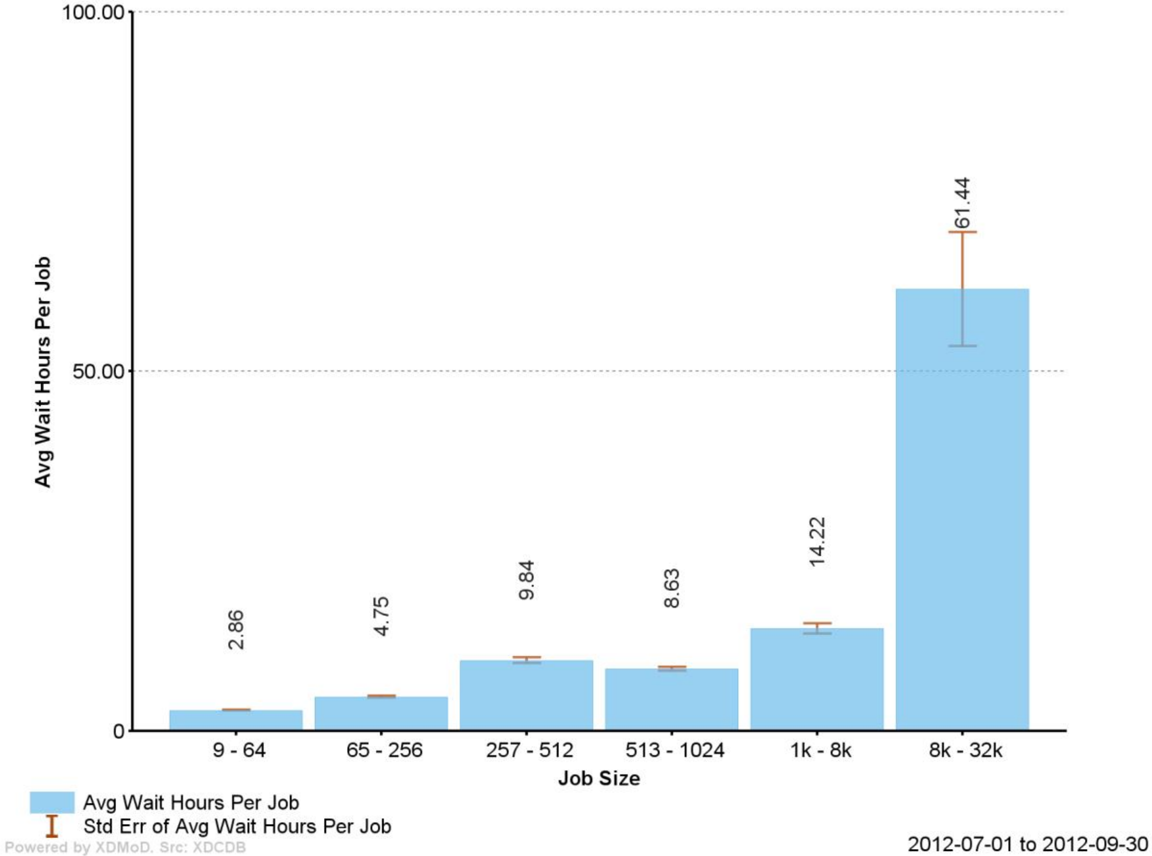
Resource = TACC-RANGER

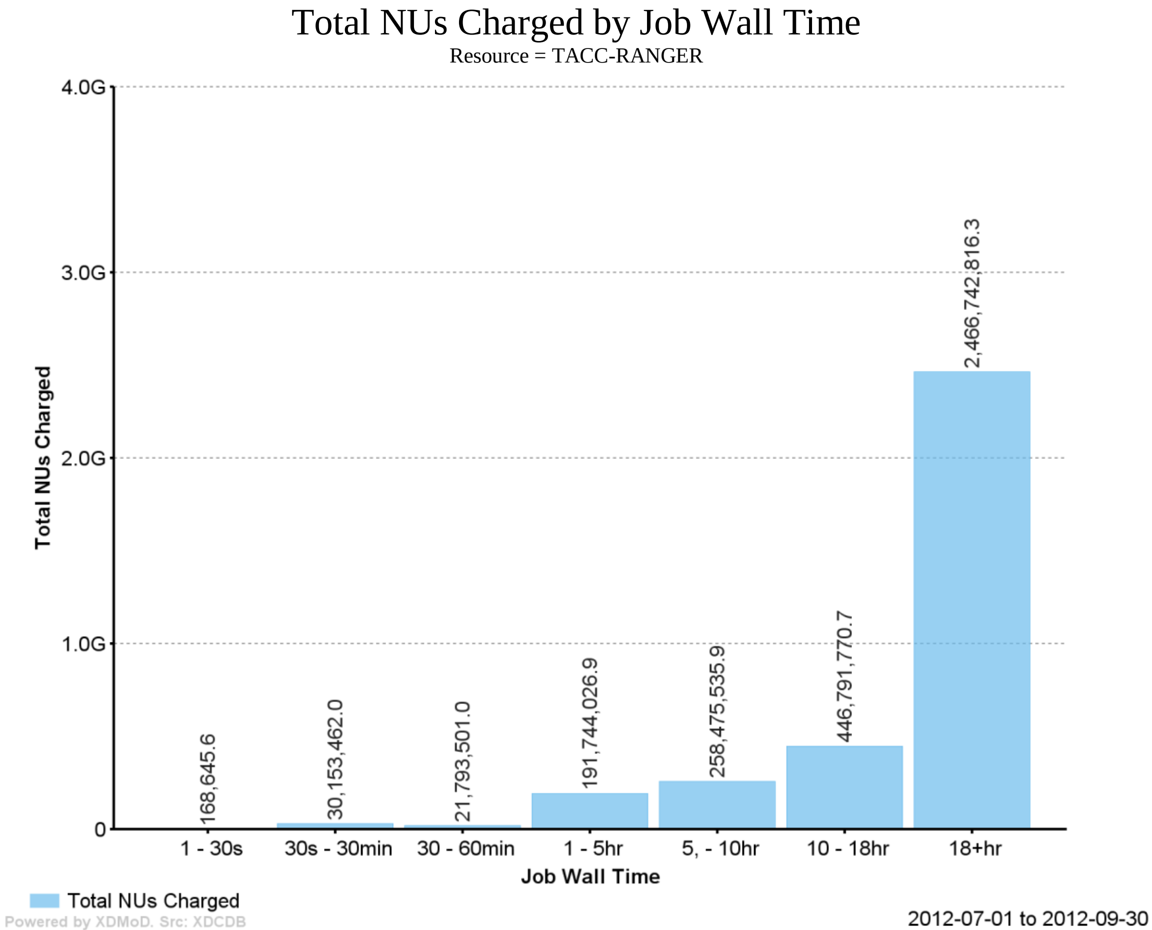



Avg Wall Hours Per Job by Job Size
Resource = TACC-RANGER
10.00
5.00
0
Avg Wall Hours Per Job
4.69
6.38
7.80
6.45
3.72
0.52
9 - 64
65 - 256
257 - 512
513 - 1024
1k - 8k
8k - 32k
Job Size
Avg Wall Hours Per Job
Std Err of Avg Wall Hours Per Job
Powered by XDMoD. Src: XDCDB
2012-07-01 to 2012-09-30

Avg Wait Hours Per Job by Job Size

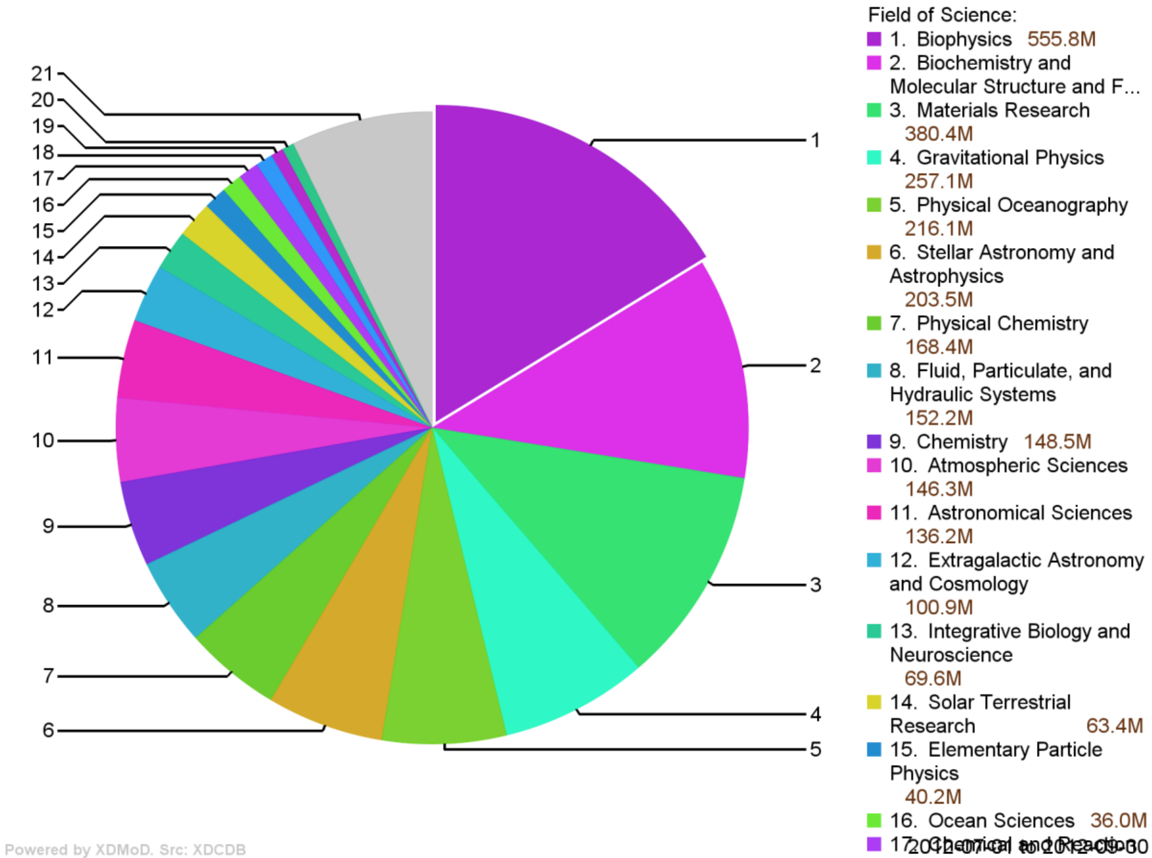
Resource = TACC-RANGER




Total NUs Charged by Job Wall Time
Resource = TACC-RANGER
4.0G
3.0G
2.0G
1.0G
0
Total NUs Charged
168,645.6
30,153,462.0
21,793,501.0
191,744,026.9
258,475,535.9
446,791,770.7
2,466,742,816.3
1 - 30s
30s - 30min
30 - 60min
1 - 5hr
5, - 10hr
10 - 18hr
18+hr
Job Wall Time
Total NUs Charged
Powered by XDMoD. Src: XDCDB
2012-07-01 to 2012-09-30

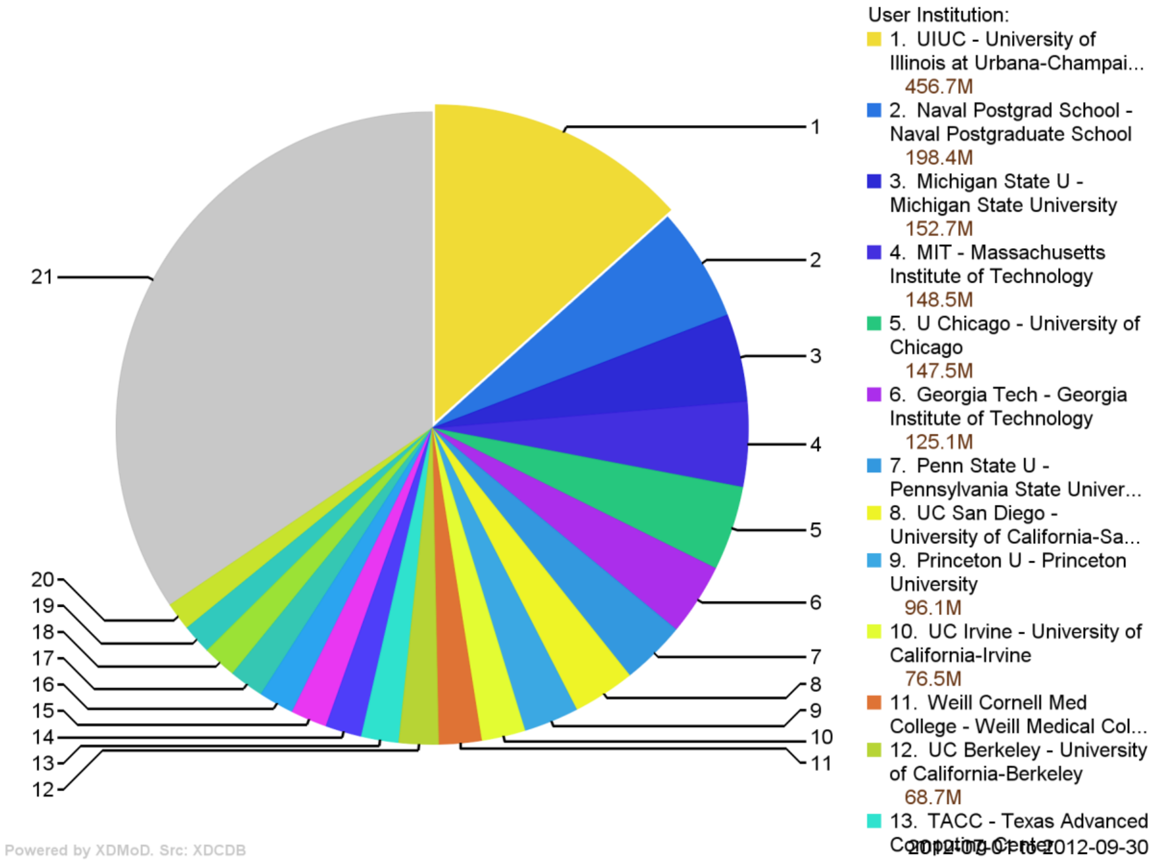
Total NUs Charged by Field of Science

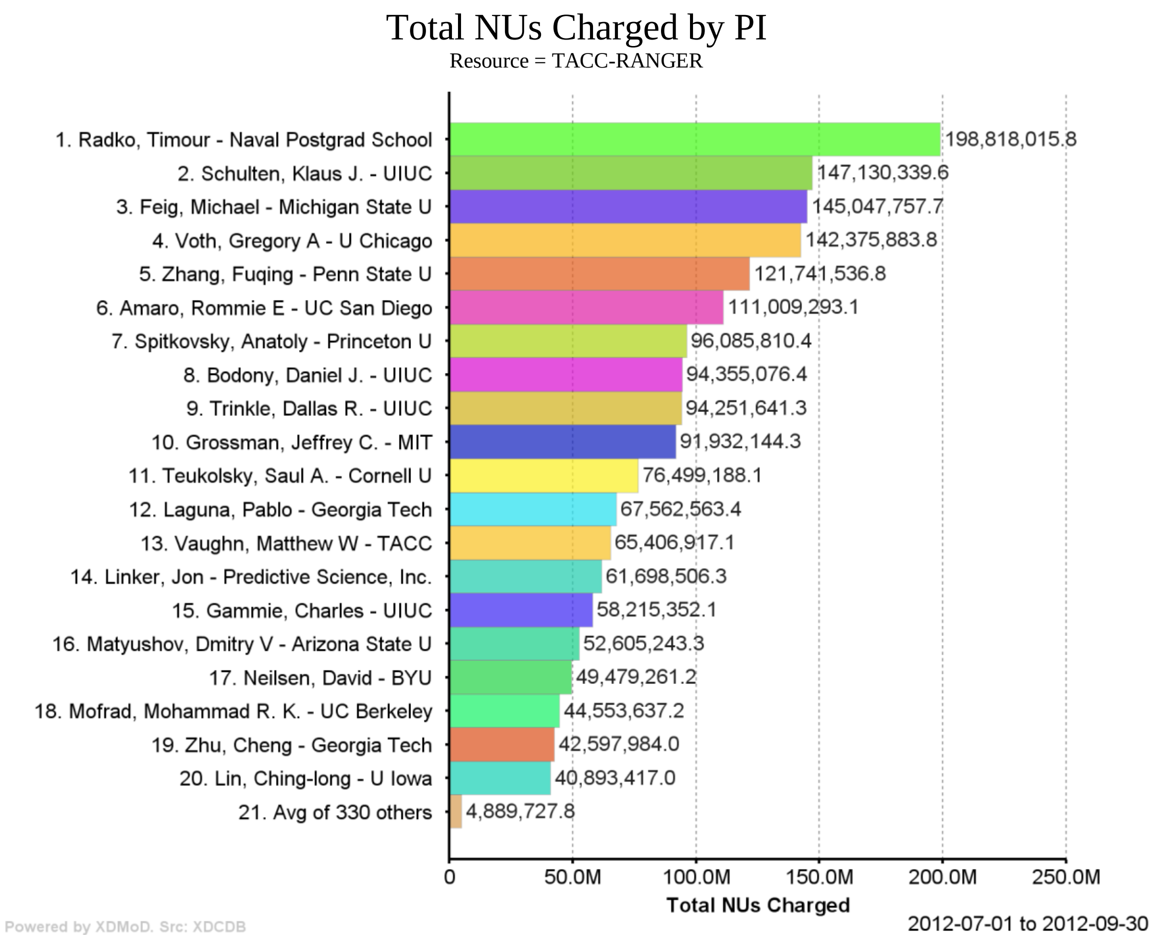
Resource = TACC-RANGER



Total NUs Charged by User Institution

Resource = TACC-RANGER

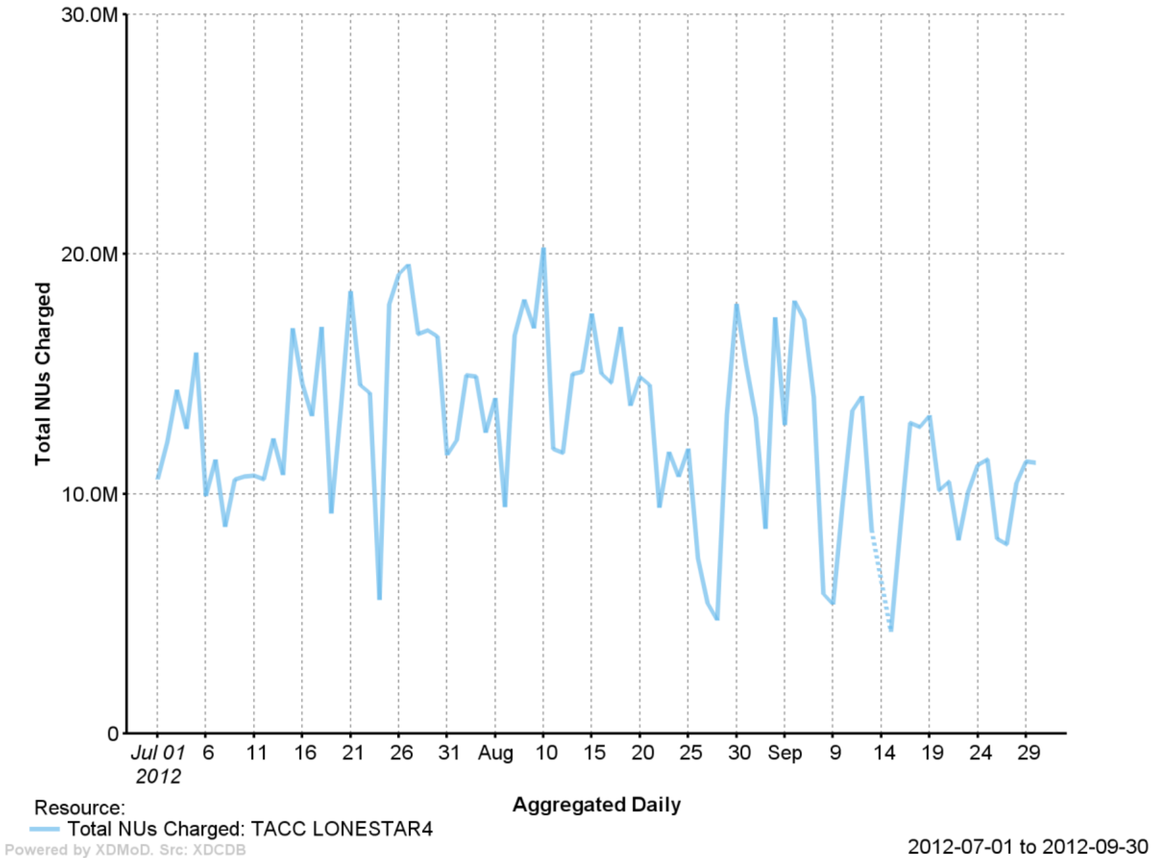



Total NUs Charged by PI
Resource = TACC-RANGER
1. Radko, Timour - Naval Postgrad School
198,818,015.8
2. Schulten, Klaus J. - UIUC
147,130,339.6
3. Feig, Michael - Michigan State U
145,047,757.7
4. Voth, Gregory A - U Chicago
142,375,883.8
5. Zhang, Fuqing - Penn State U
121,741,536.8
6. Amaro, Rommie E - UC San Diego
111,009,293.1
7. Spitkovsky, Anatoly - Princeton U
96,085,810.4
8. Bodony, Daniel J. - UIUC
94,355,076.4
9. Trinkle, Dallas R. - UIUC
94,251,641.3
10. Grossman, Jeffrey C. - MIT
91,932,144.3
11. Teukolsky, Saul A. - Cornell U
76,499,188.1
12. Laguna, Pablo - Georgia Tech
67,562,563.4
13. Vaughn, Matthew W - TACC
65,406,917.1
14. Linker, Jon - Predictive Science, Inc.
61,698,506.3
15. Gammie, Charles - UIUC
58,215,352.1
16. Matyushov, Dmitry V - Arizona State U
52,605,243.3
17. Neilsen, David - BYU
49,479,261.2
18. Mofrad, Mohammad R. K. - UC Berkeley
44,553,637.2
19. Zhu, Cheng - Georgia Tech
42,597,984.0
20. Lin, Ching-long - U Iowa
40,893,417.0
21. Avg of 330 others
4,889,727.8
0
50.0M
100.0M
150.0M
200.0M
250.0M
Total NUs Charged
Powered by XDMoD. Src: XDCDB
2012-07-01 to 2012-09-30

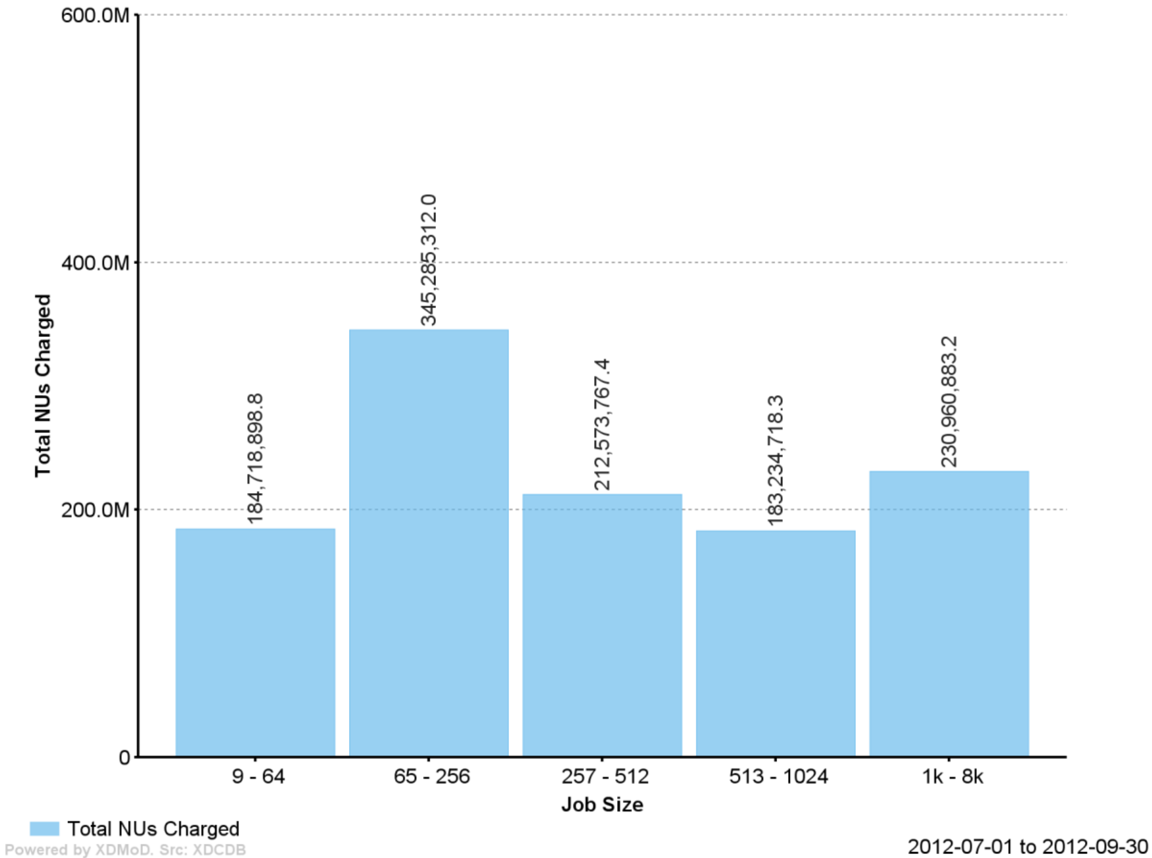
TACC-LONESTAR4 Quarterly Report

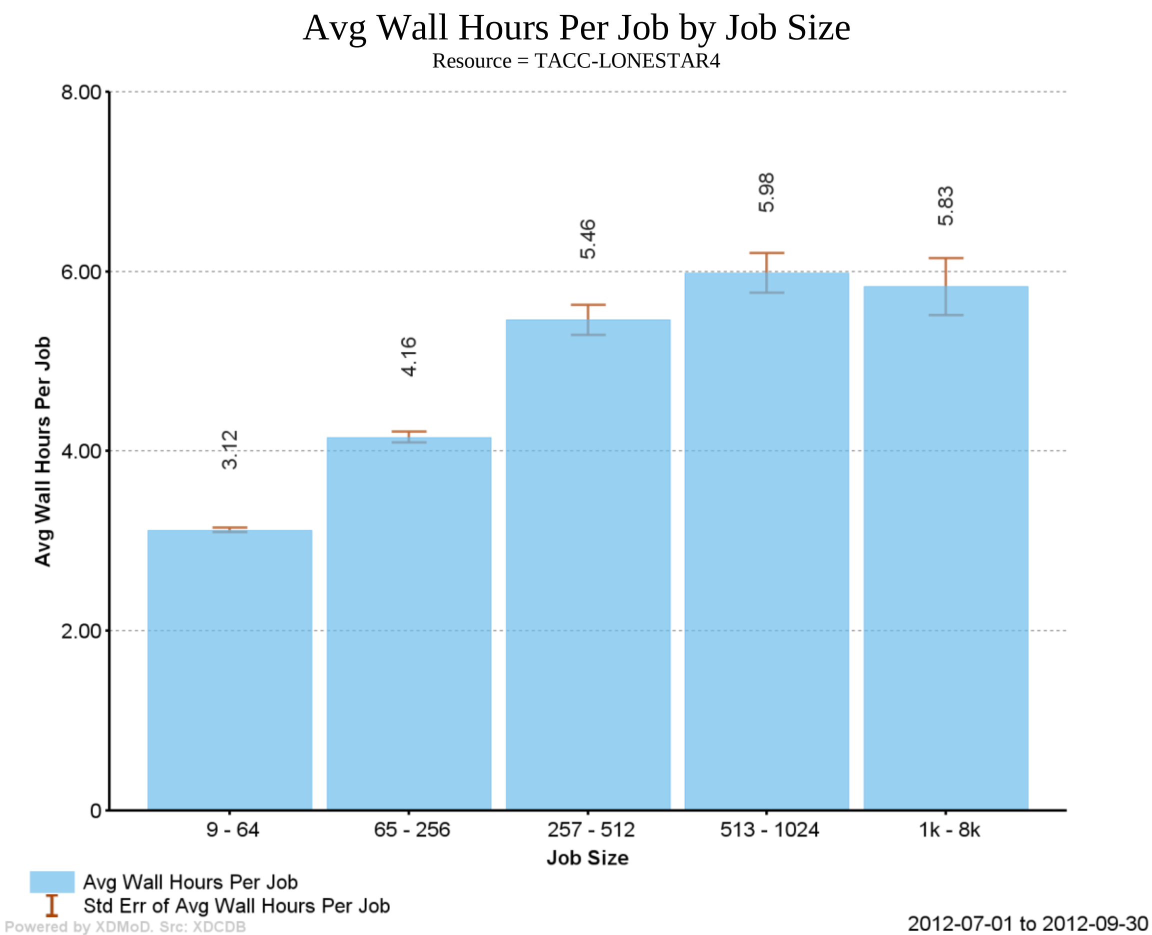
Total NUs Charged by Resource

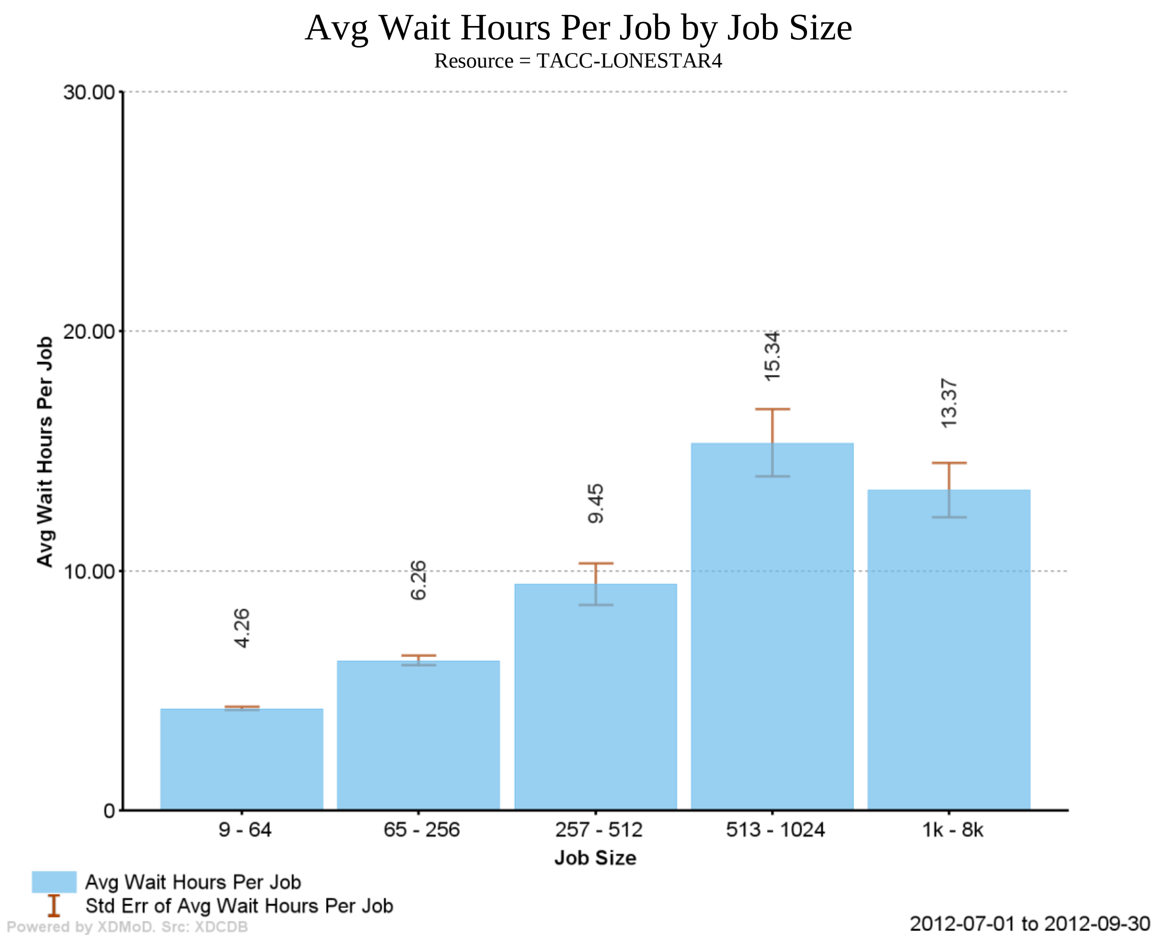
Service Provider = TACC

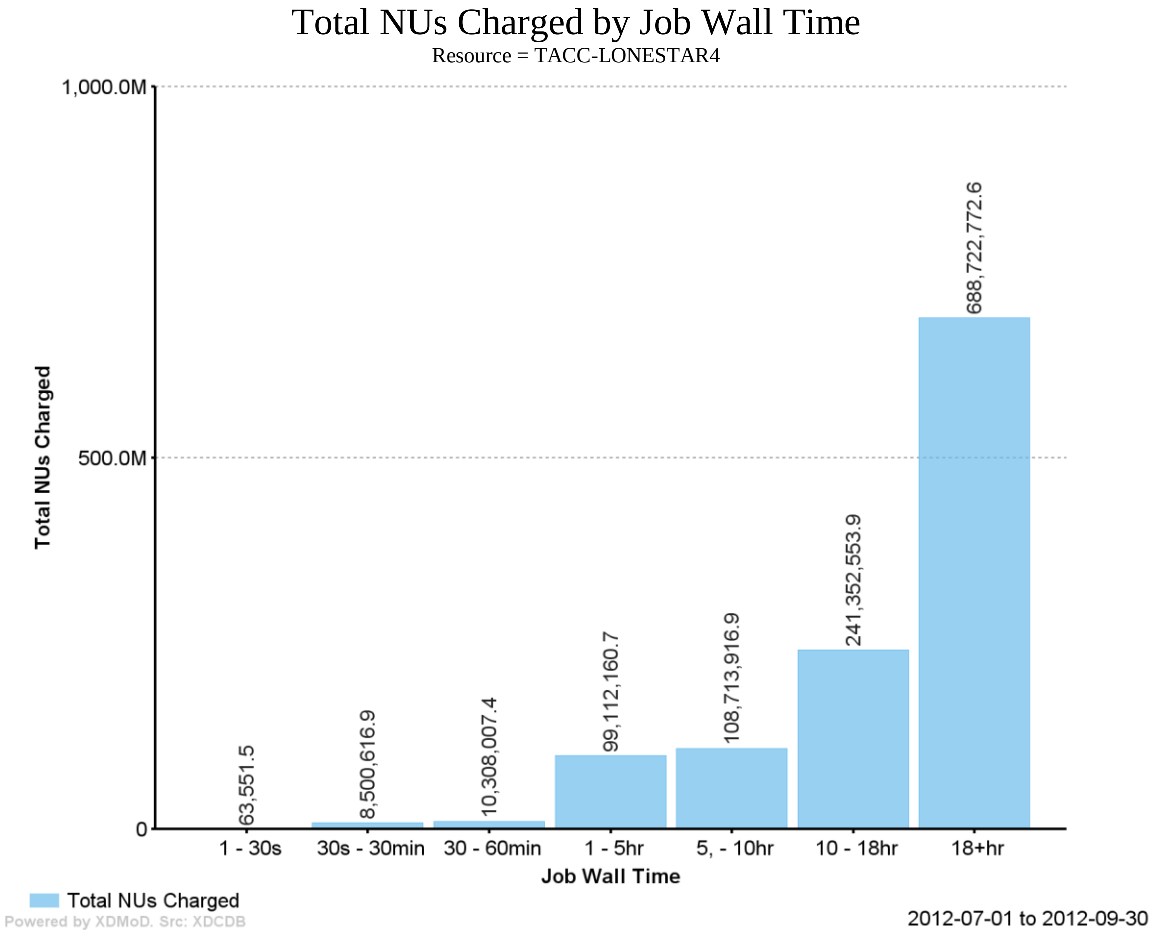


Total NUs Charged by Job Size
Resource = TACC-LONESTAR4



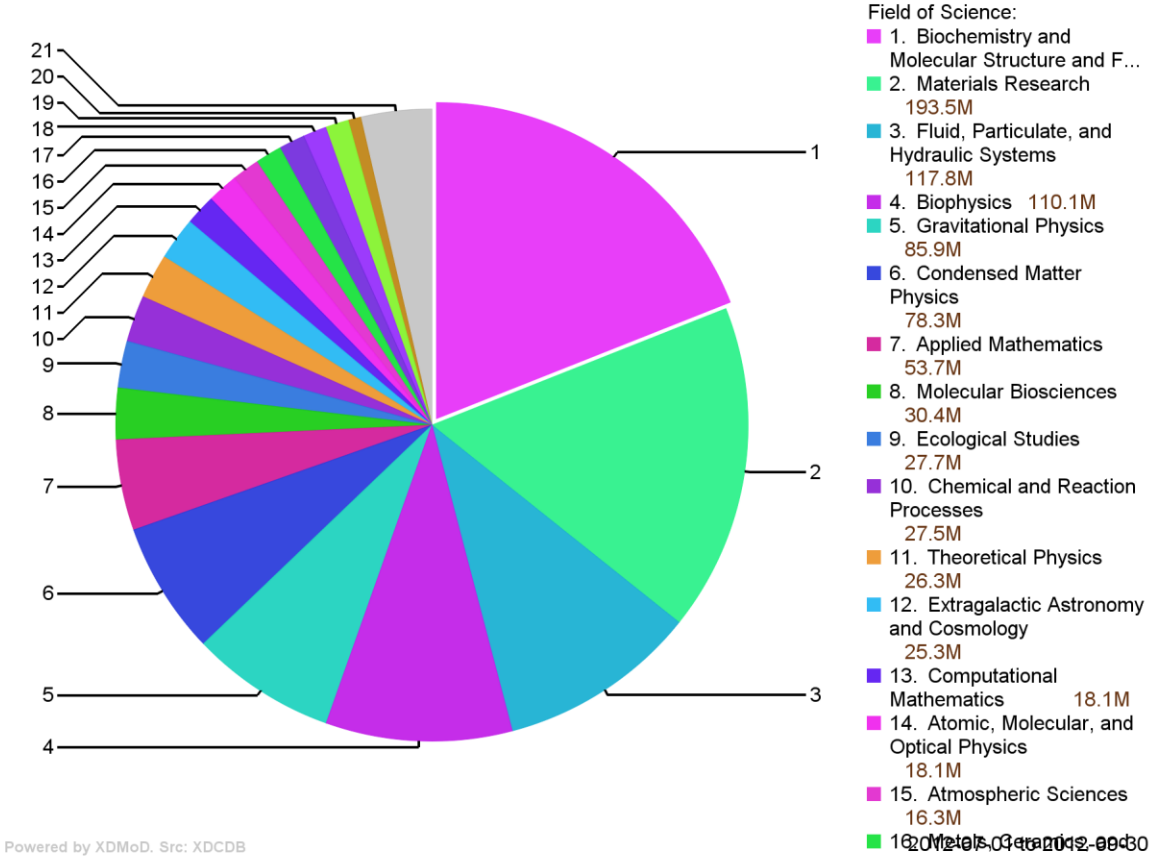

Avg Wall Hours Per Job by Job Size
Resource = TACC-LONESTAR4
8.00
6.00
4.00
2.00
0
Avg Wall Hours Per Job
3.12
4.16
5.46
5.98
5.83
9 - 64
65 - 256
257 - 512
513 - 1024
1k - 8k
Job Size
Avg Wall Hours Per Job
Std Err of Avg Wall Hours Per Job
Powered by XDMoD. Src: XDCDB
2012-07-01 to 2012-09-30

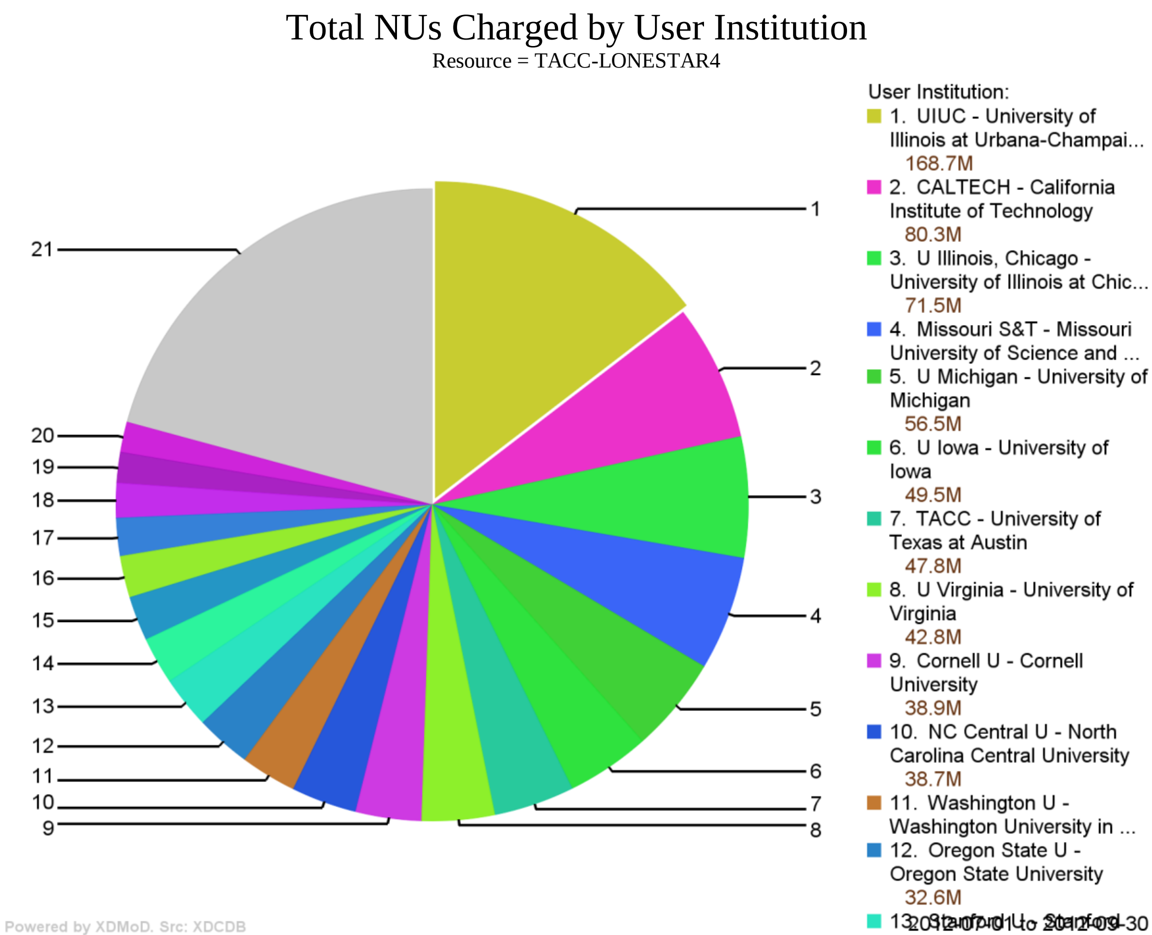

Avg Wait Hours Per Job by Job Size
Resource = TACC-LONESTAR4
Avg Wait Hours Per Job
30.00
20.00
10.00
0
4.26
6.26
9.45
15.34
13.37
9 - 64
65 - 256
257 - 512
513 - 1024
1k - 8k
Job Size
Avg Wait Hours Per Job
Std Err of Avg Wait Hours Per Job
Powered by XDMoD. Src: XDCDB
2012-07-01 to 2012-09-30


Total NUs Charged by Job Wall Time
Resource = TACC-LONESTAR4
1,000.0M
500.0M
0
Total NUs Charged
63,551.5
8,500,616.9
10,308,007.4
99,112,160.7
108,713,916.9
241,352,553.9
688,722,772.6
1 - 30s
30s - 30min
30 - 60min
1 - 5hr
5, - 10hr
10 - 18hr
18+hr
Job Wall Time
Total NUs Charged
Powered by XDMoD. Src: XDCDB
2012-07-01 to 2012-09-30

Total NUs Charged by Field of Science

Resource = TACC-LONESTAR4

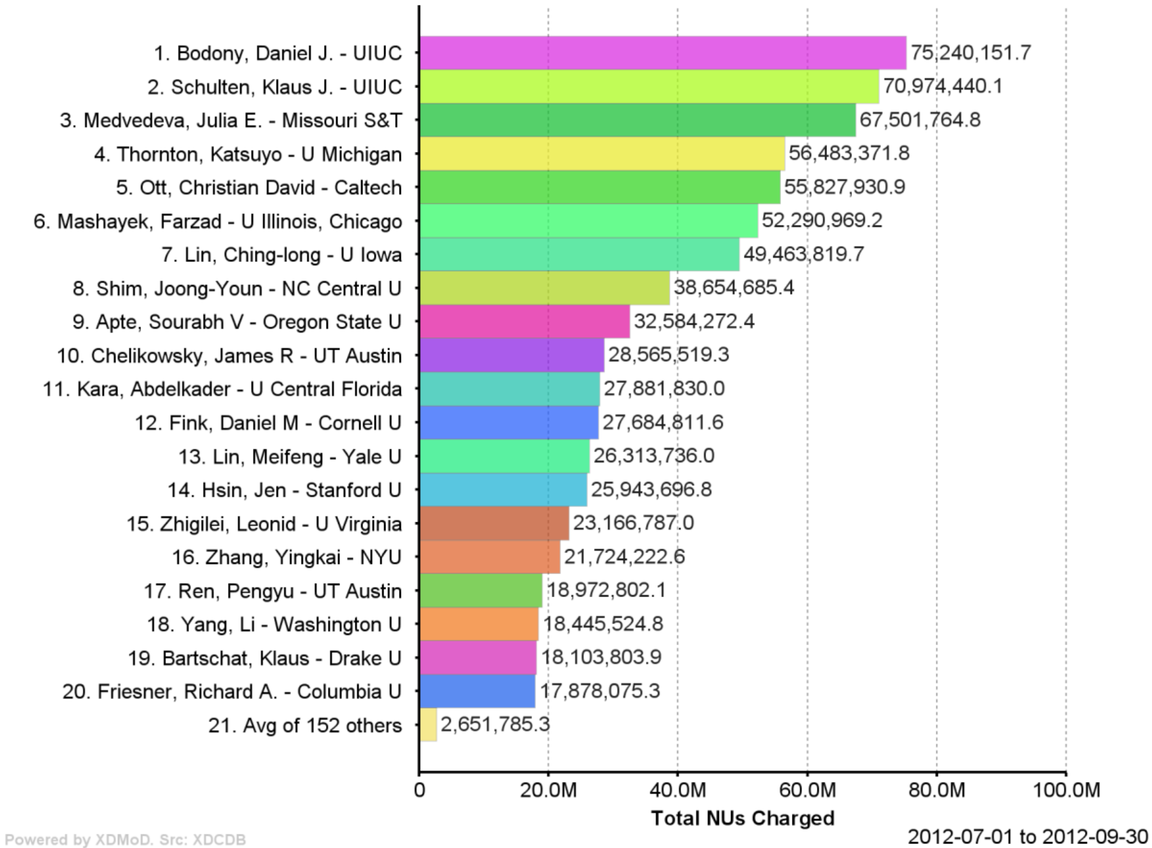




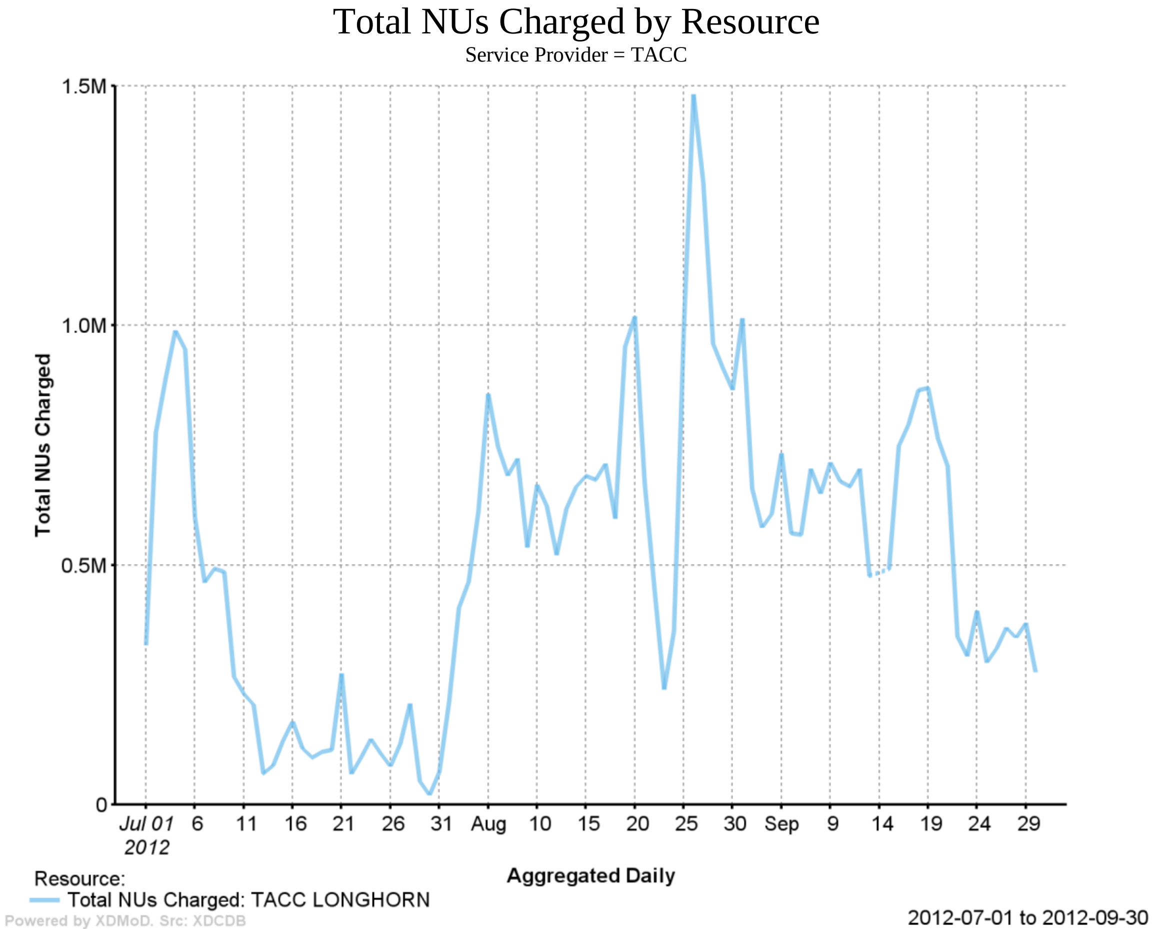
Total NUs Charged by User Institution
Resource = TACC-LONESTAR4
User Institution:
1. UIUC - University of Illinois at Urbana-Champai...
168.7M
2. CALTECH - California Institute of Technology
80.3M
3. U Illinois, Chicago - University of Illinois at Chic...
71.5M
4. Missouri S&T - Missouri University of Science and ...
5. U Michigan - University of Michigan
56.5M
6. U Iowa - University of Iowa
49.5M
7. TACC - University of Texas at Austin
47.8M
8. U Virginia - University of Virginia
42.8M
9. Cornell U - Cornell University
38.9M
10. NC Central U - North Carolina Central University
38.7M
11. Washington U - Washington University in ...
12. Oregon State U - Oregon State University
32.6M
13. Stanford U - Stanford
2012-07-01 to 2012-09-30
Powered by XDMoD. Src: XDCDB

Total NUs Charged by PI

Resource = TACC-LONESTAR4

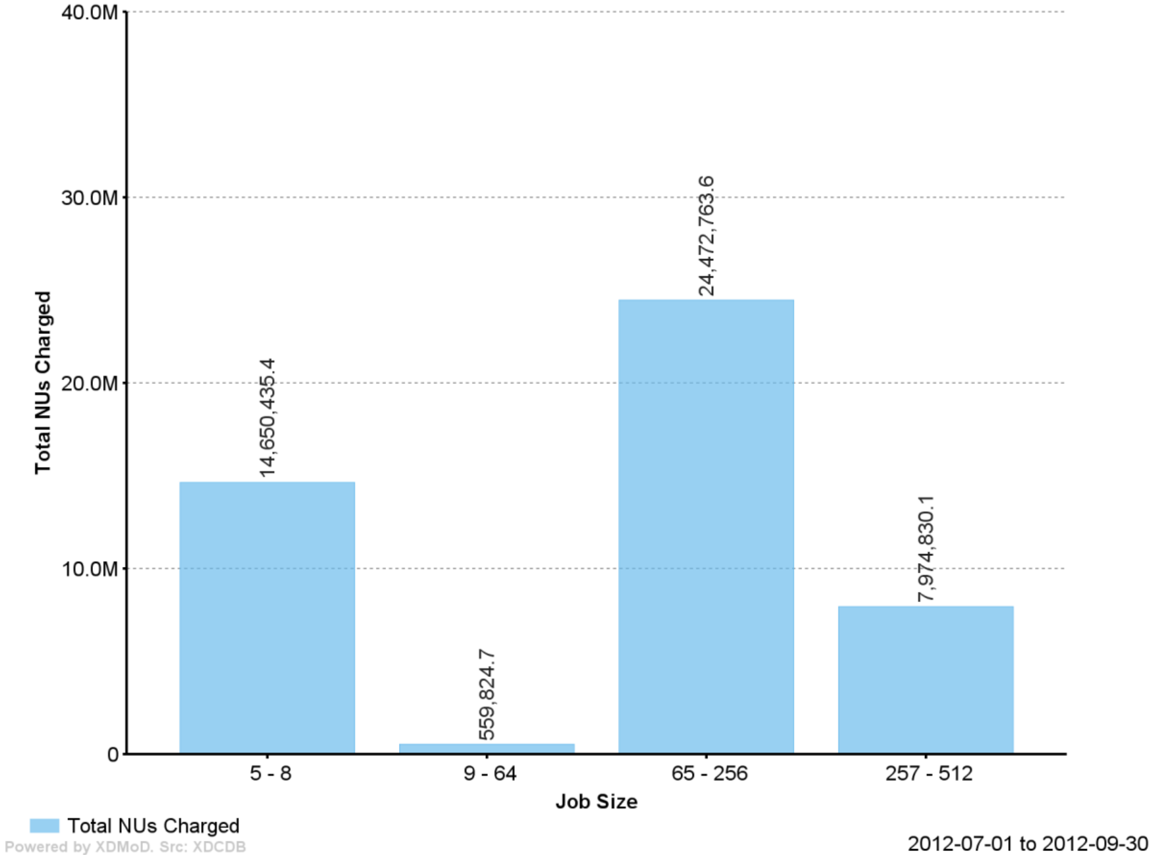


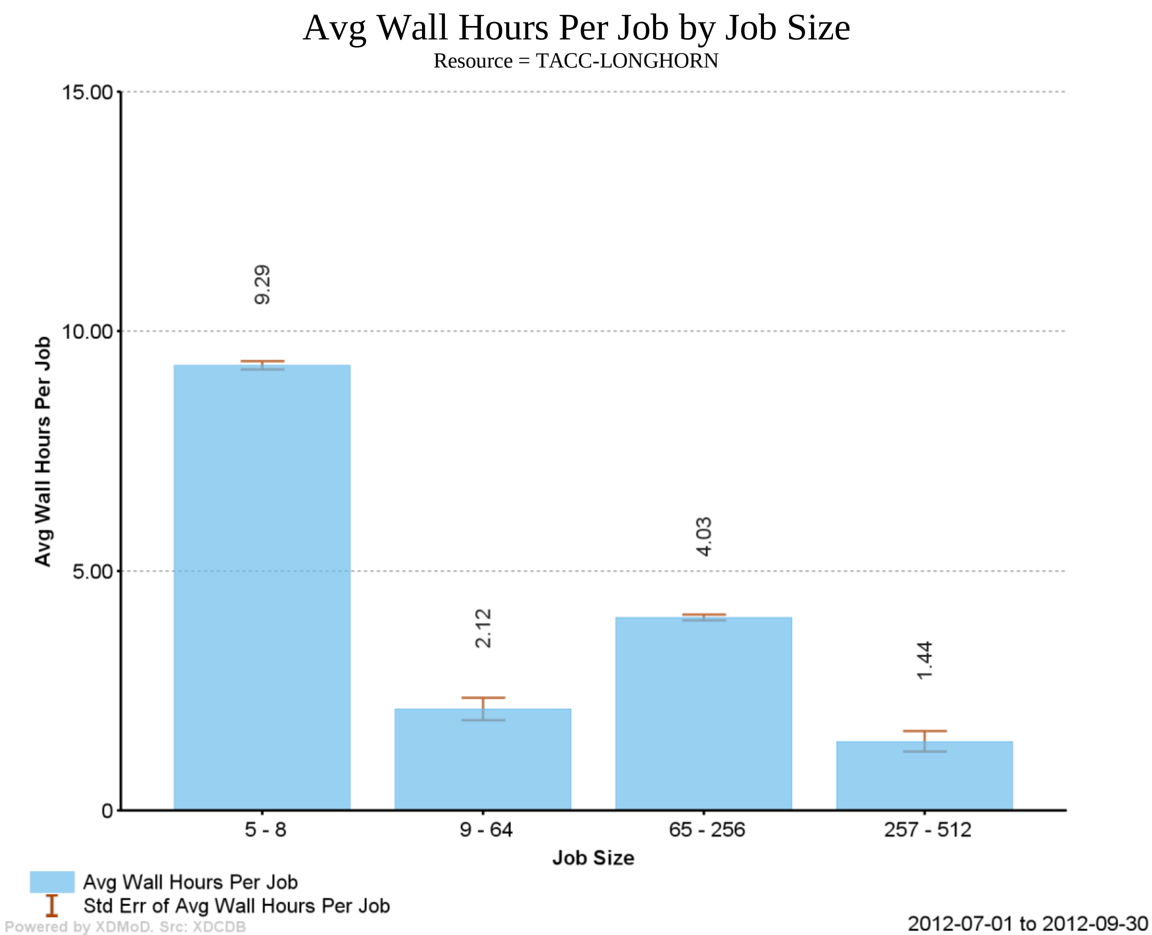
TACC-LONGHORN Quarterly Report



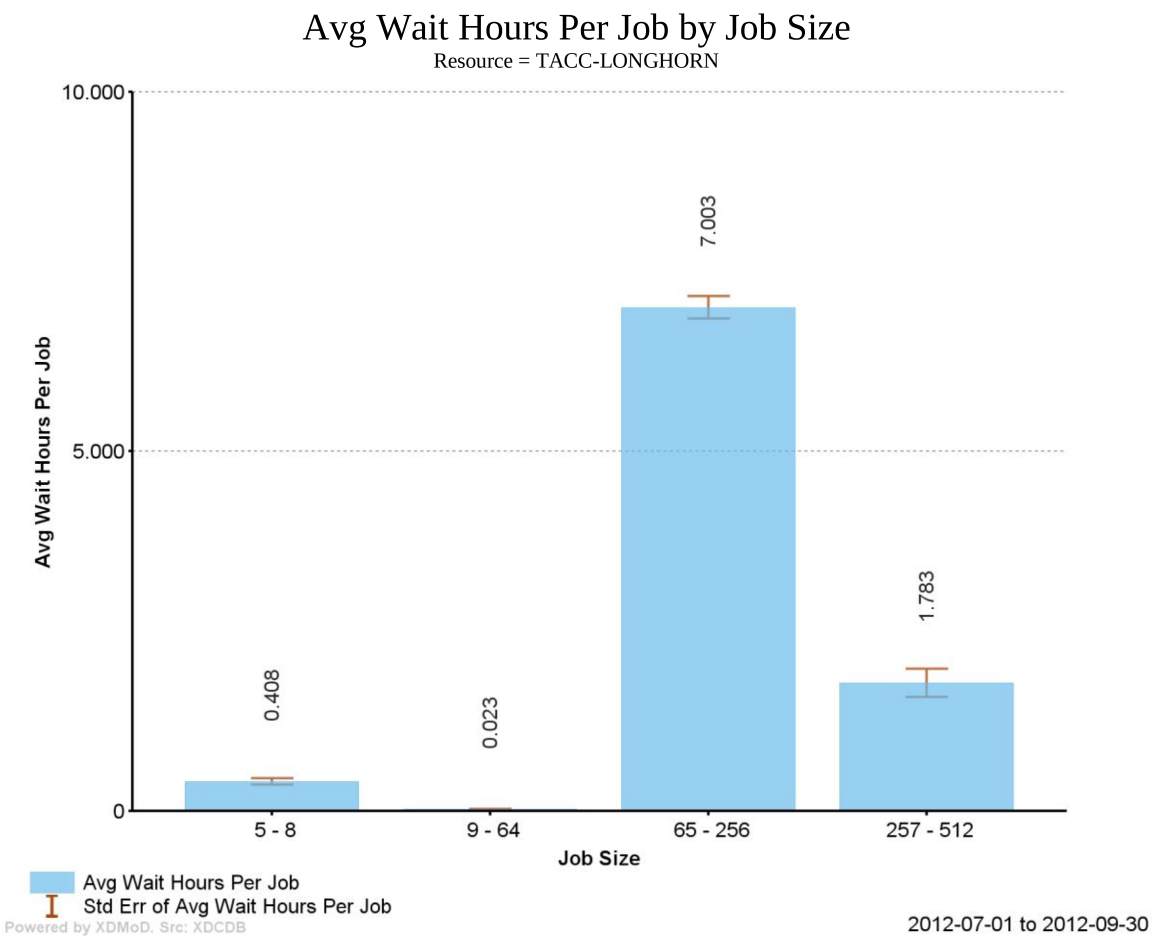
Total NUs Charged by Job Size

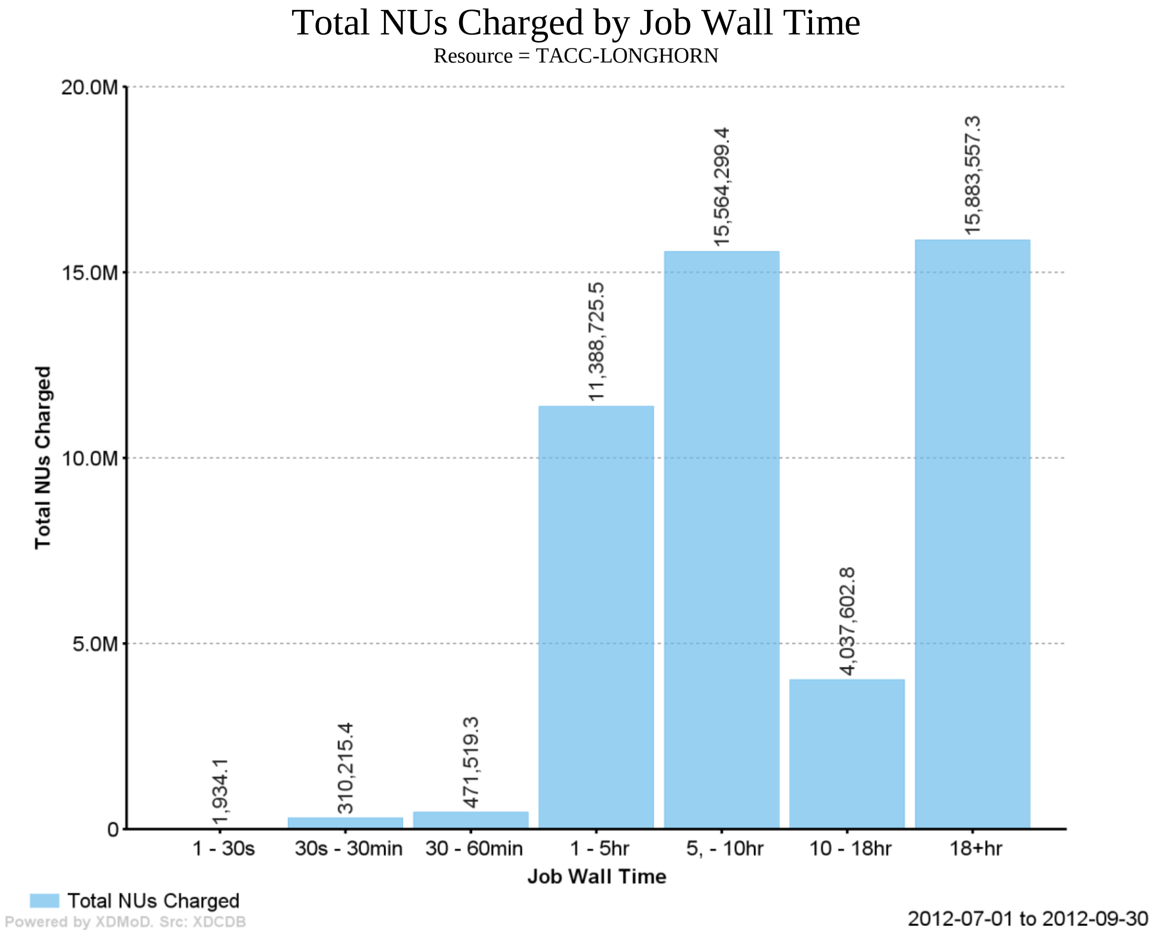
Resource = TACC-LONGHORN





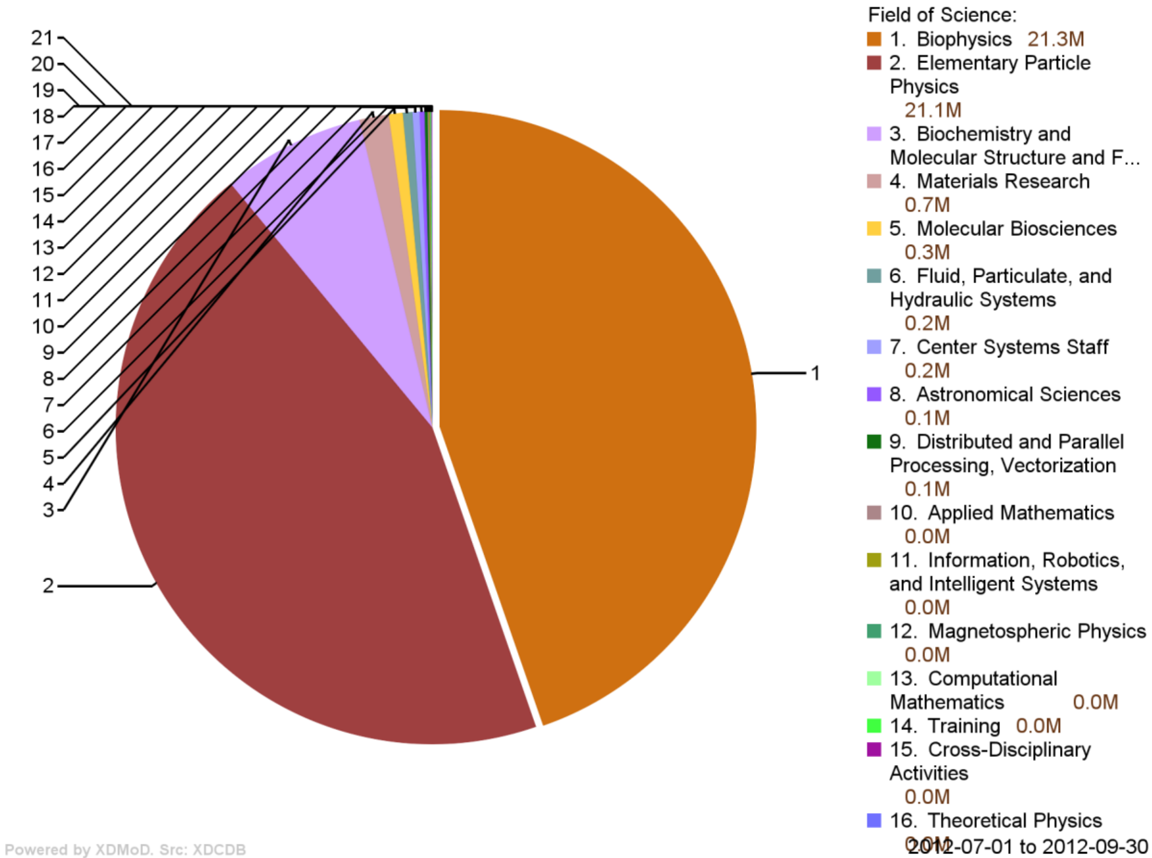
Avg Wall Hours Per Job by Job Size
Resource = TACC-LONGHORN
15.00
10.00
5.00
0
Avg Wall Hours Per Job
9.29
2.12
4.03
1.44
5 - 8
9 - 64
65 - 256
257 - 512
Job Size
Avg Wall Hours Per Job
Std Err of Avg Wall Hours Per Job
Powered by XDMoD. Src: XDCDB
2012-07-01 to 2012-09-30


Avg Wait Hours Per Job by Job Size
Resource = TACC-LONGHORN
10.000
5.000
0
Avg Wait Hours Per Job
7.003
1.783
0.408
0.023
5 - 8
9 - 64
65 - 256
257 - 512
Job Size
Avg Wait Hours Per Job
Std Err of Avg Wait Hours Per Job
Powered by XDMoD. Src: XDCDB
2012-07-01 to 2012-09-30


Total NUs Charged by Job Wall Time
Resource = TACC-LONGHORN
Total NUs Charged
20.0M
15.0M
10.0M
5.0M
0
1,934.1
310,215.4
471,519.3
11,388,725.5
15,564,299.4
4,037,602.8
15,883,557.3
1 - 30s
30s - 30min
30 - 60min
1 - 5hr
5, - 10hr
10 - 18hr
18+hr
Job Wall Time
Total NUs Charged
Powered by XDMoD. Src: XDCDB
2012-07-01 to 2012-09-30

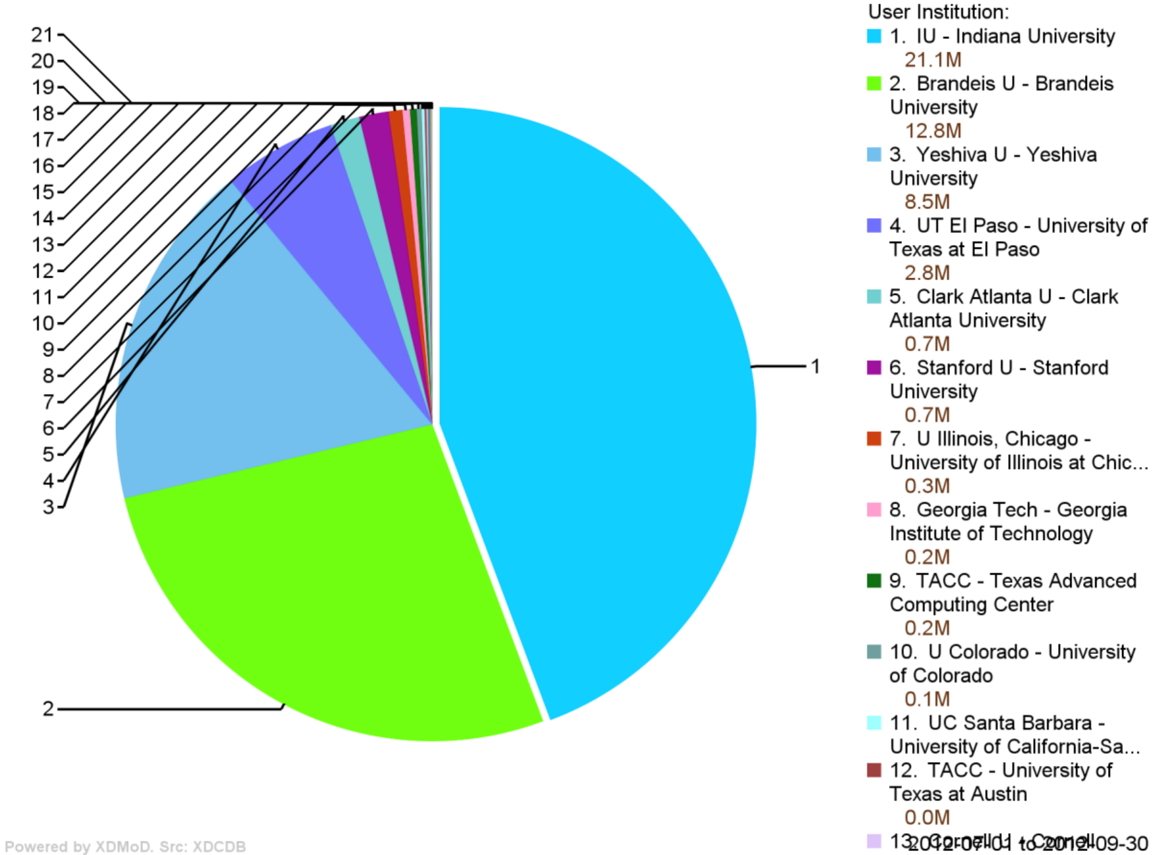
Total NUs Charged by Field of Science

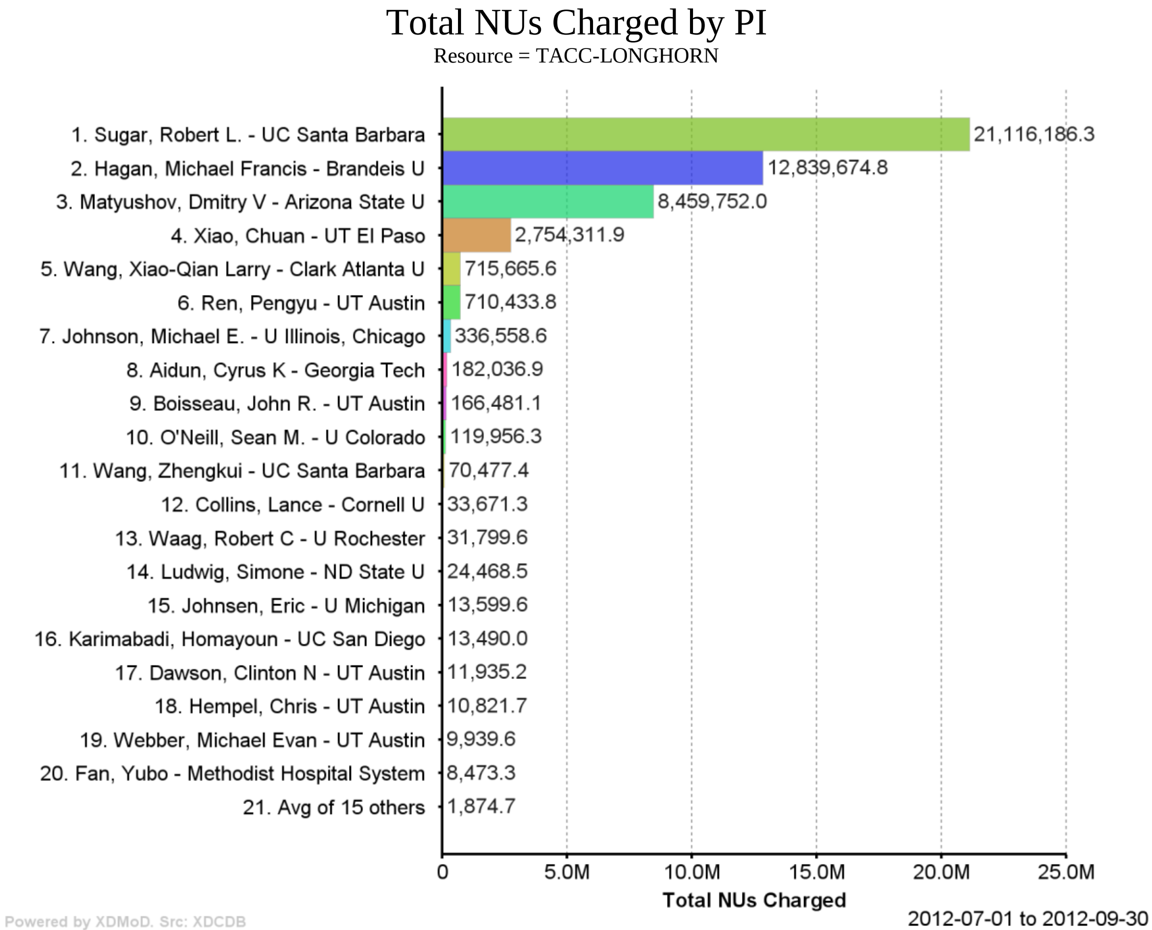
Resource = TACC-LONGHORN



Total NUs Charged by User Institution

Resource = TACC-LONGHORN





Total NUs Charged by PI
Resource = TACC-LONGHORN
1. Sugar, Robert L. - UC Santa Barbara
2. Hagan, Michael Francis - Brandeis U
3. Matyushov, Dmitry V - Arizona State U
4. Xiao, Chuan - UT El Paso
5. Wang, Xiao-Qian Larry - Clark Atlanta U
6. Ren, Pengyu - UT Austin
7. Johnson, Michael E. - U Illinois, Chicago
8. Aidun, Cyrus K - Georgia Tech
9. Boisseau, John R. - UT Austin
10. O'Neill, Sean M. - U Colorado
11. Wang, Zhengkui - UC Santa Barbara
12. Collins, Lance - Cornell U
13. Waag, Robert C - U Rochester
14. Ludwig, Simone - ND State U
15. Johnsen, Eric - U Michigan
16. Karimabadi, Homayoun - UC San Diego
17. Dawson, Clinton N - UT Austin
18. Hempel, Chris - UT Austin
19. Webber, Michael Evan - UT Austin
20. Fan, Yubo - Methodist Hospital System
21. Avg of 15 others
21,116,186.3
12,839,674.8
8,459,752.0
2,754,311.9
715,665.6
710,433.8
336,558.6
182,036.9
166,481.1
119,956.3
70,477.4
33,671.3
31,799.6
24,468.5
13,599.6
13,490.0
11,935.2
10,821.7
9,939.6
8,473.3
1,874.7
0
5.0M
10.0M
15.0M
20.0M
25.0M
Total NUs Charged
Powered by XDMoD. Src: XDCDB
2012-07-01 to 2012-09-30

A XSEDE Project Milestones Update

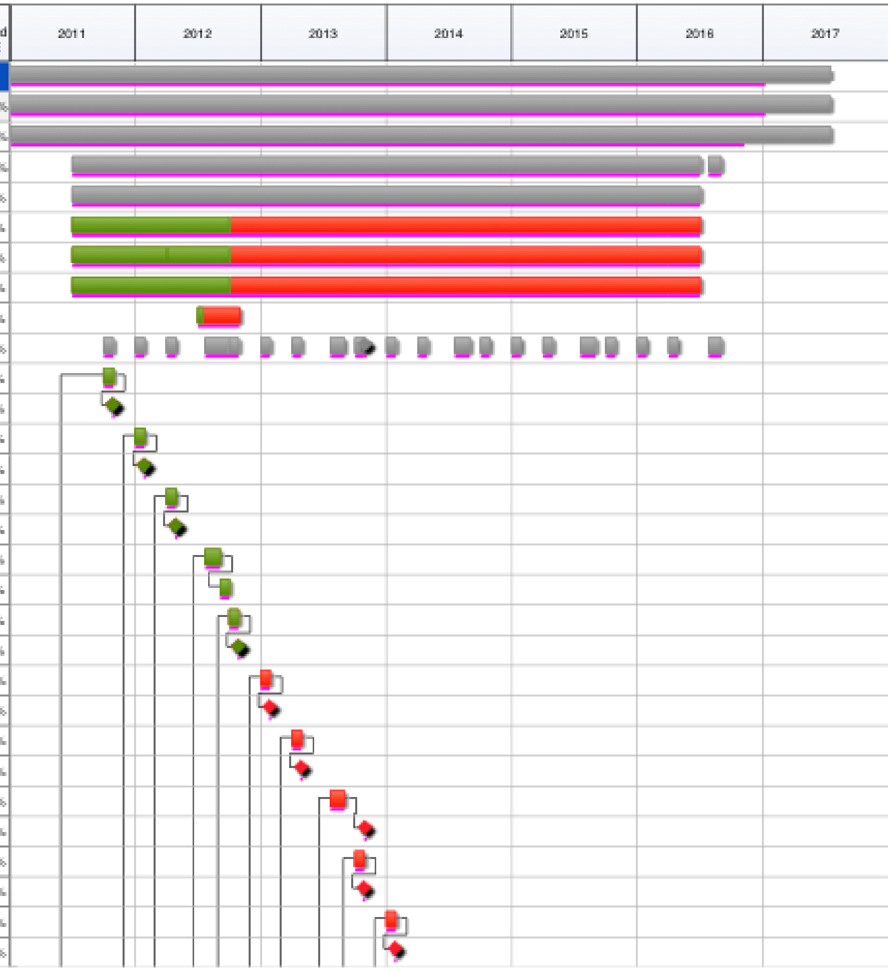
Content for this appendix is pending finalizing the XSEDE Architecture that is being reworked due to the merging of the XSEDE and XROADS proposals.

B XSEDE Schedule with Progress Update

XSEDE

Page: 1

Name	Start	Finish	% Completed - XSEDE
Prodution: XSEDE Schedule	10/6/10	7/14/17	
XSEDE	10/6/10	7/14/17	0.00%
Project Office	1/3/11	7/14/17	0.00%
Project Management and Reporting	7/1/11	8/31/16	0.00%
Management	7/1/11	7/1/16	0.00%
Ongoing: Senior Management Team - Oversight and management of XSEDE	7/1/11	6/30/16	25.00%
Ongoing: Business and finance office support - subaward management	7/1/11	7/1/16	25.00%
Ongoing: Annual Planning, Budgeting, Change Control resulting from SEMP	7/1/11	6/30/16	25.00%
Update Project Execution Plan	7/2/12	10/31/12	10.00%
Project Reporting	10/3/11	8/31/16	0.00%
Prepare 2011 Q3 Quarterly Report	10/3/11	10/28/11	100.00%
Milestone: 2011 Q3 Quarterly Report completed	10/28/11	10/28/11	100.00%
Prepare 2011 Q4 Quarterly Report	1/2/12	1/27/12	100.00%
Milestone: 2011 Q4 Quarterly Report completed	1/27/12	1/27/12	100.00%
Prepare 2012 Q1 Quarterly Report	4/2/12	4/27/12	100.00%
Milestone: 2012 Q1 Quarterly Report completed	4/27/12	4/27/12	100.00%
Prepare Y1 Annual Report	7/23/12	8/31/12	100.00%
Milestone: Y1 Annual Report completed	9/3/12	9/28/12	100.00%
Prepare 2012 Q3 Quarterly Report	10/1/12	10/26/12	100.00%
Milestone: 2012 Q3 Quarterly Report completed	10/26/12	10/26/12	100.00%
Prepare 2012 Q4 Quarterly Report	1/1/13	1/28/13	0.00%
Milestone: 2012 Q4 Quarterly Report completed	1/28/13	1/28/13	0.00%
Prepare 2013 Q1 Quarterly Report	4/1/13	4/26/13	0.00%
Milestone: 2013 Q1 Quarterly Report completed	4/26/13	4/26/13	0.00%
Prepare Y2 Annual Report	7/22/13	8/30/13	0.00%
Milestone: Y2 Annual Report completed	11/1/13	11/1/13	0.00%
Prepare 2013 Q3 Quarterly Report	10/1/13	10/29/13	0.00%
Milestone: 2013 Q3 Quarterly Report completed	10/29/13	10/29/13	0.00%
Prepare 2013 Q4 Quarterly Report	1/1/14	1/28/14	0.00%
Milestone: 2013 Q4 Quarterly Report completed	1/28/14	1/28/14	0.00%



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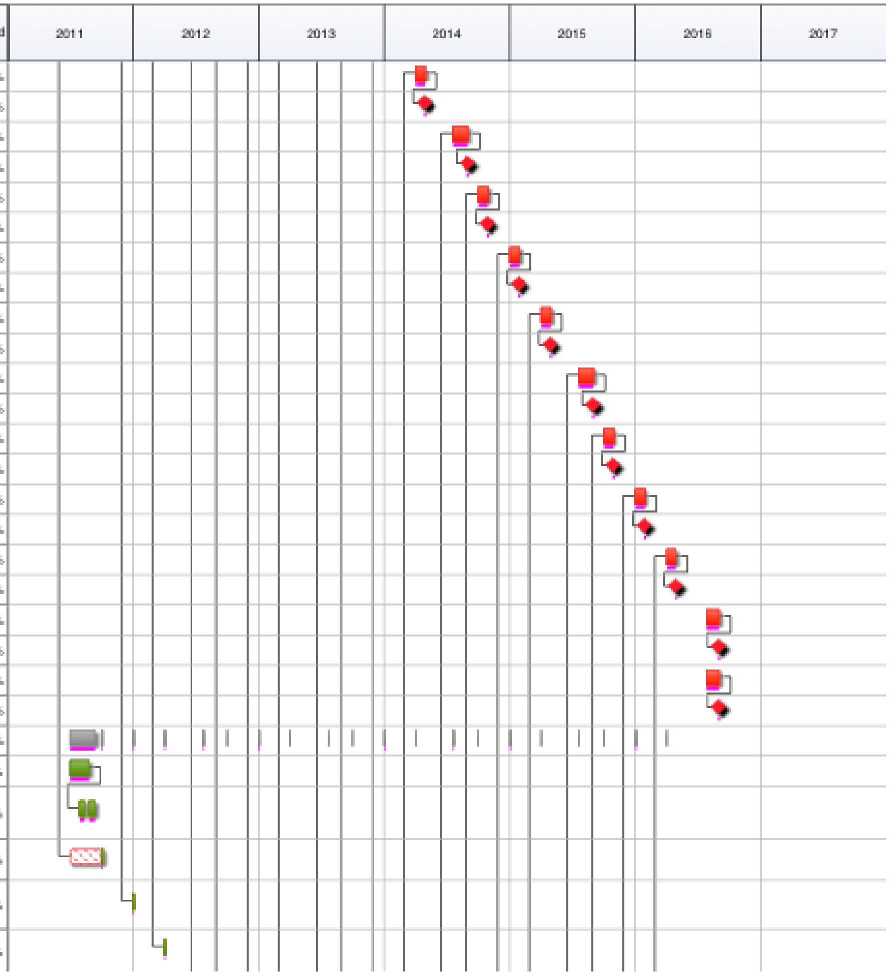
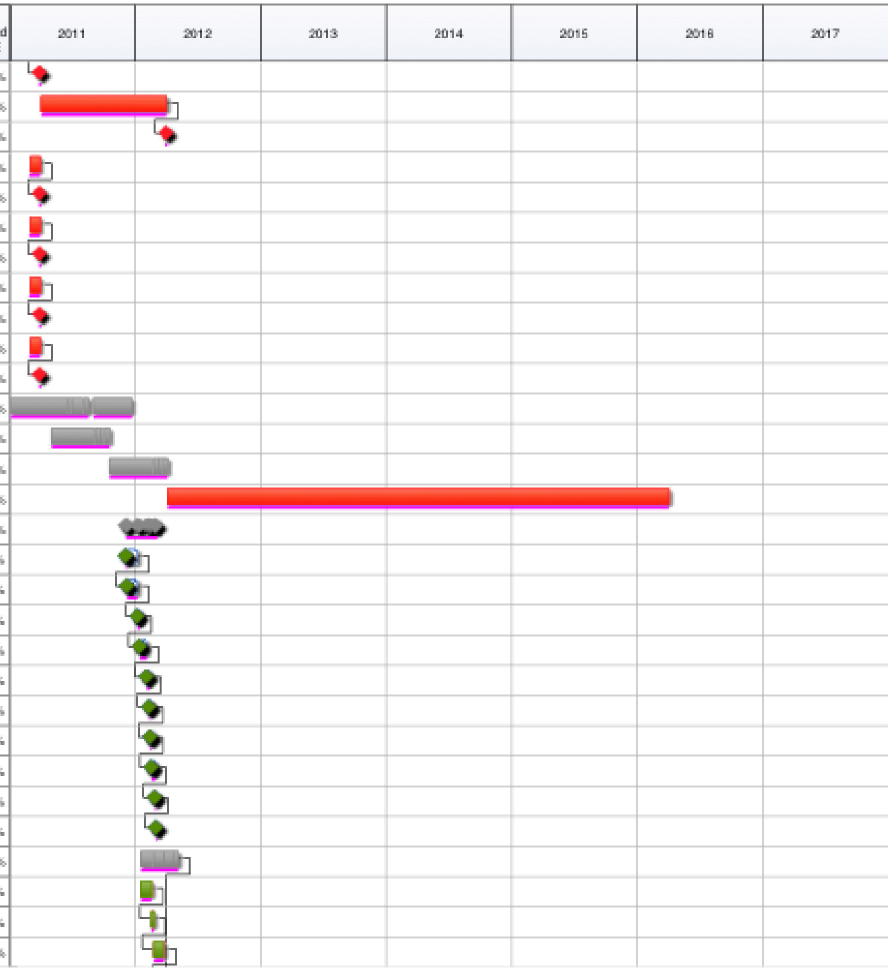
Printed on **Thursday, October 18, 2012**

Name	Start	Finish	% Completed - XSEDE
Prepare 2014 Q1 Quarterly Report	4/1/14	4/28/14	0.00%
Milestone: 2014 Q1 Quarterly Report completed	4/28/14	4/28/14	0.00%
Prepare Y3 Annual Report	7/21/14	8/29/14	0.00%
Milestone: Y3 Annual Report completed	8/29/14	8/29/14	0.00%
Prepare 2014 Q3 Quarterly Report	10/1/14	10/28/14	0.00%
Milestone: 2014 Q3 Quarterly Report completed	10/28/14	10/28/14	0.00%
Prepare 2014 Q4 Quarterly Report	1/1/15	1/28/15	0.00%
Milestone: 2014 Q4 Quarterly Report completed	1/28/15	1/28/15	0.00%
Prepare 2015 Q1 Quarterly Report	4/1/15	4/28/15	0.00%
Milestone: 2015 Q1 Quarterly Report completed	4/28/15	4/28/15	0.00%
Prepare Y4 Annual Report	7/20/15	8/31/15	0.00%
Milestone: Y4 Annual Report completed	8/31/15	8/31/15	0.00%
Prepare 2015 Q3 Quarterly Report	10/1/15	10/28/15	0.00%
Milestone: 2015 Q3 Quarterly Report completed	10/28/15	10/28/15	0.00%
Prepare 2015 Q4 Quarterly Report	1/1/16	1/28/16	0.00%
Milestone: 2015 Q4 Quarterly Report completed	1/28/16	1/28/16	0.00%
Prepare 2016 Q1 Quarterly Report	4/1/16	4/28/16	0.00%
Milestone: 2016 Q1 Quarterly Report completed	4/28/16	4/28/16	0.00%
Prepare Y5 Annual Report	7/25/16	8/31/16	0.00%
Milestone: Y5 Annual Report completed	8/31/16	8/31/16	0.00%
Prepare Final Report	7/25/16	8/31/16	0.00%
Milestone: Final Report completed	8/31/16	8/31/16	0.00%
Project Management - Risk Management	7/1/11	4/1/16	0.00%
Identify risks with Level 3 WBS Managers	7/1/11	8/25/11	100.00%
Review risk register with Level 2 WBS Managers	7/29/11	9/8/11	100.00%
Quarterly review of risk register - 2011 Q3	10/3/11	10/4/11	100.00%
Quarterly review of risk register - 2011 Q4	1/2/12	1/3/12	100.00%
Quarterly review of risk register - 2012 Q1	4/2/12	4/3/12	100.00%



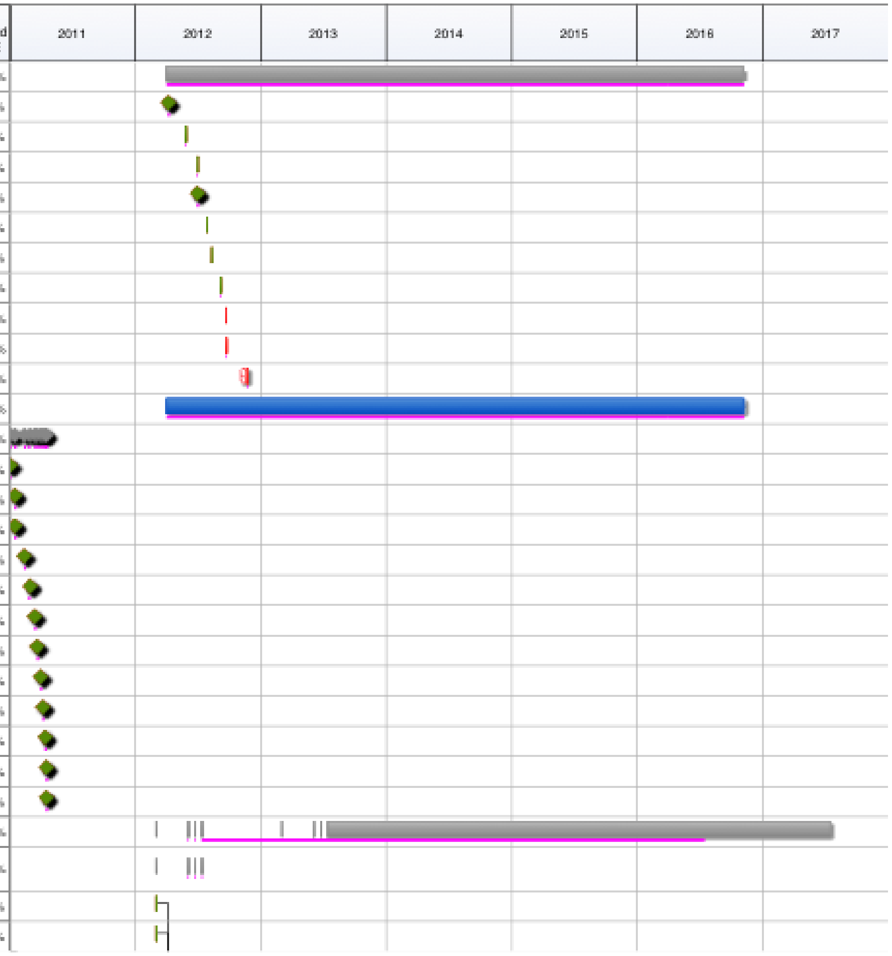
Name	Start	Finish	% Completed - XSEDE
Quarterly review of risk register - 2012 Q2	7/23/12	7/23/12	100.00%
Quarterly review of risk register - 2012 Q3	10/1/12	10/1/12	100.00%
Quarterly review of risk register - 2012 Q4	1/1/13	1/1/13	0.00%
Quarterly review of risk register - 2013 Q1	4/1/13	4/1/13	0.00%
Quarterly review of risk register - 2013 Q2	7/22/13	7/22/13	0.00%
Quarterly review of risk register - 2013 Q3	10/1/13	10/1/13	0.00%
Quarterly review of risk register - 2013 Q4	1/1/14	1/1/14	0.00%
Quarterly review of risk register - 2014 Q1	4/1/14	4/1/14	0.00%
Quarterly review of risk register - 2014 Q2	7/21/14	7/21/14	0.00%
Quarterly review of risk register - 2014 Q3	10/1/14	10/1/14	0.00%
Quarterly review of risk register - 2014 Q4	1/1/15	1/1/15	0.00%
Quarterly review of risk register - 2015 Q1	4/1/15	4/1/15	0.00%
Quarterly review of risk register - 2015 Q2	7/20/15	7/20/15	0.00%
Quarterly review of risk register - 2015 Q3	10/1/15	10/1/15	0.00%
Quarterly review of risk register - 2015 Q4	1/1/16	1/1/16	0.00%
Quarterly review of risk register - 2016 Q1	4/1/16	4/1/16	0.00%
Systems Engineering	7/2/12	6/28/13	0.00%
User needs collection	7/2/12	6/28/13	25.00%
Requirements analysis	7/2/12	6/28/13	25.00%
Managing the UREP	7/2/12	6/28/13	25.00%
Updating the Requirements Management Plan	7/2/12	9/28/12	35.00%
Updating the SEMP	7/2/12	12/14/12	0.00%
XDOR/IDEALS: establishing procedures/developing documentation	7/2/12	9/28/12	75.00%
Management of XDOR process	6/28/13	6/28/13	0.00%
Systems Architecture	1/3/11	3/30/16	0.00%
Deploy Grid Middleware Infrastructure	3/1/11	3/28/11	0.00%

Name	Start	Finish	% Completed - XSEDE
Milestone: Grid Middleware Infrastructure deployed	3/28/11	3/28/11	0.00%
Deploy Data Management software	4/1/11	3/29/12	0.00%
Milestone: Data Management software deployed	3/29/12	3/29/12	0.00%
Deploy Account Management software	3/1/11	3/28/11	0.00%
Milestone: Account Management software deployed	3/28/11	3/28/11	0.00%
Deploy Information Services Infrastructure	3/1/11	3/28/11	0.00%
Milestone: Information Services Infrastructure deployed	3/28/11	3/28/11	0.00%
Deploy Common User Environment	3/1/11	3/28/11	0.00%
Milestone: Common User Environment deployed	3/28/11	3/28/11	0.00%
Deploy System of Systems Test Environment	3/1/11	3/28/11	0.00%
Milestone: System of Systems Test Environment deployed	3/28/11	3/28/11	0.00%
Spiral 1.0	1/3/11	12/21/11	0.00%
Spiral 2.0	5/3/11	10/18/11	0.00%
Spiral 3.0	10/18/11	4/4/12	0.00%
Ongoing: Incremental improvements continue via SEMP Spiral Design Process	4/5/12	3/30/16	0.00%
Public Facing XSEDE Architecture Document	12/5/11	3/2/12	0.00%
Agreement of contents and level of detail	12/5/11	12/5/11	100.00%
Establish time frame to produce public facing architecture document	12/9/11	12/9/11	100.00%
Outline for initial level 1 & level 2-decomposition documentation	1/6/12	1/6/12	100.00%
First draft of public facing document	1/13/12	1/13/12	100.00%
Revise, comment add content to document as necessary	2/2/12	2/2/12	100.00%
Architects review first draft with Bachman	2/10/12	2/10/12	100.00%
Identify remaining steps to complete first draft	2/13/12	2/13/12	100.00%
A&D team including liaisons from SD&I, Security, Campus Bridging and	2/17/12	2/17/12	100.00%
Architects address comments/revisions and request endorsement from A&D	2/28/12	2/28/12	100.00%
First version of XSEDE Architecture Document (Level 1 & 2 Decomp)	3/2/12	3/2/12	100.00%
Campus Bridging - Architectural Response to Stakeholder Requirements	1/19/12	5/3/12	0.00%
Preliminary background work	1/19/12	2/16/12	100.00%
Documentation and review of use cases and requirements matrix completed	2/17/12	2/23/12	100.00%
Architectural response at a Level 3 Decomposition prepared by the	2/24/12	3/22/12	95.00%

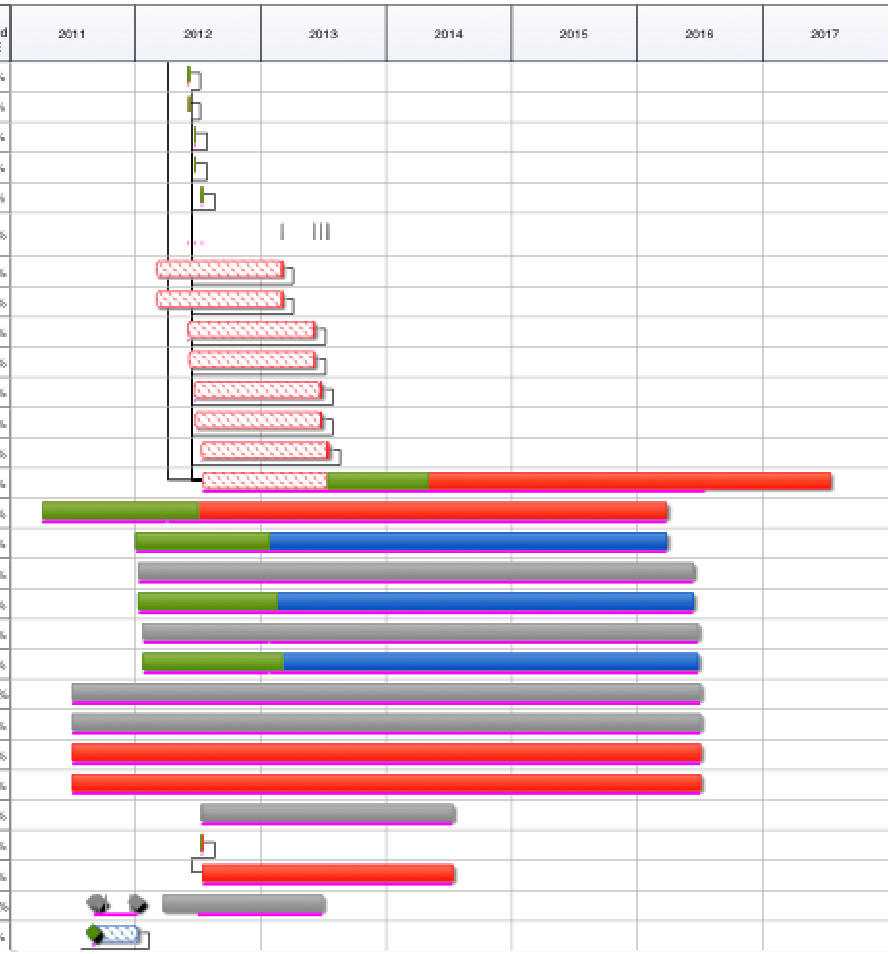


Name	Start	Finish	% Completed - XSEDE	2011	2012	2013	2014	2015	2016	2017
Stakeholder review of Architectural response	3/23/12	4/19/12	65.00%							
Stakeholder approved Arch response for Campus Bridging documented	4/20/12	5/3/12	65.00%							
Science Gateways - Architectural Response to Stakeholder Requirements	5/4/12	8/9/12	0.00%							
Documentation and review of use cases and requirements matrix completed	5/4/12	5/31/12	60.00%							
Architectural response at a Level 3 Decomposition prepared by the	6/1/12	6/28/12	0.00%							
Stakeholder review of Architectural response	6/23/12	6/29/12	0.00%							
Stakeholder review of Architectural response (cont.)	7/2/12	7/26/12	0.00%							
Stakeholder approved Arch response for Gateways documented	7/27/12	8/9/12	0.00%							
Computing - Architectural Response to Stakeholder Requirements	8/10/12	11/15/12	0.00%							
Documentation and review of use cases and requirements matrix completed	8/10/12	9/6/12	15.00%							
Architectural response at a Level 3 Decomposition prepared by the	9/7/12	10/4/12	0.00%							
Stakeholder review of Architectural response	10/5/12	11/1/12	0.00%							
Stakeholder approved Arch response for Computing documented	11/2/12	11/15/12	0.00%							
BIG Data - Architectural Response to Stakeholder Requirements	11/16/12	3/7/13	0.00%							
Documentation and review of use cases and requirements matrix completed	11/16/12	12/13/12	5.00%							
Architectural response at a Level 3 Decomposition prepared by the	12/14/12	1/25/13	0.00%							
Stakeholder review of Architectural response	1/28/13	2/21/13	0.00%							
Stakeholder approved Arch response for BIG Data documented	2/22/13	3/7/13	0.00%							
Connecting Instrumentation - Architectural Response to Stakeholder Requirements	3/8/13	6/13/13	0.00%							
Documentation and review of use cases and requirements matrix completed	3/8/13	4/4/13	5.00%							
Architectural response at a Level 3 Decomposition prepared by the	4/5/13	5/2/13	0.00%							
Stakeholder review of Architectural response	5/3/13	5/30/13	0.00%							
Stakeholder approved Arch response for Connecting Instrumention documented	5/31/13	6/13/13	0.00%							
Collaboration - Architectural Response to Stakeholder Requirements	6/14/13	9/19/13	0.00%							
Documentation and review of use cases and requirements matrix completed	6/14/13	6/28/13	9.00%							
Documentation and review of use cases and requirements matrix completed	7/1/13	7/11/13	0.00%							
Architectural response at a Level 3 Decomposition prepared by the	7/12/13	8/8/13	0.00%							
Stakeholder review of Architectural response	8/9/13	9/5/13	0.00%							
Stakeholder approved Arch response for Collaboration documented	9/6/13	9/19/13	0.00%							
External Relations	1/3/11	7/14/17	0.00%							

Name	Start	Finish	% Completed - XSEDE
Generate Publications: Highlights (Science, EOT, Digital Resources)	4/2/12	11/3/16	0.00%
SciHi subcommittee from XSEDE ER established	4/9/12	4/9/12	100.00%
Collect story ideas	5/25/12	5/25/12	100.00%
Story choices approved by XSEDE leadership	6/29/12	6/29/12	100.00%
Graphic designer selected	7/2/12	7/2/12	100.00%
About 15 science highlights stories selected, edited (incl tech review) and	7/27/12	7/27/12	100.00%
Cover-to-cover edit complete	8/10/12	8/10/12	100.00%
Overall design and test story mockup complete and reviewed	9/5/12	9/5/12	90.00%
Final design complete	9/20/12	9/20/12	0.00%
Completed book delivered to printer	9/21/12	9/21/12	0.00%
Milestone: Science Highlights published	11/21/12	11/21/12	0.00%
Ongoing: Repeat previous 10 tasks annually	4/2/12	11/3/16	0.00%
Create XSEDE website and translate relevant TG website content	1/3/11	4/18/11	0.00%
XSEDE Web-XSEDE website committee established	1/3/11	1/3/11	100.00%
Website requirements document complete	1/17/11	1/17/11	100.00%
Content requirements document complete	1/17/11	1/17/11	100.00%
First rev of design reviewed by website committee	2/15/11	2/15/11	100.00%
Rev of website reviewed by XSEDE leadership	3/1/11	3/1/11	100.00%
Short form usability test completed	3/15/11	3/15/11	100.00%
Final version of website reviewed by website committee	3/22/11	3/22/11	100.00%
Content approved	4/1/11	4/1/11	100.00%
Final build complete	4/7/11	4/7/11	100.00%
Content ported and built	4/15/11	4/15/11	100.00%
Initial version of XSEDE website launched	4/18/11	4/18/11	100.00%
Milestone: XSEDE website completed	4/18/11	4/18/11	100.00%
Generate Annual Conference Proceedings	3/1/12	7/14/17	0.00%
Genereate Annual Conference 2012	3/1/12	7/12/12	0.00%
Proceedings chair selected and incorporated into event planning	3/1/12	3/1/12	100.00%
Submission site publicized	3/1/12	3/1/12	100.00%



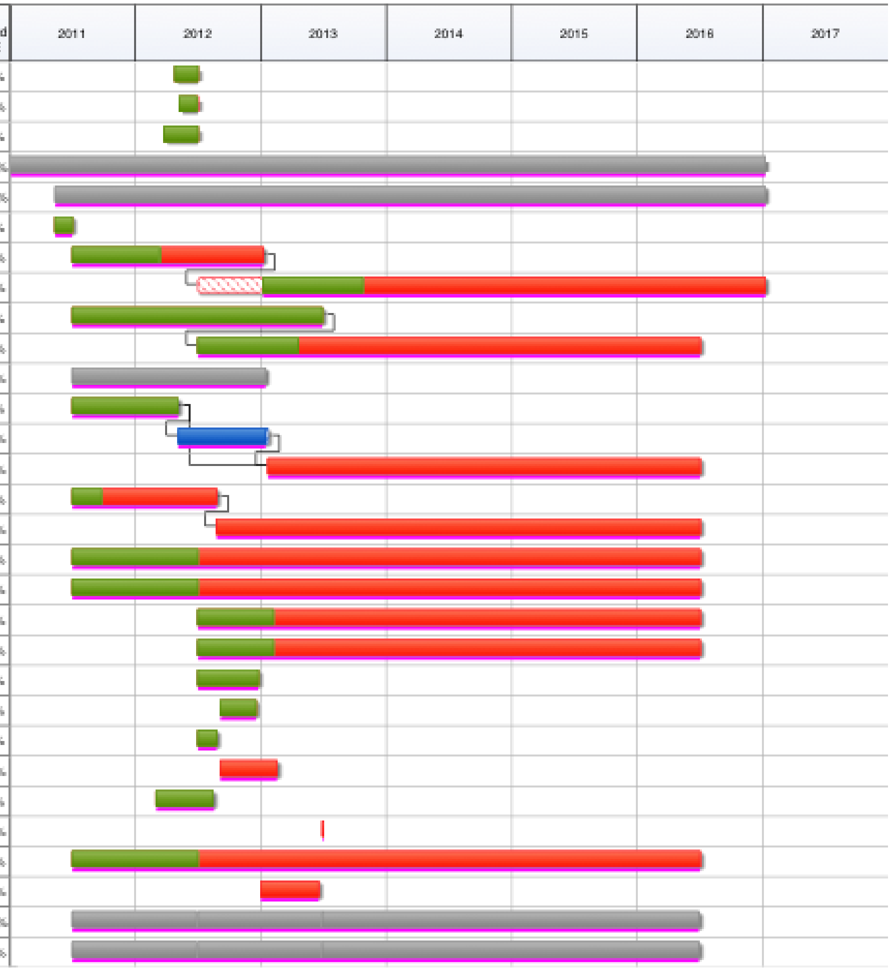
Name	Start	Finish	% Completed - XSEDE
Approval from ACM or whatever publisher received	6/1/12	6/1/12	100.00%
Templates and copyright permission forms out to authors	6/5/12	6/5/12	100.00%
All papers and copyright permission forms received from authors and	6/22/12	6/22/12	100.00%
All papers sent to production house for reproduction to USB drive	6/25/12	6/25/12	100.00%
Milestone: Annual Conference Proceedings Complete	7/12/12	7/12/12	100.00%
Generate Annual Conference 2013	3/1/13	7/12/13	0.00%
Proceedings chair selected and incorporated into event planning	3/1/13	3/1/13	0.00%
Submission site publicized	3/1/13	3/1/13	0.00%
Approval from ACM or whatever publisher received	6/1/13	6/3/13	0.00%
Templates and copyright permission forms out to authors	6/5/13	6/5/13	0.00%
All papers and copyright permission forms received from authors and	6/22/13	6/24/13	0.00%
All papers sent to production house for reproduction to USB drive	6/25/13	6/25/13	0.00%
Milestone: Annual Conference Proceedings Complete	7/12/13	7/12/13	0.00%
Ongoing: Repeat previous 7 tasks annually	7/15/13	7/14/17	20.00%
Milestone: Ongoing - Generate press releases & website content	4/4/11	3/24/16	25.00%
Milestone: Ongoing - Generate publicity via social media	1/3/12	3/24/16	25.00%
Monthly: Gather, edit and format content for internal (plain text) e-newsletter; distribute to	1/10/12	6/9/16	0.00%
Milestone: Ongoing - Generate monthly internal e-newsletter	1/10/12	6/9/16	25.00%
Monthly: Gather, edit and format content for external (HTML/designed) e-newsletter;	1/25/12	6/23/16	0.00%
Milestone: Ongoing - Generate monthly external e-newsletter	1/25/12	6/23/16	25.00%
Industry Relations	7/1/11	6/30/16	0.00%
Workforce Development	7/1/11	6/30/16	0.00%
Increase industry partners' awareness of all XSEDE SP's training opportunites	7/1/11	6/30/16	0.00%
Elicit industry partners' input to enhance training programs for workforce	7/1/11	6/30/16	0.00%
Software Development	7/12/12	7/10/14	0.00%
Hold conference call with XAB to flesh out software development activity	7/12/12	7/12/12	1.00%
Select and execute the software development project	7/13/12	7/10/14	0.00%
SD&I	9/1/11	6/28/13	0.00%
PDR	9/1/11	9/1/11	100.00%



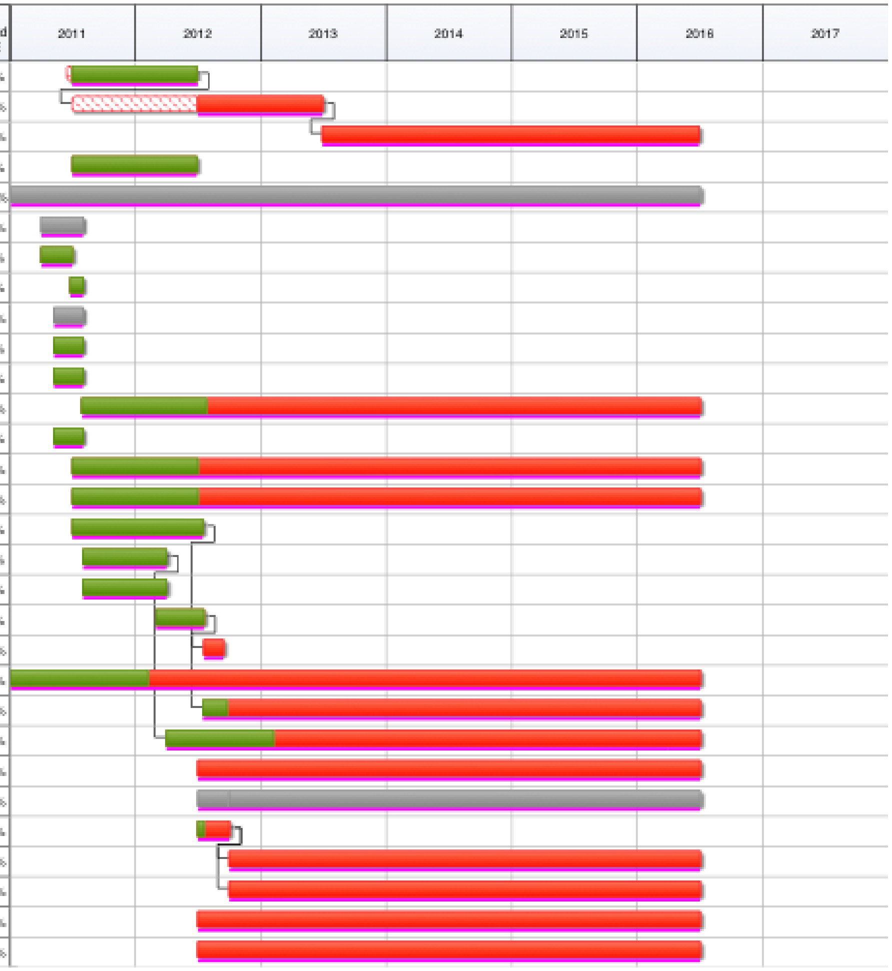
Name	Start	Finish	% Completed - XSEDE	2011	2012	2013	2014	2015	2016	2017
Increment Planning	9/1/11	9/1/11	0.00%							
develop incrment plan	9/1/11	9/1/11	100.00%							
IRR	9/7/11	9/7/11	0.00%							
conduct IRR	9/7/11	9/7/11	100.00%							
IRR complete and passed	9/7/11	9/7/11	100.00%							
CI Detailed Design	9/8/11	9/8/11	0.00%							
develop detail design	9/8/11	9/8/11	0.00%							
GFFS	9/8/11	9/8/11	100.00%							
Execution Management	9/8/11	9/8/11	100.00%							
XUAS Data	9/8/11	9/8/11	100.00%							
CDR	9/9/11	9/15/11	0.00%							
conduct CDR	9/9/11	9/9/11	100.00%							
CDR complete and passed	9/15/11	9/15/11	100.00%							
CI Development	9/16/11	9/16/11	0.00%							
develop CI	9/16/11	9/16/11	0.00%							
GFFS	9/16/11	9/16/11	100.00%							
Execution Management	9/16/11	9/16/11	100.00%							
XUAS Data	9/16/11	9/16/11	100.00%							
CI TRR	9/19/11	10/7/11	0.00%							
conduct CI TRR	9/19/11	9/19/11	0.00%							
GFFS	9/19/11	9/19/11	100.00%							
Execution Management	9/19/11	9/19/11	100.00%							
XUAS Data	9/19/11	9/19/11	100.00%							
CI TRR complete and passed	10/7/11	10/7/11	100.00%							
CI Tests	10/10/11	12/15/11	0.00%							
conduct CI tests	10/10/11	10/10/11	0.00%							
GFFS	10/10/11	10/10/11	100.00%							
Execution Management	10/10/11	10/10/11	100.00%							
XUAS Data	10/10/11	10/10/11	100.00%							
CI Tests complete and passed	12/15/11	12/15/11	100.00%							

Name	Start	Finish	% Completed - XSEDE	2011	2012	2013	2014	2015	2016	2017
STRR	12/16/11	12/16/11	0.00%							
conduct STRR	12/16/11	12/16/11	100.00%							
STRR complete and passed	12/16/11	12/16/11	100.00%							
System Integration Test	12/19/11	12/28/11	0.00%							
conduct system test	12/19/11	12/19/11	100.00%							
System test complete and passed	12/28/11	12/28/11	100.00%							
ORR	12/29/11	12/29/11	0.00%							
conduct ORR	12/29/11	12/29/11	100.00%							
ORR complete and passed	12/29/11	12/29/11	100.00%							
Increment De-brief	12/30/11	1/6/12	0.00%							
increment reflection workshop	12/30/11	12/30/11	100.00%							
reflection and practice report	1/2/12	1/2/12	100.00%							
de-brief complete	1/6/12	1/6/12	100.00%							
Implement Open, Continuous Planning	7/2/12	6/28/13	100.00%							
Implement Continuous Development and Integration	7/2/12	6/28/13	100.00%							
Implement Engineering Improvements	7/2/12	6/28/13	100.00%							
SDIACT-10 - Deliver Operational Tests with Cis	4/19/12	6/29/12	50.00%							
SDIACT-15 - Genesis II/UNICORE 6 GAML SAML	4/3/12	7/2/12	100.00%							
SDIACT-18 - Replicated/Synchronized stateful resource	4/18/12	6/18/12	100.00%							
SDIACT-28 - CANCELED: GO Transfer REST API as XSEDE Production service	4/25/12	7/2/12	100.00%							
SDIACT-31 - Improve GridFTP for SPs	4/25/12	7/2/12	85.00%							
SDIACT-43 - Genesis II Documentation	4/30/12	7/2/12	100.00%							
Activity 44. CANCELED, MERGED with SDIACT-100: Campus bridging beta support	4/30/12	7/2/12	100.00%							
SDIACT-49 - Link Globus Online into XSEDE User Portal	4/25/12	7/2/12	100.00%							
SDIACT-50 - MyProxy OAuth Limited Proxy Support	4/20/12	7/2/12	100.00%							
SDIACT-54 - Register new increment 1 components	4/19/12	6/5/12	50.00%							
SDIACT-73 - System information publishing pilot	4/24/12	6/29/12	20.00%							
SDIACT-75 - GridFTP in UNICORE 6	5/1/12	7/2/12	84.00%							
SDIACT-96 - Identify XSEDE not TeraGrid in resource names for new OSG resource	3/22/12	5/9/12	100.00%							
SDIACT-97 - Basic Execution Service	5/2/12	6/25/12	100.00%							

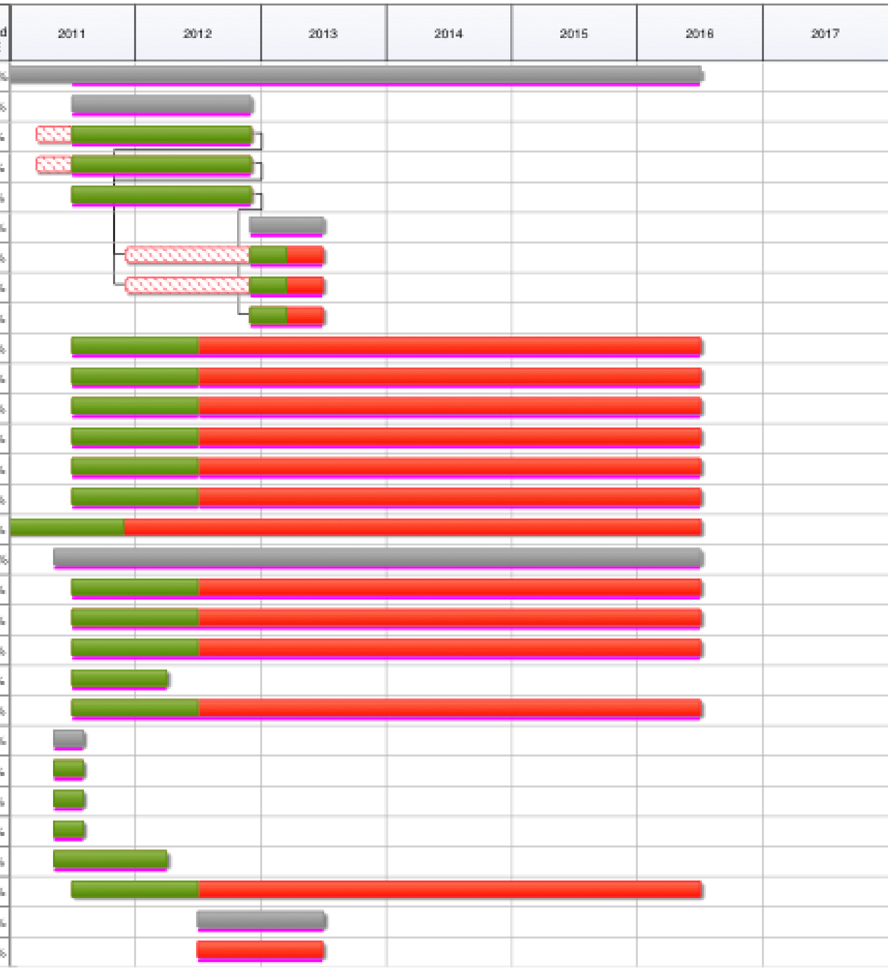
Name	Start	Finish	% Completed - XSEDE
SDIACT-100 - Globus Online Increment 2 addressing security concerns	4/25/12	7/2/12	100.00%
SDIACT-101 - EMS and GFFS Increment 2 updates	5/8/12	7/2/12	90.00%
SCIDACT-71 - Improve cmd line single sign-on access	3/27/12	6/29/12	100.00%
Operations	10/6/10	1/6/17	0.00%
Cybersecurity	5/12/11	1/6/17	0.00%
Setup coordination of XSEDE incident response	5/12/11	7/1/11	100.00%
Setup and deploy XSEDE Certificate Authority	7/1/11	1/4/13	46.00%
Ongoing: Maintain Certificate Authority	1/4/13	1/6/17	20.00%
Develop and deploy Security Awareness program	7/1/11	6/27/13	100.00%
Ongoing: Maintain Security Awareness program	7/2/12	7/1/16	20.00%
Develop and deploy two factor authentication service	7/1/11	1/11/13	0.00%
Evaluate Implementation Options	7/1/11	5/4/12	100.00%
Deploy two factor authentication	5/4/12	1/11/13	0.00%
Ongoing: Maintain two factor authentication service	1/21/13	7/1/16	0.00%
Integrate and deploy InCommon Federated Authentication service	7/1/11	8/23/12	20.00%
Ongoing: Maintain InCommon Federated Authentication service	8/24/12	6/30/16	0.00%
Ongoing: Develop and implement improvements based on SEMP Spiral Design	7/1/11	6/30/16	20.00%
Ongoing: XSEDE Incident response	7/1/11	6/30/16	20.00%
Ongoing: Conduct on-demand security reviews for SD&I	7/2/12	6/30/16	15.00%
Ongoing: Conduct security reviews for ST&D	7/2/12	7/1/16	15.00%
Conduct XSEDE security risk assessment	7/2/12	12/21/12	100.00%
Setup XSEDE Nessus vulnerability assessment capability	9/3/12	12/14/12	100.00%
Setup secure wiki	7/2/12	8/24/12	100.00%
Install and update intrusion detection capability and security monitoring	9/3/12	2/15/13	0.00%
Obtain InCommon membership for XSEDE	3/1/12	8/14/12	100.00%
Conduct annual XSEDE security meeting	6/28/13	7/2/13	0.00%
Ongoing: Participate in XSEDE communications plan	7/1/11	6/30/16	20.00%
Prototype NSFv4 wide area file system and investigate security implications	1/1/13	6/17/13	0.00%
Data Services	7/1/11	6/29/16	0.00%
XSEDE Wide File System	7/4/11	6/29/16	0.00%



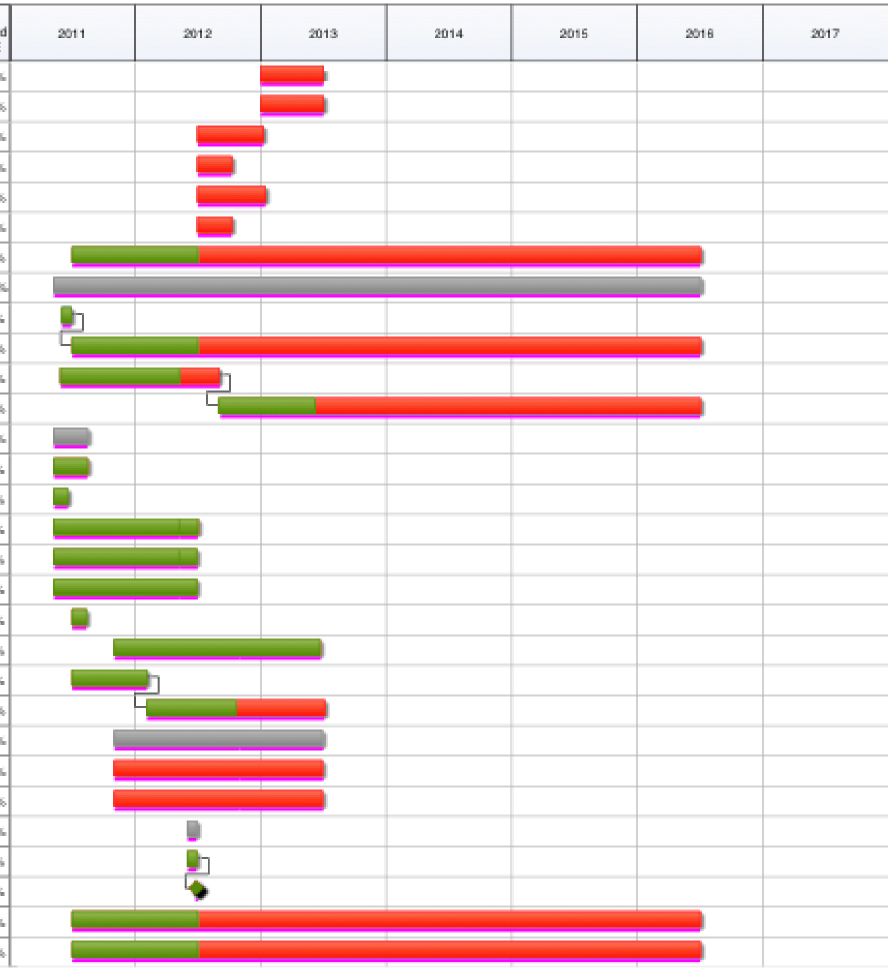
Name	Start	Finish	% Completed - XSEDE
Evaluate/Select global parallel file system(s)	7/4/11	6/28/12	100.00%
Deploy/extend global parallel file system(s)	6/29/12	6/27/13	0.00%
Ongoing: Maintain/extend global parallel file system(s)	6/28/13	6/29/16	0.00%
Evaluate and design archival replication framework	7/1/11	6/27/12	100.00%
XSEDENet Networking	1/3/11	7/1/16	0.00%
Transition current TG network to XSEDE network	4/1/11	7/29/11	0.00%
Execute NLR contracts	4/1/11	7/1/11	100.00%
Connect XSEDE sites to NLR	6/27/11	7/29/11	100.00%
xsede.org nameservice	5/9/11	7/29/11	0.00%
delegate subdomains to XSEDE partners: NICS, TACC, PSC	5/9/11	7/29/11	100.00%
establish DNS entries for non-subdomain names (network.xsede.org, etc.)	5/9/11	7/29/11	100.00%
Ongoing: Maintain and Monitor XSEDEnet	7/29/11	6/30/16	20.00%
Preserve the PSC speed page	5/9/11	7/29/11	100.00%
Ongoing: Tune end-to-end performance for user applications	7/1/11	6/30/16	20.00%
Ongoing: Develop and implement improvements based on SEMP Spiral Design	7/1/11	6/30/16	20.00%
Setup perfSONAR	7/1/11	7/13/12	100.00%
Provide Operations tools to monitor the network	8/1/11	3/30/12	100.00%
Replace network.teragrid.org functions	8/1/11	3/30/12	100.00%
Evaluate alternatives to NLR	3/1/12	7/18/12	100.00%
Execute network vendor contracts	7/19/12	9/12/12	0.00%
Ongoing: Maintain DNS entries for non-subdomain names (network.xsede.org,	1/3/11	6/30/16	20.00%
Ongoing: Maintain perfSONAR	7/13/12	7/1/16	5.00%
Ongoing: Maintain Operations tools to monitor the network	3/30/12	6/30/16	20.00%
Ongoing: Develop/Implement special ops team process for network related application	7/2/12	7/1/16	0.00%
XSEDEnet Metrics	7/2/12	7/1/16	0.00%
Determine metrics	7/2/12	9/28/12	20.00%
Ongoing: Collect data	10/1/12	7/1/16	0.00%
Ongoing: Report metrics (dashboard, quarterly report)	10/1/12	7/1/16	0.00%
SMNP Access, Layer 2 monitoring and measurement	7/2/12	7/1/16	0.00%
Develop Application Standards for Network Performance Metrics	7/2/12	7/1/16	0.00%



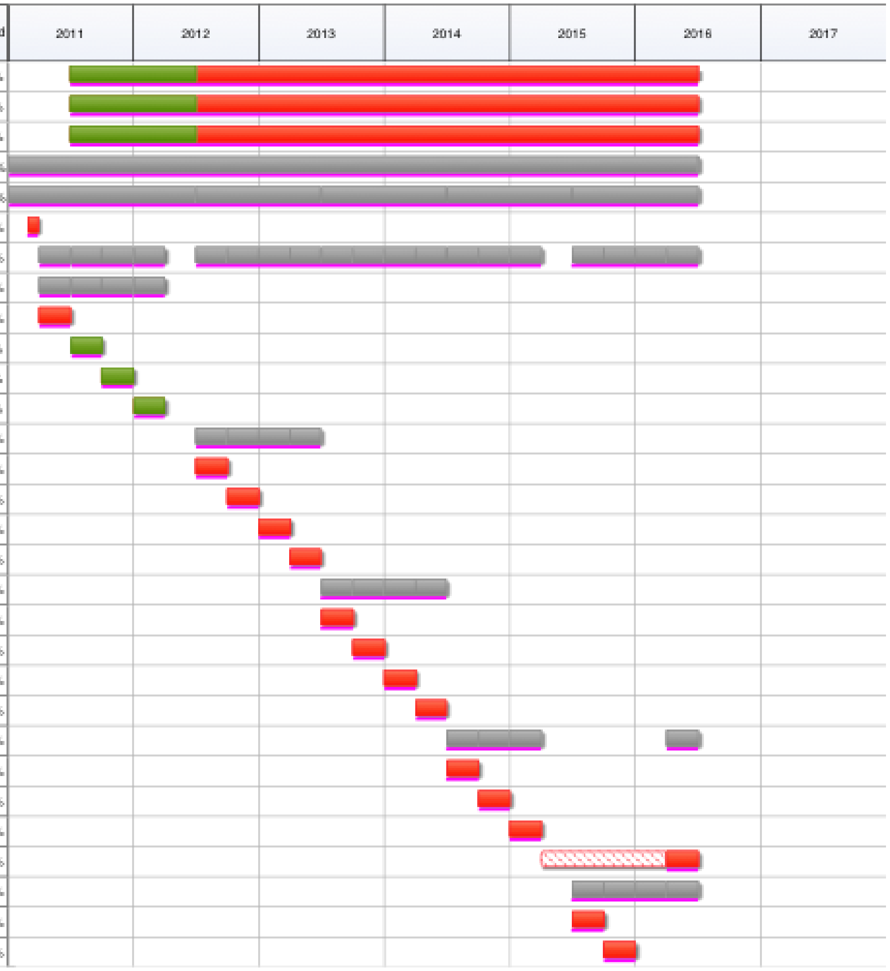
Name	Start	Finish	% Completed - XSEDE
Software Testing and Deployment	10/6/10	6/30/16	0.00%
Test XSEDE software	7/4/11	11/29/12	0.00%
Test Grid Middleware - EMS (Unicore and Genesis II client)	7/4/11	11/29/12	100.00%
Test Grid Middleware - GFSS (Genesis II)	7/4/11	11/29/12	100.00%
Test Data Movement - Globus Online	7/4/11	11/29/12	100.00%
Deploy XSEDE software	11/30/12	6/27/13	0.00%
Deploy Grid Middleware - Unicore	11/30/12	6/27/13	50.00%
Deploy Grid Middleware - Genesis II (campus bridging)	11/30/12	6/27/13	50.00%
Deploy Grid Middleware - Globus Online	11/30/12	6/27/13	50.00%
Ongoing: Coordinate operational reviews of next increment of XSEDE software on	7/1/11	6/30/16	20.00%
Ongoing: Test next increment of XSEDE Software on demand	7/4/11	6/30/16	20.00%
Ongoing: Deploy next increment of XSEDE software to SPs on demand	7/4/11	6/30/16	20.00%
Ongoing: Coordinate campus bridging deployments	7/4/11	6/30/16	20.00%
Ongoing: Develop deployment work plans and documentation	7/4/11	6/30/16	20.00%
Ongoing: Coordinate Globus Grid software support	7/4/11	6/30/16	20.00%
Ongoing: Support Deployment of Software & Services at SPs	10/6/10	6/30/16	20.00%
Accounting and Account Management	5/9/11	7/1/16	0.00%
Ongoing: Maintain existing accounting and account management databases	7/1/11	6/30/16	20.00%
Ongoing: Investigate and improve accounting/account management processes	7/1/11	6/30/16	20.00%
Ongoing: Participate in XSEDE communications plan	7/1/11	6/30/16	20.00%
Optimize and upgrade the XDCDB system	7/1/11	3/29/12	100.00%
Ongoing: Develop and implement improvements based on SEMP Spiral Design	7/1/11	6/30/16	20.00%
Make appropriate name changes to (item).xsede.org	5/9/11	7/29/11	0.00%
domain name changes	5/9/11	7/29/11	100.00%
web site changes	5/9/11	7/29/11	100.00%
documentation changes	5/9/11	7/29/11	100.00%
Complete the 2nd phase of vetted/unvetted account creation effort	5/9/11	3/30/12	100.00%
Ongoing: Maintain and enhance XSEDE-wide reporting, decision-support and	7/1/11	7/1/16	20.00%
Streamline and modernize the allocation-request and account	7/2/12	7/1/13	0.00%
Re-work and simplify the proposal submission process	7/2/12	6/28/13	0.00%



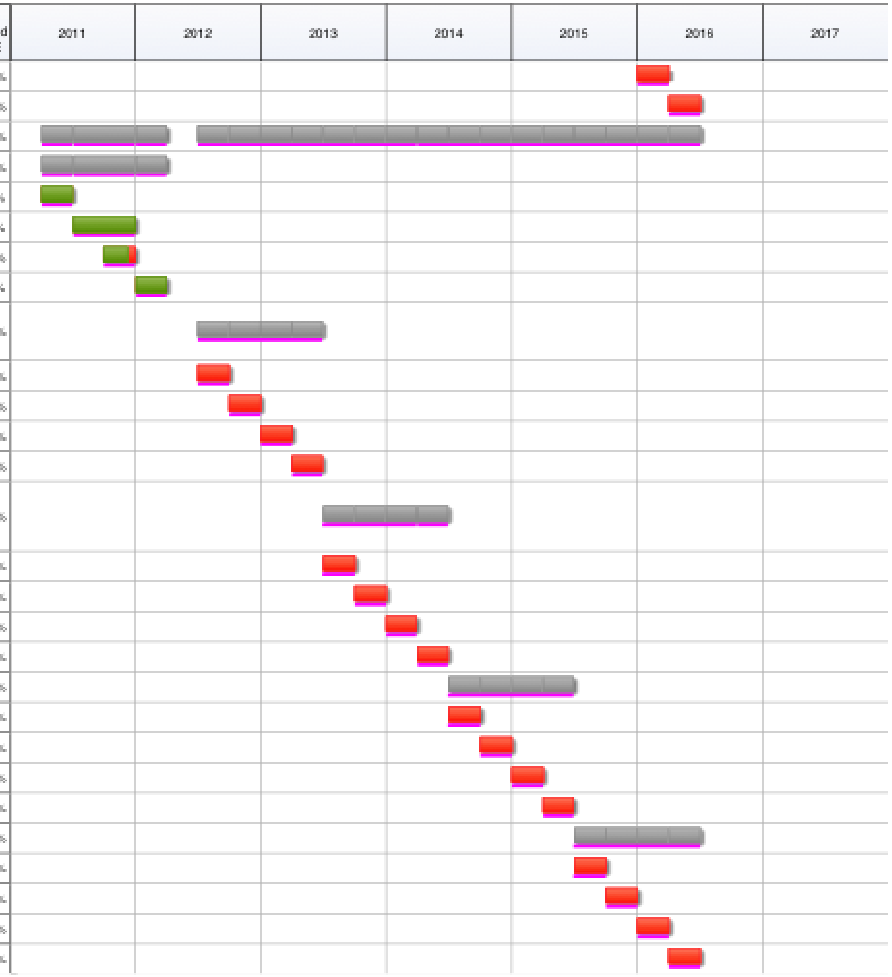
Name	Start	Finish	% Completed - XSEDE
Improve the proposal review and approval process	1/1/13	7/1/13	0.00%
Provide enhanced A&AM administrative capabilities	1/1/13	7/1/13	0.00%
Streamline account-request process	7/2/12	1/4/13	0.00%
Enhance user-based information delivery (allocation/usage info, etc.)	7/2/12	10/5/12	0.00%
Improve overall A&AM-related documentation and training	7/2/12	1/11/13	0.00%
Establish processes to improve campus bridging and new SP integration	7/2/12	10/5/12	0.00%
Ongoing: Support hardware/infrastructure integrity (server maintenace, UPS, etc.)	7/1/11	6/30/16	20.00%
System Operational Support	5/9/11	7/1/16	0.00%
Setup XSEDE Operations Center	6/1/11	6/28/11	100.00%
Ongoing: Operate XSEDE Operations Center	7/1/11	6/30/16	20.00%
Deploy centralized XSEDE cyberinfrasture servers/services	5/30/11	8/31/12	75.00%
Ongoing: Maintain centralized XSEDE cyberinfrastructure servers/services	8/31/12	7/1/16	20.00%
Upgrade XDCDB hardware and split database and AMIE parts	5/9/11	8/12/11	0.00%
upgrade hardware at SDSC and operating system at PSC	5/9/11	8/12/11	100.00%
migrate AMIE to stand alone VM server (PSC and SDSC)	5/9/11	6/17/11	100.00%
Evaluate XDCDB hardware at PSC and determine if refresh needed	5/9/11	6/29/12	100.00%
Evaluate current TG services and classify them into XSEDE HA tiers	5/9/11	6/28/12	100.00%
Plan and schedule a semi-annual XDCDB failover test (SDSC to PSC)	5/9/11	6/28/12	100.00%
TeraGrid ticket system transition	7/1/11	8/11/11	100.00%
Evaluate/Deploy XSEDE Centralized monitoring software	11/1/11	6/21/13	100.00%
Participate in Ticket System evaluation in conjunction with User Support	7/1/11	2/2/12	100.00%
Transition Ticket System: Legacy to New	2/2/12	7/4/13	50.00%
Backup XOC setup at IU	11/1/11	6/28/13	0.00%
Documentation/Training for XOC Backup	11/1/11	6/28/13	0.00%
XOC Failover Test	11/1/11	6/28/13	0.00%
Operations Annual Report	6/1/12	6/28/12	0.00%
Prepare operational metrics annual report/internal Operational Assessment	6/1/12	6/28/12	100.00%
Milestone: Operational metrics annual report completed	6/28/12	6/28/12	100.00%
Ongoing: Participate in XSEDE communications plan	7/1/11	6/30/16	20.00%
Ongoing: Provide VM support for Centralized Services	7/1/11	6/30/16	20.00%



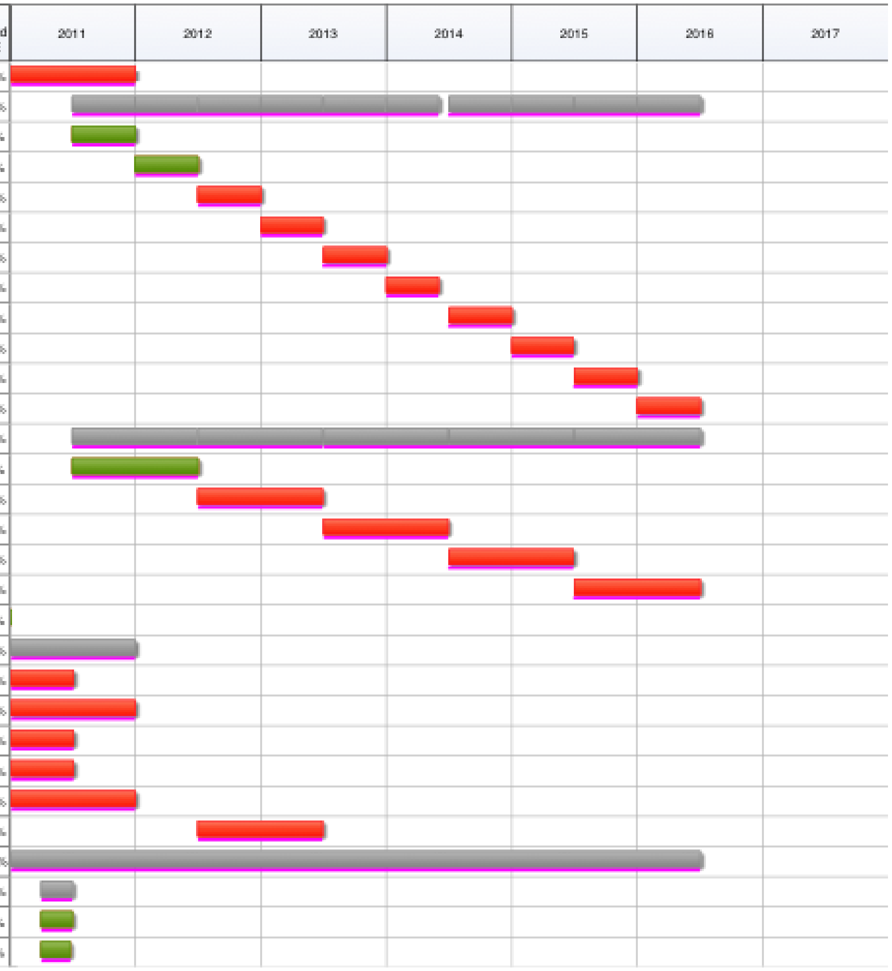
Name	Start	Finish	% Completed - XSEDE
Ongoing: Provide VM support for Science Gateway services	7/1/11	6/30/16	20.00%
Ongoing: Maintain VM server hardware	7/1/11	6/30/16	20.00%
Ongoing: Maintain other server hardware	7/1/11	6/30/16	20.00%
User Services	1/3/11	7/1/16	0.00%
Training	1/3/11	6/30/16	0.00%
Milestone: Develop guidelines for online and in-person training materials across XSEDE	3/1/11	3/28/11	0.00%
Milestone: Develop 10 Training Modules Annually	4/1/11	6/30/16	0.00%
Milestone: Develop 10 Training Modules Year 1	4/1/11	3/30/12	0.00%
Develop and Post 2 new online training tutorials	4/1/11	7/1/11	0.00%
Develop and Post 2 new online training tutorials	7/5/11	9/29/11	100.00%
Develop and Post 3 new online training tutorials	10/3/11	12/30/11	100.00%
Develop and Post 3 new online training tutorials	1/4/12	3/30/12	100.00%
Milestone: Develop 10 Training Modules Year 2	7/2/12	6/28/13	0.00%
Develop and Post 2 new online training tutorials	7/2/12	9/28/12	0.00%
Develop and Post 2 new online training tutorials	10/1/12	12/31/12	0.00%
Develop and Post 3 new online training tutorials	1/1/13	3/29/13	0.00%
Develop and Post 3 new online training tutorials	4/1/13	6/28/13	0.00%
Milestone: Develop 10 Training Modules Year 3	7/1/13	6/30/14	0.00%
Develop and Post 2 new online training tutorials	7/1/13	9/30/13	0.00%
Develop and Post 2 new online training tutorials	10/1/13	12/31/13	0.00%
Develop and Post 3 new online training tutorials	1/1/14	3/31/14	0.00%
Develop and Post 3 new online training tutorials	4/1/14	6/30/14	0.00%
Milestone: Develop 10 Training Modules Year 4	7/1/14	6/30/16	0.00%
Develop and Post 2 new online training tutorials	7/1/14	9/30/14	0.00%
Develop and Post 2 new online training tutorials	10/1/14	12/31/14	0.00%
Develop and Post 3 new online training tutorials	1/1/15	3/31/15	0.00%
Develop and Post 3 new online training tutorials	4/1/16	6/30/16	0.00%
Milestone: Develop 10 Training Modules Year 5	7/1/15	6/30/16	0.00%
Develop and Post 2 new online training tutorials	7/1/15	9/30/15	0.00%
Develop and Post 2 new online training tutorials	10/1/15	12/31/15	0.00%



Name	Start	Finish	% Completed - XSEDE
Develop and Post 3 new online training tutorials	1/1/16	3/31/16	0.00%
Develop and Post 3 new online training tutorials	4/1/16	6/30/16	0.00%
Conduct 50 Training Sessions Annually	4/1/11	6/30/16	0.00%
Milestone: Conduct 50 Training sessions Year 1	4/1/11	3/30/12	0.00%
Conduct first 10 in-person or webcast training sessions	4/1/11	7/1/11	100.00%
Conduct first 15 in-person or webcast training sessions	7/5/11	12/30/11	100.00%
Conduct first 10 in-person or webcast training sessions	10/3/11	12/30/11	75.00%
Conduct first 15 in-person or webcast training sessions	1/4/12	3/30/12	100.00%
Milestone: Conduct 50 Training sessions Year 2	7/2/12	6/28/13	0.00%
Conduct first 10 in-person or webcast training sessions	7/2/12	9/28/12	0.00%
Conduct first 15 in-person or webcast training sessions	10/1/12	12/31/12	0.00%
Conduct first 10 in-person or webcast training sessions	1/1/13	3/29/13	0.00%
Conduct first 15 in-person or webcast training sessions	4/1/13	6/28/13	0.00%
Milestone: Conduct 50 Training sessions Year 3	7/1/13	6/30/14	0.00%
Conduct first 10 in-person or webcast training sessions	7/1/13	9/30/13	0.00%
Conduct first 15 in-person or webcast training sessions	10/1/13	12/31/13	0.00%
Conduct first 10 in-person or webcast training sessions	1/1/14	3/28/14	0.00%
Conduct first 15 in-person or webcast training sessions	4/1/14	6/30/14	0.00%
Milestone: Conduct 50 Training sessions Year 4	7/1/14	6/30/15	0.00%
Conduct first 10 in-person or webcast training sessions	7/1/14	9/30/14	0.00%
Conduct first 15 in-person or webcast training sessions	10/1/14	12/31/14	0.00%
Conduct first 10 in-person or webcast training sessions	1/1/15	3/31/15	0.00%
Conduct first 15 in-person or webcast training sessions	4/1/15	6/30/15	0.00%
Milestone: Conduct 50 Training sessions Year 5	7/1/15	6/30/16	0.00%
Conduct first 10 in-person or webcast training sessions	7/1/15	9/30/15	0.00%
Conduct first 15 in-person or webcast training sessions	10/1/15	12/31/15	0.00%
Conduct first 10 in-person or webcast training sessions	1/1/16	3/31/16	0.00%
Conduct first 15 in-person or webcast training sessions	4/1/16	6/30/16	0.00%

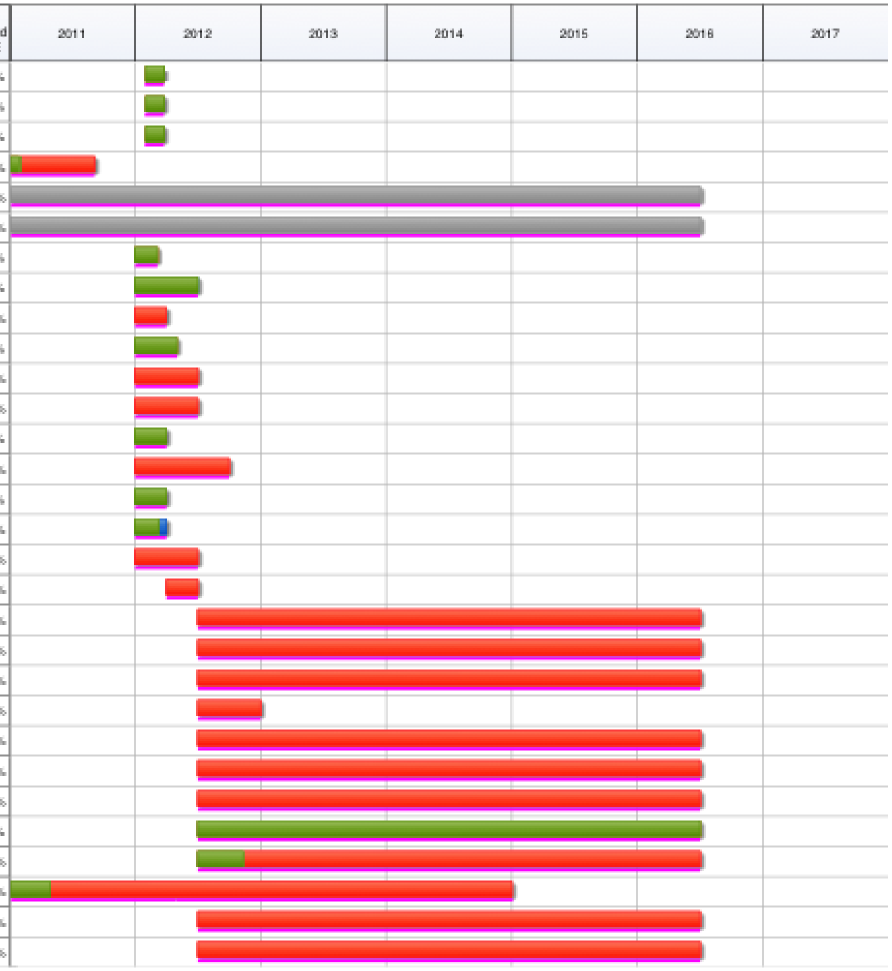


Name	Start	Finish	% Completed - XSEDE
Milestone: Complete Federation of existing online training materials with XSEDE	1/3/11	12/30/11	0.00%
Milestone: Complete 2 targeted community workshops annually	7/1/11	6/30/16	0.00%
Conduct first targeted community workshop Year 1	7/1/11	12/30/11	100.00%
Conduct second targeted community workshop Year 1	1/2/12	6/29/12	100.00%
Conduct first targeted community workshop Year 2	7/2/12	12/31/12	0.00%
Conduct second targeted community workshop Year 2	1/1/13	6/28/13	0.00%
Conduct first targeted community workshop Year 3	7/1/13	12/31/13	0.00%
Conduct second targeted community workshop Year 3	1/1/14	6/2/14	0.00%
Conduct first targeted community workshop Year 4	7/1/14	12/31/14	0.00%
Conduct second targeted community workshop Year 4	1/1/15	6/30/15	0.00%
Conduct first targeted community workshop Year 5	7/1/15	12/31/15	0.00%
Conduct second targeted community workshop Year 5	1/1/16	6/30/16	0.00%
Milestone: Conduct 4 technical training, content-based and mentoring webinars in	7/1/11	6/30/16	0.00%
Conduct 4 webinars in support of XSEDE Scholars Program Year 1	7/1/11	6/29/12	100.00%
Conduct 4 webinars in support of XSEDE Scholars Program Year 2	7/2/12	6/28/13	0.00%
Conduct 4 webinars in support of XSEDE Scholars Program Year 3	7/2/13	6/30/14	0.00%
Conduct 4 webinars in support of XSEDE Scholars Program Year 4	7/1/14	6/30/15	0.00%
Conduct 4 webinars in support of XSEDE Scholars Program Year 5	7/1/15	6/30/16	0.00%
Portfolio Review	1/3/11	1/3/11	100.00%
Focus areas	1/3/11	12/30/11	0.00%
Support of new systems (Stampede, Gordon, Keeneland, Blue Waters)	1/3/11	7/4/11	0.00%
XSEDE architecture and tools	1/3/11	12/30/11	0.00%
Security	1/3/11	7/4/11	0.00%
Train the trainers	1/3/11	7/4/11	0.00%
Training for non-traditional areas	1/3/11	12/30/11	0.00%
Portal to API for gateways	7/2/12	6/28/13	0.00%
User Information Resources	1/3/11	6/30/16	0.00%
Milestone: Release Production User Portal & Web Site	4/1/11	7/1/11	0.00%
Transition existing production portal capabilities and web site	4/1/11	7/1/11	100.00%
Define user information architecture	4/1/11	6/23/11	100.00%



Name	Start	Finish	% Completed - XSEDE	2011	2012	2013	2014	2015	2016	2017
Milestone: Maintain Production User News System	4/1/11	7/1/11	0.00%							
Transition existing user news system to production	4/1/11	7/1/11	100.00%							
Milestone: Release Allocation & User Guide for New and Transitioning Users	4/1/11	10/11/11	0.00%							
Document instructions for new users coming to XSEDE	4/1/11	7/1/11	100.00%							
Document instructions for existing users	7/4/11	9/5/11	100.00%							
Document allocation policies for resources	9/6/11	10/11/11	100.00%							
Milestone: Release new user guide with user comment capabilities	4/1/11	7/1/11	0.00%							
Create user guide template for HPC, Viz, Storage, etc.	4/1/11	6/23/11	100.00%							
Create user guide examples for each resource type	4/1/11	6/23/11	100.00%							
Ensure all user guides have been transitioned to template	4/1/11	7/1/11	100.00%							
Publish all user guides across web presence	4/1/11	7/1/11	100.00%							
Milestone: Production mobile user portal	4/1/11	6/30/11	0.00%							
Transition existing mobile framework	4/1/11	4/28/11	100.00%							
Evaluate requirements for mobile features	4/29/11	6/22/11	50.00%							
Create schedule for releasing future mobile features	4/29/11	6/30/11	50.00%							
Milestone: Release updated user news	7/1/11	9/22/11	0.00%							
Define requirements for user news system	7/1/11	7/28/11	100.00%							
Evaluate existing and alternative technologies	7/29/11	8/11/11	100.00%							
Release new user news system (if appropriate)	8/12/11	9/22/11	100.00%							
Milestone: Create new social media presence for XD	10/3/11	9/26/13	0.00%							
Define requirements for social media	10/3/11	9/3/12	50.00%							
Evaluate requirements that come out of User Engagement	10/31/11	9/26/13	0.00%							
Create twitter and facebook presence for users of XD and specifically XUP	7/2/12	12/31/12	0.00%							
Display twitter feeds on user portal	7/2/12	12/31/12	0.00%							
Milestone: Release collaborative capabilities to user portal	7/2/12	12/31/12	0.00%							
Define requirements based on User Engagement feedback	7/2/12	12/31/12	0.00%							
Enable users to be able to share calendars, chat, files, etc. with	7/2/12	12/31/12	0.00%							
Milestone: Release integrated training system	1/2/12	3/23/12	0.00%							
Define requirements for integrated training system based on TEOS and	1/2/12	1/27/12	100.00%							
Enable sites to post training courses on user portal	1/30/12	3/23/12	100.00%							

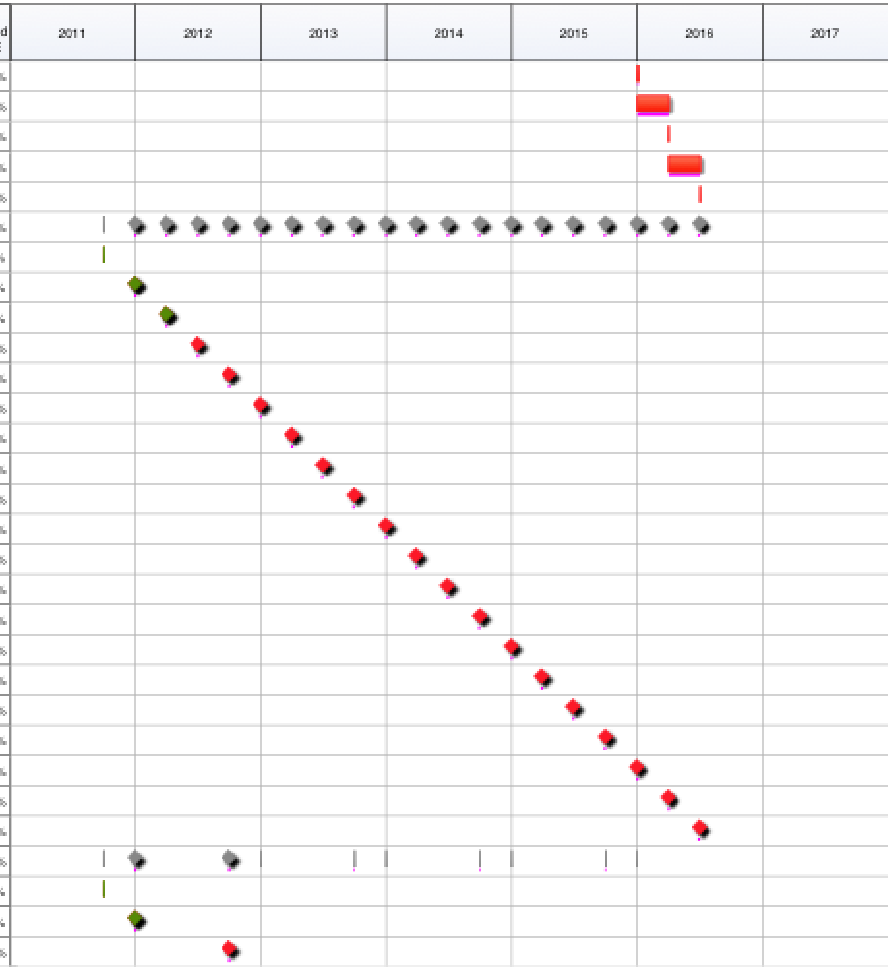
Name	Start	Finish	% Completed - XSEDE
Enable sites to add online training resources to user portal	1/30/12	3/23/12	100.00%
Enable users to register for training online via user portal	1/30/12	3/23/12	100.00%
Create one stop shop for user training on user portal with calendar, SMS	1/30/12	3/23/12	100.00%
Resource Selector	1/3/11	9/2/11	11.00%
Ongoing: Develop and implement improvements based on SEMP Spiral Design	1/3/11	6/30/16	0.00%
XSEDE User Portal	1/3/11	6/30/16	0.00%
Redesign dock at the top and apply theme	1/2/12	3/2/12	100.00%
Update profile portlet - expand with picture, publications,etc.	1/2/12	6/29/12	100.00%
Link checker for XUP & XSEDE web site	1/2/12	3/30/12	0.00%
Add forget username feature	1/2/12	4/30/12	100.00%
Integrate future grid status in XUP system monitor	1/2/12	6/29/12	0.00%
Expand system status beyond up/down/etc.	1/2/12	6/29/12	0.00%
Implement new News categories	1/2/12	3/30/12	100.00%
GridShib/InCommon integration	1/2/12	9/28/12	0.00%
Enable dynamic feedback on each page	1/2/12	3/30/12	100.00%
Migrate TGU staff queries to XUP staff area	1/2/12	3/30/12	75.00%
Compete guest homepage redesign	1/2/12	6/29/12	0.00%
Disable/gray out login link when resources are down	4/2/12	6/29/12	0.00%
Merge add/remove user page and allocation page	7/2/12	6/30/16	0.00%
Look at giving gateways a different 'view' for their community allocations	7/2/12	6/30/16	0.00%
Merge DN listing with user profile	7/2/12	6/30/16	0.00%
Integrate new ticketing system	7/2/12	12/31/12	0.00%
Chat for help	7/2/12	6/30/16	0.00%
Make hot links/bookmarking feature	7/2/12	6/30/16	0.00%
Screen sharing with support staff	7/2/12	6/30/16	0.00%
Expand allocations/usage/job history with graphs	7/2/12	6/30/16	100.00%
Integrate XDMoD services	7/2/12	6/30/16	9.00%
Custom views for communities: campus champions, gateways, fields	1/3/11	1/1/15	8.00%
Network connectivity monitor	7/2/12	6/30/16	0.00%
Dynamic visualization information in system monitor	7/2/12	6/30/16	0.00%



Name	Start	Finish	% Completed - XSEDE	2011	2012	2013	2014	2015	2016	2017
Remote visualization services	7/2/12	6/30/16	0.00%							
RSS feeds and SMS notifications for user portal functions	7/2/12	6/30/16	50.00%							
OSG documentation integration	7/2/12	6/30/16	100.00%							
Videos & interactive guide on features of XUP	7/2/12	6/30/16	0.00%							
Online training for XUP	7/2/12	6/30/16	0.00%							
Online survey for users on features	7/2/12	6/30/16	0.00%							
Workflow management interface	7/2/12	6/30/16	0.00%							
Metascheduling, job reservations, and ensemble job submission	7/2/12	6/30/16	0.00%							
Change community account form to enter information in XCDB and	7/2/12	6/30/16	10.00%							
Ongoing: Prioritize and integrate SD&I configuration items in US UII	1/3/11	12/31/15	20.00%							
User Engagement	4/1/11	7/1/16	0.00%							
Annual User Surveys	1/2/12	6/30/16	0.00%							
Develop and Implement Y1 Annual User Survey	1/2/12	3/30/12	100.00%							
Milestone: Y1 Annual User Survey report	7/2/12	7/2/12	0.00%							
Develop and Implement Y2 Annual User Survey	1/1/13	4/1/13	0.00%							
Milestone: Y2 Annual User Survey report	7/1/13	7/1/13	0.00%							
Develop and Implement Y3 Annual User Survey	1/1/14	3/31/14	0.00%							
Milestone: Y3 Annual User Survey report	6/30/14	6/30/14	0.00%							
Develop and Implement Y4 Annual User Survey	1/1/15	3/31/15	0.00%							
Milestone: Y4 Annual User Survey report	6/30/15	6/30/15	0.00%							
Develop and Implement Y5 Annual User Survey	1/1/16	3/31/16	0.00%							
Milestone: Y5 Annual User Survey report	6/30/16	6/30/16	0.00%							
XSEDE CRM	1/2/12	7/2/12	0.00%							
Document current XSEDE activities athat act as CRM	1/2/12	1/2/12	0.00%							
Design and Implemnt initial CRM system	1/2/12	6/29/12	0.00%							
Milestone: Initial CRM system deployed	7/2/12	7/2/12	0.00%							
Data Mining	10/3/11	7/1/16	0.00%							
Q1Y1 Data mining operations	10/3/11	12/30/11	100.00%							
Milestone: Q1Y1 Data mining report	12/30/11	12/30/11	100.00%							
Q2Y1 Data mining operations	1/2/12	3/30/12	100.00%							

Name	Start	Finish	% Completed - XSEDE	2011	2012	2013	2014	2015	2016	2017
Milestone: Q2Y1 Data mining report	4/2/12	4/2/12	100.00%							
Q3Y1 Data mining operations	4/3/12	7/2/12	100.00%							
Milestone: Q3Y1 Data mining report	7/2/12	7/2/12	0.00%							
Q4Y1 Data mining operations	7/3/12	10/1/12	0.00%							
Milestone: Q4Y1 Data mining report	10/2/12	10/2/12	0.00%							
Q1Y2 Data mining operations	10/2/12	12/31/12	0.00%							
Milestone: Q1Y2 Data mining report	1/1/13	1/1/13	0.00%							
Q2Y2 Data mining operations	1/2/13	4/2/13	0.00%							
Milestone: Q2Y2 Data mining report	4/2/13	4/2/13	0.00%							
Q3Y2 Data mining operations	4/1/13	6/28/13	0.00%							
Milestone: Q3Y2 Data mining report	7/1/13	7/1/13	0.00%							
Q4Y2 Data mining operations	7/1/13	9/30/13	0.00%							
Milestone: Q4Y2 Data mining report	10/1/13	10/1/13	0.00%							
Q1Y3 Data mining operations	10/1/13	12/31/13	0.00%							
Milestone: Q1Y3 Data mining report	1/1/14	1/1/14	0.00%							
Q2Y3 Data mining operations	1/1/14	3/31/14	0.00%							
Milestone: Q2Y3 Data mining report	4/1/14	4/1/14	0.00%							
Q3Y3 Data mining operations	4/1/14	6/30/14	0.00%							
Milestone: Q3Y3 Data mining report	7/1/14	7/1/14	0.00%							
Q4Y3 Data mining operations	7/1/14	9/30/14	0.00%							
Milestone: Q4Y3 Data mining report	10/1/14	10/1/14	0.00%							
Q1Y4 Data mining operations	10/1/14	12/31/14	0.00%							
Milestone: Q1Y4 Data mining report	1/1/15	1/1/15	0.00%							
Q2Y4 Data mining operations	1/1/15	3/31/15	0.00%							
Milestone: Q2Y4 Data mining report	4/1/15	4/1/15	0.00%							
Q3Y4 Data mining operations	4/1/15	6/30/15	0.00%							
Milestone: Q3Y4 Data mining report	7/1/15	7/1/15	0.00%							
Q4Y4 Data mining operations	7/1/15	9/30/15	0.00%							
Milestone: Q4Y4 Data mining report	10/1/15	10/1/15	0.00%							
Q1Y5 Data mining operations	10/1/15	12/31/15	0.00%							

Name	Start	Finish	% Completed - XSEDE
Milestone: Q1Y5 Data mining report	1/1/16	1/1/16	0.00%
Q2Y5 Data mining operations	1/1/16	3/31/16	0.00%
Milestone: Q2Y5 Data mining report	4/1/16	4/1/16	0.00%
Q3Y5 Data mining operations	4/1/16	6/30/16	0.00%
Milestone: Q3Y5 Data mining report	7/1/16	7/1/16	0.00%
Develop Focus Group Topics and conduct focus groups	9/30/11	6/30/16	0.00%
Milestone: Q1Y1 Focus Group Report	9/30/11	9/30/11	100.00%
Milestone: Q2Y1 Focus Group Report	1/2/12	1/2/12	100.00%
Milestone: Q3Y1 Focus Group Report	4/2/12	4/2/12	100.00%
Milestone: Q4Y1 Focus Group Report	7/2/12	7/2/12	0.00%
Milestone: Q1Y2 Focus Group Report	10/1/12	10/1/12	0.00%
Milestone: Q2Y2 Focus Group Report	12/31/12	12/31/12	0.00%
Milestone: Q3Y2 Focus Group Report	4/1/13	4/1/13	0.00%
Milestone: Q4Y2 Focus Group Report	7/1/13	7/1/13	0.00%
Milestone: Q1Y3 Focus Group Report	9/30/13	9/30/13	0.00%
Milestone: Q2Y3 Focus Group Report	12/31/13	12/31/13	0.00%
Milestone: Q3Y3 Focus Group Report	3/31/14	3/31/14	0.00%
Milestone: Q4Y3 Focus Group Report	6/30/14	6/30/14	0.00%
Milestone: Q1Y4 Focus Group Report	9/30/14	9/30/14	0.00%
Milestone: Q2Y4 Focus Group Report	12/31/14	12/31/14	0.00%
Milestone: Q3Y4 Focus Group Report	3/31/15	3/31/15	0.00%
Milestone: Q4Y4 Focus Group Report	6/30/15	6/30/15	0.00%
Milestone: Q1Y5 Focus Group Report	9/30/15	9/30/15	0.00%
Milestone: Q2Y5 Focus Group Report	12/31/15	12/31/15	0.00%
Milestone: Q3Y5 Focus Group Report	3/31/16	3/31/16	0.00%
Milestone: Q4Y5 Focus Group Report	6/30/16	6/30/16	0.00%
Develop and Conduct BoF Sessions	9/30/11	12/31/15	0.00%
Milestone: Conduct Y1 XSEDE BoF and Report	9/30/11	9/30/11	100.00%
Milestone: Conduct Y1 SC BoF and Report	12/31/11	1/2/12	100.00%
Milestone: Conduct Y2 XSEDE BoF and Report	9/30/12	10/1/12	0.00%



Name	Start	Finish	% Completed - XSEDE
Milestone: Conduct Y2 SC BoF and Report	12/31/12	12/31/12	0.00%
Milestone: Conduct Y3 XSEDE BoF and Report	9/30/13	9/30/13	0.00%
Milestone: Conduct Y3 SC BoF and Report	12/31/13	12/31/13	0.00%
Milestone: Conduct Y4 XSEDE BoF and Report	9/30/14	9/30/14	0.00%
Milestone: Conduct Y4 SC BoF and Report	12/31/14	12/31/14	0.00%
Milestone: Conduct Y5 XSEDE BoF and Report	9/30/15	9/30/15	0.00%
Milestone: Conduct Y5 SC BoF and Report	12/31/15	12/31/15	0.00%
Conduct Usability Panels and Testing (as needed)	4/1/11	3/31/16	20.00%
User Engagement General Operations	7/1/11	6/30/16	0.00%
Monitor tickets	7/1/11	6/30/16	20.00%
Resolve XSEDE wide tickets	7/1/11	6/30/16	20.00%
Bi-weekly User Engagement status meetings	7/1/11	6/30/16	20.00%
Quarterly reporting	7/1/11	6/30/16	20.00%
XSEDE Ticket System	4/1/11	6/29/12	0.00%
Transition existing TG ticket system to production in XSEDE	4/1/11	7/7/11	100.00%
Milestone: Release Production Ticketing System	7/7/11	7/8/11	100.00%
Deploy new/improved XSEDE Ticket System	7/1/11	6/29/12	0.00%
Define requirements for ticket system	7/1/11	8/12/11	100.00%
Evaluate candidate ticket systems	8/15/11	9/30/11	100.00%
Milestone: Select new/improved ticket system	10/1/11	10/3/11	100.00%
Develop and deploy new/improved ticket system	10/3/11	3/30/12	0.00%
Milestone: Release new/improved ticket system	3/31/12	4/2/12	0.00%
Integrate new/improved ticket system with CRM	4/2/12	6/29/12	0.00%
Milestone: Release Integrated CRM interface	6/29/12	6/29/12	0.00%
Integrate new/improved ticket system with XSEDE User Portal	4/2/12	6/29/12	0.00%
Milestone: Release Integrated XUP interface	6/29/12	6/29/12	0.00%
Consulting Policies	10/3/11	7/2/12	0.00%
Create consulting policies, procedures, and support guide	10/3/11	6/29/12	50.00%
Milestone: Deploy consulting policies, procedures, and support guide	7/2/12	7/2/12	0.00%
Contact PI at allocation start	7/15/11	4/15/16	0.00%

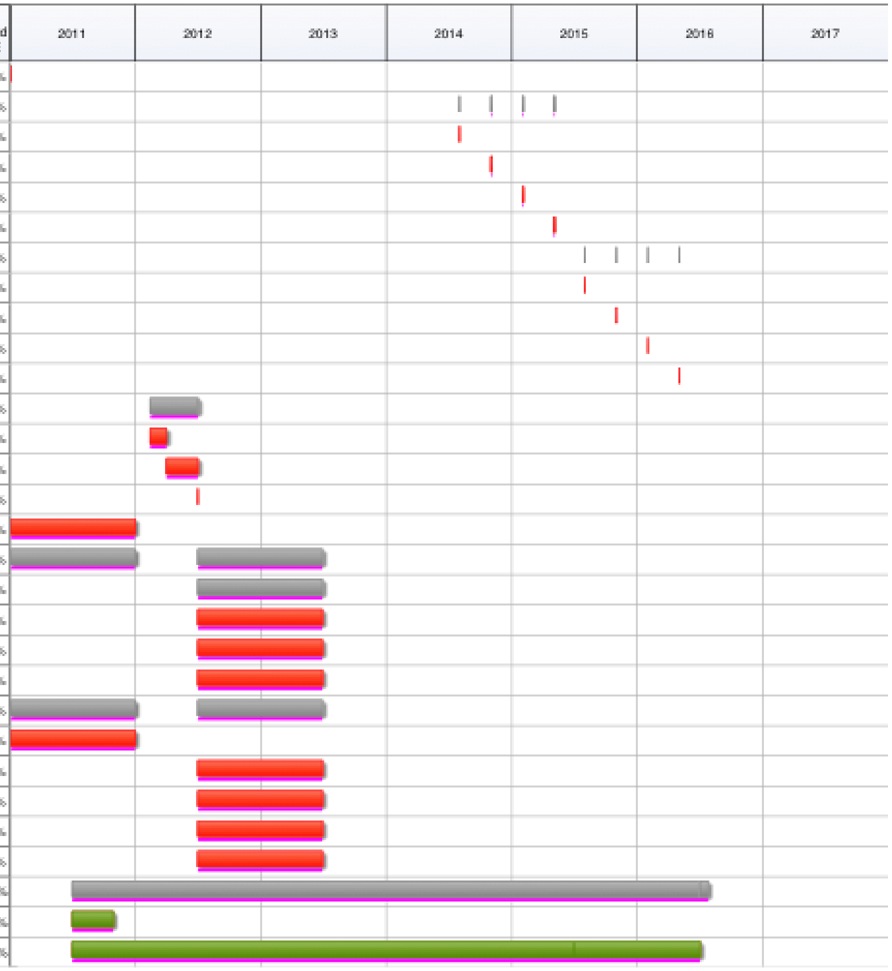
Name	Start	Finish	% Completed - XSEDE	2011	2012	2013	2014	2015	2016	2017
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	7/15/11	4/15/16	100.00%							
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	7/15/11	7/18/11	100.00%							
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	10/17/11	10/18/11	100.00%							
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	1/16/12	1/17/12	100.00%							
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	4/16/12	4/17/12	100.00%							
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	7/16/12	7/16/12	100.00%							
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	10/15/12	10/15/12	0.00%							
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	1/15/13	1/15/13	0.00%							
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	4/15/13	4/15/13	0.00%							
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	7/15/13	7/15/13	0.00%							
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	10/15/13	10/15/13	0.00%							
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	1/15/14	1/15/14	0.00%							
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	4/15/14	4/15/14	0.00%							
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	7/15/14	7/15/14	0.00%							
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	10/15/14	10/15/14	0.00%							
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	1/15/15	1/15/15	0.00%							
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	4/15/15	4/15/15	0.00%							
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	7/15/15	7/15/15	0.00%							
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	10/15/15	10/15/15	0.00%							
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	1/15/16	1/15/16	0.00%							
Contact "new"/"renewal" PIs at the beginning of each XRAC allocation	4/15/16	4/15/16	0.00%							
⊟ Contact "startup" PIs each month	7/15/11	6/15/16	0.00%							
1	7/15/11	7/18/11	100.00%							
2	8/15/11	8/16/11	100.00%							
3	9/15/11	9/16/11	100.00%							
4	10/17/11	10/18/11	100.00%							
5	11/15/11	11/16/11	100.00%							
6	12/15/11	12/16/11	100.00%							
7	1/16/12	1/17/12	100.00%							
8	2/15/12	2/16/12	100.00%							

Name	Start	Finish	% Completed - XSEDE	2011	2012	2013	2014	2015	2016	2017
9	3/15/12	3/16/12	100.00%							
10	4/16/12	4/17/12	100.00%							
11	5/15/12	5/16/12	100.00%							
12	6/15/12	6/15/12	100.00%							
13	7/16/12	7/16/12	100.00%							
14	8/15/12	8/15/12	100.00%							
15	9/17/12	9/17/12	100.00%							
16	10/15/12	10/15/12	0.00%							
17	11/15/12	11/15/12	0.00%							
18	12/17/12	12/17/12	0.00%							
19	1/15/13	1/15/13	0.00%							
20	2/15/13	2/15/13	0.00%							
21	3/15/13	3/15/13	0.00%							
22	4/15/13	4/15/13	0.00%							
23	5/15/13	5/15/13	0.00%							
24	6/17/13	6/17/13	0.00%							
25	7/15/13	7/15/13	0.00%							
26	8/15/13	8/15/13	0.00%							
27	9/16/13	9/16/13	0.00%							
28	10/15/13	10/15/13	0.00%							
29	11/15/13	11/15/13	0.00%							
30	12/16/13	12/16/13	0.00%							
31	1/15/14	1/15/14	0.00%							
32	2/17/14	2/17/14	0.00%							
33	3/17/14	3/17/14	0.00%							
34	4/15/14	4/15/14	0.00%							
35	5/15/14	5/15/14	0.00%							
36	6/16/14	6/16/14	0.00%							
37	7/15/14	7/15/14	0.00%							
38	8/15/14	8/15/14	0.00%							

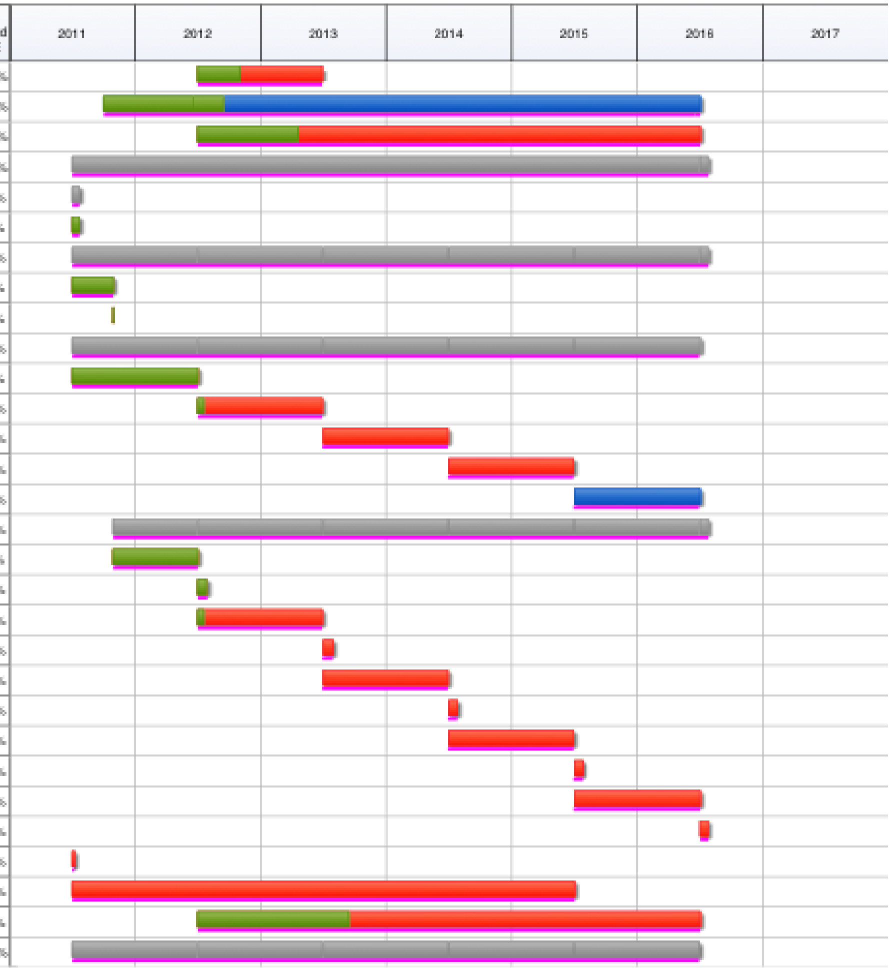
Name	Start	Finish	% Completed - XSEDE	2011	2012	2013	2014	2015	2016	2017
39	9/15/14	9/15/14	0.00%							
40	10/15/14	10/15/14	0.00%							
41	11/17/14	11/17/14	0.00%							
42	12/15/14	12/15/14	0.00%							
43	1/15/15	1/15/15	0.00%							
44	2/16/15	2/16/15	0.00%							
45	3/16/15	3/16/15	0.00%							
46	4/15/15	4/15/15	0.00%							
47	5/15/15	5/15/15	0.00%							
48	6/15/15	6/15/15	0.00%							
49	7/15/15	7/15/15	0.00%							
50	8/17/15	8/17/15	0.00%							
51	9/15/15	9/15/15	0.00%							
52	10/15/15	10/15/15	0.00%							
53	11/16/15	11/16/15	0.00%							
54	12/15/15	12/15/15	0.00%							
55	1/15/16	1/15/16	0.00%							
56	2/15/16	2/15/16	0.00%							
57	3/15/16	3/15/16	0.00%							
58	4/15/16	4/15/16	0.00%							
59	5/16/16	5/16/16	0.00%							
60	6/15/16	6/15/16	0.00%							
Allocations	1/3/11	5/2/16	0.00%							
Allocations policy in place	4/1/11	7/1/11	100.00%							
Host Quarterly Allocations Meetings Annually	9/1/11	6/1/15	0.00%							
Host Year 1 Quarterly Allocations Meetings	9/1/11	6/1/12	0.00%							
Host Quarterly Allocations Meeting	9/1/11	9/2/11	100.00%							
Host Quarterly Allocations Meeting	12/1/11	12/2/11	100.00%							
Host Quarterly Allocations Meeting	3/1/12	3/2/12	100.00%							
Host Quarterly Allocations Meeting	6/1/12	6/1/12	100.00%							

Name	Start	Finish	% Completed - XSEDE	2011	2012	2013	2014	2015	2016	2017
Host Year 2 Quarterly Allocations Meetings	9/3/12	6/3/13	0.00%							
Host Quarterly Allocations Meeting	9/3/12	9/3/12	100.00%							
Host Quarterly Allocations Meeting	12/3/12	12/3/12	0.00%							
Host Quarterly Allocations Meeting	3/4/13	3/4/13	0.00%							
Host Quarterly Allocations Meeting	6/3/13	6/3/13	0.00%							
Host Year 3 Quarterly Allocations Meetings	9/2/13	6/2/14	0.00%							
Host Quarterly Allocations Meeting	9/2/13	9/2/13	0.00%							
Host Quarterly Allocations Meeting	12/2/13	12/2/13	0.00%							
Host Quarterly Allocations Meeting	3/3/14	3/3/14	0.00%							
Host Quarterly Allocations Meeting	6/2/14	6/2/14	0.00%							
Host Year 4 Quarterly Allocations Meetings	9/1/14	6/1/15	0.00%							
Host Quarterly Allocations Meeting	9/1/14	9/1/14	0.00%							
Host Quarterly Allocations Meeting	12/1/14	12/1/14	0.00%							
Host Quarterly Allocations Meeting	3/2/15	3/2/15	0.00%							
Host Quarterly Allocations Meeting	6/1/15	6/1/15	0.00%							
Conduct How to Write a Successful Proposal Webcasts Annually	1/3/11	5/2/16	0.00%							
Conduct Year 1 How to Write a Successful Proposal Webcast	8/1/11	6/1/12	0.00%							
Conduct How to Write a Successful Proposal Webcast	8/1/11	9/1/11	100.00%							
Conduct How to Write a Successful Proposal Webcast	11/1/11	12/1/11	100.00%							
Conduct How to Write a Successful Proposal Webcast	2/1/12	3/1/12	100.00%							
Conduct How to Write a Successful Proposal Webcast	5/1/12	6/1/12	100.00%							
Conduct Year 2 How to Write a Successful Proposal Webcast	8/1/12	5/1/13	0.00%							
Conduct How to Write a Successful Proposal Webcast	8/1/12	8/1/12	100.00%							
Conduct How to Write a Successful Proposal Webcast	11/1/12	11/1/12	0.00%							
Conduct How to Write a Successful Proposal Webcast	2/1/13	2/1/13	0.00%							
Conduct How to Write a Successful Proposal Webcast	5/1/13	5/1/13	0.00%							
Conduct Year 3 How to Write a Successful Proposal Webcast	1/3/11	2/3/14	0.00%							
Conduct How to Write a Successful Proposal Webcast	8/1/13	8/1/13	0.00%							
Conduct How to Write a Successful Proposal Webcast	11/1/13	11/1/13	0.00%							
Conduct How to Write a Successful Proposal Webcast	2/3/14	2/3/14	0.00%							

Name	Start	Finish	% Completed - XSEDE
Conduct How to Write a Successful Proposal Webcast	1/3/11	1/3/11	0.00%
Conduct Year 4 How to Write a Successful Proposal Webcast	8/1/14	5/4/15	0.00%
Conduct How to Write a Successful Proposal Webcast	8/1/14	8/1/14	0.00%
Conduct How to Write a Successful Proposal Webcast	11/3/14	11/3/14	0.00%
Conduct How to Write a Successful Proposal Webcast	2/2/15	2/2/15	0.00%
Conduct How to Write a Successful Proposal Webcast	5/4/15	5/4/15	0.00%
Conduct Year 5 How to Write a Successful Proposal Webcast	8/3/15	5/2/16	0.00%
Conduct How to Write a Successful Proposal Webcast	8/3/15	8/3/15	0.00%
Conduct How to Write a Successful Proposal Webcast	11/2/15	11/2/15	0.00%
Conduct How to Write a Successful Proposal Webcast	2/1/16	2/1/16	0.00%
Conduct How to Write a Successful Proposal Webcast	5/2/16	5/2/16	0.00%
New POPS Interface	2/13/12	7/2/12	0.00%
Design new interface	2/13/12	4/2/12	0.00%
Implement and test	4/2/12	6/29/12	0.00%
Deploy	7/2/12	7/2/12	0.00%
Add Tier 2 resources to allocation process	1/3/11	12/30/11	0.00%
Implement Allocation Levels and Types	1/3/11	6/28/13	0.00%
Levels	7/2/12	6/28/13	0.00%
Small	7/2/12	6/28/13	0.00%
Standard	7/2/12	6/28/13	0.00%
XRAC	7/2/12	6/28/13	0.00%
Types	1/3/11	6/28/13	0.00%
Storage	1/3/11	12/30/11	0.00%
Visualization	7/2/12	6/28/13	0.00%
Throughput	7/2/12	6/28/13	0.00%
Advanced Support for Research Teams (ECSS)	7/2/12	6/28/13	0.00%
GPU, MIC, other non-heterogeneous x86 compute	7/2/12	6/28/13	0.00%
Extended Collaborative Support Service (ECSS)-Projects	7/1/11	7/22/16	0.00%
Create/ test proj. mgmt. framework for ECSS work plans/reporting	7/1/11	10/28/11	100.00%
Add at least 1 external FTE to fill an identified skills gap	7/1/11	6/30/16	100.00%

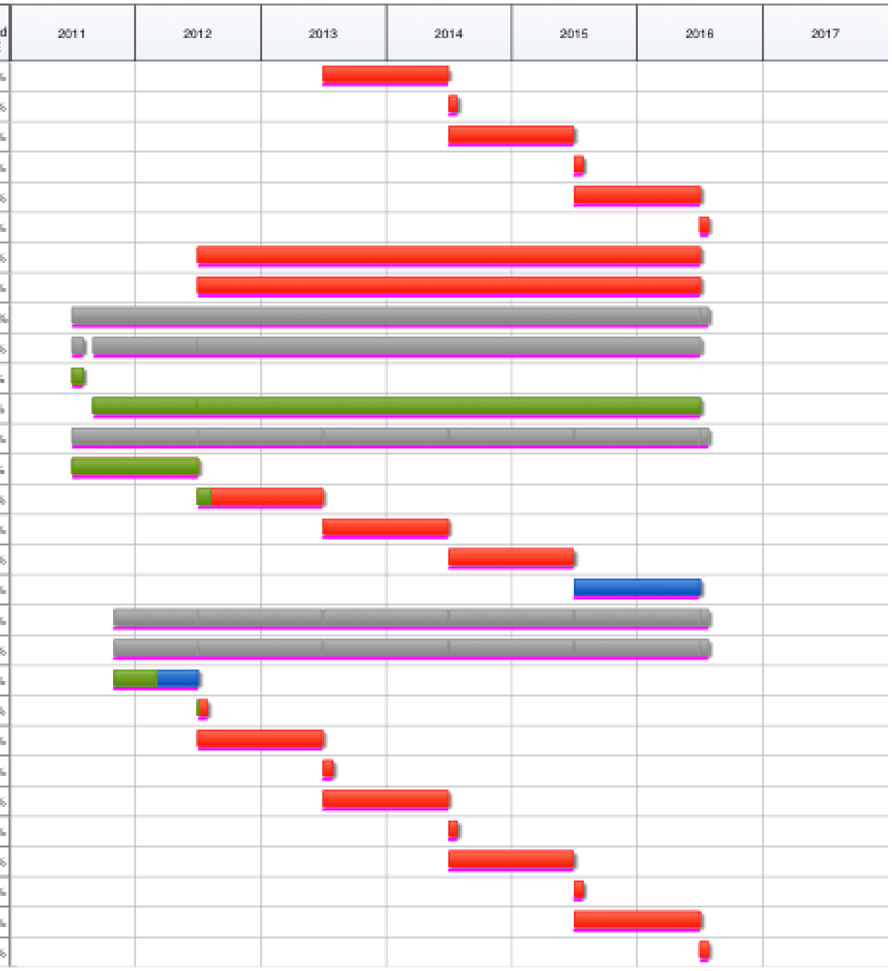


Name	Start	Finish	% Completed - XSEDE
Fill 1.5 Discretionary Hires (as needed)	7/2/12	6/28/13	33.33%
Host monthly symposium open to ECSS, XSEDE staff, and Users	10/3/11	6/30/16	20.00%
Conduct continuing training of ECSS Staff as needed	7/2/12	6/30/16	20.00%
Extended Support for Research Team (ESRT)	7/1/11	7/22/16	0.00%
Establish ESRT group	7/1/11	7/21/11	0.00%
Set up ESRT staff and management teams and communications	7/1/11	7/21/11	100.00%
Milestone: Support 20 ESRT Projects Annually	7/1/11	7/22/16	0.00%
Work w/TG AUS to transition ASTA Projs. To ESRT mgmt.	7/1/11	10/28/11	100.00%
Milestone: All TG ASTA proj. managed as XD ESRT Projs.	10/28/11	10/28/11	100.00%
Work with XD CMS to Generate 20 new XD ESRT projs. Annually	7/1/11	6/30/16	0.00%
Year 1 Generate 20 new XD ESRT projects	7/1/11	6/29/12	100.00%
Year 2 Generate 20 new XD ESRT projects	7/2/12	6/28/13	5.00%
Year 3 Generate 20 new XD ESRT projects	7/1/13	6/30/14	0.00%
Year 4 Generate 20 new XD ESRT projects	7/1/14	6/30/15	0.00%
Year 5 Generate 20 new XD ESRT projects	7/1/15	6/30/16	0.00%
20 ESRT work plans documented and actively managed annually	10/31/11	7/22/16	0.00%
Year 1 - 20 work plans documented	10/31/11	6/29/12	100.00%
milestone: Y1 prepare and complete Final Reports	7/2/12	7/27/12	80.00%
Year 2 - 20 work plans documented	7/2/12	6/28/13	5.00%
milestone: Y2 prepare and complete Final Reports	7/1/13	7/26/13	0.00%
Year 3 - 20 work plans documented	7/1/13	6/30/14	0.00%
milestone: Y3 prepare and complete Final Reports	7/1/14	7/25/14	0.00%
Year 4 - 20 work plans documented	7/1/14	6/30/15	0.00%
milestone: Y4 prepare and complete Final Reports	7/1/15	7/24/15	0.00%
Year 5 - 20 work plans documented	7/1/15	6/30/16	0.00%
milestone: Y5 prepare and complete Final Reports	7/1/16	7/22/16	0.00%
Organize and execute HPC workshop at IEEE E-Science conference	7/1/11	7/7/11	0.00%
Host Annual Workshop on Petascale Computing	7/1/11	7/1/15	0.00%
Conduct XRAC Meetings Adaptive Reviews	7/2/12	6/30/16	30.00%
Novel & Innovative Projects	7/1/11	6/29/16	0.00%

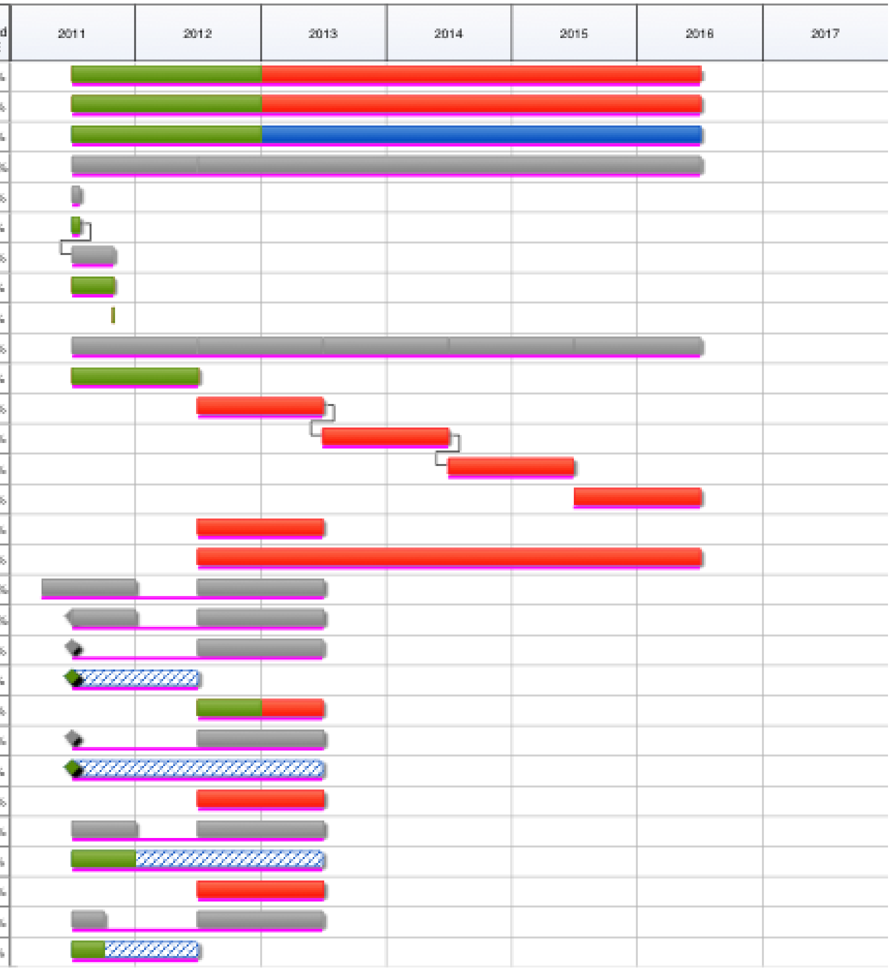


Name	Start	Finish	% Completed - XSEDE	2011	2012	2013	2014	2015	2016	2017
Establish NIP group	7/1/11	9/30/11	0.00%							
Set up NIP staff and management teams and communications	7/1/11	9/30/11	100.00%							
Milestone: Generate 20 new XSEDE+ ECS NIPs Annually	7/1/11	6/29/16	0.00%							
Year 1-work w/XD CMS,TEOS,TIS to generate 20 XD NIP projects	7/1/11	6/29/12	100.00%							
Year 2-work w/XD CMS,TEOS,TIS to generate 20 XD NIP projects	7/2/12	6/28/13	0.00%							
Year 3-work w/XD CMS,TEOS,TIS to generate 20 XD NIP projects	7/1/13	6/30/14	0.00%							
Year 4-work w/XD CMS,TEOS,TIS to generate 20 XD NIP projects	7/1/14	6/30/15	0.00%							
Year 5-work w/XD CMS,TEOS,TIS to generate 20 XD NIP projects	7/1/15	6/29/16	0.00%							
Milestone: Create ECSS Project work plans	7/1/11	12/30/11	0.00%							
Extended Collaborative Support Service - Communities	7/1/11	7/22/16	0.00%							
Create/ test proj. mgmt. framework for ESCC work plans/reporting	7/1/11	10/28/11	100.00%							
Add at least 1 external FTE to fill an identified skills gap	7/1/11	6/30/16	25.00%							
Host monthly symposium for ECSS and XSEDE staff	10/3/11	6/30/16	20.00%							
Conduct Continuing Training of ECSS Staff as needed	7/2/12	6/30/16	10.00%							
Extended Support for Community Codes (ESCC)	7/1/11	7/22/16	0.00%							
Establish ESCC group	7/1/11	7/21/11	0.00%							
Set up ESCC staff and management teams and communications	7/1/11	7/21/11	100.00%							
Transition TG ASP proj. to ESCC management	7/1/11	10/28/11	100.00%							
Milestone:Active TG ASP proj. managed as XD ESCC proj.	10/28/11	10/28/11	100.00%							
Milestone: Support 10 ESCC Projects Annually	7/1/11	7/22/16	0.00%							
Year 1-Work w/TG CMS,TEOS,TIS to generate 10 XD ESCC proj.	7/1/11	6/29/12	100.00%							
Year 2-Work w/TG CMS,TEOS,TIS to generate 10 XD ESCC proj.	7/2/12	6/28/13	10.00%							
Year 3-Work w/TG CMS,TEOS,TIS to generate 10 XD ESCC proj.	7/1/13	6/30/14	0.00%							
Year 4-Work w/TG CMS,TEOS,TIS to generate 10 XD ESCC proj.	7/1/14	6/30/15	0.00%							
Year 5-Work w/TG CMS,TEOS,TIS to generate 10 XD ESCC proj.	7/1/15	6/30/16	0.00%							
Milestone: Create 10 ESCC work plans Annually	10/31/11	7/22/16	0.00%							
Y1 - 10 work plans documented	10/31/11	6/29/12	100.00%							
milestone: Y1 prepare and complete Final Reports	7/2/12	7/27/12	10.00%							
Y2 - 10 work plans documented	7/2/12	6/28/13	10.00%							
milestone: Y2 prepare and complete Final Reports	7/1/13	7/26/13	0.00%							

Name	Start	Finish	% Completed - XSEDE
Y3 - 10 work plans documented	7/1/13	6/30/14	0.00%
milestone: Y3 prepare and complete Final Reports	7/1/14	7/25/14	0.00%
Y4 - 10 work plans documented	7/1/14	6/30/15	0.00%
milestone: Y4 prepare and complete Final Reports	7/1/15	7/24/15	0.00%
Y5 - 10 work plans documented	7/1/15	6/30/16	0.00%
milestone: Y5 prepare and complete Final Reports	7/1/16	7/22/16	0.00%
Work with the TIS group to evaluate and recommend SI2 software projects for	7/2/12	6/30/16	0.00%
Develop documentation, sample scripts, optimized builds to cover the top community	7/2/12	6/30/16	0.00%
Extended Collaborative Support Service - Science Gateways	7/1/11	7/22/16	0.00%
Establish ESSGW group	7/1/11	6/30/16	0.00%
Set up ESSGW staff and management teams and communications	7/1/11	7/29/11	100.00%
Organize bi-weekly gateway community calls open to all XSEDE users	9/1/11	6/30/16	100.00%
Milestone: Support 10 Science Gateways Annually	7/1/11	7/22/16	0.00%
Year 1-Work w/TG CMS,TEOS,TIS to generate 10 XD ESSGW proj.	7/1/11	6/29/12	100.00%
Year 2-Work w/TG CMS,TEOS,TIS to generate 10 XD ESSGW proj.	7/2/12	6/28/13	10.00%
Year 3-Work w/TG CMS,TEOS,TIS to generate 10 XD ESSGW proj.	7/1/13	6/30/14	0.00%
Year 4-Work w/TG CMS,TEOS,TIS to generate 10 XD ESSGW proj.	7/1/14	6/30/15	0.00%
Year 5-Work w/TG CMS,TEOS,TIS to generate 10 XD ESSGW proj.	7/1/15	6/30/16	0.00%
Milestone: Create ESSGW work plans	10/31/11	7/22/16	0.00%
At least 10 ESSGW work plans documented&actively managed	10/31/11	7/22/16	0.00%
Y1 - 10 work plans documented	10/31/11	6/29/12	50.00%
milestone: Y1 prepare and complete Final Reports	7/2/12	7/27/12	10.00%
Y2 - 10 work plans documented	7/2/12	6/28/13	0.00%
milestone: Y2 prepare and complete Final Reports	7/1/13	7/26/13	0.00%
Y3 - 10 work plans documented	7/1/13	6/30/14	0.00%
milestone: Y3 prepare and complete Final Reports	7/1/14	7/25/14	0.00%
Y4 - 10 work plans documented	7/1/14	6/30/15	0.00%
milestone: Y4 prepare and complete Final Reports	7/1/15	7/24/15	0.00%
Y5 - 10 work plans documented	7/1/15	6/30/16	0.00%
milestone: Y5 prepare and complete Final Reports	7/1/16	7/22/16	0.00%



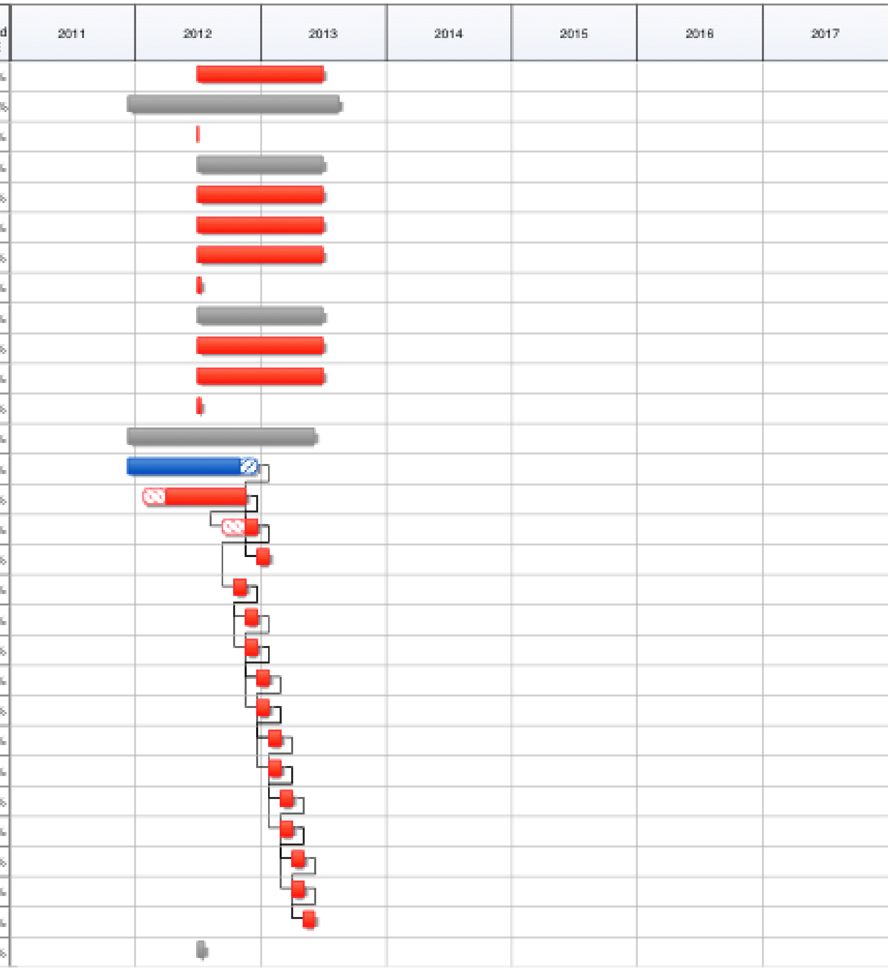
Name	Start	Finish	% Completed - XSEDE
Gateway Outreach: Constantly reach out to new potential gateways independently and	7/1/11	6/30/16	30.00%
XSEDE Requirements: Work with Gateway community in analyzing the XSEDE	7/1/11	6/30/16	30.00%
XSEDE Architecture Test Cases: Provide Test Cases to SD&I teams in nature of tests	7/1/11	6/30/16	30.00%
Extended Support for Training Education and Outreach (ESTEO)	7/1/11	6/30/16	0.00%
Establish ESTEO group	7/1/11	7/21/11	0.00%
Set up ESTEO staff and management teams and communications	7/1/11	7/21/11	100.00%
Milestone: Contribute content for TEO modules	7/1/11	10/28/11	0.00%
Work w/TG AUS to transition ASEOT projs. to XD ESTEO mgmt.	7/1/11	10/28/11	100.00%
Milestone: All TG ASEOT projs. Managed as XD ESTEO projs.	10/28/11	10/28/11	100.00%
Milestone: 50 ESTEO projects/activities supported Annually	7/1/11	6/30/16	0.00%
Year 1-work w/XD CMS, TEOS, TIS to generate 50 XD ESTEO	7/1/11	6/29/12	100.00%
Year 2- work w/XD CMS, TEOS, TIS to generate 50 XD ESTEO	7/2/12	6/28/13	0.00%
Year 3 - work w/XD CMS, TEOS, TIS to generate 50 XD ESTEO	7/1/13	6/30/14	0.00%
Year 4 - work w/XD CMS, TEOS, TIS to generate 50 XD ESTEO	7/1/14	6/30/15	0.00%
Year 5 - work w/XD CMS, TEOS, TIS to generate 50 XD ESTEO	7/1/15	6/30/16	0.00%
Test and Document initial work assignments for UCB CS class using XSEDE resouces	7/2/12	6/28/13	0.00%
Arrange ECSS Internal Training Seminars Annually	7/2/12	6/30/16	0.00%
Education and Outreach	4/4/11	7/1/13	0.00%
Education	7/1/11	7/1/13	0.00%
Milestone: 2 HPC Graduate level summer schools annually	7/1/11	6/28/13	0.00%
Milestone: 2 HPC Graduate level summer schools annually	7/1/11	7/1/11	100.00%
Milestone: 2 HPC Graduate level summer schools annually	7/2/12	6/28/13	50.00%
Milestone: 5 summer workshops annually	7/1/11	7/1/13	0.00%
Milestone: 5 summer workshops annually	7/1/11	7/1/11	100.00%
Milestone: 5 summer workshops annually	7/2/12	7/1/13	0.00%
Milestone: Add certificate programs at specific universities	7/1/11	7/1/13	0.00%
Milestone: ID univ to work with to dev vert pgm	7/1/11	12/30/11	100.00%
Milestone:Add cert and/or deg pgm @ univ and cont to ID univs for cert pgm	7/2/12	7/1/13	0.00%
Milestone: Provide online educational services	7/1/11	6/28/13	0.00%
Milestone: Provide online educational services	7/1/11	9/30/11	100.00%



Name	Start	Finish	% Completed - XSEDE	2011	2012	2013	2014	2015	2016	2017
Milestone: Provide online educational services	7/2/12	6/28/13	25.00%							
Outreach	6/1/11	7/1/13	0.00%							
Underrepresented Engagement	7/1/11	7/1/13	0.00%							
Milestone: 10 campus visits (SURA)	7/1/11	6/28/13	0.00%							
Milestone: 10 campus visits (SURA)	7/1/11	9/30/11	100.00%							
Milestone: 10 campus visits (SURA)	7/2/12	6/28/13	25.00%							
Milestone: Engage 40 underrepresented individuals (Rice)	7/1/11	6/28/13	0.00%							
Milestone: Engage 40 underrepresented individuals (Rice)	7/1/11	9/30/11	100.00%							
Milestone: Engage 40 underrepresented individuals (Rice)	7/2/12	6/28/13	25.00%							
Milestone: Create Faculty Council with 20 minority faculty (Rice)	7/1/11	7/1/13	0.00%							
Milestone: Create Faculty Council with 20 minority faculty (Rice)	7/1/11	12/30/11	100.00%							
Milestone: Create Faculty Council with 20 minority faculty (Rice)	7/2/12	7/1/13	25.00%							
Speakers' Bureau	7/1/11	6/28/13	0.00%							
Milestone: 10 National/Regional presentations	7/1/11	6/28/13	0.00%							
Milestone: 10 National/Regional presentations	7/1/11	9/30/11	100.00%							
Milestone: 10 National/Regional presentations	7/2/12	6/28/13	25.00%							
Student Engagement	7/1/11	6/28/13	0.00%							
Milestone: Recruit 20 students for training/mentoring/internship	7/1/11	6/28/13	0.00%							
Milestone: Recruit 20 students for training/mentoring/internship	7/1/11	9/30/11	100.00%							
Milestone: Recruit 20 students for training/mentoring/internship	7/2/12	6/28/13	0.00%							
Campus Champions	7/1/11	6/28/13	0.00%							
Milestone: Increase impact in Campus Champions program	7/1/11	6/28/13	0.00%							
Milestone: Increase membership in Campus Champions program	7/1/11	9/30/11	100.00%							
Milestone: Increase impact in Campus Champions program	7/2/12	6/28/13	25.00%							
XSEDE Annual Conference	6/1/11	6/28/13	0.00%							
XSEDE 12	6/1/11	9/7/11	100.00%							
XSEDE 13	7/2/12	6/28/13	25.00%							
Community Requirements	4/4/11	6/28/13	0.00%							
TEOS Advisory Commitee	4/4/11	6/28/13	0.00%							
Semi-Annual consultation with TEOS Advisory Group	4/4/11	11/16/11	100.00%							

Name	Start	Finish	% Completed - XSEDE	2011	2012	2013	2014	2015	2016	2017
TEOS Advisory Commitee	7/2/12	6/28/13	25.00%							
⊟ Collect Community Requirements	4/4/11	6/28/13	0.00%							
Annual collection and analysis of community needs and requirements	4/4/11	11/16/11	100.00%							
Collect Community Requirements	7/2/12	6/28/13	25.00%							
⊟ Infratructure	4/4/11	6/28/13	0.00%							
Curation of TEOS information on public web and XSEDE portal	4/4/11	7/26/11	100.00%							
E&O Curation	7/2/12	6/28/13	25.00%							
E&O Infrastructure Lead	7/2/12	6/28/13	25.00%							
⊟ Campus Bridging	4/4/11	6/28/13	0.00%							
⊟ Lead Campus Bridging Effort	4/4/11	6/28/13	0.00%							
Ongoing: Share information with campuses interested in campus bridging	4/4/11	7/26/11	100.00%							
Lead Campus Bridging Effort	7/2/12	6/28/13	25.00%							
Campus Bridging Travel to Pilot Program Sites	7/2/12	6/28/13	0.00%							
Pilot program, software packaging, documentation and suppport	7/2/12	6/28/13	25.00%							
Rocks Roll test cluster 10GbE at Cornell	7/2/12	6/28/13	0.00%							
Rocks Roll test cluster Infiniband at IU	7/2/12	6/28/13	0.00%							
Lead Campus Bridging Effort	7/2/12	6/28/13	25.00%							
⊟ External Evaluation	4/4/11	6/28/13	0.00%							
External Evaluator Quarterly Reports	4/4/11	7/26/11	100.00%							
External Evaluation	7/2/12	6/28/13	25.00%							
⊟ Technology Investigation Service	12/12/11	8/13/13	0.00%							
⊟ Technology Identification	7/2/12	6/28/13	0.00%							
Plan and Execute TIS Merge	7/2/12	8/10/12	0.00%							
Create QA/Testing/backup plan	7/2/12	7/2/12	0.00%							
Identify ER content coordinator for new TIS site	7/2/12	7/2/12	0.00%							
Market TIS to Technologies	7/2/12	6/28/13	0.00%							
Market TIS to user	7/2/12	6/28/13	0.00%							
Plan for increased access to TIS - ex. In common Authentication	7/2/12	11/2/12	0.00%							
Enable users to add comments to technologies - such as likes and feedbacks	7/2/12	11/2/12	0.00%							
Enable evaluators to enter evaluations for multiple pieces of a single technology	7/2/12	9/21/12	0.00%							

Name	Start	Finish	% Completed - XSEDE
Plan for future release iterations of XTED based on requirements	7/2/12	6/28/13	0.00%
Technology Evaluation	12/12/11	8/13/13	0.00%
Receive the requirements from other Level 3s.	7/2/12	7/2/12	0.00%
Providing evaluation results to the XSEDE Level 3 implementers.	7/2/12	6/28/13	0.00%
Transfer Evaluation results to the Level 3 implementers.	7/2/12	6/28/13	0.00%
Transfer TIS knowledge and deployment objects to Level 3 implementers	7/2/12	6/28/13	0.00%
Make data available to other XSEDE Level 3s about the evaluation process, data	7/2/12	6/28/13	0.00%
Maintain/update system access accounts to XSEDE RP systems for TEP members	7/2/12	7/6/12	0.00%
Maintain Test hardware	7/2/12	6/28/13	0.00%
Maintain/administer TEP acquired hardware	7/2/12	6/28/13	0.00%
Maintenance/administration of the TEL dedicated hardware	7/2/12	6/28/13	0.00%
Update XTED as appropriate	7/2/12	7/6/12	0.00%
Accomplish multiple evaluations annually	12/12/11	6/5/13	0.00%
Evaluation 5: Pegasus WMS- finish	12/12/11	10/31/12	0.00%
Evaluation 6: Unicore WMS – finish	4/1/12	11/16/12	0.00%
Evaluation 7: Medici? - star	11/19/12	12/20/12	0.00%
Evaluation 7: Medici? - finish	12/21/12	1/23/13	0.00%
Evaluation 8: GFFS Reliable File Transfer(Second Attempt) – start	10/15/12	11/15/12	0.00%
Evaluation 8: GFFS Reliable File Transfer(Second Attempt) – finish	11/16/12	12/19/12	0.00%
Evaluation 9: unspecified candidate – start	11/16/12	12/19/12	0.00%
Evaluation 9: unspecified candidate – finish	12/20/12	1/22/13	0.00%
Evaluation 10: unspecified candidate – start	12/20/12	1/22/13	0.00%
Evaluation 10: unspecified candidate – finish	1/23/13	2/25/13	0.00%
Evaluation 11: unspecified candidate – start	1/23/13	2/25/13	0.00%
Evaluation 11: unspecified candidate – finish	2/26/13	3/29/13	0.00%
Evaluation 12: unspecified candidate – start	2/26/13	3/29/13	0.00%
Evaluation 12: unspecified candidate – finish	4/1/13	5/2/13	0.00%
Evaluation 13: unspecified candidate – start	4/1/13	5/2/13	0.00%
Evaluation 13: unspecified candidate – finish	5/3/13	6/5/13	0.00%
Verify the evaluation process annually	7/2/12	7/17/12	0.00%



Name	Start	Finish	% Completed - XSEDE	2011	2012	2013	2014	2015	2016	2017
review the evaluation process	7/2/12	7/9/12	0.00%							
update the evaluation process post review as necessary	7/9/12	7/17/12	0.00%							
Assist in updating the process to identify User Requirements and the next item for	7/2/12	8/13/13	0.00%							
Maintain/update the TEP portion of the XSEDE wiki	7/2/12	8/10/12	0.00%							
Documentation	7/2/12	7/13/12	0.00%							
Document TEL Dedicated Hardware	7/2/12	7/13/12	100.00%							
Document FutureGrid systems	7/2/12	7/13/12	0.00%							
Provide short document for specific TIS activities for others	7/2/12	7/5/12	0.00%							
Create an evaluation process for hardware	7/2/12	8/24/12	0.00%							
Create a training package for new TEP members to orient them on the TEP process	10/15/12	11/15/12	0.00%							
Train new members with the training package	11/16/12	11/27/12	0.00%							
Virtual Machines	7/2/12	7/20/12	0.00%							
Create images that closely mirrors XSEDE SP systems	7/2/12	7/20/12	0.00%							

Gantt Legend

Project (Gantt Bar Styles)

Default	Completed	Scheduled	Baseline 1				

Task (Gantt Bar Styles)

Default	Completed	Scheduled	Free Float	Total Float	Negative Float	Start Delay	Baseline 1
Critical Filter	Scheduled						
Parent Filter	Scheduled						
Buffers	Scheduled						
Buffer Incursion 0% - 25%	Buffer Incursion						
Buffer Incursion 25% - 75%	Buffer Incursion						
Buffer Incursion 75% - 100%	Buffer Incursion						

Task (Gantt Symbols)

Default	Objective Start	Objective Finish	Gantt Baseline2 Finish	Gantt Baseline3 Finish	Gantt Baseline4 Finish	Gantt Baseline5 Finish

C XSEDE Risk Register

Home > Risks Register > XSEDE Risks Summary

Risks Summary

Risk Summary Stats	
Total Number of Risks:	93
Number of non-retired Risks:	73
High Impact Risks:	32
High Probability Risks:	6
High Risk-Level:	2
Key Risks:	2
Current Risks:	69
(stats count non-retired risks)	

All Risks (Probability × Impact)

1	3	3
8	16	21
9	12	20

Impact

Non-retired Risks (Probability × Impact)

1	3	2
8	14	12
4	11	18

Impact

Retired Risks (Probability × Impact)

		1
	2	9
5	1	2

Impact

Non-retired Risks

73 risks

Risk Id	Risk	Risk Level	Probability	Impact	Status	Subproject	Monitor Date	Retire Date	Owner
239	Potential equipment failure can disrupt database services.	Low	Low	Medium	Monitor	1.2.5 Accounting/Account Mgmt	Jul 01, 2011	Jul 01, 2016	Steven Quinn
241	Prohibitive Operating Costs for Hardware or Software	Low	Low	Medium	Monitor	1.2.6 Systems Operational Support	Jul 01, 2011	Jul 01, 2016	Stephen McNally
242	XRAC Meeting Costs	Medium	Low	High	Monitor	1.3.4 Allocations	Jul 01, 2011	Mar 31, 2016	Ken Hackworth
244	XD Architecture not fully implemented at an XD Service Provider	Low	Low	Medium	Monitor	1.1 Project Office	Apr 01, 2011	Mar 31, 2016	John Towns
245	Training - AUSS support	Low	Low	Medium	Monitor	1.3.1 Training	Jul 01, 2011	Mar 31, 2016	Dan Stanzione
246	Training - Sync delivery	Medium	Medium	Medium	Monitor	1.3.1 Training	Jul 01, 2011	Mar 31, 2016	Dan Stanzione
247	Education Workshops	Low	Low	Low	Monitor	1.6.1 Education	May 01, 2011	Mar 31, 2016	Steven Gordon
248	Mismatch maintained between research teams' needs, XD resources, and ECSS staff availability.	Medium	Low	High	Monitor	1.4.1 Extended Collaborative Research Teams Support	Jul 01, 2011	Mar 31, 2016	Mark Fahey
249	Student Internships	Low	Medium	Low	Monitor	1.6.2 Outreach	Jul 01, 2011	Mar 31, 2016	Laura McGinnis
250	Suitable project management framework and process is not available.	High	Medium	High	Monitor	1.4.1 Extended Collaborative Research Teams Support	Jul 01, 2011	Mar 31, 2016	Mark Fahey
251	Mentoring Program	Medium	Medium	Medium	Monitor	1.6.2 Outreach	Jul 01, 2011	Mar 31, 2016	Laura McGinnis

252	Campus Infrastructure	Medium	Medium	Medium	Monitor	1.6.5 Campus Bridging	Jul 01, 2011	Mar 31, 2016	Craig Stewart
253	Remote User Support	Medium	Medium	Medium	Monitor	1.6.5 Campus Bridging	Jul 01, 2011	Mar 31, 2016	Craig Stewart
254	Mismatch between research teams' needs, XD resources, and ECSS staff availability.	Medium	Low	High	Monitor	1.5.1 Extended Support for Community Codes	Jul 01, 2011	Mar 31, 2016	John Cazes
255	Suitable project management framework and process is not available.	Medium	Medium	Medium	Monitor	1.5.1 Extended Support for Community Codes	Jul 01, 2011	Mar 31, 2016	John Cazes
Risk Id	Risk	Risk Level	Probability	Impact	Status	Subproject	Monitor Date	Retire Date	Owner
256	Mismatch between research teams' needs, XD resources, and ECSS staff availability.	Medium	Low	High	Monitor	1.5.3 Extended Collaborative EOT Support	Jul 01, 2011	Mar 31, 2016	Jay Alameda
257	Suitable project management framework and process is not available.	Medium	Medium	Medium	Monitor	1.5.3 Extended Collaborative EOT Support	Jul 01, 2011	Mar 31, 2016	Jay Alameda
258	Mismatch between research teams' needs, XD resources, and AUSS staff availability.	High	Medium	High	Monitor	1.4 Extended Collaborative Support - Projects	Apr 01, 2011	Mar 31, 2016	Sergiu Sanielevici
259	Service Provider Non-Participation in SOC	Medium	Low	High	Monitor	1.2.1 Security	Jul 01, 2011	Mar 31, 2016	Randal Butler
260	Failure of XSEDE Operational Infrastructure	Medium	Low	High	Monitor	1.2.6 Systems Operational Support	Jul 01, 2011	Jul 01, 2016	Stephen McNally
261	UNICORE project is cancelled	Low	Low	Medium	Monitor	1.1.3 Architecture & Design	Jan 01, 2011	Mar 31, 2015	Andrew Grimshaw
262	XD Service Provider has insufficient resources to implement XSEDE Architecture	Low	Low	Medium	Monitor	1.2.4 Software Testing & Deployment	Jul 01, 2011	Jul 01, 2016	Troy Baer
264	Failure of Security Systems and Procedures	Medium	Medium	Medium	Monitor	1.2.1 Security	Jul 01, 2011	Mar 31, 2016	Randal Butler
265	Technical Obsolesence	Medium	Low	High	Monitor	1.1.3 Architecture & Design	Apr 01, 2011	Mar 31, 2016	Andrew Grimshaw
266	Architecture Obsolescence & Software Risks	Medium	Low	High	Monitor	1.1.2 Systems and Software Engineering	Apr 01, 2011	Mar 31, 2016	Janet Brown
267	Software Complexity	Low	Low	Low	Monitor	1.2.4 Software Testing & Deployment	Jul 01, 2011	Jul 01, 2016	Troy Baer
268	Software Partner Failure	Low	Low	Medium	Monitor	1.1.3 Architecture & Design	Apr 01, 2011	Mar 31, 2016	Andrew Grimshaw
269	Lack of Qualified System Administration Personnel	Low	Low	Low	Monitor	1.1.2 Systems and Software Engineering	Mar 01, 2011	Mar 31, 2016	Janet Brown
270	Loss of Senior Technical Personnel	Low	Low	Medium	Monitor	1 XSEDE	Apr 01, 2011	Mar 31, 2016	John Towns

271	Insufficient Service Provider Integration into XSEDE activities	Medium	Medium	Medium	Monitor	1.1 Project Office	Jan 01, 2011	Mar 31, 2016	John Towns
Risk Id	Risk	Risk Level	Probability	Impact	Status	Subproject	Monitor Date	Retire Date	Owner
272	Grid Software System Integration	High	High	High	Monitor	1.1.3 Architecture & Design	Apr 01, 2011	Mar 31, 2016	Andrew Grimshaw
273	Grid Software Scaling	High	High	High	Monitor	1.1.3 Architecture & Design	Apr 01, 2011	Mar 31, 2016	Andrew Grimshaw
274	Usage of deployed software and services	High	High	Medium	Monitor	1.2.4 Software Testing & Deployment	Jul 01, 2011	Jul 01, 2016	Troy Baer
275	Deviation from project management procedures	Low	Medium	Low	Monitor	1.1.1 Project Management and Reporting	Jan 01, 2011	Mar 31, 2016	Timothy Cockerill
276	Inadequate communication with SPs	Medium	Low	High	Monitor	1.1 Project Office	Jan 01, 2011	Mar 31, 2016	Timothy Cockerill
277	Noncompliant service provider	Medium	Medium	Medium	Monitor	1.1 Project Office	Apr 01, 2011	Mar 31, 2016	Timothy Cockerill
278	Implementation delays and inconsistencies	High	High	Medium	Monitor	1.2.4 Software Testing & Deployment	Jul 01, 2011	Jul 01, 2016	Troy Baer
279	Remote root compromise	High	Medium	High	Monitor	1.2.1 Security	Jul 01, 2011	Mar 31, 2016	Randal Butler
280	Local root compromise	High	Medium	High	Monitor	1.2.1 Security	Jul 01, 2011	Mar 31, 2016	Randal Butler
281	User Account Compromise	Medium	Medium	Medium	Monitor	1.2.1 Security	Jul 01, 2011	Mar 31, 2016	Randal Butler
282	Malicious Social Engineering	High	Medium	High	Monitor	1.2.1 Security	Jul 01, 2011	Mar 31, 2016	Randal Butler
283	Network Security and Operation	Medium	Low	High	Monitor	1.2.1 Security	Jul 01, 2011	Mar 31, 2016	Randal Butler
286	Reduced overall budget for the project	Medium	Low	High	Monitor	1 XSEDE	Sep 15, 2010	Feb 15, 2011	John Towns
287	Loss of Project PI or co-PI	High	Medium	High	Monitor	1 XSEDE	Jan 01, 2011	Jun 30, 2016	John Towns
288	Differing architectural views hinder deployment and operation of XSEDE	Medium	Low	High	Monitor	1.1.2 Systems and Software Engineering	Mar 01, 2011	Jun 30, 2016	Janet Brown
Risk Id	Risk	Risk Level	Probability	Impact	Status	Subproject	Monitor Date	Retire Date	Owner
295	Funds are not provided for initial network "gap" costs	Medium	Low	High	Monitor	1.2.3 XSEDEnet	Jul 01, 2011	Jun 30, 2016	Linda Winkler
296	Capacity of XSEDE reources less than demand	High	Medium	High	Monitor	1.1 Project Office	Jul 01, 2011	Jun 30, 2016	John Towns
298	XSEDE archival storage gap	High	Medium	High	Monitor	1.2.2 Data Services	Jul 01, 2011	Jun 30, 2016	Christopher Jordan
301	Opportunity: Leverage new/novel resources	High	Medium	High	Monitor	1.1 Project Office	Jul 01, 2011		John Towns
305	Federated identity management does not catch on	Medium	Medium	Medium	Monitor	1.1 Project Office	Jul 01, 2011	Jun 30, 2012	John Towns

306	Plan for long term service scaling may not meet short term needs	Low	Medium	Low	Monitor	1.1 Project Office	Jul 01, 2011	Jun 30, 2016	John Towns
307	Integrating services fail to meet standards in service level agreements	Low	Medium	Low	Monitor	1.1 Project Office	Jul 01, 2011	Jun 30, 2016	John Towns
309	Genesis II FUSE/RNS scalability and performance	Low	Low	Medium	Monitor	1.2.2 Data Services	Jul 31, 2011	Oct 31, 2012	Christopher Jordan
311	NLR Services Are Inadequate	Medium	Low	High	Monitor	1.2.3 XSEDEnet	Jul 01, 2011	Jul 01, 2016	Linda Winkler
312	Network Disruption Disables Critical Services	High	Medium	High	Monitor	1.2.3 XSEDEnet	Jul 01, 2011	Jul 01, 2015	Linda Winkler
314	XSEDE DNS Service Availability	Medium	Low	High	Monitor	1.2.3 XSEDEnet	Jul 01, 2011	Jul 01, 2016	Linda Winkler
315	XSEDE RS Service Availability	Medium	Low	High	Monitor	1.2.3 XSEDEnet	Jul 01, 2011	Jul 01, 2015	Linda Winkler
316	Prohibitive Cost for Required Software	Medium	Low	High	Monitor	1.2.4 Software Testing & Deployment	Jul 01, 2011	Jul 01, 2016	Troy Baer
317	TeraGrid Domain Name Hardcoded into SP Software	Medium	High	Low	Monitor	1.2.6 Systems Operational Support	Jul 01, 2011	Jul 01, 2016	Stephen McNally
318	Communication Breakdown	Medium	Medium	Medium	Monitor	1.2.6 Systems Operational Support	Jul 01, 2011	Jul 01, 2016	Stephen McNally
Risk Id	Risk	Risk Level	Probability	Impact	Status	Subproject	Monitor Date	Retire Date	Owner
319	Overloading XSEDE Operations Center Staff	Low	Medium	Low	Monitor	1.2.6 Systems Operational Support	Jul 01, 2011	Jul 01, 2016	Stephen McNally
320	Security Compromise of XSEDE Infrastructure	High	Medium	High	Monitor	1.2.1 Security	Jul 01, 2011	Jul 01, 2016	Randal Butler
321	Mismatch between non-traditional users' needs, XSEDE services, and NIP staff allocation.	Low	Medium	Low	Monitor	1.4.2 Novel & Innovative Projects	Jul 01, 2011	Jun 30, 2016	Sergiu Sanielevici
322	Suitable project management framework and process is not available	Medium	Medium	Medium	Monitor	1.5.2 Extended Collaborative Science Gateways Support	Jul 01, 2011	Mar 31, 2016	Suresh Marru
325	Delay in program implementation	Medium	Medium	Medium	Monitor	1.6.1 Education	Sep 19, 2011	Sep 30, 2012	Steven Gordon
326	NLR Business Focus Changes	Low	Low	Medium	Monitor	1.2.3 XSEDEnet	Sep 01, 2011	Jul 01, 2016	Linda Winkler
327	Namespace collisions between XSEDE software and local software	Low	Medium	Low	Monitor	1.2.4 Software Testing & Deployment	Oct 03, 2011	Jul 01, 2016	Troy Baer
328	Campus Bridging expectation management	High	High	Medium	Monitor	1.6.5 Campus Bridging	Oct 01, 2012	Dec 31, 2013	Craig Stewart
329	Delay in ticketing system interface release	Low	Low	Low	Monitor	1.3.2 User Information & Interfaces	Jan 01, 2012	Jan 01, 2013	Maytal Dahan

330	Lack of Testing Resources	Low	Medium	Low	Monitor	1.2.4 Software Testing & Deployment	Jan 10, 2012	Jul 01, 2016	Troy Baer
331	Program Plan	High	Medium	High	Monitor	1.1.1 Project Management and Reporting	Feb 16, 2012	Jul 01, 2015	Timothy Cockerill
332	Failure of XDCDB failover process	Medium	Low	High	Monitor	1.2.6 Systems Operational Support	Jun 18, 2012	Jul 01, 2016	Stephen McNally
333	Outdated Critical Documents	Low	Low	Medium	Monitor	1.2 XSEDE Operations	Aug 16, 2012	Jul 01, 2016	Justin Whitt

Retired risks

Retired Risks

D XSEDE Change Control Report

Nothing to report this quarter.

E Metrics

To demonstrate its success and help focus management attention on areas in need of improvement, XSEDE monitors a wide range of metrics in support of different aspects of "success" for the program. The metrics presented in the quarterly reports provide a view into XSEDE's user community, including its success at expanding that community, the projects and allocations through which XSEDE manages access to resources, and the use of the resources by those projects (§E.1). In addition, XSEDE has identified metrics describing the program's success at delivering centralized services to this community, including operations, user support, advanced user support, and education and outreach activities (§E.2). Together, these metrics provide perspectives on how XSEDE works to ensure that the XSEDE-associated services and resources deliver science impact for the science and engineering research community.

E.1 XSEDE Resource and Service Usage Metrics

and allocations, and resource utilization for the quarter. Expanded information and five-year historical trends are shown in three corresponding subsections.

Notably for Q3 2012, XSEDE saw a continued increase in open user accounts and active individuals, with 863 individuals getting new XSEDE accounts during the quarter, the third highest quarterly total on record. Gateways continued to represent a major part of the XSEDE community, with a new high of 1,624 users submitting jobs via science gateways. More user community details are in §E.1.1.

Table 16. Quarterly activity summary

User Community	Q4 2011	Q1 2012	Q2 2012	Q3 2012
Open user accounts	5,829	6,313	6,636	6,964
Active individuals	1,819	2,165	2,245	2,148
Gateway users	1,389	1,039	1,580	1,624
New user accounts	545	1,063	760	863
Active fields of science	26	26	29	29
Active institutions	316	340	375	354
Projects and Allocations				
NUs available at XRAC	16.780B	17.377B	17.939B	22.429B
NUs requested at XRAC	28.012B	36.959B	37.539B	57.611B
NUs recommended by XRAC	16.268B	20.562B	23.194B	19.738B
NUs awarded at XRAC	16.268B	18.230B	17.502B	18.149B
Open projects	1,560	1,545	1,600	1,612
Active projects	917	979	1,027	1,044
Active gateways	16	17	16	16
New projects	188	216	247	212
Closed projects	254	219	207	218
Resources and Usage				
Resources open (all types)	23	23	24	24
Total peak petaflops	2.50	2.92	2.92	3.54
Resources reporting use	15	14	13	14
Jobs reported	1.13M	1.04M	1.70M	1.32M
NUs delivered	15.21B	14.76B	16.67B	17.9B
Avg wtd run time (hrs)	22.5	23.3	20.9	22.4
Avg wtd wait time (hrs)	26.8	23.2	32.6	36.5
Avg wtd slow down	3.5	3.3	4.7	4.1

Project and allocation activity showed continued high demand, with XSEDE resources requested at 257% of what was available. The XRAC recommendations, however, fit within the resources available. During the quarter, open projects climbed to 1,612, and an increased number (1,044) made use of the resources. More details are in §E.1.2.

XSEDE computing resources represented more than 3.5 Pflops (peak) at the end of the quarter, due to the Georgia Tech Keeneland system entering production near the end of the quarter. The central accounting system showed 14 resources reporting activity, and together they delivered 17.9 billion NUs of computing. This represents an decrease of approximately 7% over the previous quarter. At the same time, XSEDE users experienced slightly longer wait times, on average, but the average slow down for jobs decreased. More details are in §E.1.3.

E.1.1 User community metrics

Figure 37 shows the five-year trend in the XSEDE user community, including open user accounts, total active XSEDE users, active individual accounts, active gateway users, the number of new accounts, and the total number of unvetted user accounts (i.e., portal-only accounts) at the end of each quarter. (Unvetted user accounts can be used for training course registration and other functions.) The 863 new user accounts created represents one of the busiest quarters in the past two years.

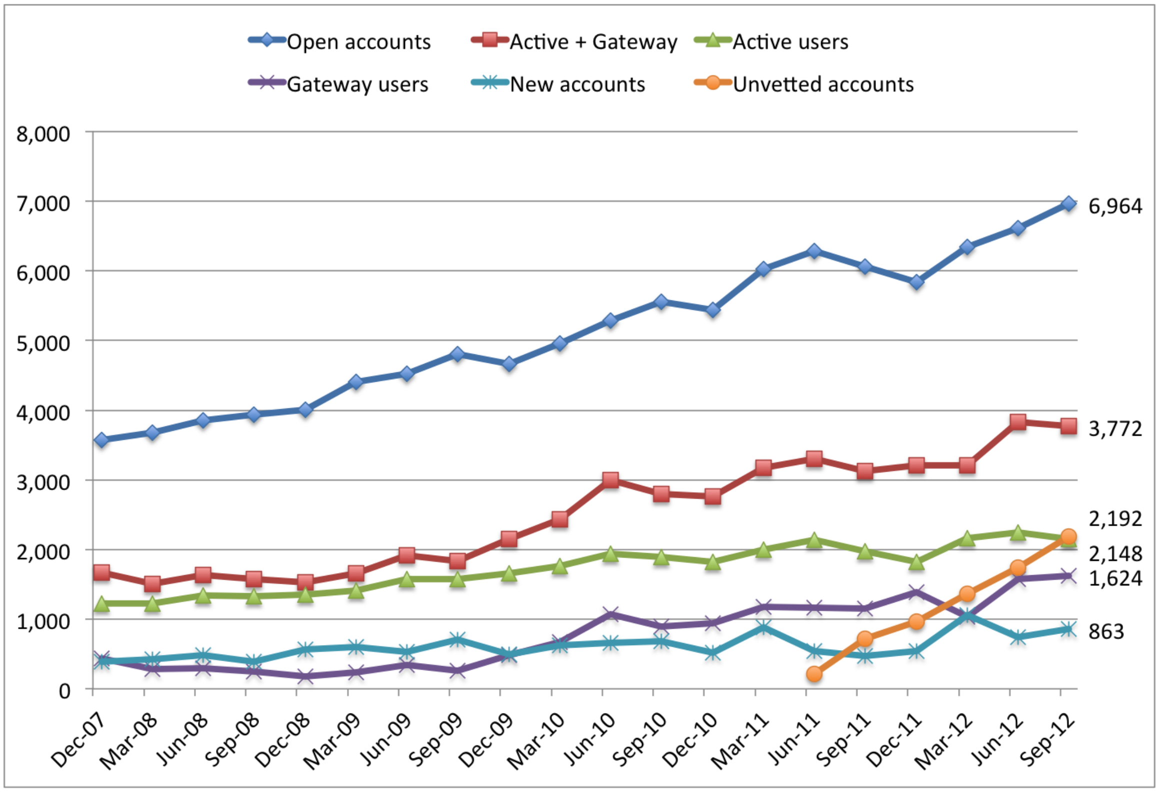


Figure 37. XSEDE user census, excluding XSEDE staff.

Figure 38 shows the activity on XSEDE resources according to field of science, including the relative fraction of PIs, open accounts, active users, allocations, and NUs used according to discipline. For consistency across quarters, we show (and will show in future quarters) the nine fields of science that typically consume ~2% or more of delivered NUs per quarter. PIs and users are counted more than once if they are associated with projects in different fields of science. The Q3 data show that the percentages of PIs and accounts associated with the “other” disciplines represent nearly 30% of all PIs and more than 30% of user accounts, and more than 20% of active users. Collectively the “other” fields of science represent 7.5% of total quarterly usage, an increase from the previous quarter and led by activity in ocean sciences and environmental biology. Figure 39 shows the publications, conference papers, and presentations reported by XSEDE users each quarter, including the 775 reported for Q3; Appendix F lists these publications according to allocated project.

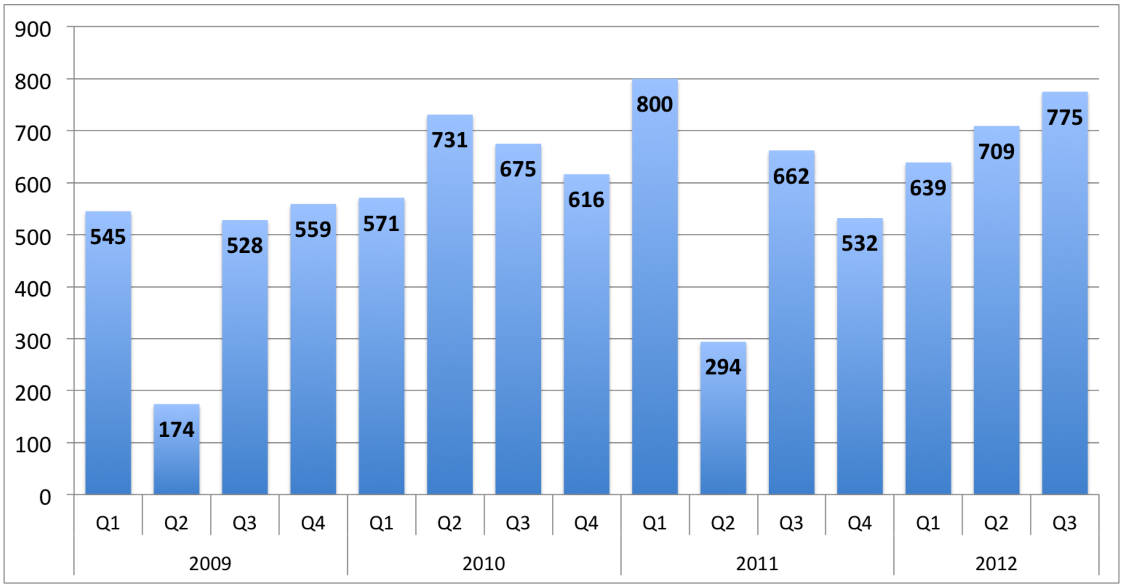


Figure 39. Publications, conference papers, and presentations reported by XSEDE users

Table 17 and Table 18 highlight aspects of the broader impact of XSEDE. The former shows that graduate students, post-doctoral researchers, and undergraduates make up 65% of the XSEDE user base. The latter table shows XSEDE's reach into targeted institutional communities. Institutions with Campus Champions represent a large portion of XSEDE's usage (this table shows all users at Campus Champion institutions, not just those on the champion's project). The table also shows XSEDE's reach into EPSCoR states, the MSI community, and internationally.

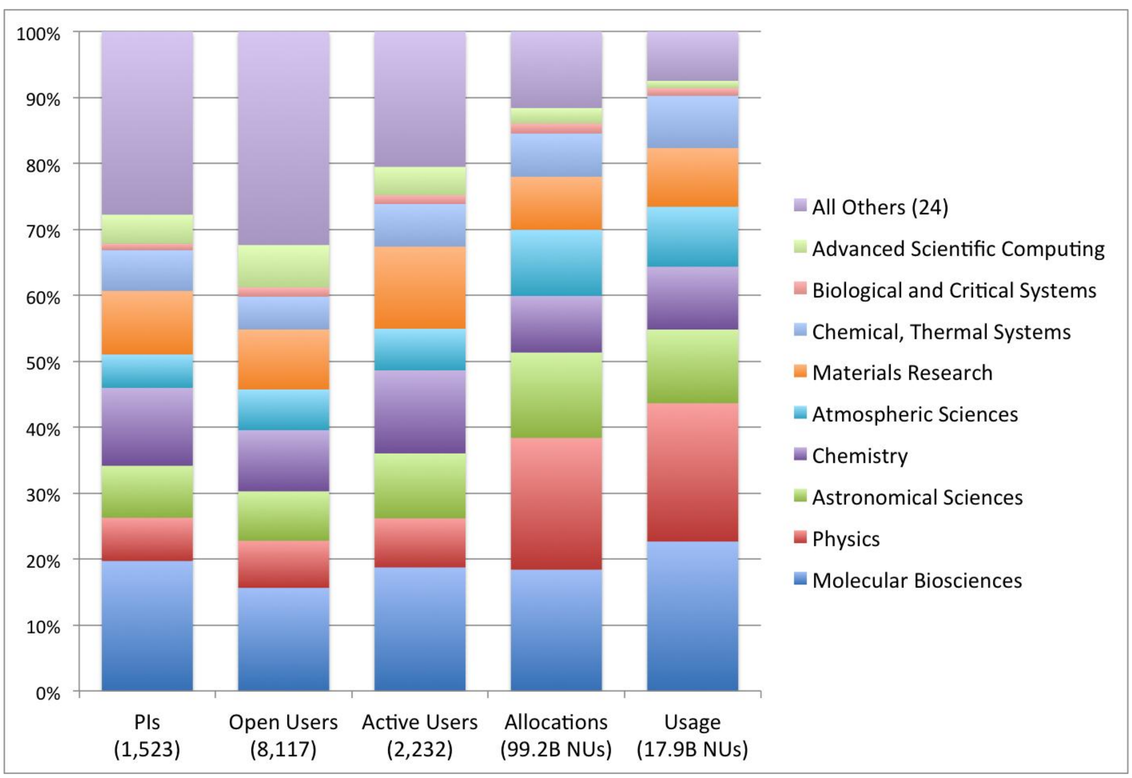


Figure 38. Quarterly XSEDE user, allocation, and usage summary by field of science, in order by usage, excluding staff projects. Note: PIs, users may appear under more than one field of science.

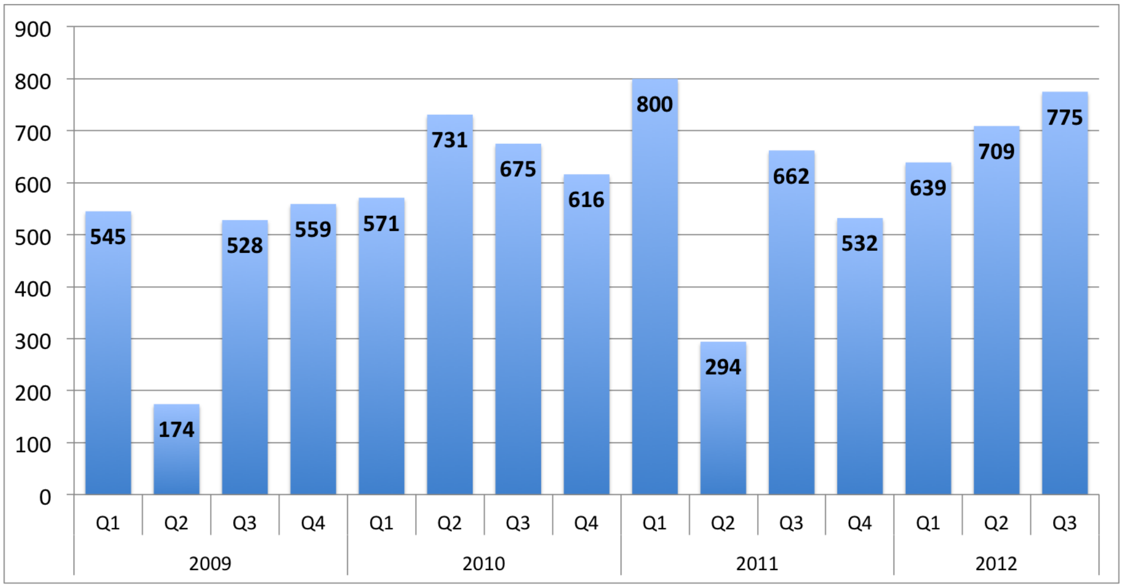


Figure 39. Publications, conference papers, and presentations reported by XSEDE users

Table 17. End of quarter XSEDE open user accounts by type, excluding XSEDE staff.

Category	Q4 2011	Q1 2012	Q2 2012	Q3 2012
Graduate Student	2,275	2,466	2,574	2,678
Faculty	1,299	1,293	1,344	1,386
Postdoctorate	1,002	1,059	1,075	1,109
Undergraduate Student	416	587	639	733
University Research Staff (excluding postdocs)	501	509	535	559
High school	5	5	4	10
Others	331	394	465	489
TOTALS	***5,829***	***6,313***	***6,636***	***6,964***

Table 18. Active institutions, overall and in selected categories. Notes: “Total” reflects institutions not in any specially designated category. Institutions may be in more than one category.

Category	Institutions	Users	NUs	% NUs
Campus Champion site	69	812	6,981,899,233	39%
EPSCoR state	66	324	2,615,793,283	15%
MSI	17	37	97,288,760	1%
International	44	70	432,097,445	2%
Total	354	2,148	17,863,853,747	100%

E.1.2 Project and allocation metrics

Figure 40 shows the historical trends for requests and awards at XSEDE quarterly allocation meetings. The figure shows the continued strong growth in demand against the relative plateau in available resources; the requests at the September 2012 XRAC meeting totaled more than 1 billion SUs for the first time. NUs requested were 257% of NUs available, although the XRAC recommendations were 88% of the NUs available. XSEDE was able to award fewer NUs than recommended because requests could not be moved to alternate resources in all cases, due to architectural differences.

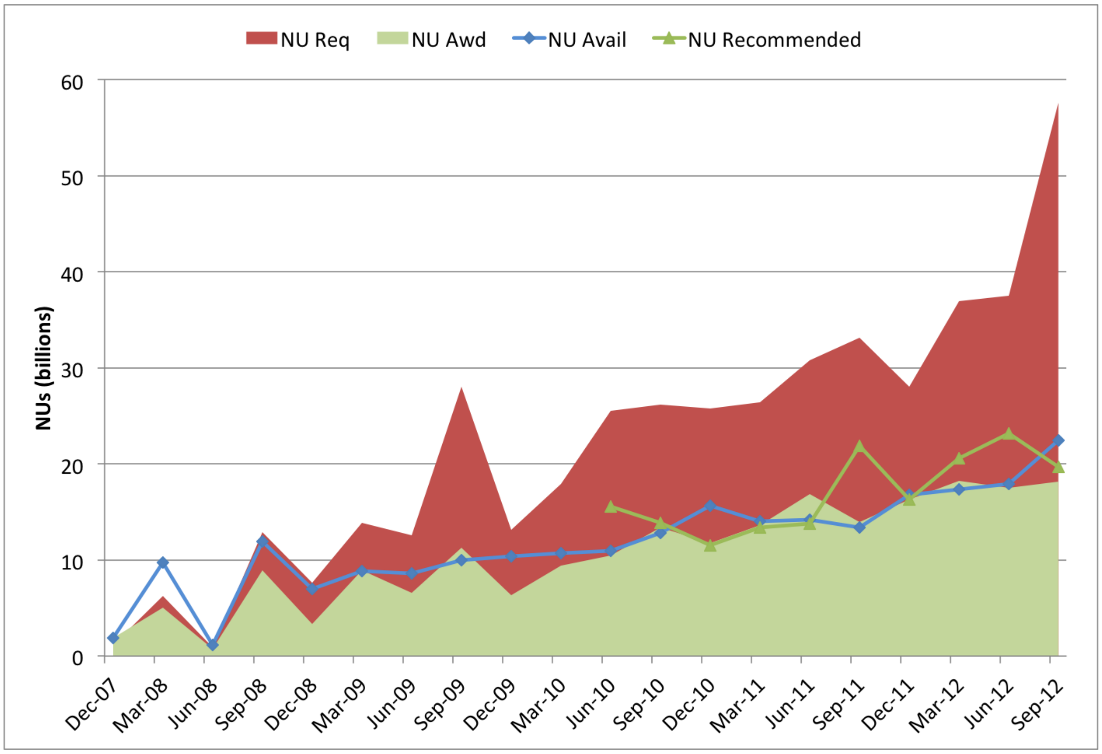


Figure 40. Allocation meeting history, showing NUs requested, awarded, available, and recommended. December 2007 and June 2008 were the last MRAC meetings, i.e. only had "medium" requests.

Table 19 presents a summary of overall project activity. Notably, 87% of XRAC requests received an award, and 36% were new awards.

Table 20 and Table 21 show projects and activity in key project categories—Campus Champion, Staff, and Science Gateways—and by allocation board type. (Science Gateways may appear under any board.) Table 20 also shows new and closed projects for the quarter, while Table 21 shows the number of open and active user accounts with each type of project. Table 22 shows detailed information about allocations activity for the various request types available for the different classes of projects. Notably, XSEDE had 158 Research (XRAC) requests, of which 137 (87%) received awards, including 50 new projects. There were also 176 Startup requests, of which 142 (81%) received awards; 20 Education requests with 19 awards; and 21 Campus Champion requests with 20 awards.

As a special class of projects, science gateway activity is detailed in Figure 41 showing continued high levels of usage and users from these projects. Table 23 shows gateway activity supported by specific XSEDE resources.

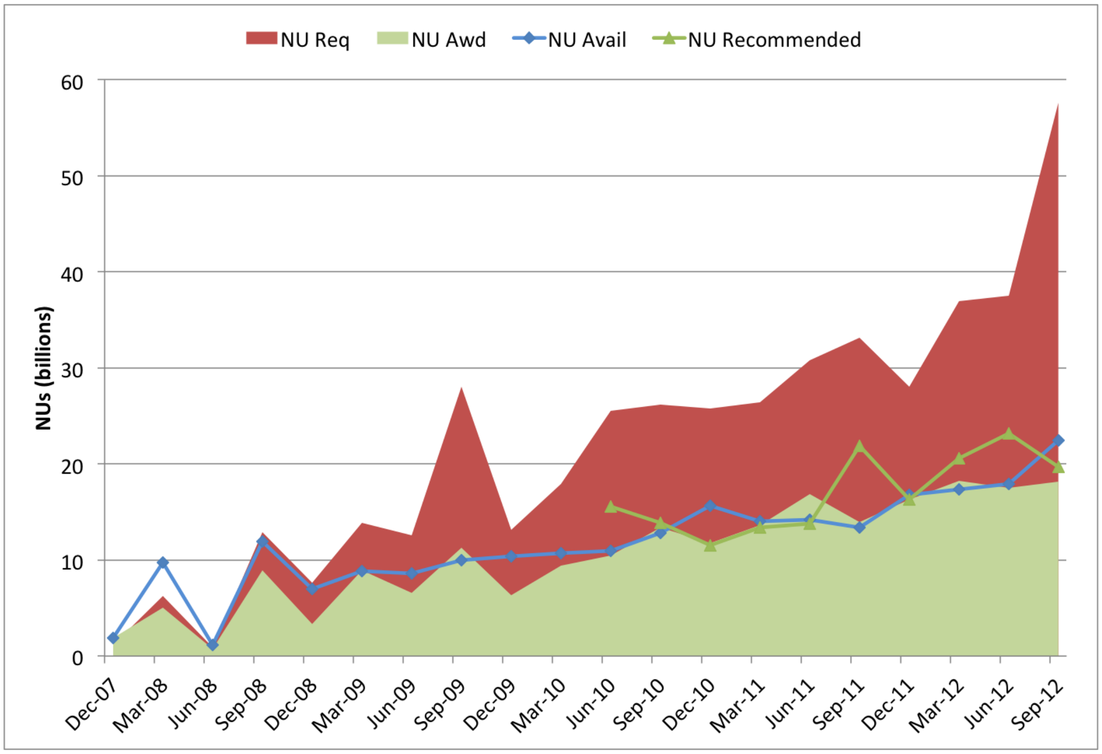


Figure 40. Allocation meeting history, showing NUs requested, awarded, available, and recommended. December 2007 and June 2008 were the last MRAC meetings, i.e. only had "medium" requests.

Table 19. Project summary metrics

Project metric	Q4 2011	Q1 2012	Q2 2012	Q3 2012
XRAC requests	138	123	147	158
XRAC request success	88%	96%	90%	87%
XRAC new awards	29%	36%	39%	36%
Startup requests	129	168	206	176
Startup request success	89%	89%	82%	81%
Projects open	1,560	1,545	1,600	1,612
Projects new	188	216	247	212
Projects active	917	979	1,027	1,028
Projects closed	254	219	207	218
Resource diversity (wtd)	1.4 (2.1)	1.4 (1.9)	1.5 (2.0)	1.5 (2.1)
SP diversity (wtd)	1.3 (1.7)	1.3 (1.6)	1.3 (1.7)	1.3 (1.7)

Table 20. Project activity in designated categories.

Type	Open	New	Closed	Active	NUs	% NUs
Campus Champion	97	10	8	39	64,793,893	0.4%
Science Gateway	22	0	2	22	811,202,997	4.5%
TG Staff Project	29	1	2	16	127,457,965	0.7%
Other	1,464	201	206	967	16,987,856,849	94.4%
Totals	1,612	212	218	1,044	17,991,311,704	100.0%

Table 21. Project activity by allocation board type.

Board	Open projects	Open users	Active projects	Active users	NUs
XRAC	628	4,416	540	1,535	17,141,479,682
Startup	784	1,852	411	534	583,980,110
Staff	29	527	16	130	127,457,964
Campus Champions	96	522	38	74	64,670,607
Educational	74	1,308	37	191	49,439,673

Board	Open projects	Open users	Active projects	Active users	NUs
Discretionary	1	19	2	11	24,283,668
Totals	1,612	8,644	1,044	2,475	17,991,311,704

Table 22. Allocations activity in POPS, excluding staff and discretionary projects.

	Research				Startup			
	# Req	SUs Req	# Awd	SUs Awd	# Req	SUs Req	# Awd	SUs Awd
New	63	217,740,159	50	100,040,537	158	23,248,424	129	16,550,113
Prog. Report	1	1,000,000	1	700,000	n/a			
Renewal	94	585,485,478	86	279,574,869	18	2,489,527	13	1,379,003
Advance	30	34,657,356	24	13,596,905	n/a			
Justification	4	22,394,000	2	368,000	n/a			
Supplemental	29	53,223,328	19	42,515,809	22	2,227,024	19	1,492,012
Transfer	87	35,232,555	76	19,141,240	38	2,534,179	34	1,504,928
Extension	67	n/a	60	n/a	53	n/a	51	n/a
	Education				**Campus Champions**			
	# Req	**SUs Req**	**# Awd**	**SUs Awd**	**# Req**	**SUs Req**	**# Awd**	**SUs Awd**
New	19	1,441,013	18	1,344,002	12	9,464,030	11	8,426,003
Prog. Report	n/a				n/a			
Renewal	1	50,001	1	50,002	9	7,953,114	9	6,125,013
Advance	n/a				n/a			
Justification	n/a				n/a			
Supplemental	0	0	0	0	5	410,010	4	245,001
Transfer	5	106,566	4	42,500	1	2,600,000	5	190,000
Extension	1	n/a	1	n/a	1	n/a	1	n/a

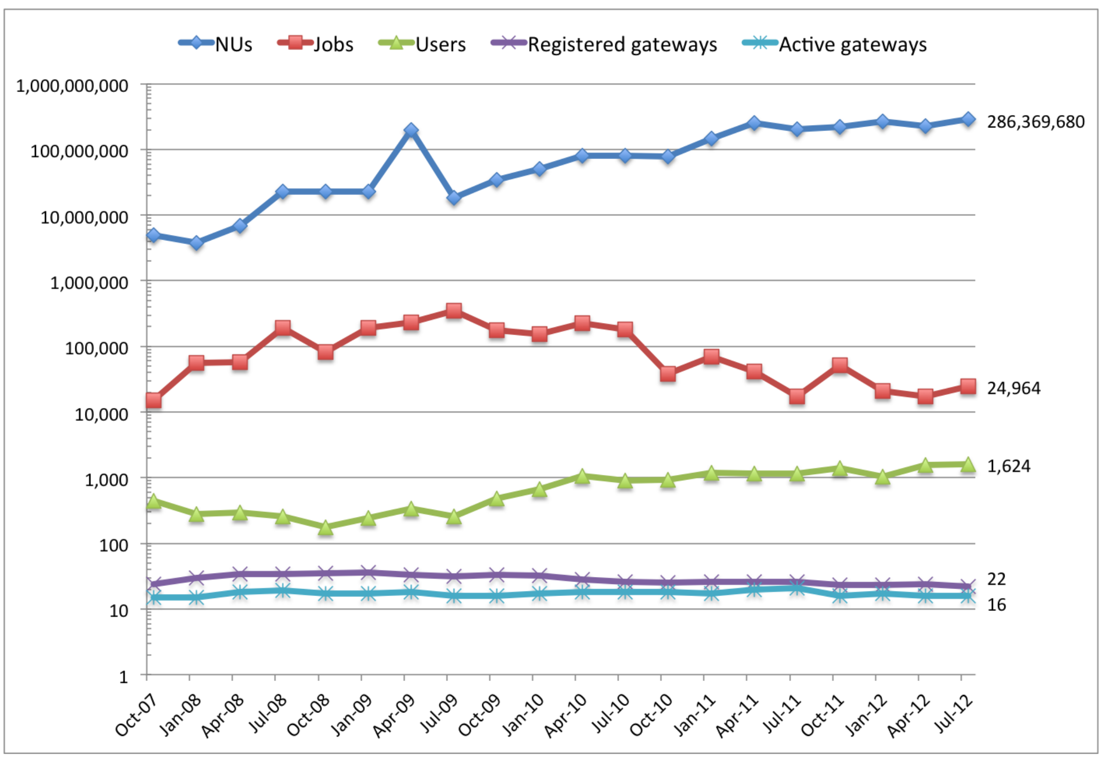


Figure 41. Quarterly gateway usage (NUs), jobs submitted, users (reported by ECSS), registered gateways, and active gateways.

Table 23. Gateway activity by resource.

Resource	Gateways	Jobs	NUs
SDSC Gordon	4	5,027	121,958,683
SDSC Trestles	7	13,703	111,329,158
NICS Kraken	4	3,264	30,328,875
TACC Ranger	8	1,036	16,011,353
TACC Lonestar	3	422	6,047,371
PSC Blacklight	1	69	431,072
NCSA Forge	1	718	252,624
Purdue Steele	3	725	10,545

E.1.3 Resource and usage metrics

Figure 42 shows the total NUs delivered by XSEDE computing systems, as reported to the central accounting system over the past five years. In Q3, the systems delivered 17.9 billion NUs, an increase of about 7% from the previous quarter, and 21% more NUs than the year-ago quarter. Table 24 breaks out the resource activity according to different resource types.

Figure 43 presents a perspective of the capacity and capability use of XSEDE resources by project. The figure shows the cumulative percentage of projects and resource usage according to each project's largest reported job size (in cores). The point at which the proverbial 80/20 rule holds precisely is at 75/25; that is the 75% of projects whose largest jobs were between 512 and 1,024 cores consumed only 25% of the delivered NUs, while the remaining 25% of projects consumed the remaining 75% of delivered NUs.

Finally, Table 25 presents some summary metrics to reflect aggregate "usage satisfaction," including the average run time, wait time, response time (run + wait), and slow down (or expansion factor). These values are presented as unweighted averages, which show the impact of small jobs, and as averages weighted by each job's portion of the workload (in core-hours), which show responsiveness to the jobs responsible for most of the delivered NUs. Notably for Q3, while the "average" job is only 2 hours long, the average weighted job is just more than 22 hours long. On most of the weighted usage satisfaction metrics, larger jobs saw increases in average weighted wait time and average weighted response time, although the average weighted slow down decreased. The weighted average for slow down (4.1) eliminates the skew in the job slow down attributed to small jobs and shows a much more realistic average perceived slowdown for the work delivered.

XSEDE provides central monitoring of GRAM5 job submission activity at XSEDE SP sites (Figure 44). GRAM has been deprecated in favor of GRAM5, and thus we are no longer reporting pre-GRAM5 jobs separately.

Table 24. Resource activity, by type of resource, excluding staff projects.
Note: A user will be counted for each type of resource used.

Type	Resources	Jobs	Users	NUs
High-performance computing	7	981,054	1,747	15,686,958,399
Data-intensive computing	2	149,623	491	2,088,819,963
Visualization system	3	9,263	126	66,997,811
High-throughput computing	2	175,567	22	23,533,845
Totals	14	1,315,507	2,386	17,866,310,018

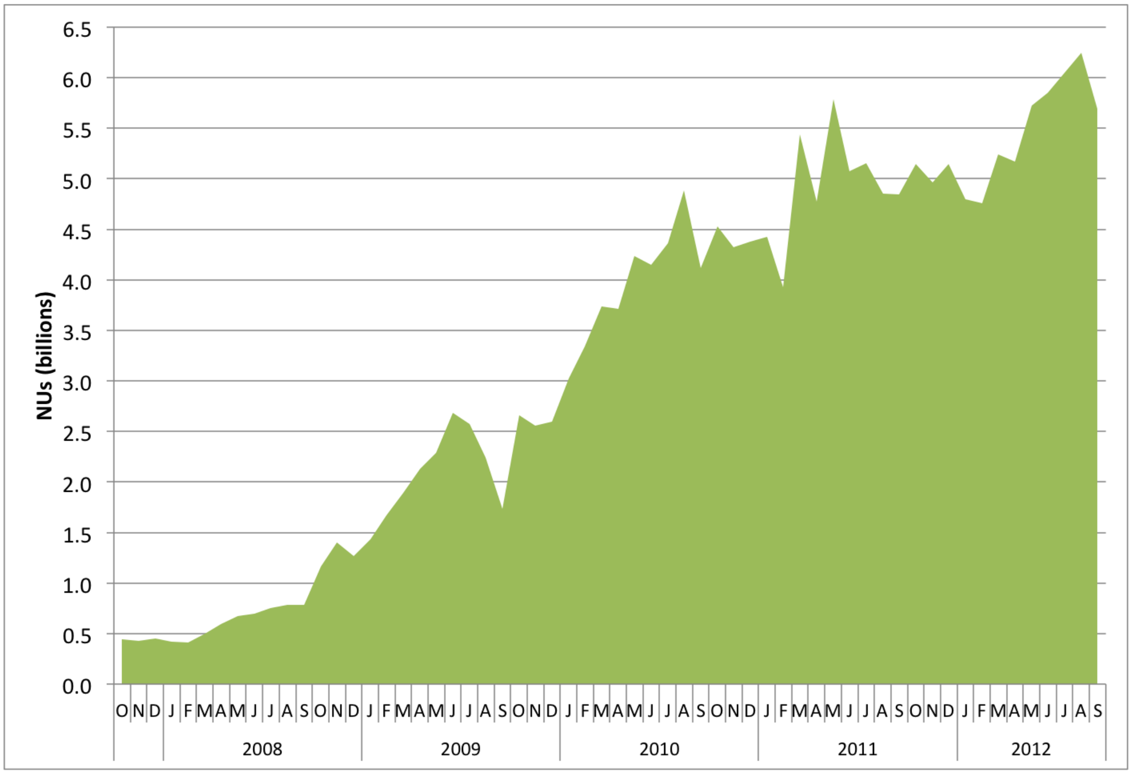


Figure 42. Total XSEDE resource usage in NUs.

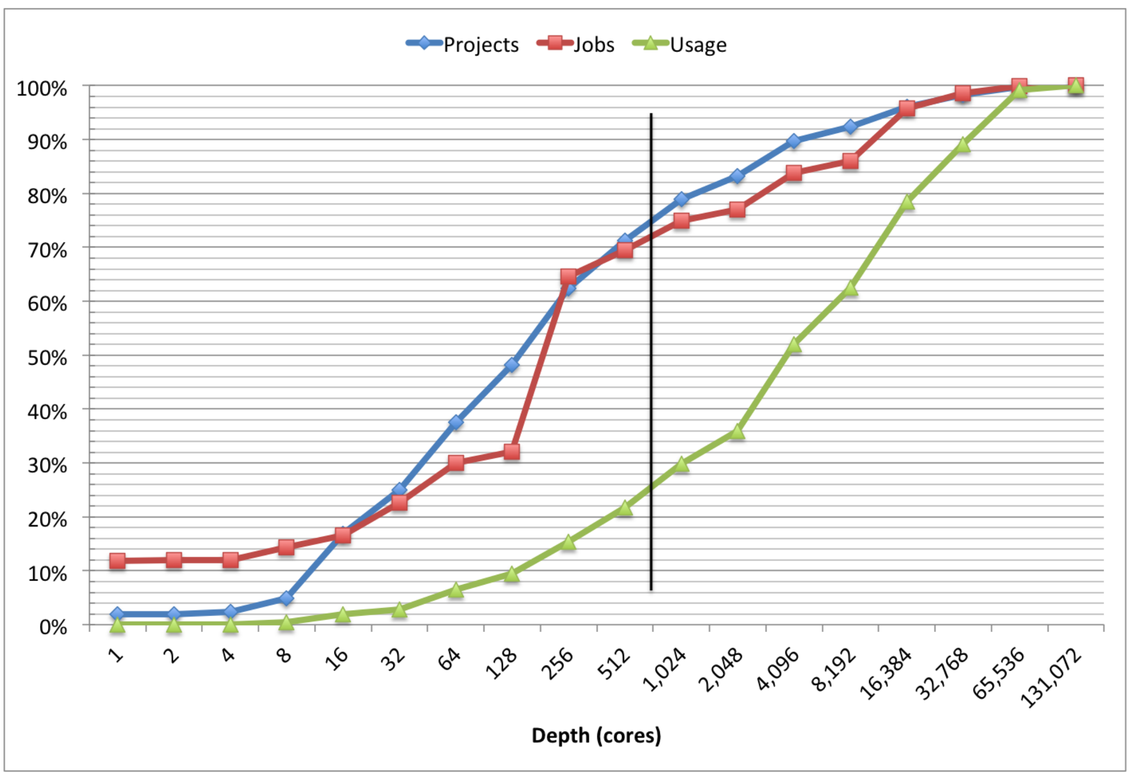


Figure 43. Cumulative distribution of projects, jobs, and usage according to project's maximum job size in cores (excludes staff projects). Vertical line (black) shows "joint ratio" of 75/25 at between 512 and 1,024 cores. I.e., 75% of projects use fewer than 1,024 cores and consume 25% of XSEDE NUs; the other 25% of projects have jobs larger than 1,024 cores and consume the other 75% of XSEDE NUs.

Table 25. Usage satisfaction metrics, for HPC and data-intensive computing resources only, excluding staff projects.

	Job attribute	Q4 2011	Q1 2012	Q2 2012	Q3 2012
Unweighted average	Run time (hrs)	3.0	5.0	2.0	2.0
	Wait time (hrs)	3.1	6.1	4.4	6.2
	Response time (hrs)	7.0	12.1	7.3	9.7
	Slow down	252.3	334.4	324.7	512.2
Weighted average	Wtd run time (hrs)	22.5	23.3	20.9	22.4
	Wtd wait time (hrs)	26.8	23.2	32.6	36.5
	Wtd response time (hrs)	49.4	46.5	53.5	58.9
	Wtd slow down	3.5	3.3	4.7	4.1

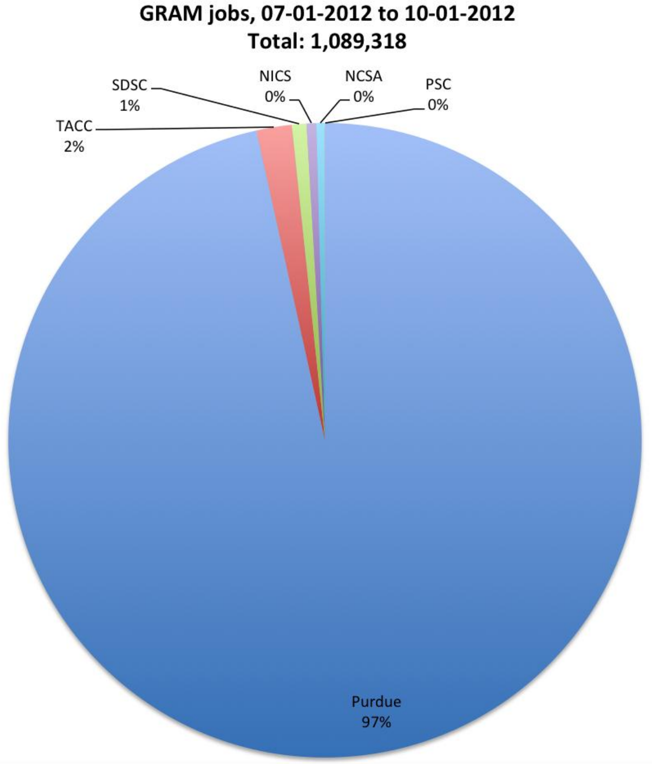


Figure 44. GRAM5 jobs by site 07-01-2012 to 10-01-2012

E.2 XSEDE Program Metrics

E.2.1 Project Office 1.1

1.1.4 External Relations

The XSEDE External Relations team reported the following media hits for the quarter.

Table 26. XSEDE media hits.

Date	Source	Headline	Notes
9/27/12	PhysOrg	One Degree Imager: Bigger, sharper images to be refined, processed and stored at IU	
9/25/12	E-Commerce News	Dell Takes the Long View with Hyper Scale Computing	
9/21/12	InsideHPC	Multisite OpenACC workshop Oct.16-17	Also in NVIDIA blog
9/20/12	NVIDIA blog	U.S. scientists, NSF to host nationwide GPU computing workshop	

Date	Source	Headline	Notes
9/20/12	NVIDIA	Kepler GPUs: The right tool for new high-density Dell servers	
9/19/12	ISGTW	Keeping on top of the data deluge	
9/18/12	HPCWire	Kevin Franklin joins XSEDE advisory board	
9/18/12	HPCWire	Supercomputer does deep dive into election day effect of Facebook post	
9/18/12	Lab Manager Magazine	National Science Foundation Award Bolsters "Big Data" Research at NDSU	
9/14/12	HPCwire	North Dakota State University awarded $400,000 NSF grant	
9/13/12	HPCWire	Globus and grid: Blazing trails for future discovery	
9/12/12	HPCWire	Gregory Peterson named project director at National Institute of Computational Sciences	
9/11/12	Phys.Org	SEED project to enable rapid video encoding and dissemination	Also in Digital Manufacturing Report
9/11/12	HPCWire	SDSC awarded NSF grant to facilitate sharing and streaming of scientific visualizations	
9/10/12	Phys.Org	SDSC awarded NSF grant to facilitate sharing and streaming of scientific visualizations	
9/10/12	HPCwire	XSEDE, NSF Call for Cloud Computing Research Use Cases	Also in HPC in the Cloud
9/8/12	New Mexico EPSCoR	NM EPSCoR Hosts Free XSEDE Webinar!	
9/10/12	HPCwire	XSEDE, NSF call for cloud computing research use cases	Also in HPC in the Cloud and its weekly digest.
9/6/12	HPCwire	Indiana University, partners awarded funding by NSF for Science Gateway Institute	
		0	
8/30/12	UI website	Green awarded XSEDE grant to study data mining and network analysis of library collections	Also on the UI Library and I-CHASS sites
8/30/12	HPCwire	University at Buffalo, TACC receive funding to evaluate XSEDE clusters	
8/29/12	ISGTW	Women, technology, and feminism -- reflections from India	
8/28/12	InsideHPC	SDSC to lead development of NSF Science Gateway Institute	
8/27/12	Data Center Knowledge	Tracking hurricanes with supercomputers	References and links to Zhang study on Ranger at TACC.
8/23/12	InsideHPC	XSEDE12 student programming challenge showcases tomorrow's HPC leaders	
8/22/12	equities.com	Appro is No. 4 on the Top 500 list by total systems deployed	Also in HPCwire, Virtual Strategy magazine, insideHPC, and Prweb
8/21/12	HPCwire	Pittsburgh Supercomputing Center deploys disk-based data repository	
8/15/12	ISGTW	Record-breaking U.S. drought set to become the norm	
8/10/12	InsideHPC	Researchers encouraged to take XSEDE Cloud Use Survey	
8/8/12	Phys.Org	UC San Diego, Yale awarded collaborative NSF grant for Neuroscience Gateway	Also in Equities.com, HPCwire, UC Health
8/78/12	ISGTW	Building a new bridge between XSEDE and PRACE	
8/7/12	HPCwire	XSEDE brings in NCSA's Alan Craig as Digital Humanities Specialist	
8/7/12	HPCwire	Steven Reiner urges scientists to tell their stories	
8/2/12	HPCwire	Proving the case for climate change with hi-res models	

Date	Source	Headline	Notes
8/1/12	HPCwire	XSEDE identifies Fellows for Campus Champions program	
		0	
7/30/12	HPCwire	Deeper collaboration between PRACE and XSEDE proposed	
7/30/12	HPC In the Cloud	New API delivers science as a service	
7/27/12	genomeweb	TACC's API for scientific computing on the web	
7/26/12	HPCwire	Lack of minority representation in science and engineering endangering US economic health	
7/26/12	PhysOrg	Chasing science as a service	Also in: EurekAlert!, ECN
7/25/12	NSF	XSEDE project brings advanced cyberinfrastructure, digital services and expertise to nation's scientists and engineers	
7/25/12	HPCwire	XSEDE gaining speed as year two begins	
7/20/12	HPCwire	PRACE, XSEDE issue call for Expressions of Interest	
7/23/12	ISGTW	PRACE and XSEDE call for expressions of interest for joint access by international teams	
7/18/12	HPCwire	Penguin computing offers on-demand cycles to university partners	
7/18/12	HPC In the Cloud	Penguin Computing offers HPC compute clouds build for academia and research	
7/18/12	ISGTW	Field of Dreams: How are the XSEDE users using the infrastructure?	
7/17/12	ISGTW	Building bridges: XSEDE and PRACE announce joint call at XSEDE'12	
7/17/12	Clarkson University News & Events	Clarkson University's Maria Gracheva edits nanopore book	
7/17/12	HPCwire	Indiana University team accelerates gene expression software	
7/17/12	HPCwire	PRACE, XSEDE team up to promote trans-Atlantic collaboration	
7/16/12	insideHPC	Video: David Lifka on Red Cloud -- On Demand Research Computing	
7/16/12	ISGTW	Video: David Lifka on Red Cloud -- on demand research computing	
7/16/12	ISGTW	Bridging from the eXtreme to the campus and beyond at XSEDE12	
7/16/12	ISGTW	Third Annual HPC Summer School welcomes 60 students from 4 continents	
7/16/12	HPCwire	PRACE-XSEDE summer school hosts students from 4 continents	
7/9/12	Medicalxpress.com	Small molecule may play big role in Alzheimer's disease	Also in: EurekAlert!, HPCwire, ScienceDaily, eScienceNews, Biospace.com, on Twitter, and several blogs
7/5/12	HPCwire	Pittsburgh Supercomputing Center delivers training to minority institutions	
7/4/12	ISGTW	Five ways to anticipate natural disasters	
7/4/12	HPCwire	Supercomputing gateway helps researchers discover evolutionary relationships	
7/3/12	Newswise	SDSC's CIPRES science gateway clarifies branches in evolution's 'tree of life'	
7/3/12	EurekAlert!	SDSC's CIPRES science gateway clarifies branches in evolution's 'tree of life'	

E.2.2 Operations 1.2

1.2.1 Security

The XSEDE security team has identified the following metrics for tracking security incidents and response. summarizes the metrics, and details on any incidents are provided in the main body of the report. Of the two compromised accounts, one was reactivated after a password change, while the other user never responded to emails/calls from staff and remains suspended.

Table 27. XSEDE security metrics and incident response

	Q4 2011	**Q1 2012**	**Q2 2012**	**Q3 2012**
XSEDE-wide notice of vulnerability	0	0	0	0
Compromised user accounts	5	0	0	2
Other incident response	1	0	0	0
Critical rollout of vulnerability patches	0	0	0	0
Security enhancement rollouts	0	0	1	0

1.2.2 Data Services

XSEDE supports monitoring for two central data movement services: the gridFTP service connecting the XSEDE service providers and the Globus Online service for connecting XSEDE service providers as well as external sites. Table 28 shows quarterly summary metrics and increasing Globus Online adoption over the past four quarters, while Figure 45 and Figure 46 show Globus Online and GridFTP activity, respectively, by SP site.

Table 28. Globus Online activity to and from XSEDE endpoints, excluding GO XSEDE speed page user.

		Q4 2011	**Q1 2012**	**Q2 2012**	**Q3 2012**
To/from XSEDE endpoint	Files to XSEDE	8 million	27.6 million	34.8 million	57.1 million
	TB to XSEDE	216	232	824	311
	Files from XSEDE	21.8 million	17.8 million	23.9 million	44.9 million
	TB from XSEDE	180	242	185	325
	Faults detected	573,000	584,000	971,000	985,000
	Users	124	149	187	218
To/from XSEDE via Globus Connect	Files to XSEDE	1.5 million	6.3 million	2.5 million	24.9 million
	TB to XSEDE	19	45	18	37
	Files from XSEDE	1.4 million	0.6 million	2.2 million	9.4 million
	TB from XSEDE	20	25	11	34
	Faults detected	102,000	242,000	381,000	575,000
	Users	74	87	97	138

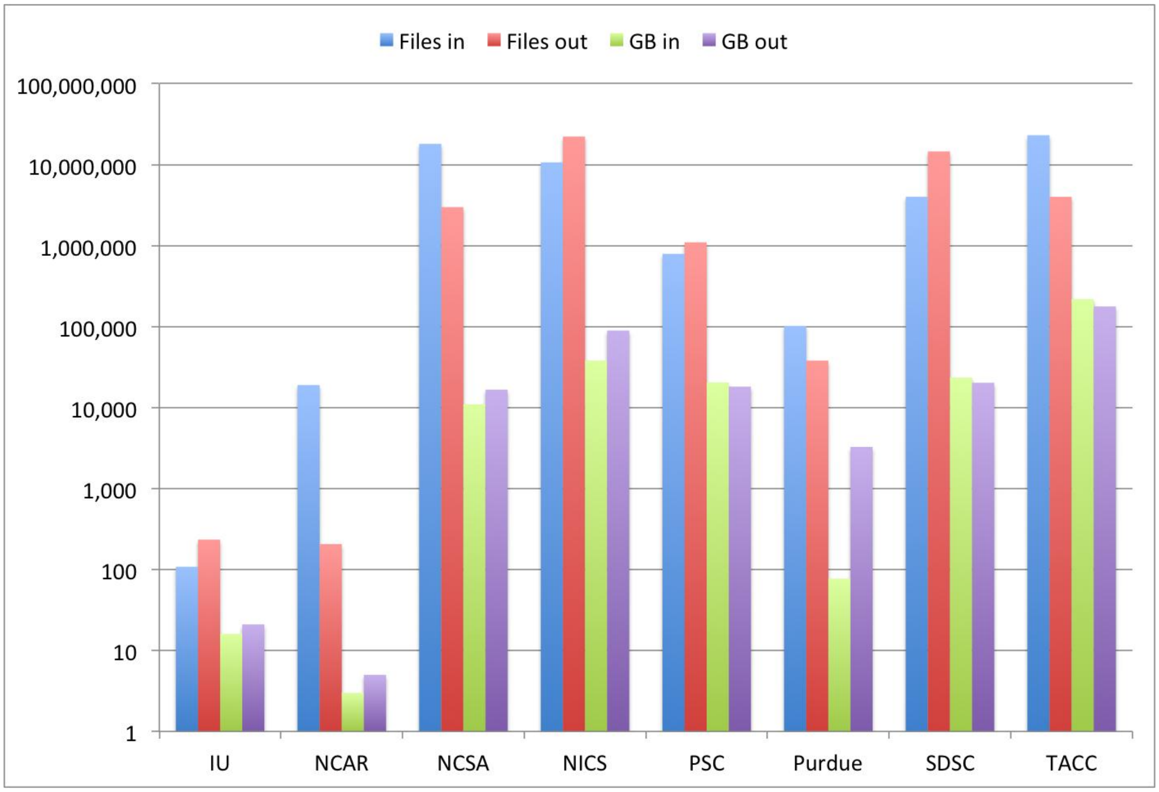


Figure 45. Globus Online activity into and out of XSEDE SP end points

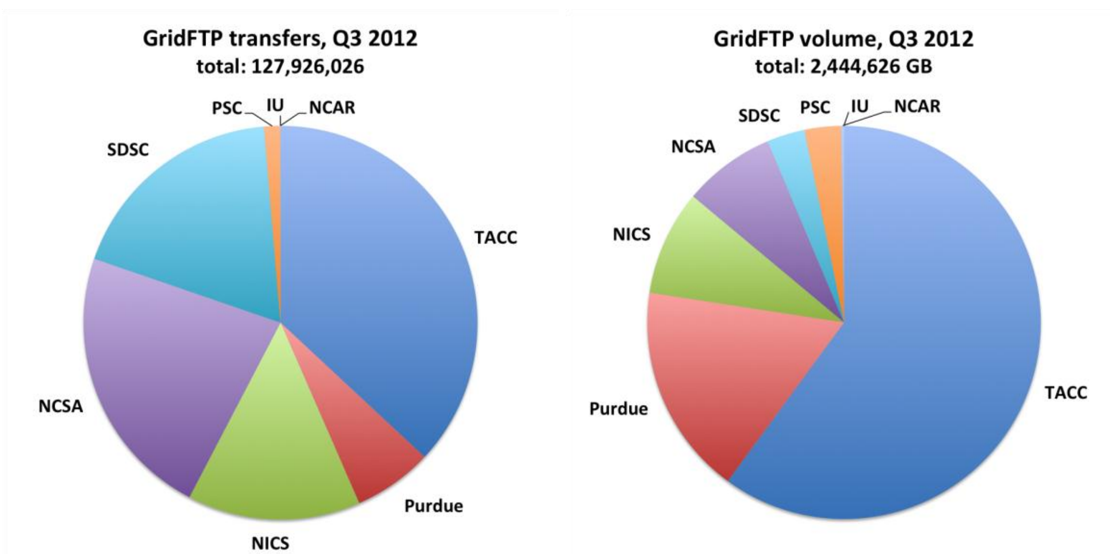


Figure 46. GridFTP volume and file transfers, per SP site.

1.2.3 XSEDEnet

Traffic utilization of the Chicago-Denver XSEDEnet link is shown in two figures below. Figure 47shows the peak bandwidth across the link for the period. Figure 48 shows link utilization as a percentage. Traffic across all XSEDEnet links is shown in Figure 49.

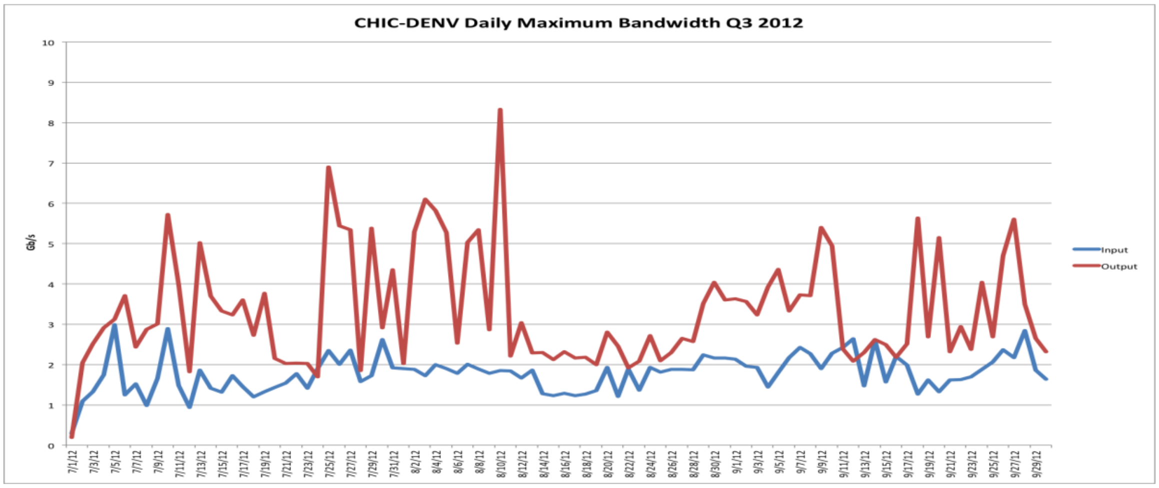


Figure 47. XSEDEnet Chicago-Denver peak bandwidth

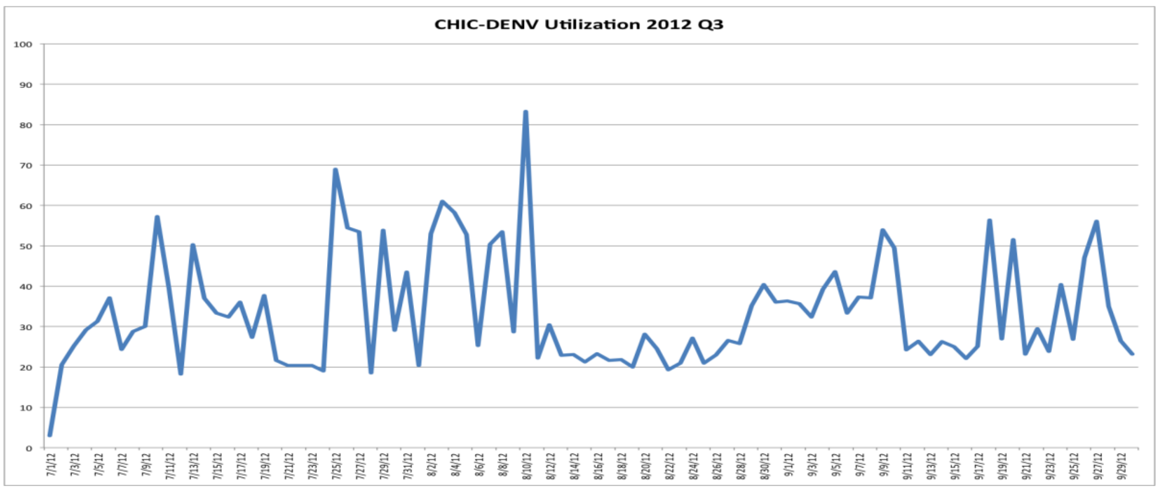


Figure 48. XSEDEnet Chicago-Denver utilization (as a percentage)

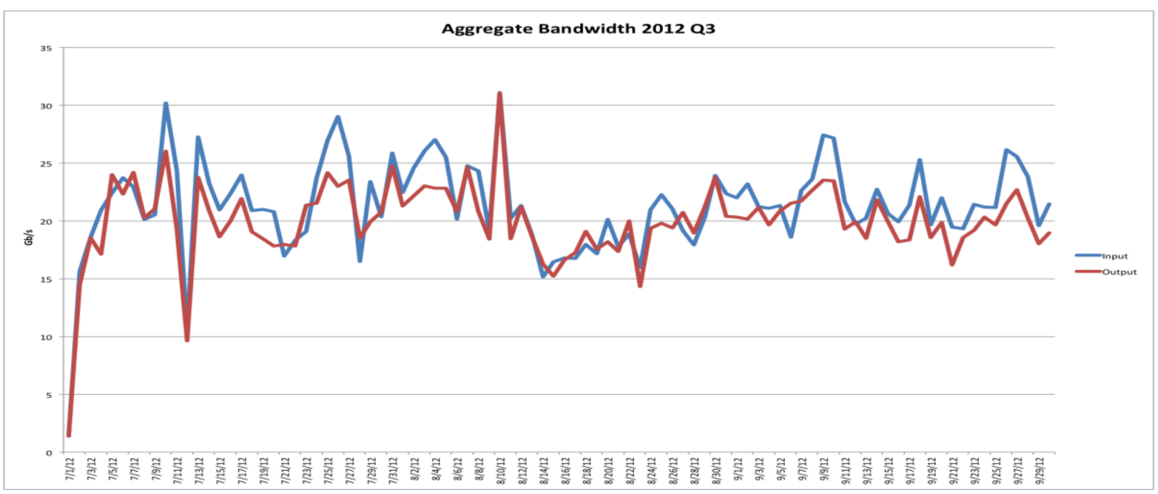


Figure 49. XSEDEnet Q3 2012 aggregate bandwidth across all links

1.2.5 Accounting and Account Management

The Accounting and Account Management group administers and operates the software for the XSEDE allocations system (POPS), the accounting system, and user account management. Table 29 shows the processing time for ongoing allocation requests outside of the quarterly XRAC requests. XSEDE reduced the account creation time to a matter of minutes with the deployment of POPS and User Portal components that allow users to create their own portal logins.

Table 29. Average time to process allocation requests and account creation requests, in days. (Excludes quarterly XRAC requests; "n/a" indicates none submitted.)

ALLOCATION REQUESTS		**Q4 2011**	**Q1 2012**	**Q2 2012**	**Q3 2012**
Research	Advance	12	6	7	5
	Transfer	4	3	3	5
	Supplement	27	25	14	7
	Justification	54	15	n/a	44
Startup, Education, Campus Champions, Discretionary	New	13	9	9	10
	Renewal	11	10	6	3
	Transfer	4	3	3	4
	Supplement	11	4	4	8
Account creation requests		4.6	1.8	0.03	0.03

1.2.6 Systems Operational Support

The Systems Operational Support group encompasses the XSEDE Operations Center (XOC), which includes front-line user support and the ticket system, and the system administration of all XSEDE centralized services. In the ticket system, XSEDE tracks total ticket volume and responsiveness (Table 30), which groups ("resolution centers") field the tickets (Table 31), and the numbers of tickets in seven common categories (Table 32 and Figure 50). The totals by resolution center and by category do not add up to the total number of tickets opened and closed because some tickets are resolved by staff not in a resolution center and some resolution centers have non-standard categories.

For the central services, XSEDE tracks the uptime reported by system administrators (Table 33) as well as the Inca-reported uptime for seven key user-visible services (Table 34). The Inca-reported uptime better reflects "user-visible outages," that is, what the average user would experience, and typically exceeds the actual system uptime, reflecting the effectiveness of XSEDE's backup systems, failover capabilities, and operational responsiveness.

Table 30. XSEDE Operations Center ticket system metrics.

	Q4 2011	**Q1 2012**	**Q2 2012**	**Q3 2012**
Total tickets opened	2,140	2,651	2,744	2,421
Tickets opened – email	1,318	2,381	2,448	2,175
Tickets opened – portal	684	254	26	18
Tickets opened – phone	138	16	270	228
Total tickets closed	2,111	2,335	2,394	2,028
Tickets, response in 24 hrs	1,550 (72%)	2,263 (85%)	2,326 (85%)	2,021 (83%)
Tickets closed within 2 bus. days	739 (35%)	1,044 (39%)	1,050 (38%)	880 (36%)

Table 31. Ticket breakdown (opened/closed) for each major resolution center.

	Q4 2011		**Q1 2012**		**Q2 2012**		**Q3 2012**	
	Opened	**Closed**	**Opened**	**Closed**	**Open**	**Closed**	**Open**	**Closed**
NICS	413	372	670	605	657	640	481	458
XOC	398	278	427	305	415	298	349	231
TACC	336	300	330	295	276	251	292	257
Proposal issues	142	97	343	251	408	376	403	358
SDSC	118	100	218	182	379	327	313	251
PSC	160	147	115	108	89	87	75	64

	Q4 2011		Q1 2012		Q2 2012		Q3 2012	
	Opened	**Closed**	**Opened**	**Closed**	**Open**	**Closed**	**Open**	**Closed**
Purdue	68	64	69	58	118	115	82	82
NCSA	45	36	60	42	89	72	83	81
User facing services	64	51	88	68	73	65	25	22
UST	16	14	12	9	11	11	11	11
IU	7	0	7	1	10	7	3	3
OSG	1	0	2	1	3	3	1	1
Others	*535*	*430*	*335*	*258*	*215*	*135*	*303*	*209*

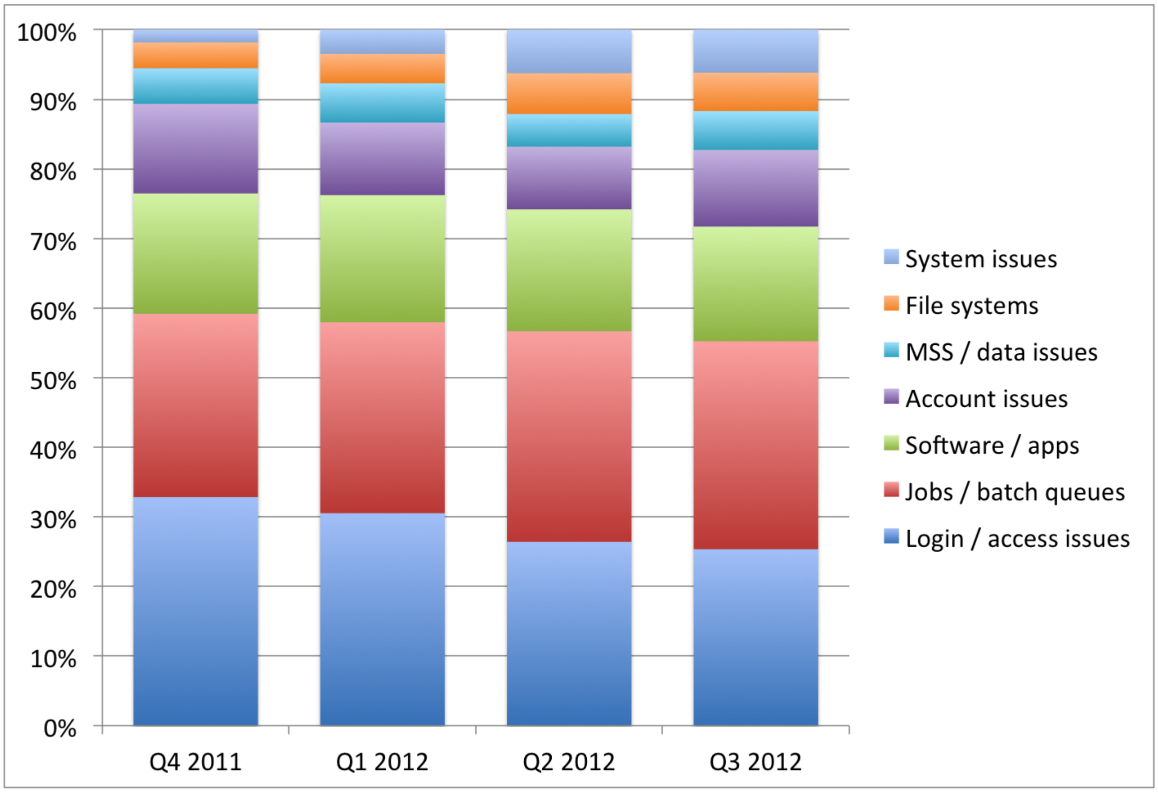


Figure 50. Tickets in seven primary problem categories. This chart represents a significant portion of tickets but does not represent the entire range. Tickets largely fit in the seven displayed categories; other categories are not significant enough to visually represent.

Table 32. Ticket counts for the seven primary problem categories shown in Figure 50.

	Q4 2011	Q1 2012	Q2 2012	Q3 2012
Login / access issues	416	483	445	345
Jobs / batch queues	334	434	510	407
Software / apps	219	289	295	224
Account issues	163	165	152	150
MSS / data issues	65	89	79	76
File systems	47	67	99	75
System issues	23	55	105	84

Table 33. XSEDE centralized service uptime and outages. Empty cells indicate *no outages (100% up)*. "% Up" is percent uptime; "Hrs (P|U)" shows outage hours, planned and unplanned.

Service	Q4 2011		Q1 2012		Q2 2012		Q3 2012	
	% Up	Hrs (P|U)	% Up	Hrs (P|U)	% Up	Hrs (P|U)	% Up	Hrs (P|U)
AMIE					99.91%	0|2		
AMIE backup	99.77%	5|0	99.98%	0.5|0				
Bugzilla			97.46%	0|56	99.82%	4|0		
Build and Test			97.46%	0|56	99.82%	4|0		
Certificate Authority			99.62%	8.5|0				
Data Movement Service								
Globus Listener			97.46%	0|56	99.82%	4|0		
IIS Metrics			97.46%	0|56	99.82%	4|0		
Inca	98.44%	3.75|30.75			99.31%	0|15	98.71%	26|2.5
Inca backup					99.50%	11|0		
Information Services	99.95%	0|1	97.46%	0|56	99.82%	4|0		
Karnak	98.60%	0|31	97.40%	0|57.5	99.82%	4|0	99.98%	0|0.5
Kerberos backup	99.91%	2|0	99.91%	2|0.08				
Knowledgebase								
MyProxy	99.73%	6|0						
Openfire Jabber								
POPS								
RDR	99.77%	5|0	98.69%	5|24				
Sciforma							99.84%	3.5|0
Secure Wiki								
SELS								
Sharepoint								
Software Distribution			97.46%	0|56	99.82%	4|0		
Source Repository			97.46%	0|56	99.82%	4|0		
Speedpage	99.91%	2|0	99.91%	2|0			99.95%	1|0
TG Wiki			97.46%	0|56	99.82%	4|0		
Ticket System								
Usage Reporting Tools								
User Portal	99.99%	0|0.17	99.97%	0|0.75				
User Portal backup			99.62%	8.5|0	99.95%	1|0		
User Profile Service			97.46%	0|56				
XDCDB	99.99%	0.25|0			99.91%	0|2	99.97%	0|0.75
XDCDB backup	99.77%	5|0	99.98%	0.5|0	99.91%	2|0	98.91%	0|24

Table 34. Inca-monitored XSEDE central services, Inca-detected uptimes, and outages.

Service	Outage definition. Test frequency.	Q4 2011	Q1 2012	Q2 2012	Q3 2012
Inca	Inca status pages unavailable or test details page fails to load. Every 5 min.	98.4%	100%	99.3%	98.71%
Information Services	Information web pages unavailable. Every 15 min.	99.95%	99.97%	99.9%	100%
Karnak	Karnak front page fails to load. Every 30 min.	98.6%	99.93%	99.9%	99.98%
MyProxy	MyProxy server does not respond to credential check. Every hour.	99.7%	100%	100%	100%
User Portal	Portal home page fails to load correctly. Every 30 min.	100%	99.98%	100%	99.98%
XDCDB	Connection to database refused or slow (using check_postgres.pl script). Every 5 min.	100%	100%	99.99%	99.96%

E.2.3 User Services 1.3

The User Information and Interfaces group provides XSEDE users with central information and services via the XSEDE User Portal (XUP), web site, XUP mobile, and knowledgebase. Table 35 shows increasing activity on most user information interfaces, as well as increases in the numbers of logged-in users accessing these interfaces. Table 36 shows the most popular XUP applications, by visits.

Table 35. XSEDE web site, user portal and XUP Mobile activity. (Note: "Users" indicates logged-in users.)

UII Activity	Q4 2011	Q1 2012	Q2 2012	Q3 2012
Web hits	1,924,648	2,667,120	2,676,532	2,362,105
Web visitors	24,208	38,502	33,362	33,053
XUP hits	1,164,994	1,340,704	1,465,537	1,540,402
XUP visitors	10,346	14,913	13,787	16,118
XUP accounts	4,205	6,159	7,563	9,015
XUP users (logged in)	3,024	3,919	3,976	4,399
XUP users (logged in and running jobs)	1,219	1,554	1,552	1,552
XUP Mobile hits	1,702	1,307	1,693	1,931
XUP Mobile users	48	37	25	20
KB docs retrieved	64,679	68,619	57,451	87,987
Total KB docs	405	478	497	538
New KB docs	25	73	19	62

Table 36. XUP and Web site application visits. "Users" indicates logged-in users.

	Q4 2011		Q1 2012		Q2 2012		Q3 2012	
Application	**Visits**	**Users**	**Visits**	**Users**	**Visits**	**Users**	**Visits1**	**Users**
Allocations/Usage	69,290	2,991	49,261	3,803	50,998	3,724	45,899	3,773
File Manager	60,009 (transfers)	60 (3.9 TB)	31,952 (transfers)	79 (2.5 TB)	21,375 (transfers)	78 (20 TB)	42,219 (transfers)	97 (3.6 TB)
User News	4,312	25	62,784	526	47,194	2,013	25,707	263
GSI-SSH	34,132	1,083	24,714	1,343	28,317	1,354	22,411	1,286
Resource Listing	100,544	864	36,244	1,104	22,483	1,265	16,934	1,391
System Accounts	13,457	1,609	12,897	1,841	12,235	1,813	10,919	1,731
Training Registration	12,648	345	19,535	828	11,642	631	10,556	650
Software Search	14,812	176	8,204	265	8,879	316	9,903	318
Knowledge Base	17,454	261	11,436	377	10,964	338	8,269	156
System Monitor	13,350	1,050	8,213	1,257	9,401	1,034	6,819	985
POPS Submit					5,639	1,204	5,982	1,117
User Profile			1,954	833	5,476	1,262	5,930	1,345
Science Gateways List	51,684	180	16,338	229	8,914	234	5,470	158
Help Desk (Consulting)	6,206	557	4,659	748	4,815	733	4,704	652
Add User Form	8,406	611	5,751	626	4,628	617	4,446	547
Publications ***(added Sep. 10, 2012)***							2,908	595
My Jobs	5,640	908	3,500	960	3,195	900	2,634	788
Ticketing System	3,708	609	2,366	682	2,600	654	2,229	609
Online Training Listing	2,720	215	2,093	347	1,668	437	1,414	220
SU Calculator (web)	4,376	180	2,048	243	1,466	239	1,240	109
Karnak Q Prediction	1,770	212	1,108	222	871	264	643	182
Feedback form	1,174	57	791	53	426	39	333	17
Community Accounts					436	311	318	259
Gateway Registration					243	16	238	8
DN Listing	1,092	399	554	371	450	326	127	99

E.2.4 Extended Collaborative Support Service 1.4, 1.5

The Extended Collaborative Support Service pairs members of the XSEDE user community with expert staff in projects lasting up to a year to solve challenging science and engineering problems. Table 37 shows project and staffing metrics. Table 38 shows metrics for Extended Support for Training, Education, and Outreach.

Table 37. Extended Collaborative Support project and staffing activity

		Q4 2011	Q1 2012	Q2 2012	Q3 2012
Project requests	XRAC	16	22	20	14
	Supplemental/Startups	21	41	28	30
	ECSS In-house project		1	0	0
Projects initiated	Research Team	18	19	14	15
	Community Codes	9	8	7	3
	Science Gateways	4	6	6	2
	Unassigned		7	0	2
Projects cancelled/no-go	XRAC	1	4	5	5
	Supplemental/Startups	9	20	16	17
Projects active	Research Team (XRAC)	7	27	29	26
	Research Team (S/S)	4	17	20	19
	Research (TG)	29	12	1	0
	Subtotal	**40**	**56**	**50**	**45**
	Community Codes (XRAC)	3	6	10	9
	Community Codes (S/S)	3	9	17	18
	Community Codes (TG)	2	2	2	1
	In-house		1	1	1
	Subtotal	**8**	**18**	**30**	**29**
	Science Gateways (XRAC)		4	9	9
	Science Gateways (S/S)		7	10	8
	Science Gateways (TG)	10	4	1	0
	Subtotal	**10**	**15**	**20**	**17**
	Total Projects Active	**58**	**89**	**100**	**91**
Work plans		6	14	10	14
Projects completed		11	16	15	11
Novel, Innovative Projects (NIP)	User groups engaged	15	20	47	65
	NIP-led ECS planning efforts	8	9	9	3
	NIP ECS requests (prospective user groups)	14	23	38	42
	NIP ECS projects active	5	7	9	10
	NIP outreach events	9	9	16	21
ECSS staffing (FTE)	Research Team	13.72	13.28	12.8	13.19
	Community Codes	6.73	7.11	8.24	8.14
	Science Gateways	4.83	4.92	4.73	4.63
	NIP	5.30	5.79	5.64	5.64
	TEO	4.02	4.42	3.53	3.43
	Total	**34.60**	**35.52**	**34.94**	**35.03**

Table 38. Extended Support for Training, Education and Outreach 1.5.3

	Q4 2011		Q1 2012		Q2 2012		Q3 2012	
Description	**#**	**Staff**	**#**	**Staff**	**#**	**Staff**	**#**	**Staff**
Requests for service	1	1	4	4	2	2	0	0
User meetings and BOFs	7	9	2	2	18	20	11	12
Mentoring	3	3	3	2	12	12	9	9
Talks and presentations	7	8	12	9	20	20	15	22
Tutorials	3	3	21	25	31	32	12	18
Online tutorials and webinars	1	3	4	6	0	0	3	3
Online tutorial reviews	5	4	6	6	17	17	2	2

F XSEDE Publications Listing

F.1 XSEDE Staff Publications

F.1.1 Project Office 1.1

1. D. L. Hart, Longitudinal user and usage patterns in the XSEDE user community. Proceedings of the 1st Conference of the Extreme Science and Engineering Discovery Environment on Bridging from the eXtreme to the campus and beyond - XSEDE '12. Chicago, Ill.. 2012.
2. Foster, I., Kettimuthu, R., Martin, S., Tuecke, S., Hauser, T., Milroy, D., Palen, B. and Braden, J., “Campus Bridging Made Easy via Globus Services”, XSEDE 2012, Chicago, IL, USA, 2012.
3. Stewart, C., Knepper, R., Ferguson, J., Bachmann, F., Foster, I., Grimshaw, A., Hazlewood, V. and Lifka, D., “What is Campus Bridging and what is XSEDE doing about it?”, XSEDE, Chicago, IL, USA, 2012, ACM Press.
4. Ian Foster, XSEDE panel: SaaS for Science, XSEDE’12, Chicago, IL, July 18, 2012
5. I. Foster, "Big process for big data: Process automation for data-driven science", Keynote, Latin American HPC Conference, Buenos Aires, Argentina, July 24, 2012.
6. Bo Liu, “Integrating Galaxy with Globus Online: Lessons learned from the CVRG project” Presentation at the Galaxy Community Conference, Chicago, July 26, 2012.
7. S. Tuecke, “Globus Online for NCAR Users”, NCAR Live webcast, August 16, 2012.
8. K. Wallnau, F. Bachmann, M. Konrad, J. Brown, J.-P. Navarro, “Improving XSEDE Software Quality Using Software Engineering Best Practices”, XSEDE 12 Conference, Chicago Illinois, July 18, 2012.

F.1.2 Operations 1.2

9. C. Stewart, F. Bachmann, V. Hazlewood, et al., What is campus bridging and what is XSEDE doing about it?. Proceedings of the 1st Conference of the Extreme Science and Engineering Discovery Environment on Bridging from the eXtreme to the campus and beyond - XSEDE '12. Chicago, Illinois. 2012.
10. Foster, S. Tuecke, T. Hauser, et al., Campus bridging made easy via Globus services. Proceedings of the 1st Conference of the Extreme Science and Engineering Discovery Environment on Bridging from the eXtreme to the campus and beyond - XSEDE '12. Chicago, Illinois. 2012.
11. B. Allen, K. Pickett, S. Tuecke, et al., Software as a service for data scientists. Communications of the ACM. 55 / 2. 2012.
12. Moore, R. L.; Carson, L.; Ghadersohi, A.; Jundt, A.; Yoshimoto, K.; Young, W.; “Optimization of Throughput and Utilization on Trestles.” XSEDE’12, July 2012, Chicago, IL, USA. ACM TBD.

F.1.3 User Services 1.3

F.1.4 Extended Collaborative Support Service –1.4, 1.5

13. Rane A., Browne J., Koesterke L. “A Systematic Process for Efficient Execution on Intel’s Heterogeneous Computation Nodes” *Presentation at XSEDE12 Conference*
14. Schulz K. “A Distributed Memory Out-of-Core Method on HPC Clusters and its Application to Quantum Chemistry Applications” *Presentation at XSEDE12 Conference*
15. Hanning C., Zhu X. “Electrostatic Screening Effects on a Model System for Molecular Electronics” *Presentation at XSEDE12 Conference*
16. Willmore F. “Tools for the Visualization and Analysis of Free Volume in Materials” *Presentation at XSEDE12 Conference*
17. V. Betro, E. Duque, N. Wyman, Meshing, Visualization, and Computational Environments Technical Committee Year In Review. AIAA Aerospace America. December 2012. 2012.
18. W. E. Brock, S. L. Karman, C. Burdyshaw, et al., Adjoint-Based Design Optimization Using CAD Parameterization Through Capri. AIAA ASM. Nashville, TN. 2012.
19. Betro, V., Brook, G., and Hulguin, R. "Hybrid Message Passing and Threading for Heterogeneous Use on CPUs and the Intel Many Integrated Core (MIC) Architecture". Proceedings of the XSEDE Extreme Scaling Workshop 2012: Chicago, IL. July 15-16, 2012.
20. Chourasia, Amit (2012). “Memory Layout Experiments for Common Visualization Tasks” Presented at XSEDE 12 Conference, Chicago, Jul 2012.
21. Chourasia, Amit; Ogden, D.; Choi, D. J.; and Wohletz, K. (2012) “Snapshots of a Volcano Eruption Simulation". Presented at Visualization Showcase at XSEDE 12 conference, Chicago, July 2012.
22. Chourasia,Amit, Zhou, J. ; Cui, Y.; Choi, D.J. ; Olsen, K. B. ; (2012)"Role of visualization in porting a seismic simulation from CPU to GPU architecture". Presented at Visualization Showcase at XSEDE 12 conference, Chicago, July 2012.

23. Dickson, C.J.; Rosso, L.; Betz, R.M.; Walker, R.C.; Gould, I.R., "GAFFlipid: a General Amber Force Field for the accurate molecular dynamics simulation of phospholipid.", Soft Matter,2012, 8, 9617-9627, DOI: 10.1039/C2SM26007G
24. Isborn, Christine; Goetz, Andreas W.; Walker, Ross C.; Martinez, Todd - “Ab Initio QM/MM Molecular Dynamics with TeraChem and AMBER: Exploring Environmental Effects on the Absorption Spectrun of Photoactive Yellow Protein”, Gordon Research Conference in Computational Chemistry, Mount Snow, VT., July 2012. (Poster).
25. Pierce, L.C.T.; Salomon-Ferrer, R.; de Oliveira, C.A.F.; McCammon, J.A.; Walker, R.C., "Routine access to millisecond timescale events with accelerated molecular dynamics.", Journal of Chemical Theory and Computation, 2012, 8(9), 2997-3002, DOI: 10.1021/ct300284c
26. Salomon-Ferrer, R.; Case, D.A.; Walker, R.C.; "An overview of the Amber biomolecular simulation package", WIREs Comput. Mol. Sci., 2012, in press, DOI: 10.1002/wcms.1121
27. Skjevik, A.A,; Madej. B.D.; Walker, R.C.; Teigen, K.; "LIPID11: A Modular Framework for Lipid Simulations Using Amber", Journal of Physical Chemistry B, 2012, 116 (36), pp 11124-11136, DOI: 10.1021/jp3059992
28. Walker, R. C., “Extreme acceleration of AMBER molecular dynamics: Sampling for the 99%”, Gordon Research Conference in Computational Chemistry, Mount Snow, VT, Invited Speaker. July 2012.
29. Walker, R. C., “Transforming Molecular Biology through Extreme Acceleration of Molecular Dynamics”, XSEDE 12 Conference, Chicago, Il, July 2012.
30. Walker, R. C.; “Extreme acceleration of AMBER molecular dynamics.” Joint Charmm/Amber meeting, NIH, MD. July 2012, Invited Speaker.

F.1.5 Education and Outreach 1.6

31. C. Wigal, V. Betro, Engineering Education’s Role in Improving Student Understanding and Learning of Mathematics and Sciences. ASEE SE Section Meeting. Starkville, MS. 2012.
32. Baxter, Diane, (2012). “Building Collaborations for Computing Principles Education” Presented at XSEDE 12 Conference, Chicago, July 2012

F.2 Publications from XSEDE Users

The following publications were gathered from Research submissions to the September 2012 XSEDE Resource Allocations Committee (XRAC) meeting. Renewal submissions are required to provide a file specifically to identify publications resulting from the work conducted in the prior year. The publications are organized by the proposal with which they were associated. This quarter, users identified 775 publications and conference papers that were published, in press, accepted, submitted, or in preparation.

ASC040046

1. Situ, Y., Liu, L., Martha, C. S., Louis, M., Li, Z., Sameh, A. H., Blasidell, G. A., and Lyrintzis, A. S., “A communication-efficient linear system solver for large eddy simulation of jet engine noise.” Cluster Computing, published on-line 10 Sept. 2011, DOI 10.1007/s10586-011-0180-9. (Selected papers from the Proceedings of the IEEE Cluster 2010 Conference held September 20-24, 2010 in Heraklion, Crete.) [Revised and expanded version of the conference paper reported last year.]
2. Blaisdell, G., Lyrintzis, A., Situ, Y., Martha, C., Louis, M., Li, Z., “Recent Advances in Large Eddy Simulations for Jet Noise Predictions,” Inter-Noise 2011 Conference, September 4-7, Osaka, Japan, 2011. [Reported last year as to be presented, but now as a published conference paper.]
3. Martha, C., Situ, Y., Louis, M., Blaisdell, G., Lyrintzis, A., Li, Z., “Development of an Efficient, Multiblock 3- D Large Eddy Simulation Tool for Jet Noise,” AIAA Paper 2012-0833, AIAA Aerospace Sciences Meeting, Nashville, TN, January 2012. [Reported last year as a submitted abstract, but now as published conference paper.]
4. Situ, Y., Liu, L., Martha, C. S., Louis, M. E., Li, Z., Sameh, A. H., Blasidell, G. A., and Lyrintzis, A. S., “Petascale Large Eddy Simulation of Jet Engine Noise based on the Truncated SPIKE Algorithm,” submitted to Parallel Computing, May 2012. [submitted journal paper]
5. Lo, S.-C., Aikens, K., Blaisdell, G., and Lyrintzis, A., “Numerical Investigation of 3-D Supersonic Jet Flows using Large-Eddy Simulation,” submitted to the International Journal of Aeroacoustics June 2012. [submitted journal paper]

ASC070008

6. Tiwari A, Laurenzano M, Carrington L, Snavely A: Modeling Power and Energy Usage of HPC Kernels. High Performance Power-Aware Computing (HPPAC12) 2012.
7. Tiwari A, Laurenzano M, Carrington L, Snavely A: Auto-tuning for Energy Usage in Scientific Applications. In: Proceedings of Workshop on Productivity and Performance (PROPER 2011): 2011; Bordeaux, France; 2011.
8. Laurenzano M, Meswani M, Carrington L, Snavely A: Reducing Energy Usage with Memory and Computation-Aware Dynamic Frequency Scaling. In: Euro-Par 2011: 2011; France; 2011.
9. Carrington L, Ffrench P, Hawkins R, Snavely A: Performance Estimation of HPCMP Applications on General Purpose Graphics Processing Units (GPGPUs). In: UGC2011: 2011; Portland, OR; 2011.
10. Meswani M, Carrington L, Unat D, Snavely A, Baden S, Poole S: Modeling and Predicting Performance of High Performance Computing Applications on Hardware Accelerators. Proc of the 2nd Int'l Workshop on Accelerators and Heterogenous Exascale Systems (AsHES 2012) 2012.
11. Meswani M, Carrington L, Unat D, Peraza J, Snavely A, Baden S, Poole S: Modeling and Predicting Application Performance on Hardware Accelerators. In: IEEE International Symposium on Workload Characterization (IISWC-2011): 2011; Austin, TX; 2011.
12. Proceedings of the Tools for Benchmarking, Tracing, and Simulating SHMEM Applications: 2012; Stuttgart, Germany.

ASC090058

13. Zhuhua Cai, Yener Kuru, Jeong Woo Han, Yan Chen, and Bilge Yildiz, "Surface Electronic Structure Transitions at High Temperature on Perovskite Oxides: The Case of Strained La0.8Sr0.2CoO3Thin Films", J. Am. Chem. Soc.133(2011) 17696-17704.
14. Jeong Woo Han and Bilge Yildiz, "Enhanced one dimensional mobility of oxygen on strained LaCoO3(001) surface", J. Mater. Chem.21(2011) 18983-18990
15. Jeong Woo Han and Bilge Yildiz, "Mechanism for enhanced oxygen reduction kinetics at the (La,Sr)CoO3-δ/(La,Sr)2CoO4+δhetero-interface", Energy Environ. Sci.Advance Article (2012) DOI:10.1039/C2EE03592H.
16. Jennifer L. M. Rupp, Emiliana Fabbri, Jeong Woo Han, Dario Marrochelli, Daniele Pergolesi, Enrico Traversa, Bilge Yildiz, and Harry L. Tuller, "Strain Toolbox to Play with Metal Oxides Lattice", in preparation for Nature Mater.(2012).
17. Jeong Woo Han and Bilge Yildiz, "Driving Forces for Segregation of Dopants on the LnMnO3(Ln=La, Sm) Surface", in preparation for J. Am. Chem. Soc.(2012).
18. Jeong Woo Han and Bilge Yildiz, "Driving Forces for Segregation of Dopants on the LnMnO$_3$(Ln=La, Sm) Surface", E-MRS Meeting, Strasbourg, France, May 14-18, 2012.
19. Dario Marrocchelli, Jennifer L.M. Rupp, Jeong Woo Han, and Bilge Yildiz, "Strain and Defect Ordering in doped CeO$_2$thin films", E-MRS Meeting, Strasbourg, France, May 14-18, 2012.
20. Wonyoung Lee, Jeong Woo Han, Zhuhua Cai, and Bilge Yildiz, "The Role of Chemical Heterogeneities on Oxygen Reduction Kinetics on the Surface of Thin Film Cathodes", 221st ECS Meeting, Seattle, WA, May 6-10, 2012.
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412. T.C. Luu, Lattice QCD and Nuclear Physics: Petascale, Exascale, and Beyond", Bi-annual Meeting of the Norwegian Physical Society, Oslo Norway June, 2011.
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414. A. Walker-Loud, Applications of Lattice QCD to Low Energy Nuclear Physics, Theoretical Hadron Physics Seminar, University of Tokyo, Japan (Nov. 2011).
415. A. Walker-Loud, 2-Hadron Interactions from Lattice QCD, Invited Seminar for the 4th Berkeley School on Collective Dynamics in High-Energy Collisions (May 2012).
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437. Invited talk Magnetized Turbulence in the Multiphase ISM" (Presenter: Alexei Kritsuk), KITP Program: The Nature of Turbulence, Santa Barbara, California, May 13, 2011.
438. Invited talk Comparing Numerical Methods for Isothermal Magnetized Supersonic Turbulence" (Presenter: Alexei Kritsuk), ASTRONUM 2011: 6th International Conference on Numerical Modeling of Space Plasma Flows, Valencia, Spain, June 13, 2011.
439. Contributed talk On the Density Distribution in Star-forming Interstellar Clouds" (Presenter: Mike Norman), 2011 TeraGrid Conference: Extreme Digital Discovery, Salt Lake City, Utah, July 2011.
440. Contributed talk What Shapes the Structure of Molecular Clouds: Turbulence or Gravity?" (Presenter: Alexei Kritsuk), CCAT Meeting: Formation and Development of Molecular Clouds, Cologne, Germany, October 5, 2011.
441. Invited talk, The Two States of Star Forming Clouds" (Presenter: David Collins), Center for Magnetic Self-Organization, University of New Hampshire, October 2011.
442. Invited talk, An Introduction to Star Formation and Magnetic Fields" (Presenter: David Collins), Young CMSO, University of New Hampshire, October 2011.
443. Invited talk, ISM Turbulence: Effects of Compressibility and Gravity" (Presenter: Alexei Kritsuk), 6th Korean Astrophysics Workshop: Fundamental Processes in Astrophysical Turbulence, Pohang, South Korea, November 17, 2011.
444. Contributed talk, Turbulence and Gravity in Molecular Cloud Structure Formation" (Presenter: Alexei Kritsuk), Turbulence in Cosmic Structure Formation, ASU, Tempe, Arizona, March 5, 2012.
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446. Invited talk, Compressible Turbulence in the Interstellar Medium" (Presenter: Alexei Kritsuk), KITPC Program: New Directions in Turbulence, KITPC, Beijing, China, April 4, 2012.
447. Invited talk Strong Magnetic-field Fluctuations in Supersonic Turbulence" (Presenter: Alexei Kritsuk), ASTRONUM 2012: 7th International Conference on Numerical Modeling of Space Plasma Flows, Kona, Hawaii, June 25, 2012.

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628. MD SIMULATIONS REVEAL ULTRAFAST DIELECTRIC COMPENSATION BY WATER OF LARGE STOKES SHIFTS FROM CHARGED GROUPS IN STAPHYLOCOCCAL NUCLEASE. Poster Presentation Time: February 29 2012 10:30 AM Session Title: Molecular Dynamics II, Location: Hall FGH, J. Nathan Scott, Patrik R. Callis. Montana State University, Bozeman, MT, USA.
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G XSEDE Citation Report

Content for this appendix is pending the publication and subsequent citation of a research paper on the XSEDE project. XSEDE allocated users will be requested to cite this paper in their publications, thus enabling a more comprehensive analysis of the science impact of the XSEDE project.

H XSEDE EOT Event Details

Type	Title	Location	Date(s)	Hours	Number of Participants	Number of Under-represented people	Method	Funding Sources
Workshop	Computational Biology for Biology Educators	Montogmery College Germantown, MD	July 16-18, 2012	14	21	5	Synchronous	XSEDE
Workshop	Computational Chemistry for Chemistry Educators	University of Pittsburgh, Pittsburgh, PA	June 11-15, 2012		22	5	Synchronous	XSEDE
Workshop	Introduction to Computational Thinking with a Parallel Perspective	Southern University, BatonRouge, LA	June 11-14, 2012		21	11	Synchronous	XSEDE
Workshop	Introduction to Parallel Programming and Cluster Computing	University of Oklahoma, Norman, OK	July 29 – Aug 4		41	18	Synchronous	XSEDE OK
Workshop	Kinder, Gentler Supercomputing: Using HPC Resources and Visualization Tools	Kean University, Union, NJ	July 23 - 25		12	5	Synchronous	XSEDE
Workshop	PICUP Summer 2012 Workshop for Computational Physics	California State Polytechnic University, Pomona, CA	June 27 – July 2, 2012		8	1	Synchronous	XSEDE AAPT/NSF/ComPADRE, and Bradley University
Workshop	Berkeley PARLAB Bootcamp	University of California, Berkeley	Aug 16-17, 2012		397		Synchronous	XSEDE
Paper Presentation	Petascale I/O: Challenges, Solutions, and Recommendations Crosby, L. D.; Mohr, R.	Extreme Scaling Workshop, Des Plaines, IL.	July 15, 2012	1.0			In-Person	
Tutorial	Metrics and Measurement for Understanding usage of a Visualization and Analysis HPC System	Texas Advanced Computing Center, Austin TX	September 27, 2012	1.0	7		In-person	

	Szczepanski, Amy							
Presentation	Extending Parallel Scalability of LAMMPS and Multiscale Reactive Molecular Simulations Peng, Y.; Knight, C.; Blood, P.; Crosby, L.; Voth G. A.	ECSS Symposium	September 18, 2012	1.5			Remote	
Presentation	JICS resources and centers	University of Tennessee Knoxville TN	September 12, 2012	1.5	8		In-person	
Presentation, Panel moderator	Welcome to UT – Resources and Centers Yost, Christal	University of Tennessee Knoxville TN	August 21, 2012	2.0	20		In-person	
Paper Presentation	Achieve Better Performance with PEAK on XSEDE Resources You, Haihang	XSEDE12, Chicago IL	July 18, 2012	0.5	30		In-person	
Tutorial	TIPS: Toward Improved Performance Solutions on XSEDE Resources You, Haihang	XSEDE12, Chicago IL	July 16, 2012	8.0	5		In-person	
Presentation	NICS and UTK Art collaborations Yost, C.; Ahern, S.; Ferguson, J.	University of Tennessee Knoxville TN	July, 2012	2.0	8		In-person	