

Indiana University Pervasive Technology Institute – Research Technologies: XSEDE Service Provider and XSEDE subcontract report (PY 1: 1 July 2011 to 30 June 2012)

3 October 2012

Version 1.0



Table of Contents

A.	Document History.....	v
B.	Document Scope.....	vi
C.	General introduction	1
D.	Indiana University Pervasive Technology Institute – Research Technologies Service Provider report.....	1
D.1.	Executive summary.....	1
D.2.	Indiana University Level 2 Service Provider systems: Resource descriptions.....	2
D.3.	Science highlights	3
D.4.	User-facing activities	4
D.4.1.	System activities	4
D.4.2.	Services activities	5
D.5.	Security	6
D.6.	Education, outreach, and training (EOT) activities	6
D.6.1.	IU SP EOT metrics	6
D.6.2.	EOT highlight: PTI Ready, Set, Robots Workshop 2012.....	12
D.7.	SP collaborations	12
D.8.	SP-specific activities.....	13
D.8.1.	IU Cyberinfrastructure Newsletter	13
D.8.2.	100 Gbps networking.....	13
D.9.	Publications.....	13
D.9.1.	Journal articles.....	13
D.9.2.	Peer-reviewed papers.....	14
D.9.3.	Other publications, not peer-reviewed.....	15
D.9.4.	Presentations	16
D.9.5.	Tutorials and courses taught	18
D.9.6.	Major conference displays	18
D.9.7.	Lay / business press placements	18
D.10.	Metrics	18
D.10.1.	Standard user assistance metrics	18
D.10.2.	SP-specific metrics	18
E.	Indiana University Pervasive Technology Institute – XSEDE subcontract report.....	20
E.1.	WBS 1.2.2 Data Services	20
E.2.	WBS 1.2.6 Systems Operational Support	20
E.2.1.	Virtual machines	20
E.2.2.	XD Operations Center Fail-over	20
E.3.	WBS 1.3.2 User Information and Interfaces	21
E.3.1.	Knowledge Base	21
E.3.2.	Other documentation activities	23
E.4.	WBS 1.3.3 User Engagement.....	23
E.5.	WBS 1.4/1.5 ECSS.....	24
E.6.	WBS 1.4.2 Novel & Innovative Projects	24
E.7.	WBS 1.5.2 Extended Support for Science Gateways.....	24
E.7.1.	Gateway Leadership.....	24
E.7.2.	UltraScan Science Gateway	24
E.8.	WBS 1.5.3 Extended Support for Training, Education, and Outreach	25

E.8.1.	Gateway Training and Outreach	25
E.8.2.	Dark Energy Survey Simulation Working Group.....	25
E.8.3.	Petascale computations in mineral physics with Quantum ESPRESSO (VLAB)...	26
E.9.	WBS 1.6.5 Campus Bridging	26
E.9.1.	Discussion of campus bridging within XSEDE and within the national cyberinfrastructure community.....	27
E.9.2.	Definition of use cases and quality attributes for XSEDE's Campus Bridging efforts	27
E.9.3.	GFFS Pilot Project	29
E.9.4.	Challenges in Program Year Two	29
E.10.	Peer-reviewed publications, technical reports, and presentations funded by XSEDE subcontract (exclusively or primarily)	29
E.10.1.	Peer-reviewed Publications	29
E.10.2.	Technical reports (not peer reviewed).....	30
E.10.3.	Presentations	30

List of Figures

Figure 1. Example workflow to optimize dihedral angles.....	3
Figure 2. Jamberoo Molecule editor with molecule and table of initial guesses from CGenFF program.....	4
Figure 3. Visualization of the parameterization validation results and history file retrieval.....	4
Figure 4. Ready, Set, Robots participants program their robot.	12
Figure 5. Total Knowledge Base accesses by month, current program year to date.....	21
Figure 6. XSEDE and TeraGrid Knowledge Base annual accesses. (Data are not available for 2009/2010.)	22
Figure 7. Knowledge Base editing activity (new entries added; existing entries modified or removed) by month, current program year to date.....	22
Figure 8. Total number of documents in XSEDE Knowledge Base by month, current program year to date.....	23

A. Document History

Relevant Sections	Version	Date	Changes	Author
Entire Document	1.00	09/28/2012	Baseline	IU XSEDE team

B. Document Scope

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C. General introduction

This document is a summary of the activities of the Research Technologies division of UITS, a Service & Cyberinfrastructure Center affiliated with the Indiana University Pervasive Technology Institute, as part of the eXtreme Science and Engineering Discovery Environment (XSEDE) during XSEDE Program Year 1 (1 July 2011 – 30 June 2012).

This document consists of three parts:

- Section 2 of this document describes IU's activities as an XSEDE Service Provider, using the format prescribed by XSEDE for reporting such activities.
- Section 3 of this document describes IU's activities as part of XSEDE management, operations, and support activities funded under a subcontract from the National Center for Supercomputer Applications (NCSA), the lead organization for XSEDE. This section is organized by the XSEDE Work Breakdown Structure (WBS) plan.
- Appendix 1 is a summary table of IU's education, outreach, and training events funded and supported in whole or in part by IU's subcontract from NCSA as part of XSEDE.

D. Indiana University Pervasive Technology Institute – Research Technologies Service Provider report

D.1. Executive summary

During XSEDE Program Year 1, Indiana University Pervasive Technology Institute – Research Technologies made a transition from being a TeraGrid Resource Provider to being a Service Provider with one Level 2 system (Quarry), one system proposed as a Level 3 system (Rockhopper), one system being phased out of XSEDE availability (Data Capacitor), and one system that may or may not yet be available on a continuing basis for allocation via XSEDE. IU's involvement in XSEDE providing the Quarry virtual machine (VM) service and access to Penguin-On-Demand via the Rockhopper cluster are consistent with IU's general history in TeraGrid. Our expertise makes us well able to implement novel and new systems.

Quarry is an IBM Intel-based cluster that continues and expands services available under TeraGrid. IU was the first Resource Provider within TeraGrid to offer a VM service. Quarry has become the premier hosting site for VMs that deliver science gateways for XSEDE, as well as serving as a VM hosting site for many operational XSEDE activities. Quarry is very actively used as a host for virtual machines and science gateways. Some of the most significant science gateways supported on Quarry include:

- ParamChem (Dr. Sudhakar Pamidighantam, National Center for Supercomputer Applications)
- Galaxy (Dr. Louise Laurent, the Scripps Research Institute)
- Dark Energy Survey (Prof. August Evrard, University of Michigan)
- Einstein Genome Gateway (Dr. Joseph Hargitai, Einstein Medical School)

IU and Cornell are leading within XSEDE in experimenting with “___ as a service” models coordinated with XSEDE. Rockhopper is available on a “fee for service” basis, providing a user-funded complement to XSEDE services. Rockhopper (rockhopper.uits.iu.edu) is Penguin Computing’s Penguin-On-Demand (POD) supercomputing cloud appliance hosted by Indiana University. 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 cloud services in a secure US facility.

During the current reporting period there were no unscheduled outages of network connectivity from the Indiana University Pervasive Technology Institute – Research Technologies SP resources and XSEDE.

IU has played a leadership role in the creation of the Service Providers Forum (SPF), with David Hancock as the inaugural vice chair of the SPF.

D.2. 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. 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 VMs. The front-end systems host the KVM-based virtual machines. 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 inputting credit card information on a web form to 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.

Being phased out from XSEDE allocations: Data Capacitor – The Data Capacitor and Data Capacitor WAN are a high speed/high bandwidth Lustre storage system for research computing that serves all IU campuses. Each comprises 6 servers (2 MDS, 4 OSS). The total usable storage capacity is 1.1 PB for the Data Capacitor and 339 TB for Data Capacitor WAN.

Fate relative to XSEDE yet unclear: Scholarly Data Archive (HPSS) – HPSS forms the core of IU’s Scholarly Data Archive, a tape-based archival data storage service. It comprises 23 IBM x3650 M2

servers, two TS3500 tape libraries, a total of 48 Jaguar4 tape drives, 500TB disk cache, and 15PB of tape. Data are replicated between the Indianapolis and Bloomington campuses. While TeraGrid allocations will be provisioned until at least the end of 2012, currently HPSS is not accepting new XSEDE allocations. (The possibility of new allocations of one particular type remains under discussion.)

D.3. Science highlights

Empirical Force Field Dihedral Parameter Optimization through Airavata Workflows under ParamChem

Researchers at the University of Illinois and University of Maryland (Baltimore) have collaborated with the Indiana University Science Gateway Group to deploy services and workflows to automate the process of parameterization of Dihedral Parameters used in CGenFF (Charmm General Molecular Forcefield (FF)) in an extensible framework using XSEDE resources. The Apache Airavata workflow toolkit is used for registering workflow components, prefabricated automation steps, and workflow execution management. Asynchronous workflow monitoring enables long running optimization procedures.

Molecular Forcefield Parametrization is critical in enabling the simulation of large molecular systems and their interactions as a way of understanding their behavior. Study of biomolecules and their interactions including how they are modulated by pharmaceuticals is essential to rapid drug prototype development and reducing toxicity. Including various models in the process enables testing the validity of the models and corroborating experimental observations. The workflow infrastructure will benefit a large community of modeling scientists who deal with large and novel molecular systems for which transferable parameters can be generated that enable simulation of new systems including chemical cures of cancer and other diseases and to understand how biomolecules work in physiological and pathological states.

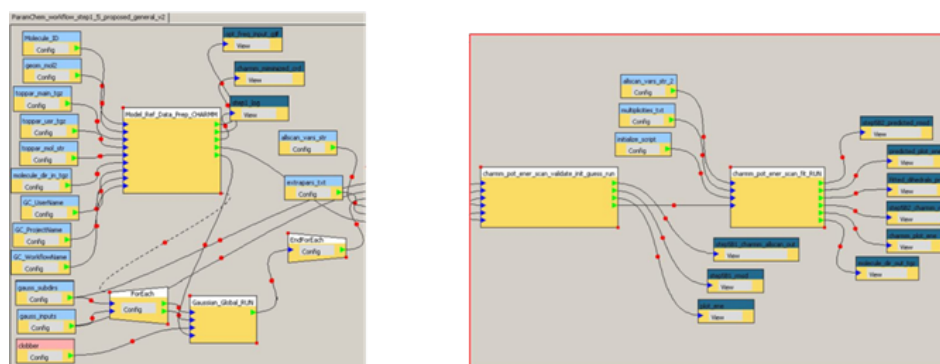


Figure 1. Example workflow to optimize dihedral angles.

configured with dual quad-core Intel E5603 processors, 24 GB of RAM, and a 10 gigabit Ethernet adapter. The front-end systems host the KVM-based virtual machines; previously OpenVZ was used, but it had limitations in hosting VMs with extensive java environments. 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. The storage is provided to the virtual machines using iSCSI on top of ZFS and is replicated between campuses using DRBD, which will support manual failover between campuses.

Due to extensive quality assurance testing of the new environment and making a late design decision to change the storage architecture from a parallel block storage environment (CEPH) to iSCSI for increased reliability, the final migrations of all VMs from OpenVZ to the KVM environment have been delayed until PY2 instead of occurring in Q4 of PY1 as planned.

D.4.1.2. Level 3 (pending) – Rockhopper (Penguin on Demand commercial cluster as a service)

The system has been deployed and is running smoothly.

D.4.2. Services activities

D.4.2.1. Level 2 – Quarry

During February 2012 the Quarry gateway hosting environment experienced an outage of all virtual machine (VM) resources that had been migrated to the new environment, affecting 10 VMs total. Unfortunately, the server crashed between VM migrations that were underway at IU. The VM admins at IU were migrating off of old hardware and technology to more robust systems. During these migrations VM redundancy at IU was disabled. Typically there is redundancy between the Bloomington and Indianapolis campuses in two different data centers separated by 50 miles. The new hardware did not have this redundancy implemented at the time because the Indianapolis storage array was still in use by the VMs that had not yet been migrated. The server encountered a fatal crash, and during recovery triggered a bug in the underlying file system that caused the admins to restore to the last known good state of the VM's. This date from the restore was one week old for most VMs. IU restored all VM's as of February 9th at 3:00 PM.

Since this outage a new service level document has been created and vetted by XSEDE operations. Migrations were also paused while the new hardware was hardened and we went through a two-month testing phase where Quarry users put both real and artificial load on the new systems. Regular nightly backups were always run on the old OpenVZ environment. The new environment has implemented the same policy but is now leveraging Tivoli Storage Manager (TSM) instead of HPSS to back up individual files inside each VM as opposed to taking full tar snapshots at each backup, which made the restores difficult. Restore time was bound to I/O for concurrent restores from HPSS and should be reduced by moving to TSM. Some of the services affected were XSEDE central resources such as SVN, Bugzilla, DOORS, and TeraGrid CVS and access to CTSS software.

A standard VM now consists of 1 virtual CPU, 4 GB of memory, and 10 GB of persistent local storage. Service owners are granted root access to their virtual machine. The 339 TB Data Capacitor WAN (Lustre) file system can also be mounted for larger project and scratch space if requested. Support for the XSEDE Wide File System will be explored as the system is developed. The host operating system is CentOS 6 and a variety of guest operating systems are supported.

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. An external request form can be found at:
<http://pti.iu.edu/hps/vm-account-request>

D.4.2.2. Level 3 (pending) – Rockhopper

Usage of Rockhopper has picked up significantly during PY1 of XSEDE. The Rockhopper “cluster on demand” service was first deployed at IU on 5/1/2012. From 7/1/2011-6/30/2012 usage on Rockhopper was as follows, indicating significant uptake in this new service (which was still experimental during the first part of PY1):

- Number of user logins: 28,520
- Number of unique users: 54
- Number of jobs run: 28,520

D.5. Security

There were no security issues during PY1.

D.6. Education, outreach, and training (EOT) activities

D.6.1. IU SP EOT metrics

Type	Title	Location	Date(s)	Hours	Number of Participants	Number of individuals from traditionally under-represented groups ¹	Method	Funding Sources ²
Tour	2011 DEMA Middle School STEM Camp: AVL	IUPUI	Jul '11	1	62	46	S	IU/PTI
Tour	RICTC Tour	IUPUI	Jul '11	1	24	23	S	IU/PTI
Tour	#59078: IUPUI food service	IUPUI	Jul '11	1	4	0	S	IU/PTI
Workshop / training event	DEMA Middle School STEM Camp		July '11		62		S	IU/PTI

¹ Traditionally Underserved Groups as defined by the National Science Foundation: women, African Americans, Hispanic Americans, Native Americans, Native Pacific Islanders

² Funding sources include IU/PTI (general funds and Student Technology Fees and support from the Lilly Endowment for the Pervasive Technology Institute at Indiana University); XSEDE – IU subcontract from the University of Illinois Champaign-Urbana for support of eXtreme Science and Engineering Discovery Environment (XSEDE), which is supported by National Science Foundation grant number OCI-1053575; NCGAS – National Center for Genome Analysis Support – NCGAS, which is supported by NSF grant 1062432 to Indiana University

Type	Title	Location	Date(s)	Hours	Number of Participants	Number of individuals from traditionally under-represented groups ¹	Method	Funding Sources ²
Workshop / training event	MEAP Summer Camp	Indiana University Purdue University Indianapolis (IUPUI)	July '11		50		S	IU/PTI
Workshop / training event	UITS Research Technologies Fair Fall 2011	IUPUI & IUB	August '11	1	12	0	S	IU/PTI
Workshop / training event	Bugbots Workshop (Wonderlab)	Bloomington	Aug '11		18		S	IU/PTI
Tour	ICTC Summer Tours	IUPUI	September '11	1	13	0	S	IU/PTI
Tour	Craig Kemp & Eli Lilly Co. representatives	IUPUI	Sep '11	1	5	1	S	IU/PTI
Tour	IUPUI HCI students Fall tour	IUPUI	Sep '11	1	10	2	S	IU/PTI
Tour	Anacore visit to Advanced Visualization Lab	IUPUI	Sep '11	1	4	0	S	IU/PTI
Tour	Job Shadow - Student Oct. 18th Afarin Pirzadeh	IUPUI	Sep '11	1	1	0	S	IU/PTI
	2011 Statewide IT Conference Family Night		Sep '11		150		S	IU/PTI
Tour	Craig Kemp		Sep '11		5		S	IU/PTI
Tour	IUPUI Human-Computer Interaction Students	IUPUI	Sep '11		10		S	IU/PTI
Presentation	XSEDE Campus Bridging	CASC Fall Meeting	Sep' 2011	1	45	10	S	XSEDE
Presentation	Regional CI Support for Bridging and Research Engagement	Internet2 Fall Member's Meeting	October 2011	1	50	8	S	XSEDE
Tour	Tour for Dean Garland Elmore with new School of Science Dean	IUPUI	Oct '11	1	10	8	S	IU/PTI
Tour	#Tour for Dean Garland Elmore with Vice Chancellor for Student Life	IUPUI	Oct '11	1	1	1	S	IU/PTI
Tour	Tour for MURI students Oct. 24th 12:30pm	IUPUI	Oct '11	1	7	0	S	IU/PTI
Tour	iQ-Wall for CIB dedication	IUB	Oct '11	1	300		S	IU/PTI
Booth / Display at Event	Celebrate Science Indiana	Indiana State Fairgrounds	Oct '11	7	130		S	IU/PTI
Booth / Display at Event	CIB Dedication	IUB	Oct '11		300		S	IU/PTI
Booth / Display at Event	Family Night at the CIB	IUB	Oct '11		60		S	IU/PTI
Tutorial	HPC Systems for IU Researchers: Advanced Topics		Oct '11		11		S	IU/PTI
Tutorial	HPC Systems for IU Researchers: An Introduction		Oct '11		22		S	IU/PTI
Conference hosted	HPSS User Forum	IUB	Oct '11	30	70	8	S	IU/PTI
Tour	Job Shadow Student Extern		Oct '11		1		S	IU/PTI
Tour	Tour for MURI Students		Oct '11		1		S	IU/PTI

Type	Title	Location	Date(s)	Hours	Number of Participants	Number of individuals from traditionally under-represented groups ¹	Method	Funding Sources ²
BOF	Campus Bridging GFFS Pilot Program	SC11	November 2011	1	28	5	S	XSEDE
Tour	Learning Communities Class Tours	IUPUI	Nov '11	1	40	8	S	IU/PTI
Booth / Display at Event	Display for GIS day at the Wells Library November 16th	IUB	Nov '11	1	100	0	S	IU/PTI
Booth / Display at Event	IQ-Wall for 2011 Statewide IT event at the CIB	IUB	Nov '11	1	60		S	IU/PTI
Booth / Display at Event	AVL gear for Family Night at the CIB	IUB	Nov '11	1	75		S	IU/PTI
Tour	Stonebelt visit / use IC-105 for a meeting using VC	IUB	Nov '11	1	25		S	IU/PTI
Tour	Tour for Albert William and Mark Phaff Nov. 18th	IUPUI	Nov '11	1	1	0	S	IU/PTI
Tour	Prospective Student Tour Nov. 21st	IUPUI	Nov '11	1	10	0	S	IU/PTI
Tour	Tour group for Joan Savage	IUPUI	Nov '11	1	8	0	S	IU/PTI
Tour	Tour for Todd Shelton's N100 Class	IUPUI	Nov '11	1	60	12	S	IU/PTI
Tour	Polly Baker STARS group tour	IUPUI	Nov '11	1	6	4	S	IU/PTI
Tour	Host people visitors from IDAH in IC-105 for a tour	IUB	Nov '11	1	4	0	S	IU/PTI
Tour	Physics-Astronomy open house on Nov. 5, 2011	IUB	Nov '11	1	100		S	IU/PTI
Tour	AVL gear for Family Night at the CIB	IUB	Nov '11	1	60		S	IU/PTI
Tour	Prospective Student Tour Nov. 18th	IUPUI	Nov '11	1	11	0	S	IU/PTI
Tour	#69820: Host insurance presentation on the IQ-wall (open enrollment)	IUB	Nov '11	1	200		S	IU/PTI
Booth / Display at Event	2011 IEEE/ACM Supercomputing Conference	Seattle, WA	Nov '11		2500		S	IU/PTI
Event	CREST Ribbon Cutting Ceremony	IUB	Nov '11		40		S	IU/PTI
Workshop / Professional or scientific	Gateway Computing Environment 11 held at SC11		Nov '11		40		S	IU/PTI
Tour	IUPUI School of Science Dean Tour	IUPUI	Nov '11		10		S	IU/PTI
Booth / Display at Event	Physics/Astronomy Open House	IUB	Nov '11		100		S	IU/PTI
Tour	Polly Baker STARS Tour	IUPUI	Nov '11		6		S	IU/PTI
Tour	Tour Group for Joan Savage		Nov '11		8		S	IU/PTI
Tour	Tour Group for Todd Shelton N100 Class		Nov '11		60		S	IU/PTI
Major Event hosted	GIS Day	IUB	Nov '11		300	150	S	IU/PTI
Tour	Tour for Prof. Acheson's TECH10400 Lab 18646 Dec. 12th	IUPUI	December '11	1	14	1	S	IU/PTI
Performances	3D Showcase show into the IU Cinema	IUB	Dec '11		100	10	S	IU/PTI
Tour	#67172: EOT: Nursing K-12 Tour	IUPUI	Dec '11	1	24	17	S	IU/PTI

Type	Title	Location	Date(s)	Hours	Number of Participants	Number of individuals from traditionally under-represented groups ¹	Method	Funding Sources ²
Tour	Adobe representative visit to use the IQ-Wall	IUB	Dec '11	1	25		S	IU/PTI
Tour	ICTC Tour	IUPUI	Dec '11	1	8	1	S	IU/PTI
Tour	ICTC Tour	IUPUI	Dec '11	1	22	3	S	IU/PTI
Tour	ICTC Tour	IUPUI	Dec '11	1	9	1	S	IU/PTI
Booth / Display at Event	Reception at IQ-wall following Gerry Bernbom bench dedication	IUB	Dec '11	1	30		S	IU/PTI
Tour	Tour for Albert Williams N444 Class Jan. 18th	IUPUI	January '12	1	17	0	S	IU/PTI
Tour	AVL tour for Student IT Ambassadors Jan 27	IUPUI	Jan '12	1	9	2	S	IU/PTI
Tour	#68711: Visit by Meadowwood to CIB, using the IQ-wall	IUB	Jan '12	1	44	0	S	IU/PTI
Tour	Tour for representatives of Indonesia University	IUPUI	Jan '12	1	3	0	S	IU/PTI
Tour	Tour for Vice Chancellor for Research student group	IUPUI	Jan '12	1	44	23	S	IU/PTI
Tour	Tour for UITs staff	IUPUI	Jan '12	1	8	0	S	IU/PTI
Presentation	Campus Bridging	ACTI-CCI/ACTI-CSG	Jan '12	1	25	3	S	XSEDE
Tour	Microsoft visitors tour	IUPUI	Feb '12	1	3	1	S	IU/PTI
Performance	3D movie performance at Indiana Filmmakers Network Indy meeting	Noblesville, IN	Feb '12	1	55	0	S	IU/PTI
Tour	Tour for Brian Benedict's N299 class	IUPUI	Feb '12	1	15	0	S	IU/PTI
Presentation	Penguin at IU and Cloud Services	CASC Spring Meeting	March '12	2	50	10	S	XSEDE
Tour	Tour for Sun Yat-Sen University Delegation	IUPUI	Mar '12	1	31	0	S	IU/PTI
Tour	Tour for King Mongkut's Institute of Technology	IUPUI	Mar '12	1	20	0	S	IU/PTI
Tour	Tour for International Peer Mentoring Program March 23rd	IUPUI	Mar '12	1	9	0	S	IU/PTI
Tour	Tour for High School Teachers (Computer Science)	IUPUI	Mar '12	1	6	0	S	IU/PTI
Tour	IQ-wall tour for Univ. of Kentucky visitors	IUB	Mar '12	1	12	0	S	IU/PTI
Tour	Tour for new Communications Staff		Mar '12		1	0	S	IU/PTI
Tour	Career Shadow Tour for Pike K-12 Student	IUPUI	Mar '12	1	4	2	S	IU/PTI
Tour	Quick tour for new Communications Staff	IUPUI	Mar '12	1	1	0	S	IU/PTI
Tutorial	Bioinformatics Support for Experimental Biologists	Jordan Hall, Indiana University	26 Mar '12	1	30	15	S	NCGAS, IU/PTI
Presentation	Campus Bridging in XSEDE, OSG, and beyond	Internet2 Spring Members meeting	April 2012	1	42	8	S	XSEDE
Tour	Tours for Prospective informatics students.	IUPUI	Apr '12	1	72	6	S	IU/PTI
Tour	SLIS InfoVis Class	IUB	Apr '12	1	10	1	S	IU/PTI
Tour	Digital Connectors Field Trip April 23rd 3:30pm-4:30pm	IUPUI	Apr '12	1	14	12	S	IU/PTI

Type	Title	Location	Date(s)	Hours	Number of Participants	Number of individuals from traditionally under-represented groups ¹	Method	Funding Sources ²
Tour	Zheng CS Undergrad Tour April 10th	IUPUI	Apr '12	1	26	2	S	IU/PTI
Tour	Tour for high school students from George Washington High	IUPUI	Apr '12	1	60	28	S	IU/PTI
Tour	Tour for IUPUI Admissions representatives Mon April 16th	IUPUI	Apr '12	1	7	0	S	IU/PTI
Tour	Tour for Polly Baker's N220 Media Programming class	IUPUI	Apr '12	1	11	0	S	IU/PTI
Tour	Tech 104 Class Tour	IUPUI	Apr '12	1	19	4	S	IU/PTI
Tour	MICI-AHEC Tours	IUPUI	Apr '12	1	14	12	S	IU/PTI
Tour	Jon Racek Interior Design Class Spring 2012	IUPUI	Apr '12	1	14	0	S	IU/PTI
Booth / Display at Event	IUPUI Research Day	IUPUI	Apr '12		200	50	S	IU/PTI
Presentation	Lustre User Group Meeting	Austin, TX	Apr '12		200	25	S	IU/PTI
Panel	Campus Bridging in XSEDE, OSG, and Beyond	Internet2 Spring Members' Meeting	Apr '12	1.25	32	10	S	XSEDE
Presentation	National Infrastructure for High Speed Data	Bio-IT World	Apr '12		100	0	S	IU/PTI, NCGAS
Tour	Tour for CDW-G intern Erik Hencier	IUB	May '11	1	1		S	IU/PTI
Tour	IUPUI Math Dept. EOT event in May 2012	IUPUI	May '12	1	69	5	S	IU/PTI
Tour	Tour for University College Academic Advising staff	IUPUI	May '12	1	28	4	S	IU/PTI
Tour	EDUCAUSE Security Conference Tours	IUPUI	May '12	1	62	7	S	IU/PTI
Tour	Tour for Will Potter from Herron School of Fine Art May 17th	IUPUI	May '12	1	2	0	S	IU/PTI
Tour	Tour of CIB IQ-wall for Rotary Club	IUB	May '12	1	23	0	S	IU/PTI
Tour	Geek Camp tour of the VCT and stereographs	IUPUI	May '12	1	10	1	S	IU/PTI
Tutorial	Research File System (RFS) Training	IUB	May '12		20	0	S	IU/PTI
Tutorial	Research File System (RFS) Training	IUPUI	May '12		20	0	S	IU/PTI
Presentation	Data Management? I'm a Biologist	Research Computing Day, U. of Florida	May '12	1	50	20	S	NCGAS, IU/PTI
Tutorial	Designing RNA-Seq Experiments	Daphnia Genomics Jamboree, Indiana University	May '12	3	22	14	S	NCGAS, IU/PTI
Workshop / Training Event	Ready, Set, Robots Summer Camp	IU Bloomington (IUB)	Jun '12		40		S	IU/PTI
Tour	Nanotechnology Discovery Academy Summer Program	IUPUI	June '12	1	20	4	S	IU/PTI

Type	Title	Location	Date(s)	Hours	Number of Participants	Number of individuals from traditionally under-represented groups ¹	Method	Funding Sources ²
Tour	#74573: tour for IUPUI Nanotechnology Discovery Academy Summer Program	IUPUI	Jun '12	1	22	7	S	IU/PTI
Tour	#78214: MEAP Tour Sessions June 22nd	IUPUI	Jun '12	1	34	15	S	IU/PTI
Tour	#78310 (Game On! Summer Workshop Tour June 14th 12pm)	IUB	Jun '12	1	22	2	S	IU/PTI
Tour	#78311: Game On! Summer Workshop Tour June 19th 11:30am	IUB	Jun '12	1	29	3	S	IU/PTI
Tour	#78312: Web Design Summer Workshop Tour June 28th 11:30am	IUPUI	Jun '12	1	11	0	S	IU/PTI
Tour	#78558: Tour LSAMP Summer Field Trip June 22nd 11:45am	IUPUI	Jun '12	1	16	4	S	IU/PTI
Tour	#79885: Tour for New Covenant Church June 21 at 11am.	IUPUI	Jun '12	1	13	12	S	IU/PTI
Tour	#80020: EOT: Tour for GIS NEH Institute	IUB	Jun '12	1	25	0	S	IU/PTI
Tour	#80313: EOT: Girls Inc and Nursing tour	IUPUI	Jun '12	1	55	39	S	IU/PTI
Tour	#80375 (Tour for Matt Farmer (prospective Student))	IUPUI	Jun '12	1	2	0	S	IU/PTI
Webinar	“What is campus bridging and why should XSEDE Campus Champions Care?”	Michigan City, IN	8 Jun 2012	1	15	7	S	XSEDE
Booth / Display at Event	Smithsonian Institution Folklife Festival (part 1)	Washington D.C.	Jun 27, 2012 – Jun 30, 2012	28	1356	828	S	IU/PTI with special support from Office of the President and Office of the VP for Research

Table 1. Listing of Education, outreach, and training events.

Type of event	Total number of individual events	Total Number of Participants	Total Number of individuals from traditionally under-represented groups ³
BOF (Birds of a Feather) Session	1	28	5
Booth / Display at Event	11	4911	878
Conference hosted	1	70	8
Event	1	40	0
Major Event hosted	2	450	150
Panel	1	32	10
Performance	2	155	10
Presentation	8	562	84
Tour	82	2,087	324
Tutorial	6	125	29
Webinar	1	15	7
Workshop / Professional or scientific	1	40	0
Workshop / Training Event	5	182	0
GRAND TOTAL	122	8,697	1,505

Table 2. Listing of total number of events and participants in IU / PTI education, outreach, and training events.

³ Traditionally Underserved Groups as defined by the National Science Foundation: women, African Americans, Hispanic Americans, Native Americans, Native Pacific Islanders

D.6.2. EOT highlight: PTI Ready, Set, Robots Workshop 2012

A particular highlight in IU education, outreach, and training activities was the offering of the sixth occurrence of an annual workshop titled “Ready, Set, Robots.” This year eight PTI staff worked with 52 future engineers and scientists programming LEGO Mindstorms™ robots. In anticipation of the NASA Curiosity landing later in the summer, the workshop adopted a Mars rover theme. Students ranging from seventh grade to high school juniors programmed robots to simulate a Mars sample return rover mission. The test arena contained several swatches of colored tape that represented different mineral deposits of interest to scientists back on earth. The challenge was to detect a minimum number of the minerals and then dock with the return vehicle by homing in on an infrared signal.

The students worked in teams of three or four. Each team was paired with a PTI staff member as a mentor. The tasks were broken down into sub-tasks with mini-evaluations for each sub-task. The mini-evaluations gave the teams a chance to explain their algorithms they developed and used as well as exchange ideas about challenges they all found. The evaluations contained several criteria, but the students excelled in the creativity criteria.

On the second day of the two-day workshop, each team presented and demonstrated its solution to an assembled group of parents, siblings, and PTI staff. The interest in this workshop remains high and PTI continues to seek ways to bring this material to even more future researchers next year.



Figure 4. Ready, Set, Robots participants program their robot.

D.7. SP collaborations

IU collaborated with the Technische Universitaet Dresden (Germany) on optimization of the Trinity RNA sequencing software, resulting in substantial improvement in the performance of that application. This work is described in a paper that was submitted to and accepted for publication at XSEDE12.

IU has an ongoing collaboration with Cummins, Inc. to aid Cummins in design of diesel engine pistons to help improve fuel efficiency and decrease productions of emissions. During PY1 IU worked with Cummins on experiments in analysis workflows, and production design of new improved diesel engine components.

D.8. SP-specific activities

D.8.1. IU Cyberinfrastructure Newsletter

IU publishes a monthly newsletter that often features news and activities related to XSEDE. It reaches a total of 6,968 individuals. Back issues are archived at:
<http://pti.iu.edu/ci/cyberinfrastructure-news/archives>

D.8.2. 100 Gbps networking

The SCinet Research Sandbox (SRS) at the Supercomputing 2011 (SC11) conference encouraged institutions to showcase new and innovative technologies in the area of networking. For the demonstration SCinet, in collaboration with ESnet and Internet2, provided SRS participants with a 100 Gbps network connection from the SC11 show floor to the Internet2 backbone. The 100 Gbps link provided an end-to-end connection from the IU booth on the SC11 show floor to the IU Data Center in Indianapolis, Indiana. Our SRS entry was as much an experiment at the network layer as it was at the file system or applications layer. Indiana University used a dedicated 100 Gbps wide area network (WAN) link spanning more than 3,500 km (2,175 mi) to demonstrate the capabilities of the Lustre high performance parallel file system in a high bandwidth, high latency WAN environment. This demonstration functioned as a proof of concept and provided an opportunity to study Lustre's performance over a 100 Gbps WAN. To characterize the performance of the network and file system, a series of benchmarks and tests were undertaken. These included low level iperf network tests, Lustre networking (LNET) tests, file system tests with the IOR benchmark, and a suite of real-world applications reading and writing to the file system. All of the benchmarks were run over the WAN link with a latency of 50.5 ms.

D.9. Publications

D.9.1. Journal articles⁴

- Kluge, M., S. Simms, T. William, R. Henschel, A. Georgi, C. Meyer, M.S. Mueller, C.A. Stewart, W. Wunsch and W.E. Nagel. "Performance and quality of service of data and video movement over a 100 Gbps testbed." (In press) *Future Generation Computer Systems*, 29(1), 230-240. 2013.
<http://dx.doi.org/10.1016/j.future.2012.05.028> (Preprint: <http://hdl.handle.net/2022/14620>)
- Foroud, T., L. Wetherill, S. Vinci-Booher, E. S. Moore, R. E. Ward, H. E. Hoyme, L. K. Robinson, J. Rogers, E. M. Meintjes, C. D. Molteno, et al., "Relation Over Time Between Facial Measurements and Cognitive Outcomes in Fetal Alcohol-Exposed Children" *Alcohol Clinical and Experimental Results*, Mar 08 2012.
- Guha, R., G. D. Wiggins, D. J. Wild, M. - H. Baik, M. E. Pierce, and G. C. Fox, "Improving usability and accessibility of cheminformatics tools for chemists through cyberinfrastructure and education" *In Silico Biology*, vol. 11, no. 1-2, pp. 41-60, Jan 2012.

⁴ Peer-reviewed, includes print and online.

D.9.2. Peer-reviewed papers⁵

- Michael, S., L. Zhen, R. Henschel, S. Simms, E. Barton, M. Link, A study of lustre networking over a 100 gigabit wide area network with 50 milliseconds of latency, Proceedings of the fifth international workshop on Data-Intensive Distributed Computing, June 18-22, Pages 43-52, ISBN: 978-1-4503-1341-4, 10.1145/2286996.2287005.
- Knepper, R., W. Johnson, S. Michael, R. Henschel and M. Link. Wide-area 100Gb Networking at the SCinet Research Sandbox. Proceedings of the 7th IEEE International Conference on Networking, Architecture, and Storage, Xiamen, China June 28-30, 2012.
- Welch, V., A. Walsh, W.K. Barnett, C. A. Stewart. 2011. A Roadmap for Using NSF Cyberinfrastructure with InCommon.
<http://dl.acm.org/citation.cfm?id=2016771&dl=ACM&coll=DL&CFID=143501349&CFTOKEN=70704554>
- Wernert, E., W. Sherman, P. O'Leary, and E. Whiting, "A common path forward for the immersive visualization community" Workshop: Immersive Visualization Revisited – Challenges and Opportunities, Orange County, CA, IEEE VR 2012, Mar 2012.
- Huang, H., X. Wu, M. Sonachalam, S. N. Mandape, R. Pandey, K. F. MacDorman, P. Wan, and J. Y. Chen, "PAGED: A Pathway and Gene-set Enrichment Database to Enable Molecular Phenotype Discoveries" BMC Bioinformatics, Feb 2012.
- Zhang, H., M. Korayem, E. You, and D. Crandall, "Beyond co-occurrence: Discovering and visualizing tag relationships from geo-spatial and temporal similarities" ACM International Conference on Web Search and Data mining, Seattle, Washington, Feb 2012.
- Donnellan, A., J. Parker, R. Granat, E. DeJong, S. Suzuki, M. Pierce, G. Fox, J. Rundle, D. McLeod, R. Al-Ghanmi, et al., "QuakeSim: Integrated Modeling and Analysis of Geologic and Remotely Sensed Data" 2012 IEEE Aerospace Conference, Big Sky, Montana, Mar 2012.
- Dolinsky, M., W. Sherman, E. Wernert, and Y. C. Chi, "Reordering virtual reality: recording and recreating real-time experiences" The Engineering Reality of Virtual Reality 2012, vol. 8289: SPIE Electronic Imaging, Jan 2012.
- Glasscoe, M., R. Blom, G. Bawden, G. Fox, M. Pierce, J. Rundle, J. Wang, R. Granat, M. Burl, Y. Ma, et al., "E-DECIDER: Earthquake Disaster Decision Support and Response Tools. Development and Experiences" Fall AGU Meeting, San Francisco, CA, Dec 2011.
- Hayashi, S., A. Gopu, and R. Quick, "GOC-TX: A Reliable Ticket Synchronization Application for the Open Science Grid" Computing in High Energy Physics (CHEP), Taipei Taiwan, IOP Publishing, Dec 2011.
- Parker, J. W., A. Donnellan, R. A. Granat, G. A. Lyzenga, M. T. Glasscoe, D. McLeod, R. Al-Ghanmi, M. Pierce, G. Fox, L. G. Ludwig, et al., "QuakeSim: a Web Service Environment for Productive Investigations with Earth Surface Sensor Data" Fall AGU Meeting, San Francisco, CA, Dec 2011.
- Eller, C., "Stereoscopic 3D Storytelling" Department of Telecommunications, vol. Masters, Bloomington, Indiana University, May 2012.
- Frend, C., "SARGE: Spatial Augmented Reality Game Equipment" School of Informatics, vol. Masters, Indianapolis, Indiana University-Purdue University Indianapolis, May 2012.

⁵ Includes abstracts and papers in conference proceedings, as well as any other peer-reviewed item that is not a journal article.

D.9.3. Other publications, not peer-reviewed⁶

- Donnellan, A., J. W. Parker, E. DeJong, M. Pierce, G. Fox, D. McLeod, J. Rundle, and L. Grant, A Distributed Approach to Computational Earthquake Science: Opportunities and Challenges , Bloomington, IN, Indiana University, Jan 2012.
- Henschel, R., S.C. Simms, D. Hancock, S. Michael, T. Johnson, N. Heald, T. William, D.K. Berry, M. Allen, R. Knepper, M. Davy, M.R. Link and C.A. Stewart. Technical Report: Report on Lustre use across an experimental 100Gb network spanning 2,175 mi. Indiana University. 2012. Available from: <http://hdl.handle.net/2022/14137>
- Henschel, R., C. A. Stewart, W. Thomas, M. Mueller, and W. E. Nagel, Report About the collaboration between UITS/Research Technologies at Indiana University and the Center for Information Services and High Performance Computing at Technische Universitat Dresden, Germany , Dresden, Germany, Mar 2012.
- McRobbie, M. A., B. C. Wheeler, B. Plale, and C. A. Stewart, Indiana University Pervasive Technology Institute Report to the Lilly Endowment, Inc. 36 Month Program Report Jun 1, 2011 - Nov 30, 2011 : Indiana University, Dec 2011.
- Miller, T., B. Plale, and C. A. Stewart, 2011 annual report on training, education, and outreach activities of the Indiana University Pervasive Technology Institute and affiliated organizations : Indiana University, Jan 2012.
- Stewart, C.A.; Link, M.R.; Henschel, R.; Hancock, D.Y.; Li, H. 2012. Technical Report: Benchmarking an HP DL580 cluster at Indiana University (Mason). <http://hdl.handle.net/2022/14078>
- Stewart, C.A., M.R. Link, D.S. McCaulay, R. Henschel, D. Hancock. "Technical Report: Acceptance Test for FutureGrid Cray XT5m at Indiana University (Xray)," Indiana University, Bloomington, IN. PTI Technical Report PTI-TR12-005, Mar 2012. <http://hdl.handle.net/2022/14267>
- Stewart, C.A. and T. Miller. Economic development by the Indiana University Pervasive Technology Institute, Pervasive Technology Labs, and the Research Technologies Division of University Information Technology Services September 1999 – June 2011: a public report. Indiana University, Bloomington, IN. 2011. <http://hdl.handle.net/2022/13559>
- Donnellan, A., G. Fox, D. McLeod, M. Pierce, and J. Rundle, OpenQuake Social Networking for EarthCube , Jan 2012.
- Stewart, C. A., R. Knepper, A. Grimshaw, I. Foster, F. Bachmann, D. Lifka, M. Riedel, and S. Tuecke, Campus Bridging Use Case Quality Attribute Scenarios , May 2012.
- Stewart, C. A., R. Knepper, A. Grimshaw, I. Foster, F. Bachmann, D. Lifka, M. Riedel, and S. Tuecke, XSEDE Campus Bridging Use Cases , May 2012.
- Wang, J., M. E. Pierce, Y. Ma, G. C. Fox, A. Donnellan, J. W. Parker, and M. Glasscoe, Using Service-Based Geographical Information System to Support Earthquake Research and Disaster Response , Bloomington, IN, Indiana University, Jan 2012.
- William, T., D. Berry, and R. Henschel, Analysis and Optimization of a Molecular Dynamics Code Using PAPI and the Vampir Toolchain , Jan 2012.

⁶ Includes workshop and technical reports, position papers, data sets, and blogs.

D.9.4. Presentations⁷

- Barnett, W. K., A Nation-Wide Area Networked File System for Very Large Scientific Data, Bio-IT World, Boston, MA, Apr 2012.
- Barnett, W., The NCGAS Model for Genomics Support, The Daphnia Genomics Jamboree, Bloomington, IN, May 22, 2012.
- Doak, T.G., L.-S. Wu, C.A. Stewart, R. Henschel and W.K. Barnett. National Center for Genome Analysis Support (Poster). 2012. Presentation. Available from: <http://hdl.handle.net/2022/14539>
- Doak, T. G., L. - S. Wu, C. A. Stewart, R. Henschel, and W. K. Barnett, National Center for Genome Analysis Support, Plant and Animal Genomes, San Diego, CA., Jan 2012.
- Doak, T. G., L. - S. Wu, C. A. Stewart, R. Henschel, and W. K. Barnett, National Center for Genome Analysis Support, Pacific Symposium on Biocomputing, Big Island, HI, Jan 2012.
- Glasscoe, M., R. Blom, G. Bawden, G. Fox, M. Pierce, J. Rundle, J. Wang, R. Granat, M. Burl, Y. Ma, et al., E-DECIDER: Earthquake Disaster Decision Support and Response Tools. Development and Experiences, Fall AGU Meeting , <http://sites.agu.org/fallmeeting/>, San Francisco, CA USA, Dec 2011.
- Hedstrom, M., and R. H. McDonald, An Overview of the National Science Foundation DataNet Funded Sustainable Environment-Actionable Data Project, Coalition for Networked Information (CNI) Fall Members Meeting, <http://www.cni.org/events/membership-meetings/past-meetings/fall-2011/project-briefings/>, Arlington, VA, Dec 2011.
- Hancock, D.Y. 2012. HPC 101 (Presentation) InCNTRE Internship Program - Summer of Networking (Bloomington, IN, 21 June, 2012).
- Jacobs, M. and C.A. Stewart. 2012. Penguin Computing / IU Partnership HPC “cluster as a service” and Cloud Services. (Presentation) Coalition for Academic Scientific Computation (Arlington, VA, 29 Feb). Available from: <http://hdl.handle.net/2022/14441>
- Kowalczyk, S., J. Unsworth, B. Plale, R. H. McDonald, and Y. Sun, The HathiTrust Research Center: An Overview, <http://dlib.indiana.edu/education/brownbags/index.shtml>, Indiana University, Bloomington, IN, Apr 2012.
- LeDuc, R., RNA-seq Analysis, The Daphnia Genomics Jamboree, Bloomington, IN, May 22, 2012.
- LeDuc, R., "Data Management? I'm a Biologist !" Research Computing Day, University of Florida, Gainesville, Apr 2012.
- LeDuc, R., "Biology Brown Bag" UITS Bioinformatic Support for Experimental Biologists, Indiana University Bloomington, Mar 2012.
- McDonald, R. H., M. Winkler, and B. Johnson, An Update on Quali OLE, State Assisted Academic Libraries of Kentucky (SAALCK) Director's Council Meeting, May 2012.
- McDonald, R. H., Bleeding, Leading, or Not Competing: A Theme and Variations on Current Emerging Technologies, Pennsylvania State System of Higher Education (PASSHE) 2012 Virtual Conference, Feb 2012.

⁷ Includes poster presentations and Congressional testimony.

- McDonald, R. H., B. Plale, M. Hedstrom, A. Zimmerman, P. Kumar, and J. Myers, SEAD: A System to Support Active and Social Data Curation in Sustainability Science, Research Data Access & Preservation (RDAP) Summit 2012, <http://rdap12.posterous.com/>, New Orleans, LA, Mar 2012.
- McDonald, R. H., M. Tamarkin, and M. Winkler, Quali Open Library Environment: Reflections on Our First Year of Collaborative Software Development, Educause Live, Jan 2012.
- Pierce, M., and G. Fox, IU QuakeSim/E-DECIDER Effort, Indiana University, Bloomington, Indiana, Feb 2012.
- Steinhart, G., M. Hedstrom, R. H. McDonald, P. Schaeffer, and O. Reiger, SIG-DL Sustainability Panel, Research Data Access & Preservation (RDAP) Summit 2012, New Orleans, LA, Mar 2012.
- Simms, S.C. 2012. Using the Lustre File System at 100Gb across 2,300 Miles,(Presentation) N-Wave Stakeholder Meeting (Boulder, CO, 22-23 May, 2012).
- Simms, S.C. 2012. Secure Identity Management for Lustre 2.X (Presentation), Lustre Roadmap BOF at ISC 2012 (Hamburg, Germany, 19 June, 2012).
- Steinhart, G., M. Hedstrom, R. H. McDonald, P. Schaeffer, and O. Reiger, SIG-DL Sustainability Panel, Research Data Access & Preservation (RDAP) Summit 2012, New Orleans, LA, Mar 2012.
- Stewart, C.A. 2012. Cyberinfrastructure Begins at Home. (Presentation) Rutgers University (New Brunswick, NJ, 20 Feb). Available from: <http://hdl.handle.net/2022/14442>
- Stewart, C.A. 2011. Management and organizational structure of large scale innovative projects. (Presentation) FLEET Working Group Meeting (Vienna, Austria, 19 July 2011). <http://hdl.handle.net/2022/13403>
- Stewart, C.A. 2011. Communicating with government & public stakeholders. (Presentation) FLEET Working Group Meeting (Vienna, Austria, 19 July 2011). <http://hdl.handle.net/2022/13404>
- Stewart, C.A. 2011. A tale of two grids -- Open Science Grid & TeraGrid. (Presentation) FLEET Working Group Meeting (Vienna, Austria, 20 July 2011). <http://hdl.handle.net/2022/13405>
- Stewart, C.A., R. Henschel, W.K. Barnett and T. Doak. 2011. Experiences with a large-memory HP cluster – performance on benchmarks and genome codes. (Presentation) HP-CAST 17 - HP Consortium for Advanced Scientific and Technical Computing World-Wide User Group Meeting (Seattle, WA, 12 Nov 2011). <http://hdl.handle.net/2022/13879>
- Stewart, C.A., M.R. Link, G. Turner and W.K. Barnett. 2011. Penguin Computing and Indiana University partner for "above campus" and campus bridging services to the community. (Presentation) IEEE/ACM SC11 Conference (Seattle, WA, 14-17 Nov 2011). <http://hdl.handle.net/2022/13880>
- Stewart, C.A. and B.C. Wheeler. 2011. Cyberinfrastructure Begins at Home. (Presentation) IBM Multi-customer Briefings, IEEE/ACM SC11 Conference (Seattle, WA, 15 Nov 2011). <http://hdl.handle.net/2022/13888>
- Stewart, C. A., Cyberinfrastructure Begins at Home, Rutgers University, New Brunswick, NJ, Feb 2012.
- Stewart, C. A., "Campus Bridging" XSEDE (eXtreme Enviroment for Science and Engineering Discovery) Advisory Board Meeting, Chicago, Il, Apr 2012.
- Stewart, C. A., S. Marru, R. Knepper, D. Y. Hancock, J. Wernert, C. Aikman, J. Bolte, P. Brown, and T. M. Miller, "Indiana University collected XSEDE update" XSEDE (eXtreme Enviroment for Science and Engineering Discovery) Quarterly Meeting, Austin, TX., Mar 2012.

Walgenbach, J. 2012. Secure Identity Mapping for Lustre 2.X. (Presentation) Lustre User Group (Austin, TX, 23-25 April, 2012).

D.9.5. Tutorials and courses taught

None this PY.

D.9.6. Major conference displays

Moving fast, thinking big. Indiana University. Exhibit floor display, IEEE/ACM SC11. 2011. <http://pti.iu.edu/sc11>.

D.9.7. Lay / business press placements

"IU to Establish Genome Research Center." *Inside Indiana Business*. 20 Oct 2011. <http://www.insideindianabusiness.com/newsitem.asp?id=50370>

D.10.Metrics

D.10.1. 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										
1-24 hr										
1-7 d										1
1-2 wk										
> 2 wk	1	1				2		1		1
Still Open						1			1	1

Table 3. IU ticket resolution times by category from the XSEDE ticket system.

D.10.2. SP-specific metrics

D.10.2.1. Quarry

Quarry remains a very actively used system as a host for virtual machines and science gateways. There are a total of 50 allocated VMs active at present on Quarry, including 21 for science gateways, 12 for IU internal gateway efforts, and 17 to support XSEDE core services.

D.10.2.2. Rockhopper

During the past quarter a total of 32 distinct individuals used Rockhopper.

D.10.2.3. Data Capacitor

There remain a total of 53 XSEDE allocations, for a total of 2.25 TB, on the Data Capacitor, either held over from TeraGrid or provided under XSEDE upon special request, due to need for particular capabilities provided uniquely by the Data Capacitor.

D.10.2.4. Scholarly Data Archive – HPSS

There remain a total of 23 XSEDE allocations, for a total of 53TB, on the IU Scholarly Data Archive (HPSS) tape archival storage system.

D.10.2.5. Networking connectivity to XSEDE

During the current quarter, there were zero (0) unscheduled outages and two (2) scheduled maintenance events that directly affected Indiana University's connection to XSEDE. Maintenance accounted for 301 minutes of maintenance downtime. There were 131,040 minutes during the current quarter, yielding a 99.770299% uptime. During the outages and maintenance events, Indiana University's XSEDE connectivity failed over to our Internet2 and NLR connectivity, giving an actual site-to-site XSEDE uptime of 100%.

D.10.2.6. Usage metrics – current quarter

System	# Allocations	# VMs allocated	# TB allocated	# accesses	Storage high water mark	TB written	TB read
Quarry VM	21	50					
Rockhopper				1,383			
Data Capacitor WAN	53		2.25	1.2 B	314 TB	114	180
Scholarly Data Archive – HPSS	23		53				

Table 4. Service Provider system key usage metrics for the current quarter (Q4 of PY1 – Apr-Jun 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	97.4%	1	240			240
Rockhopper						
Data Capacitor WAN	99.61%	1	510	0	0	510
Scholarly Data Archive – HPSS						

Table 5. Service Provider system key usage metrics for the current quarter (Q4 of PY1 – Apr-Jun 2012).

D.10.2.7. Usage metrics – project year one

System	# Allocations	# VMs allocated	# TB allocated	# accesses	Storage high water mark	TB written	TB read
Quarry VM	21	50					
Rockhopper				1,383			
Data Capacitor WAN	53		2.25	696 B	331	1,520	1,612
Scholarly Data Archive – HPSS	23		53				

Table 6. Service Provider system key usage metrics for PY1 (Jul 2011 – Jun 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	99.3%	1	240	2	3600	3840
Rockhopper						
Data Capacitor WAN	99.86%	2	642	2	92	734
Scholarly Data Archive – HPSS						

Table 7. Service Provider system key usage metrics for PY1 (Jul 2011 – Jun 2012).

E. Indiana University Pervasive Technology Institute – XSEDE subcontract report

Section 3 of this document describes IU's activities as part of XSEDE management, operations, and support activities funded under a subcontract from the National Center for Supercomputer Applications (NCSA), the lead organization for XSEDE. This section is organized by the XSEDE Work Breakdown Structure (WBS) plan.

E.1. WBS 1.2.2 Data Services

This is an activity that begins in PY2; no activities to report yet.

E.2. WBS 1.2.6 Systems Operational Support

E.2.1. Virtual machines

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

E.2.2. XD Operations Center Fail-over

The IU GlobalNOC continued work on implementation activities in preparation for as a failover site for the XSEDE Operations Center. The status of various failover preparations follows:

- Phones – completed XSEDE NOC Greeting on IU phone system
- Email – completed setup of e-mail acceptance for failover on IU side. Pending XSEDE/NCSA setup, policy, procedures and documentation before further implementation.
- Ticketing – IU awaits final decision on new trouble ticket system for XSEDE. Pending XSEDE.
- Monitoring – currently SNAPP monitoring from Pittsburgh. Steven McNally looking at how IU NOC to get access to current monitoring. Pending XSEDE.
- Process and Procedure Documentation – XSEDE evaluating moving all documentation to XSEDE staff wiki. Pending XSEDE.
- Fail-over Documentation – Fail-over documentation is part of process and procedure documentation above – pending move to XSEDE staff wiki. Pending XSEDE.
- Training – Training for IU NOC staff pending finalization of trouble ticket system. Pending XSEDE.

E.3. WBS 1.3.2 User Information and Interfaces

E.3.1. Knowledge Base

Summary statistics for the XSEDE Knowledge Base:

Metric	For current quarter
Number of KB documents available at end of quarter	476
Number of new KB documents added	83
Total number of retrievals	76,401
Total number of retrievals minus bots	62,044

Table 8. High-level XSEDE Knowledge Base metrics for current quarter.

Metric	PY to date (when applicable)
Number of KB documents available at end of quarter	476
Number of new KB documents added	476
Total number of retrievals	407,735
Total number of retrievals minus bots	256,964

Table 9. High-level XSEDE Knowledge Base metrics for current quarter.

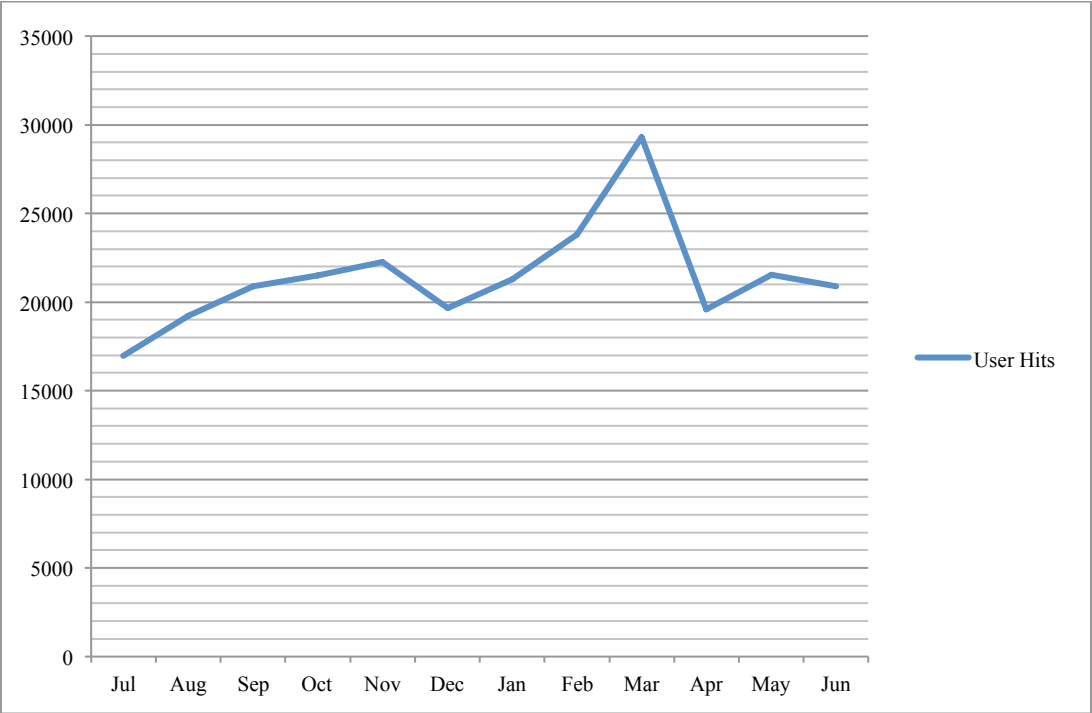


Figure 5. Total Knowledge Base accesses by month, current program year to date.

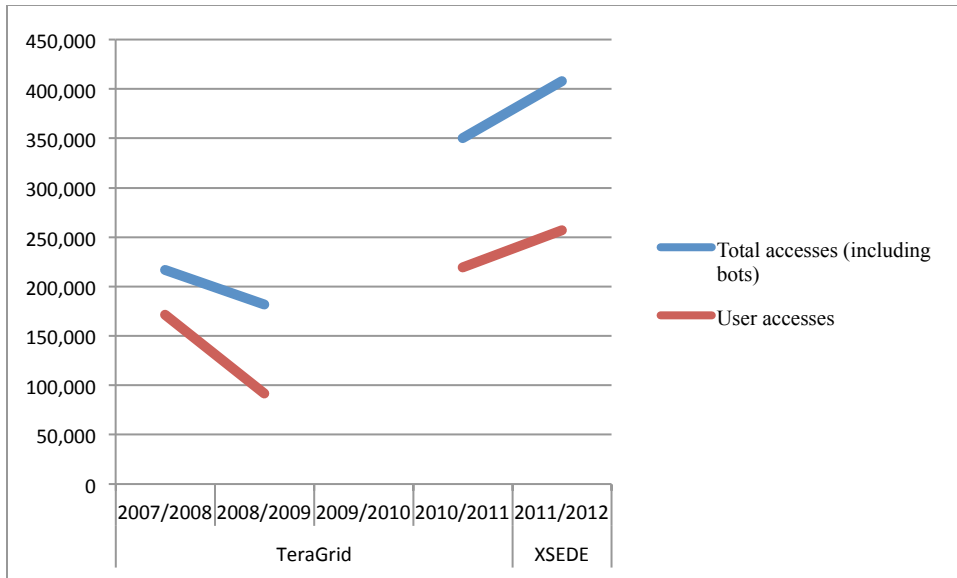


Figure 6. XSEDE and TeraGrid Knowledge Base annual accesses. (Data are not available for 2009/2010.)

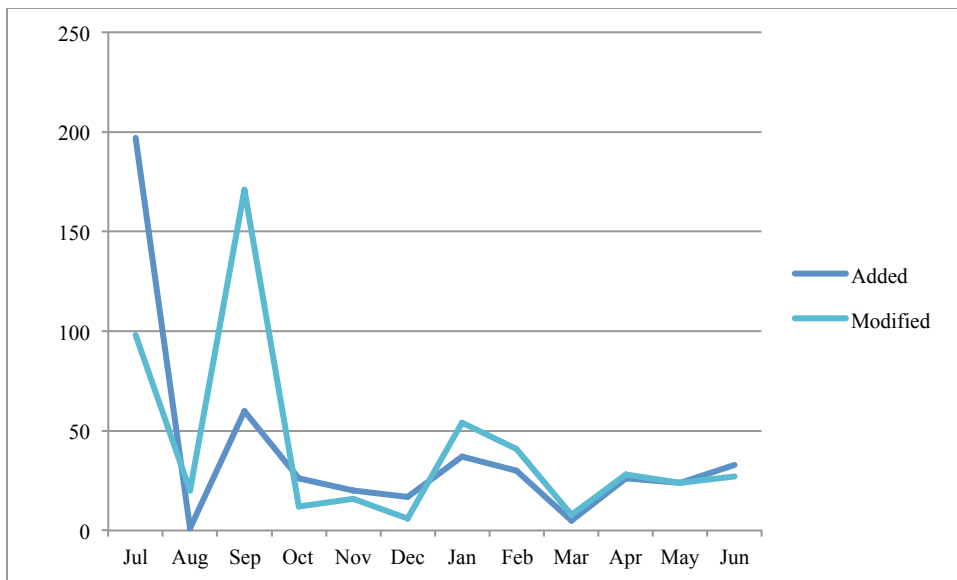


Figure 7. Knowledge Base editing activity (new entries added; existing entries modified or removed) by month, current program year to date.

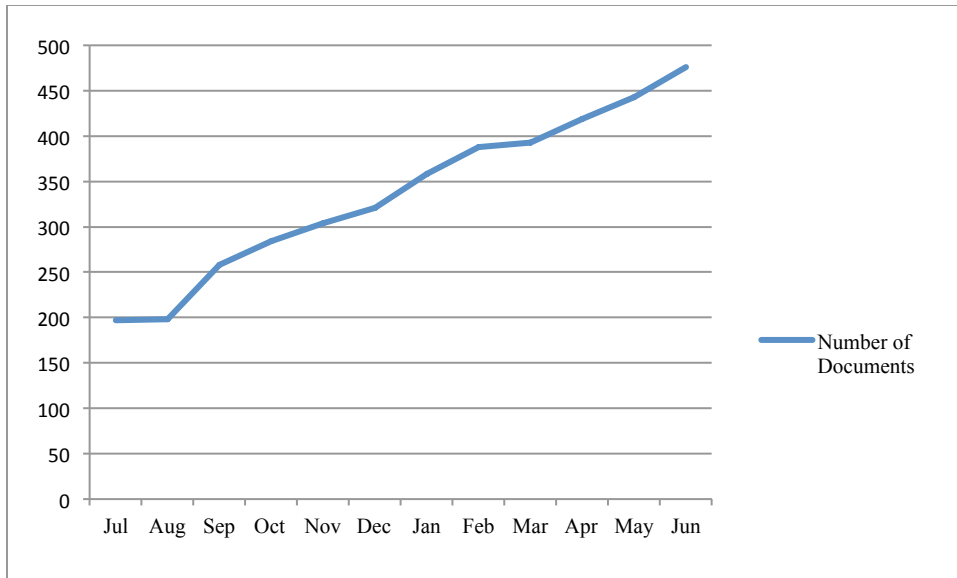


Figure 8. Total number of documents in XSEDE Knowledge Base by month, current program year to date.

E.3.2. Other documentation activities

Jeremy Fischer was hired in April 2012 to fill the vacant IU position in Online Information and Interfaces. Since becoming active with XSEDE at the beginning of 2Q 2012, he has taken part in several projects. One of the first items was working with Susan Lindsey to update the Quarry Gateway documentation. Part of this update was to also introduce a "hybrid" systems template that may get adapted for future use with other resources. This will join the existing templates for HPC systems and storage systems that are already finalized and published.

In addition, an internal wiki was brought online for Indiana University XSEDE members for archiving plans, problems, and progress related to XSEDE projects. This wiki has been useful for tracking all IU specific activity so that consistent reporting may happen and will probably expand to cover more IU activities in the future. Plans for the future include expanding the documentation features developed for IU to be more generally accessible to XSEDE.

A new draft system description for hybrid systems has been drafted and is being reviewed and refined by relevant leaders within XSEDE.

E.4. WBS 1.3.3 User Engagement

Survey Support

The 2012 XSEDE User Satisfaction Survey was launched on May 1, 2012, after receiving approval from XSEDE leadership and IU IRB, and closed on June 11, 2012. The survey sample population was generated randomly from (1) a complete list of XSEDE users and (2) a list of NSF-funded principal investigators from the NSF award database. As of June 11 there were 734 responses representing just over 7% of the total survey population (400+ were current XSEDE users). The final survey report will be available no later than August 31, 2012.

E.5. WBS 1.4/1.5 ECSS

E.6. WBS 1.4.2 Novel & Innovative Projects

Startup gateway projects

The Einstein Genome Gateway is targeted to provide large-scale computational interface between XSEDE compute and storage resources and the national community with large-scale computational needs in genomics and related fields.

The IU science gateways group is recently assigned to initiate the ECSS support on this project and had initial discussions with the project team. Quarry gateway hosting infrastructure is set up as a development testbed and targeted production platform. Next quarter will focus on job management and workflow abstractions to seamlessly migrate from Einstein medical school's computational resources to XSEDE.

E.7. WBS 1.5.2 Extended Support for Science Gateways

E.7.1. Gateway Leadership

The IU Science Gateways Group contributed to the ongoing gateway coordination and to development and execution of work plans for gateway-related requests made through ECSS. Activities include the community engagement and coordination of gateway support personnel across all the sites.

Continuing from the previous quarter, the IU group has led the gateway use case requirements sessions, a collaborative requirement gathering exercise involving all funded science gateway ECSS staffers. Early versions were presented to the XSEDE Architecture and Design team for initial feedback and guidance. Gateway use cases will be finalized during Q3.

E.7.2. UltraScan Science Gateway

The UltraScan Science Gateway provides access to data analysis and modeling applications to support experimental biophysics research. This ECSS project with the IU gateway team will enable UltraScan jobs to be submitted to SDSC's Trestles (in addition to Ranger, Lonestar, and campus resources) and will enable the new UltraScan Solution Modeling (SOMO) analysis codes to run on XSEDE. SOMO applications will represent a major increase in UltraScan's user base.

Efforts during the current reporting period are as follows:

- Worked with UltraScan developers to deploy the code on Trestles and Gordon.
- Helped Ultrascan developers to test the code using PBS scripts to figure out *work* and *scratch* locations on SDSC resources.

- Tested the Grid services on SDSC resources and ran into several issues.
 - GridFTP transfer was not working from Gateway machine to Trestles. (XSEDE ticket No. 215410 – Closed)
 - Gram5 RSL properties were not configured in standard parameters. (XSEDE ticket No. 216752 – Closed)
 - Trestles Gram5 is not configured to run MPI jobs. (XSEDE ticket No. 217698 – Open)
 - Gordon does not have Gram5 to interface running the jobs from Gateway portal. (XSEDE ticket No. 215409 – Open)
- Worked with UltraScan Gateway to enable new code US-SOMO on exiting resources.
- Submitted/Published/Presented XSEDE 12 paper on US-SOMO work.

E.8. WBS 1.5.3 Extended Support for Training, Education, and Outreach

E.8.1. Gateway Training and Outreach

The IU Science Gateway Group and its collaborators spearheaded two tutorials that were accepted for XSEDE12: “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).

E.8.2. Dark Energy Survey Simulation Working Group

The Dark Energy Survey (DES) is an upcoming international experiment that aims to constrain the properties of dark energy and dark matter in the universe using a deep, 5000-square degree survey in five optical bands. The production of a suite of large N-body simulations will allow the development of a Blind Cosmology Challenge (BCC) process for the DES collaboration. The IU gateway group’s extended support is focusing on developing workflow solutions for N-body production process executing 2LPT and L-GADGET codes using the Apache Airavata software suite. The workflow will prepare input files for these tasks, submit 2LPT initial conditions (ICs) code, verify correct execution, archive ICs, submit L-gadget simulation code, verify correct execution, archive output, re-submit and verify until code terminates successfully. This project recently completed its first ECSS support period and was granted a second phase for Quarters 3 and 4.

In previous work, initial versions of the workflow were implemented and tested. During this quarter, work focused 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 environment; and providing automatic processing steps within the workflow.

The goal for the next quarter is to extend the current workflow, adding capabilities to trigger data movement to persistent storage, to manage XSEDE and off-XSEDE post-processing steps, and to launch multiple jobs on TACC and SDSC machines. Improvements to provenance and output handling under the current workflow system will also be implemented.

The initial results of this collaboration were documented in an XSEDE12 submission: Raminderjeet Singh, Suresh Marru, Brandon Erickson, August Evrard, Matthew Becker, Michael Busha, Andrey Kravtsov, Marlon Pierce, Risa Wechsler, "A High throughput workflow environment for cosmological simulations," XSEDE 2012, Chicago IL 2012.

E.8.3. Petascale computations in mineral physics with Quantum ESPRESSO (VLAB)

The IU gateways group 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 will optimize the execution of the Quantum ESPRESSO software for materials simulations in XSEDE systems.

During the current period of performance, the IU gateways team hosted Pedro da Silveira (primary VLAB gateway developer) for a three-day developer retreat at IU. These meetings included detailed discussions of VLAB workflows, job submission requirements, and software architecture so that integration with Apache Airavata software could be planned. The VLAB codes were installed on Trestles and Lonestar, queue submission and remote invocation issues were resolved. IU and VLAB developers also developed a prototype client for submission of VLAB applications through Airavata.

During the next quarter, the goals will be to complete integration of basic VLAB job submission to XSEDE resources using Apache Airavata and to begin implementing some of VLAB's advanced job submission requirements (such as job collections) on XSEDE.

E.9. WBS 1.6.5 Campus Bridging

The critical and overarching theme for program year one was transforming campus bridging⁸ from a very amorphous state of "sounds like a great idea . . . what is it?" to a point where we have a clear definition of what the XSEDE Campus Bridging team would like to accomplish over the course of the five-year XSEDE award. The Campus Bridging team engaged in three major iterative and overlapping activities during this year:

- Discussion of campus bridging within XSEDE and within the national cyberinfrastructure community
- Preparation of documents and presentations defining and describing campus bridging
- Work on pilot projects for testing the Global Federated File System (GFFS) software on campuses

⁸ Note that campus bridging is not capitalized when used to describe a general type of activity, but when referring to the organizational unit the Campus Bridging team, it is capitalized.

E.9.1. Discussion of campus bridging within XSEDE and within the national cyberinfrastructure community

One of the side effects of the very great deal of public input and public attention that surrounded the activities of the National Science Foundation Advisory Committee for Cyberinfrastructure was that community expectations about XSEDE's Campus Bridging efforts ran far ahead of actual planning work related to campus bridging within XSEDE, or the preparation of products useable in a campus bridging context. To address this, a tremendous amount of effort was spent addressing the question "what does campus bridging mean to you?" Such discussions were held in BOFs and panels at SC11, Internet2 meetings, XSEDE organizational and planning meetings (including several meetings with Campus Champions), computing organizations (e.g. Coalition for Academic Scientific Computation, EDUCAUSE), participants in and leaders of the Open Science Grid, and many other community members.

Formal liaisons were established to foster on-going communications as follows:

- Open Science Grid (Dan Fraser assigned as liaison from OSG to XSEDE Campus Bridging)
- EDUCAUSE ACTI (Rich Knepper assigned as liaison from XSEDE Campus Bridging to EDUCAUSE ACTI)
- XSEDE Architecture & Design (Craig Stewart assigned as primary liaison to A&D; Knepper secondary).

The Campus Bridging team also set up discussion areas in the community forums of the XSEDE User Portal. The Campus Bridging team provided seven presentations describing campus bridging and facilitating discussions about Campus Bridging in XSEDE, that are included in section E.10.3.

E.9.2. Definition of use cases and quality attributes for XSEDE's Campus Bridging efforts

Working with the Architecture & Design (A&D) team, the XSEDE Campus Bridging team finalized two technical reports on XSEDE's Campus Bridging use cases. These documents serve two purposes. First, they define the functions that the XSEDE Campus Bridging team would like XSEDE as an organization be able to fulfill during the five-year XSEDE award. Second, they have now become the model for the use case development process within XSEDE. These documents are:

Stewart, C.A., Knepper, R., Grimshaw, A., Foster, I., Bachmann, F., Lifka, D., Riedel, M. and Tuecke, S. Campus Bridging Use Case Quality Attribute Scenarios, 2012. <http://hdl.handle.net/2022/14476>

Stewart, C.A., Knepper, R., Grimshaw, A., Foster, I., Bachmann, F., Lifka, D., Riedel, M. and Tuecke, S. XSEDE Campus Bridging Use Cases, 2012. <http://hdl.handle.net/2022/14475>

The Campus Bridging team is working with Architecture & Design on Level 3 decomposition documents, which are nearly complete as of the end of the current reporting period.

With these use cases defined, the Campus Bridging team put a great deal of effort into defining a proposed plan of action for the remaining four years of the initial XSEDE award. Discussions and a variety of informal and formal presentations gave rise to the paper “What is Campus Bridging and what is XSEDE doing about it?” which was accepted for inclusion in the XSEDE12 conference. Presentations were given to the XSEDE Advisory Board, the XSEDE TEOS Advisory Board, the NSF review panel that conducted the first annual review of XSEDE, and a teleconference of the Campus Champions.

The completion of the paper the paper “What is Campus Bridging and what is XSEDE doing about it?” – which was presented at XSEDE12, after the end of the reporting period but distributed in preprint form during the current reporting period, is a major milestone. It constitutes a suggested work plan, which may now be used as input into the normal XSEDE prioritization and budgeting plan for the remaining four years of XSEDE. It presents a succinct and clear answer to the questions “what does XSEDE mean by campus bridging?” and “how does the Open Science Grid relate to campus bridging?”

In addition to this paper, the Campus Bridging team proposed two panels that were accepted for presentation at XSEDE12:

- Security for Science Gateways and Campus Bridging (Jim Basney, Randy Butler, Dan Fraser, Suresh Marru, Craig Stewart)
- Campus Bridging and the GFFS Pilot: Pilot site reports (Jin Ferguson, Guy Almes, Toby Axelsson)

The evaluation of the pilot projects will be conducted in collaboration with the XSEDE TEOS evaluation group. Key criteria for evaluation will be:

- Did the software work as described in the documentation and did it work properly and consistently?
- Did it improve the ability of campus-based users to interact with XSEDE – particularly those who were not already users of XSEDE services?
- Was the training related to the software of high quality and did it make effective use of learners’ time?
- Were the training, information, and documentation such that local support experts on campus were well able to aid their local users?

The XSEDE12 conference was very definitely a defining moment for XSEDE Campus Bridging. We have a plan: now the questions are 1) where do our plans fit into the overall picture of XSEDE plans, priorities, and constraints; and based on the tasks and goals that are approved and set by XSEDE leadership as prioritized and funding Campus Bridging activities, can we have positive impact on how XSEDE supports the national open research community and how that community works to support itself?

E.9.3. GFFS Pilot Project

Working with the A&D team, Software Development and Integration team, and Operations team, the XSEDE Campus Bridging team initiated a pilot program to test the XSEDE Global Federated File System software (GFFS). The four pilot sites and main themes of their work are as follows:

Texas A&M University: using GFFS to move between users on campus and the Brazos file systems and to the TACC Ranger system.

University of Kansas: using GFFS for cosmology, molecular modeling, and polar research to share data between KU, NCSA, Purdue, and Indiana University.

University of Miami: using GFFS to simplify data transfer between Miami and XSEDE resources as well as data sharing within UM.

City University of New York: using GFFS to facilitate researcher use of CUNY Center resources. Data will be shared via GFFS between the College of Staten Island, Miami, and Delaware with the CUNY Center to transfer large files. CUNY's team also plans to make use of GFFS to expand the capacity of existing CUNY Center file systems.

Just as the reporting period ended the latest version of the GFFS software passed XSEDE readiness review, so we will pursue completion of these pilot projects during PY2.

E.9.4. Challenges in Program Year Two

The XSEDE12 conference, held just after the end of PY1, was a watershed event for Campus Bridging: we presented a clear vision for what we wanted to do, and got a very positive reaction. Now the challenge in PY2 will be to demonstrate some tangible and positive change in the way researchers in the US do their research as a result of XSEDE Campus Bridging efforts. Key metrics in PY2 will be:

Are the community as a whole, and XSEDE and OSG in particular, able to clearly enunciate what campus bridging means and what PY2 plans are?

Are the GFFS pilots successful, and do they lead to wide and rapid deployment of these tools?

Is XSEDE able to deliver a "Rocks Roll" distribution of a generic XSEDE-like cluster and have some early adoption of that distribution on campuses in the US?

E.10. Peer-reviewed publications, technical reports, and presentations funded by XSEDE subcontract (exclusively or primarily)

E.10.1. Peer-reviewed Publications

Chathura Herath, Fang Liu, Suresh Marru, Lahiru Gunathilake, Masha Sosonkina, James P. Vary, Pieter Maris, Marlon Pierce, "Web Service and Workflow Abstractions to Large Scale Nuclear

Physics Calculations,” (SCC2012-2101). Proceedings of ICWS 2012, Honolulu, HI June 24-29, 2012.

E.10.2. Technical reports (not peer reviewed)

Lindsey, S.; M. Dahan, J.L. Fischer, C.A. Stewart, J. Boisseau. 2012. XSEDE system description template. <http://hdl.handle.net/2022/14521>

Stewart, C.A., Knepper, R., Grimshaw, A., Foster, I., Bachmann, F., Lifka, D., Riedel, M. and Tuecke, S. Campus Bridging Use Case Quality Attribute Scenarios, 2012. <http://hdl.handle.net/2022/14476>.

Stewart, C.A., Knepper, R., Grimshaw, A., Foster, I., Bachmann, F., Lifka, D., Riedel, M. and Tuecke, S. XSEDE Campus Bridging Use Cases, 2012. <http://hdl.handle.net/2022/14475>.

E.10.3. Presentations

Stewart, C.A. 2012. Campus Bridging. (Presentation) XSEDE (eXtreme Environment for Science and Engineering Discovery) Advisory Board Meeting (Chicago, IL, 23 Apr). <http://hdl.handle.net/2022/14443>

Stewart, C.A., S. Marru, R. Knepper, D.Y. Hancock, J. Wernert, C. Aikman, J. Bolte, P. Brown and T.M. Miller. 2012. Indiana University collected XSEDE update. (Presentation) XSEDE (eXtreme Environment for Science and Engineering Discovery) Quarterly Meeting (Austin, TX, 6-7 Mar). <http://hdl.handle.net/2022/14444>

Stewart, C.A. 2012. “What is campus bridging and why should XSEDE Campus Champions Care?” Presentation. Presented to XSEDE Campus Champions 8 June 2012. Presented to campus champions virtual meeting from Michigan City, IN.

Stewart, C.A. 2012. “WBS 1.6.5 Campus Bridging Program Plan” Presentation. Presented to NSF review panel 14 June 2012. Arlington VA.

Appendix 1: Aggregate XSEDE report Appendix H (EOT events done under XSEDE subcontract)

The following are events conducted during the quarter.

Type	Title	Location	Date(s)	Hours	Number of Participants	Number of Under-represented people	Method	Funding Sources
Panel	Campus Bridging in XSEDE, OSG, and Beyond	Internet2 Spring Members' Meeting	24 Apr 2012	1.25	32	10	Live	XSEDE
Webinar	"What is campus bridging and why should XSEDE Campus Champions Care?"	Michigan City, IN	8 Jun 2012	1	15	7	Webcast	XSEDE
Presentation	XSEDE Campus Bridging	CASC Fall Meeting	September 2011	1	45	10	Live	XSEDE
Presentation	Regional CI Support for Bridging and Research Engagement	Internet2 Fall Member's Meeting	October 2011	1	50	8	Live	XSEDE
BOF	Campus Bridging GFFS Pilot Program	SC11	November 2011	1	28	5	Live	XSEDE
Presentation	Campus Bridging	ACTI-CCI/ACTI-CSG	January 2012	1	25	3	Live	XSEDE
Presentation	Penguin at IU and Cloud Services	CASC Spring Meeting	March 2012	2	50	10	Live	XSEDE
Presentation	Campus Bridging in XSEDE, OSG, and beyond	Internet2 Spring Members meeting	April 2012	1	42	8	Live	XSEDE