User Support & Campus Grids

OSG area coordinators meeting 9/30/15 Bala Desinghu

Topics

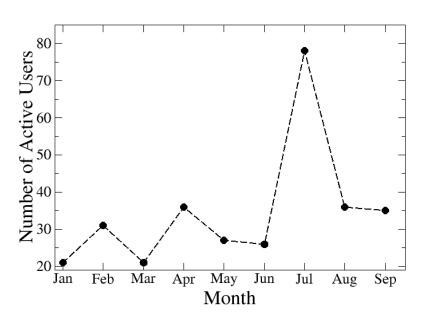


- Last Three Months:
 - Recent Users, Projects and Active users
 - Users supported
- Joint OSG Software Carpentry Workshop at Duke University
- Computational Neuroscience Freesurfer
- Connect Client updates

New Users: July 1st 15 - Sept 29th 15



- 110 new users joined OSG
 Connect
- 60 from UserSchool15
- We had nearly 150 active users, during the last three months



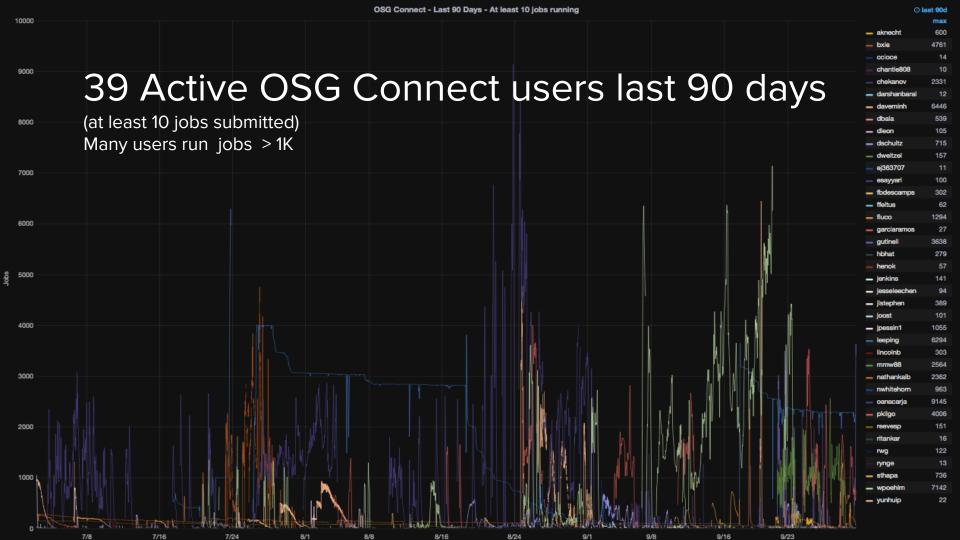
New Projects: July 1st 15 - Sept 29th 15

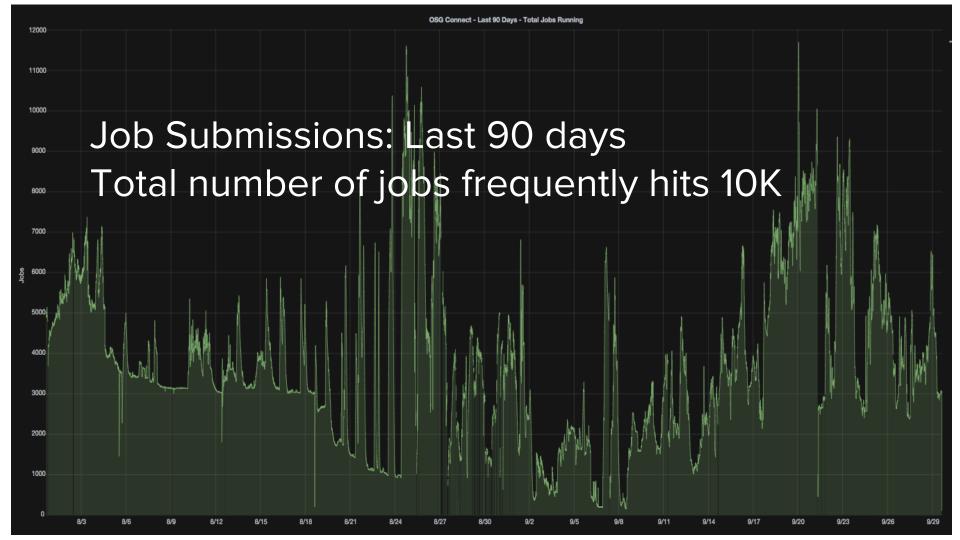


- 19 projects created during the last three months
- Approximately, six projects/month
- From 15 universities:
 - Clemson University, Texas A&M University, University
 of Illinois at Urbana-Champaign, University of
 Wisconsin-Madison, University of Wyoming, Argon
 National Lab, MIT, University of Maryland Baltimore,
 National Research Council of Canada, University of
 Hawaii at Manoa, BNL, Florida State University, UCSD,
 University of Kentucky, University of Central Florida

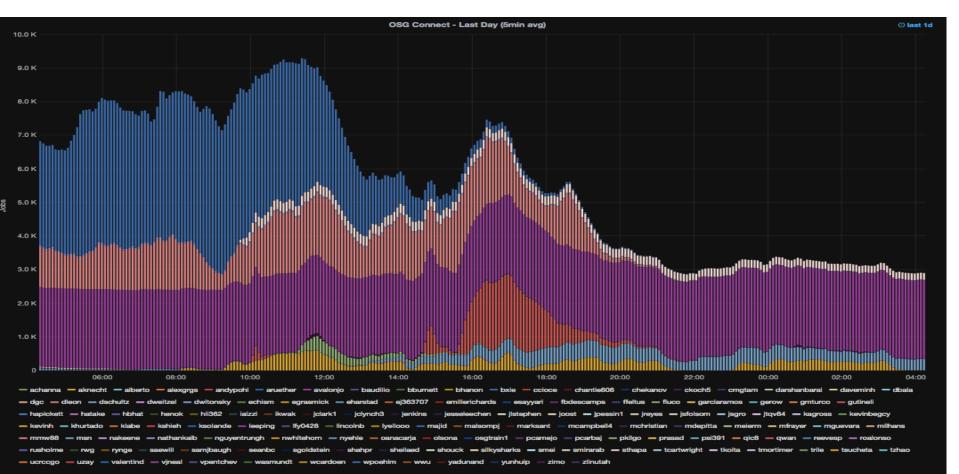
osg.BioGraph	Alex Feltus	Clemson Univ.	Bioinformatics	constructing gene interaction graphs
osg.MCP	C. S. Raman	Univ. of Maryland Baltimore	Structural Biology	finding molecular replacement solutions
osg.numfpi	Jerry Tessendorf	Clemson Univ.	Computer Science	Multiple Scattering volume renderer
osg.oclab	Dave OConnor	Univ. of Wisconsin Madison	Pathology	Cell Image Analysis
osg.DemandSC	Fernando Luco	Texas A&M Univ.	Economics	welfare under the different scenarios
osg.BGAgenomics	Sucheta Tripathy	Indian Institute of Chemical Biology	Bioinformatics	cyanobacteria genomics program
osg.ProbTracx	Bruce P. Hermann	Univ. of Wisconsin Madison	Neurology	Brain image analysis to understand idiopathic epilepsy
osg.EvolvingAl	Jeff Clune	Univ. of Wyoming	Computer Science	Evolving artificial intelligence mimicking natural systems
osg.FutureColliders	Sergei Chekanov	ANL	HEP	Simulations beyond LHC

osg.Phylo	Siavash Mirarab	UCSD	Bioinformatics	Reconstructing tree of life
osg.NSLS2ID	Dean Hidas	BNL	HEP	Beamline simulation
osg.peers	Jessica Folsom	Florida State Univ.	Sociology	Quantitative analysis of student achievements
osg.ncidft	Alberto Roza	National Research Council of Canada	Chemistry	Modelling non-covalent interactions
osg.TextLab	James Evans	Univ. of Chicago	Sociology	Data analytics on text
osg.mab	Vivek Farias	MIT	Management	Multi-Armed Bandit problem
osg.QEvolBiol	Jeremy Cleve	Univ. of Kentucky	Biology	population dynamics under evolutionary forces
osg.NeoflAnnot	Petra Lenz	Univ. of Hawaii	Marine Biology	transcriptome for the flamingeri
osg.SciSim	Amit Goe	Univ. of Central Florida	Computer Science	Support for research computing
osg.EHEC	Chuck Kaspar	Univ. of Wisonsin Madison	Microbiology	transmission and evolution of pathogens



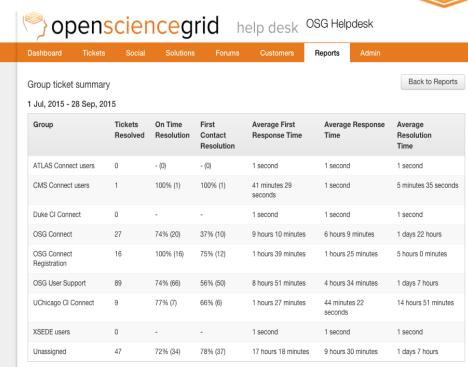


Job submission patterns - one day



Help Desk: July 1st 15 - Sept 29th 15

- Helped more than one user/day. This includes answering simple questions related job submission and all the way to set up their workflow towards production run
- On an average, a new user account was created within 1.5 hours from the sign-up time
- On-line chat opened recently
 - We find that new users
 like to use the chat service



Solution Center: July 1st -Sept 29th



- Tutorials:
 - Matlab runtime examples
 - linear algebra solver
 - ordinary differential equation
 - optimization tool box
 - Pegasus-Blast for bioinformatic applications
 - Gromacs for molecular dynamics simulations
- Forum article on re-trying failed jobs
- Multicore and GPU jobs

OSG-Duke Workshop



- OSG-Duke Workshop front page: http://swc-osg-workshop.github.io/2015-10-27-duke/index.html
- A three day workshop that covers shell scripting, version control, python programming and distributed high throughput computing
- Special lecture and informal discussion on the evening of the second day
- For each session, an average of 30 students registered out of 40 seats

Freesurfer project - S.Thapa, D.Krieger



- Project to build a simple submission service for computational neuroscientists
- Background: Freesurfer is a suite of image processing utilities that process MRI data. Since image processing is fully independent, this fits well with a DHTC environment.
- This project aims to provide an easy to use web based gateway that will allow the Freesurfer community to process batches of MRI data using resources on OSG.

Freesurfer, II



- Web piece by CS students at Pitt
- User registration, upload of MRI images for processing, monitor jobs, and download results
- Backend processing handled by OSG staff

Freesurfer, III



- Replicated original workflow on COMET using Don Krieger's scripts
- Installed Freesurfer 5.3.0 on OASIS
- Set up Pegasus workflow and DAX generation scripts (https://github.com/OSGConnect/freesurfer_workflow/tree/master/python)
 - Supports both single job and diamond dag workflows
 - Supports using single and multicore jobs
- Currently testing workflows and middleware
- Requirements document for students

Connect Client status - Overview



David Champion

- Bug fixes based on user feedback
- Improvement: ClassAds to track the connectclient jobs
- Ongoing site deployment testing
 - on UChicago-RCC
 - on Palmetto-Clemson

Connect Client status



- several bug fixes and minor new features in release 0.5; nothing world-shifting
 - bug fixes in tutorial command
 - o add ConnectClient* classads to submits:
 - ConnectClientVersion
 - ConnectClientServer
 - ConnectClientUser
 - ConnectClientLocalUser
 - ConnectClientLocalNode
 - ConnectClientLocalDir
 - o add a connect release command.

Connect Client status



connect status: pool names mapped to meaningful aliases — mapping in Gratia pending [tbi]

OLD NEW

\$ c	connect	status					connect	status					
Sum	mary of	availa	able resou	rces for al	l HTCondo	or pools:	Summary of	availa	able resou	rces for al	l HTCondo	r pools:	
	Total	Owner	Claimed	Unclaimed	Matched	Preempting	Total	Owner	Claimed	Unclaimed	Matched	Preempting	
===	rccf-o	sg.ci-c	connect.ne	t:11012?soc	k=collect	or ===	=== Clemso	on Palme	tto ===				
	249	0	195	54	0	0	249	0	195	54	0	0	
===	rccf-o	sg.ci-c	connect.ne	t:11011?soc	k=collect	or ===	=== Syracu	ise Oran	ngeGrid ==	=			
	646	29	510	105	2	0	646	29	510	105	2	0	
===	osg-fl	ock.gri	d.iu.edu	===		=	=== OSG Gr	rid ===					
	5498	0	5424	74	0	0	5498	0	5424	74	0	0	
===	uc3-mo	n.mwt2.	org ===			=	=== UChica	igo UC3					
	791	3	732	51	1	4	791	3	732	51	1	4	

Connect Client status



- various internal flow, config mgt changes
- allocate pty for server aliases
 - helps with some server-side commands that use keyboard interaction
- install: disable module "dependencies" by default
- install: Rename -site option to -oasis
- o q, rm, history, and release act on own jobs
 - connect q ~ condor q \$ (whoami)
- remove osgconnect-specific URL from setup directions

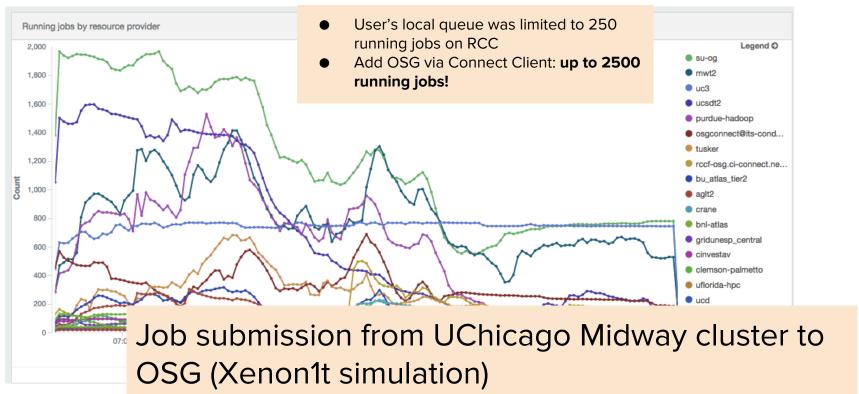
Deployments, testing & user feedback



- UChicago RCC Midway
 - XENON1T (Dark Matter, Gran Sasso) testing
 - Geant4, ROOT installed in OASIS
 - Have run multiple successful test sequences:
 - 10k runs, 85-100k events each; 850m-1b events
 - "1tb data output working on data collection models
 - globus and xroot access methods in development
 - Next: local Midway allocation as resource target to UChicago CI Connect

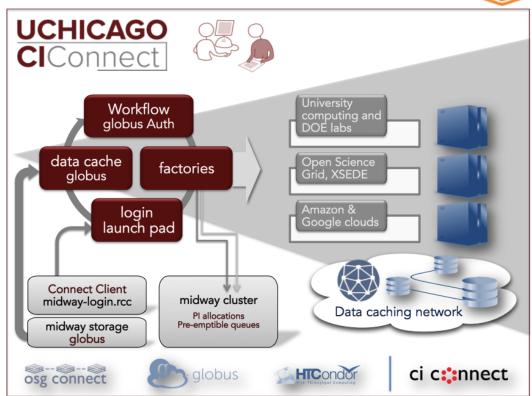
Show users power of sharing



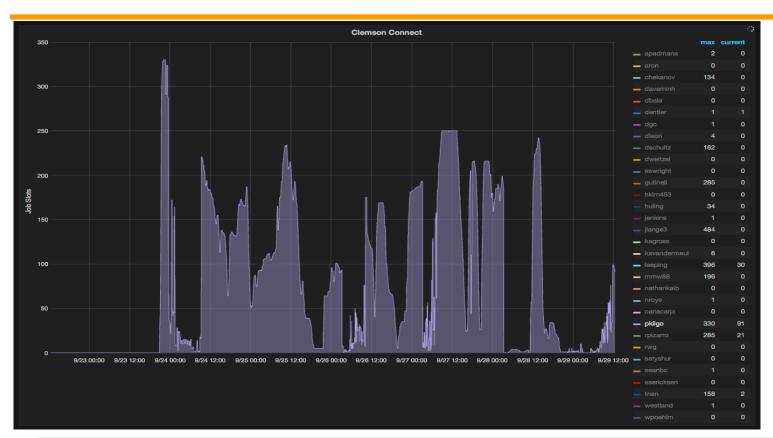


Pattern for Campus Grids

- Connect client installed locally
- OSG Connect (or CI Connect) to bring remote resources to the local cluster
- Potentially flocking back to campus (e.g. Palmetto)
- One campus-based queue



Connect Client from Palmetto & back





User: P.Kligo Inst: Clemson Project: numfpi

Started on login. osgconnect.net

Moving to connect-client on Palmetto

Connect Client release schedule



- v0.5 released yesterday
- Next release foci:
 - Paul Kilgo's (Palmetto user) feedback
 - extensions/improvements to data transfer capability
 - automatability of Globus xfer for large datasets (e.g. xenon1t)
 - possible improvements to push/pull technique
- Will aim for incremental releases at 2-week intervals. Next: Oct 13.

- Ongoing
 - a. OSG Connect account and Project requests (Bala)
 - b. Respond to user forum "how-do-1?" questions, feature requests, errors (full team)
 - c. Software and packaging of user applications in the modules + OASIS service (Bala, Suchandra)
 - d XD Progra
 - Support users with XRAC allocations (Mats)
 - Attend quarterly XRAC allocations meetings (Rob, Mats)
 - e. Operation of user infrastructure
 - Maintenance of Cobbler build and Puppet configuration rules (Lincoln, Judith)
 - Maintenance of KVM-based virtual machine infrastructure (Lincoln, Judith)
 - login01.osgconnect.net (login service) (Lincoln)
 - i. schedd, collector, Gratia probe
 - login02.osgconnect.net (remote campus connect clients server) (Lincoln)
 - i. schedd, collector, Gratia probe
 - NSF file server for /home directories (Lincoln)
 - i. 50 GB/user quota
 - ii. Backup service
 - hosted campus factory services (Syracuse, Clemson, St. Louis resource targets) (Lincoln)
 - Ceph object store (750 TB usable capacity shared with ATLAS Connect users) (Lincoln)
 - GaneshaFS for Posix access to the Stash RBD (RADOS Block Device, variable capacity)
 - ii. 14 Xrootd doors at 20 Gbps to SciDMZ (100 Gbps to OmniPoP)
 - iii. 14 Gridftp doors at 20 Gbps to SciDMZ (100 Gbps to OmniPoP)
 - stash.osgconnect.net services (Lincoln)
 - i. http server
 - ii. xrootd origin server
 - iii. stash cache server
 - iv. Globus gridftp server endpoint
 - v. Management of user and project stash areas for quasi-transient job data

- 2. Lowering Barriers to Usabiliy
 - a. Campus Connect Client [David, ongoing: bug support and progressive releases]
 - c. Create GitHub-backed help desk service [Rob, David, July 2015]
 - c. Create user community-focused website [Rob, Student, Aug 2015]
 - . Create publication database and upload service [Rob, Student, Aug 2015]
 - e. Create domain specific HTC recipes [Bala, Mats, Emelie, on-going]
 - . Provide NX server interface to login.osgconnect.net [Judith, July 2015]
 - g. Reducing friction between user data and resources [Rob, on-going]
 - Campus to Stash; Stash to Campus [Suchandra, on-going]
 Document and benchmar high priority data access use cases with StashCache
 - (copy, "Posix", etc.) [Suchandra, Dec 2015]

 iii. Development of stash-cp [Student, Lincoln, on-going]
 - h. Assessment of XSEDE user community application workflows, suitability for HTC (Mats. Bala)
 - Demonstrated HTC conversion and reach of traditionally HPC applications in MD (Molecular Dynamics) such as NAMD, GROMACS
 - Perform HTC analog to XRAC MPI scaling demonstrator to determine performance equivalent → common currency for XRAC proposals
 - ii. Same, bioinformatics (BLAST), docking (Auto Vina)
 - i. Support for the NIH community (Rob, Mats, Emelie, Bala)
 - Create Project and necessary software components to support users of FreeSurfer, an open source software suite for processing and analyzing human brain MRI images
 - ii. Adapt basic FreeSurfer tutorial modules to Condor, support in the OSG Connect tutorial collection
 - Work with Don Krieger to identify a research group actively analyzing MRI data with FreeSurfer, potentially partnering with XSEDE ECSS, and explore issues of support on OSG
 - iv. Support BLAST applications
 - v. Support molecular docking applications (drug discovery)

owering Barriers to Sharing Resources (small campus integration) [Suchandra, Lincoln]

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Progress against metrics



Campus and User Support Metrics							
OSG Connect	2015	2016	2017				
Active users	50	100	150				
Active projects	25	50	75				
Avg (active users / week)	5	10	20				
Avg (active projects / week)	3	6	12				
Campus connect client users	2015	2016	2017				
Downloads	10	50	100				
Active users	5	10	50				
Campuses	2	5	10				
Avg (active users / week)	5	10	20				
Avg (active projects / week)	3	6	12				
OSG Quick Connect Campuses	2015	2016	2017				
Campus as resource targets	3	5	10				