User Support, XD & Campus Infrastructures

Rob Gardner • University of Chicago



User Support and Campus Team

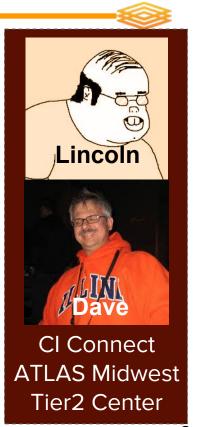












38M 52M 24M 200 XSEDE cpu-Direct cpu-Connect cpu-Active users hrs hrs hurs 96 29 190 **Training** PI/Projects **Publications** app modules events 81 3.0 Campus FTE Submit hosts Institutions

grids



Feild of Science

Nuclear Physics

High Energy Physic

Computer and Infor

Physics and astron

Feild of Science

Molecular and Stru

Feild of Science

Multi-Science Com

Multi-Science Com

Community Grid

Multi-Science Com

Multi-Science Com

Multi-Science Com

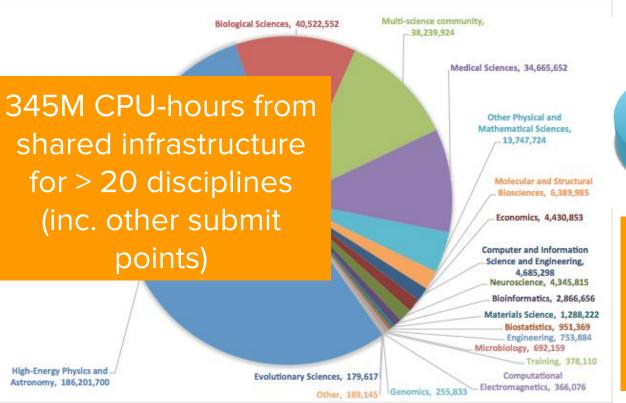
Feild of Science Wall Hours

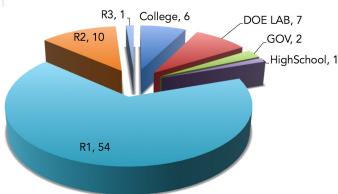
Wall Hours

Wall Hours

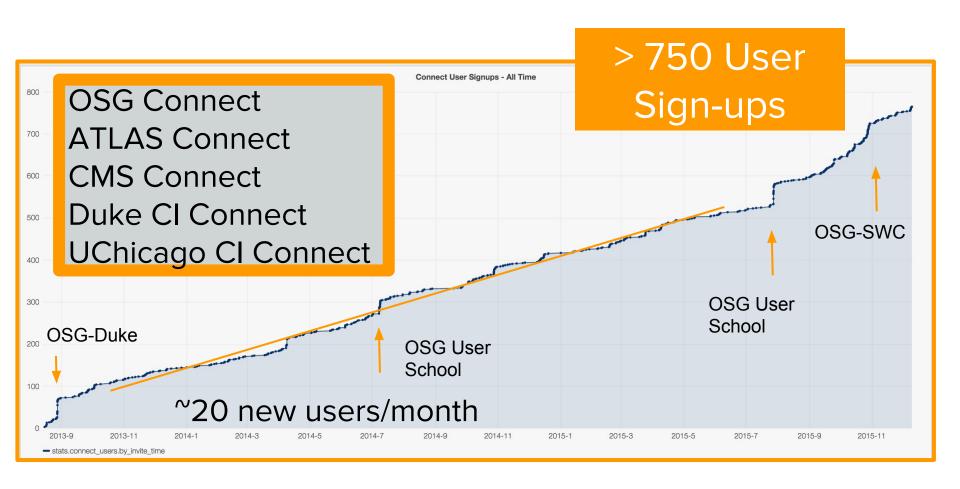
Wall Hours

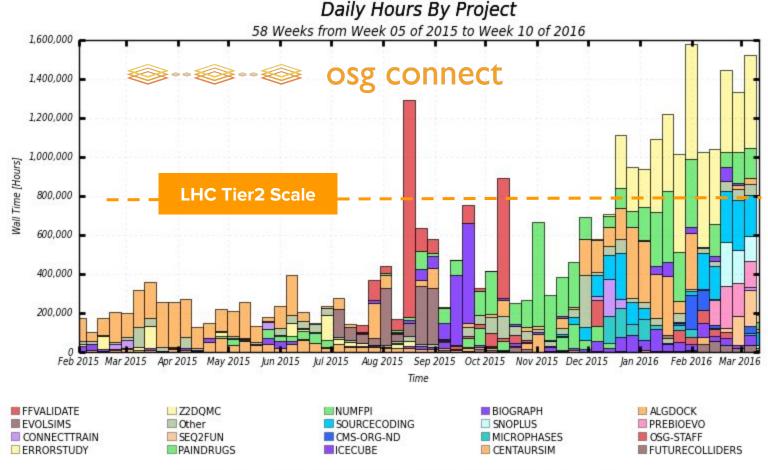
Impact across disciplines and institutions





Pls by Institution
Carnegie
classification
(opportunistic users)





Maximum: 1,580,233 Hours, Minimum: 104,823 Hours, Average: 520,720 Hours, Current: 191,775 Hours

Science



Science publications (partial list)



Project: ProtEvol

1. Shah P, McCandlish DM, and Plotkin JB. "Contingency and entrenchment in protein evolution under purifying selection". PNAS 112: E3226–E3235 2. Otwinoski J, McCandlish DM, Shah P, and Plotkin JB. "Identifying site-specific amino acid preferences for modeling protein evolution" (In Prep)

Project: AIGDock

- 1. Trung Hai Nguyen and David D. L. Minh, "Intermediate Thermodynamic States Contribute Equally to Free Energy Convergence: Demonstration with Replica Exchange." (In preparation)
- 2. David D. L. Minh, "Protein-Ligand Binding Potential of Mean Force Calculations with Hamiltonian Replica Exchange on Alchemical Interaction Grids" (http://arxiv.org/pdf/1507.03703.pdf

Project: ErrorStudy

1. Patrick A. Reeves, Cheryl L. Bowker, Christa E. Fettig, Luke R. Tembrock, and Christopher M. Richards, "Effect of error and missing data on population structure inference using microsatellite data" (In preparation)

Project: numpfi

- Paul Kilgo and Jerry Tessendorf. "Accelerated path generation and visualization for numerical integration of Feynman path integrals for radiative transfer". Joint International Conference on Mathematics and Computation, Supercomputing in Nuclear Applications and the Monte Carlo Method, April 2015.
- 2. Paul Kilgo and Jerry Tessendorf. Toward validation of a Monte Carlo rendering technique. Special Interest Group on Graphics and Interactive Techniques, August 2015. (Poster).

Project: FutureColliders

- 1) S.V. Chekanov, I. Pogrebnyak, D. Wilbern, Cross-platform validation and analysis environment for particle physics, arXiv:1510.06638
- 2) S.V.Chekanov, J.Dull. Energy range of hadronic calorimeter towers a and cells for high-pT jets at a 100 TeV collider, arXiv:1510.06638

Project: CentaurSim

Kaib, Nathan A.; Chambers, John E. "The fragility of the terrestrial planets during a giant-planet instability", Monthly Notices of the Royal Astronomical Society, Volume 455, Issue 4, p.3561-3569 (2016)

Project: SPT

N. Whitehorn, T. Natoli et al, "Millimeter Transient Point Sources in the SPTpol 100 Square Degree Survey," (to be submitted to The Astrophysical Journal).

Project: RicePhenomics

Knecht, AC, Campbell, MT, Caprez, A, Swanson, DR: Image Harvest: An open source platform for high-throughput plant image processing and analysis. Journal of Experimental Botany. [Accepted, pending minor revision].

XD-Project: TG-CHE130091

- 1. Paul D. Siders, "Conformational free energy of alkylsilanes by nonequilibrium-pulling Monte Carlo simulation," Molecular Simulation, accepted September 2015. doi: 10.1080/08927022.2015.1083101
- 2. Presented "Conformational free energy in a chromatographic stationary phase by nonequilibrium pulling within Gibbs-Ensemble Monte Carlo simulation" at the Virtual Conference on Computational Chemistry, University of Mauritius, August 2015.

Optical data communication & compression

- David Mitchell, New Mexico State
 - Ahmad Golmohammadi (EE graduate student)
 - Important for digital space and satellite communication & wireless data transmission
 - Whole system simulations transmitter, decoder, receiver & stochastic noise, data compression
 - I am so happy that could do my simulation that much fast. Instead of waiting for several weeks, right now I am getting them in hours. Thank you very much, Best wisehs





Randomness in Evolution



- Understanding evolution at molecular scale in DNA with combination of mathematical modeling and simulation
- How quickly does a genome fix a mutation?
- Role of randomness versus natural selection?

Joshua Plotkin, Penn

"We use the OSG to run computer simulations for complex processes. By simulating evolution in populations, we can study hypothetical situations that you can't study in the wet lab or field."

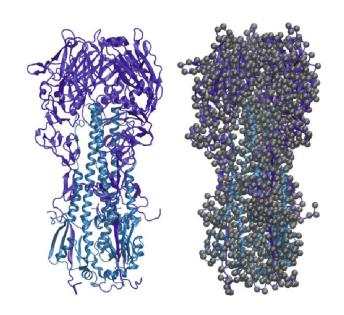
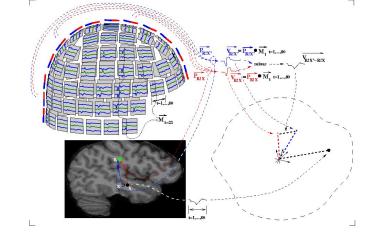


Image courtesy Joshua Plotkin. A computationally predicted structure of an influenza virus protein. Plotkin's research group uses the Open Science Grid to study questions in evolutionary biology and ecology.

Human Neuroimaging on the Open Science Grid

(c.f. Don Krieger's talk this week)

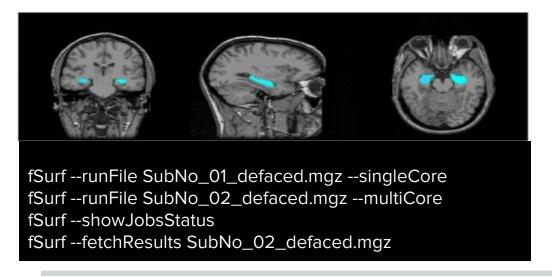


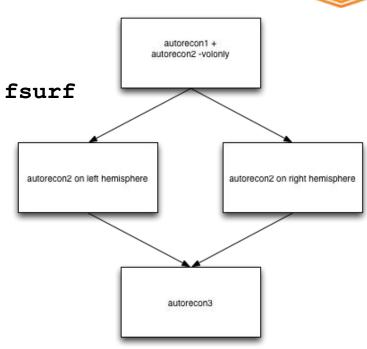
Referee consensus is a new approach to solving large systems of simultaneous mixed linear/nonlinear equations (<u>ACM</u>, <u>Intl J Adv Comp Sci</u>, <u>Explanation of the figure on YouTube</u>).

- Solution of the equations requires search of a high dimensional space.
- The discovery and use of a cost function computed in the "source" space rather than in the "measurement" space enables:
 - solution for a single source at a time,
 - efficient implementation on the grid.

Computational Neuroimaging Service

 OSG partnership with University of Pittsburgh Medical School to provide open computational brain image analysis platform FreeSurfer analysts

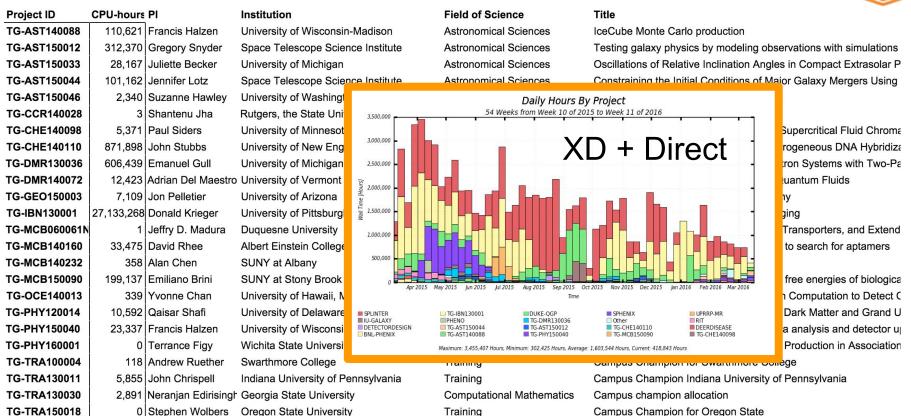




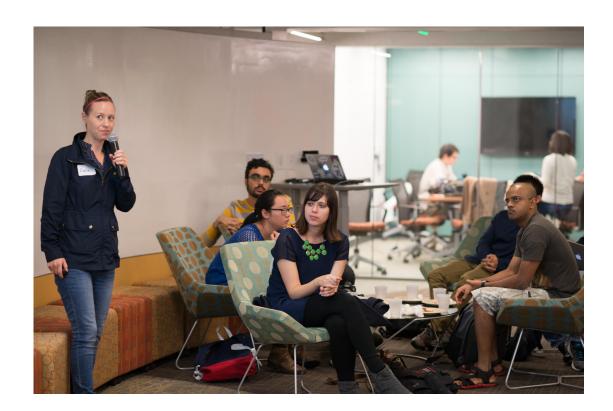
Command line and web API - S. Thapa

OSG XSEDE - 24 active projects





User Support

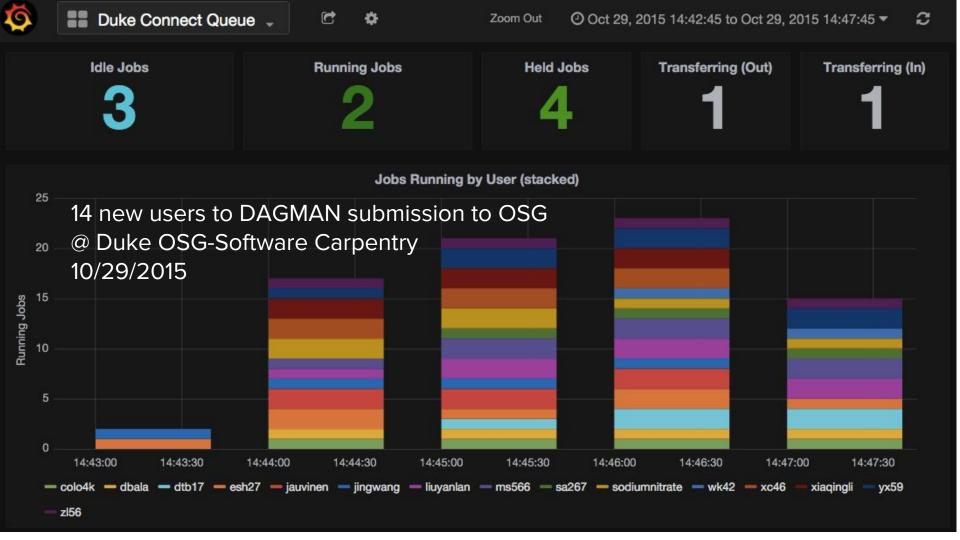


Joint OSG Software Carpentry Workshops



- Two members of OSG User Support team are Software Carpentry instructors
- Extended standard core curriculum with a day of HTC computing best practices





OSG Connect Service



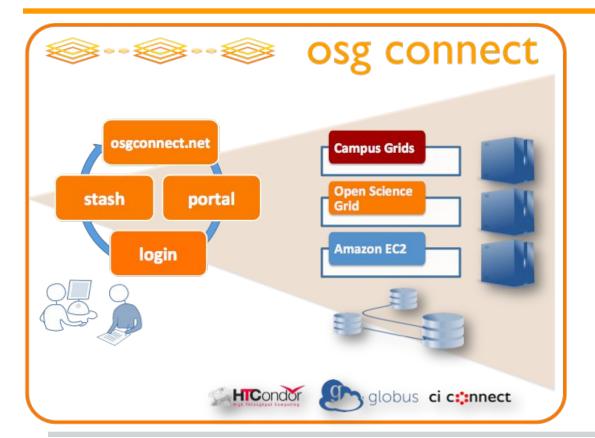
Local campus identity (CILogon) • OSG Connect identity (Globus) • virtual organization (OSG) • HTCondor Glidein





OSG Connect is an easy way to get started





OSG as a campus cluster

- **★** Login host
- ★ Job scheduler
- **★** Software
- **★** Storage

OSG Connect Service



- For users without an institutional submission point
- login node for job management,

```
login.osgconnect.net
```

- Stash is a temporary storage service
 - Globus Online, HTTP, Xrootd
 - Posix accessible from login nodes
 - Origin server for StashCache
- Uses OASIS software repository for user-installed software

User software Installed on the OSG

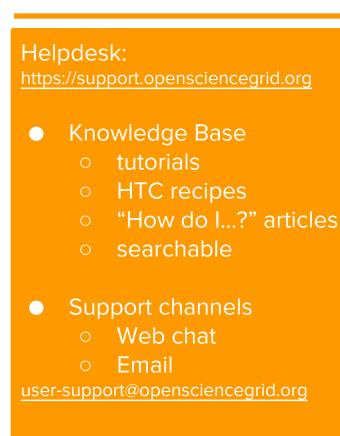
Repository for common, pre-installed user installed software

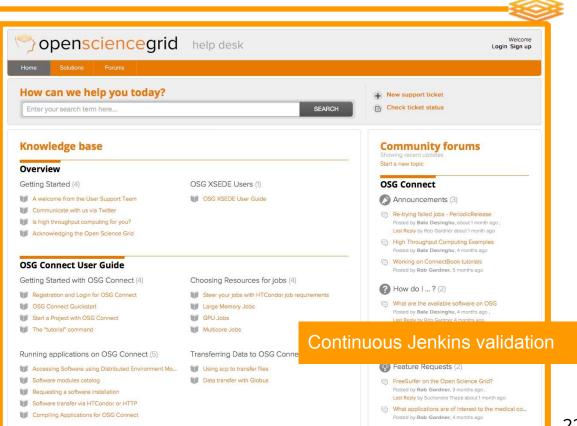
- Accessed with a module command
 - identical software on all clusters
 - apps/libraries installed

```
#!/bin/bash
switchmodules oasis
module load R
module load matlab
```



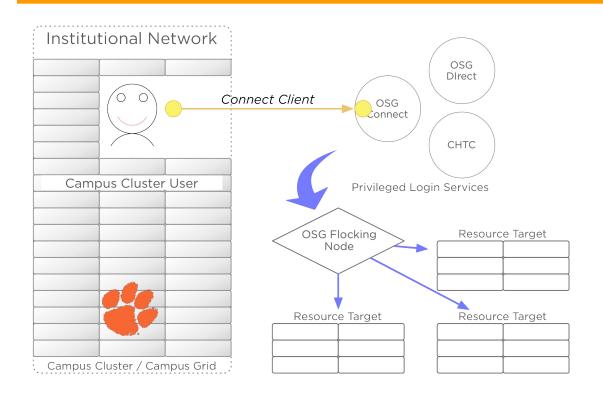
Integrated KB, tutorials, github-managed





Connect Client brings OSG pools to campus





Work from "home"

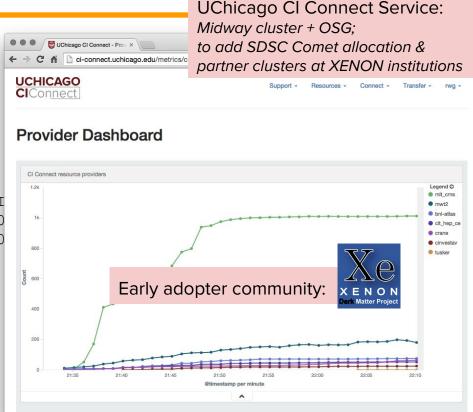
Submit locally, run globally

> Workshop Thursday OSG + ACI-Ref

Organized into a 'local' queue

```
module load connect-client
  connect setup
  connect test
  connect submit myjob.sub
  connect q rwq
-- Submitter: login.ci-connect.uchicago.edu:
uchicago.edu
                                      RUN TI
 TD
        OWNER
                         SUBMITTED
                                      0+00:0
252624.0
                          9/2 14:21
          rwa
                                      0+00:0
252624.1
                          9/2 14:21
          rwa
  connect status
  connect pull (results)
```

Submitted from UChicago Research Computing Center cluster "Midway"

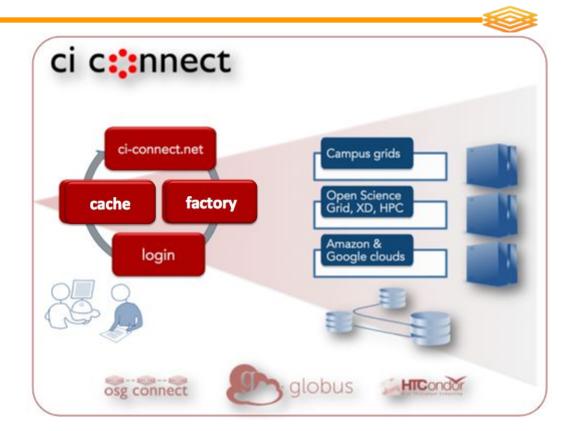


Campus Cyberinfrastructure

mwt2.org

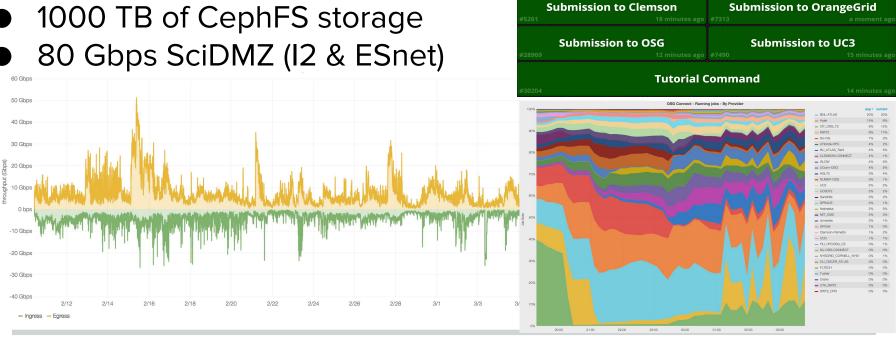
CI Connect

- Integration of mature software
- Concetrated expertise
- Minimize footprint on resources
- Deliver as service



*-Connect Support Infrastructure

- 6 login servers (schedd's)
- 25 Connect (bosco) factories
- 1000 TB of CephFS storage



Monitor

Stash Cache Access

Stash Web Access

Distributed Software Service

Stash Filesystem

Campus Users (@ Clemson) + OSG



Submission to Palmetto cluster (local)



add OSG nodes



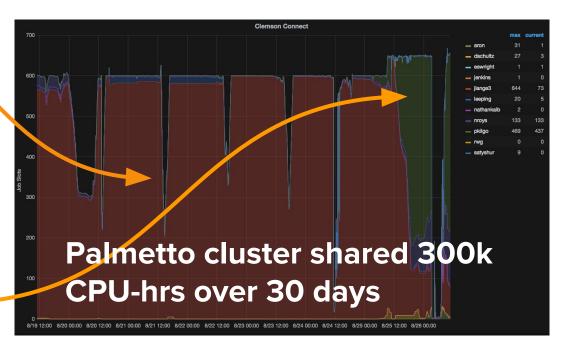
Sharing local resources with communities

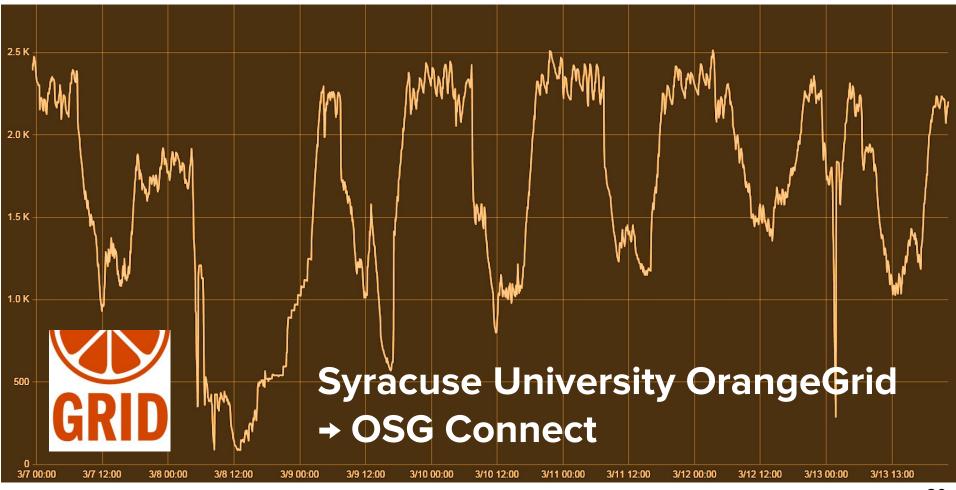


GLOW (UWisconsin-based campus researchers)



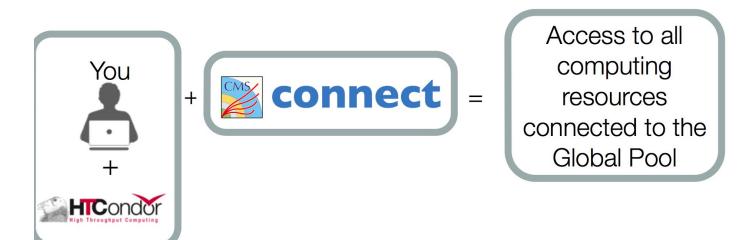
OSG Connect





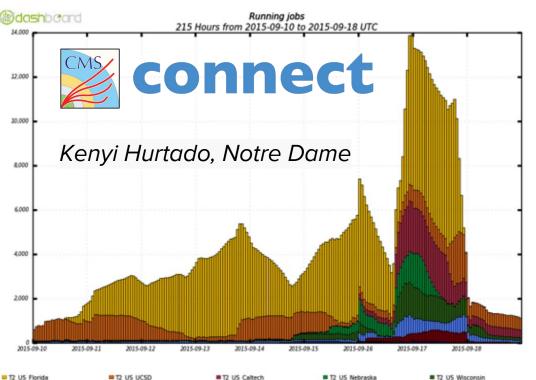
CMS Connect

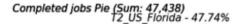
Kenyi Hurtado, Notre Dame

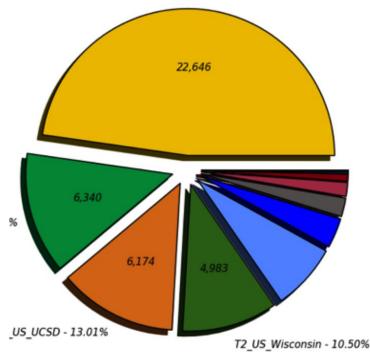


This is a complement to the existing tools in CMS with access to the same CMS Global resources for condor-like workflows that are frequently submitted to local clusters like e.g the LPC CAF at Fermilab or local University CMS analysis clusters.

T2 US Sites historical view example







Maximum: 13.916 , Minimum: 601.00 , Average: 4,229 , Current: 1.108

T2 US MIT

T3 US UCD

T3 U5 Omaha

T2"U5"Purdue

T3 U5 Colorado

T2 US Vanderbilt

T3 US UMiss

T2_US_Wisconsin - 10.50% (4,983)
T3_US_Omaha - 2.06% (976.00)

T3 US PuertoRico

T2_US_MIT - 0.20% (97.00) T3_US_UCD - 0.00% (1.00)

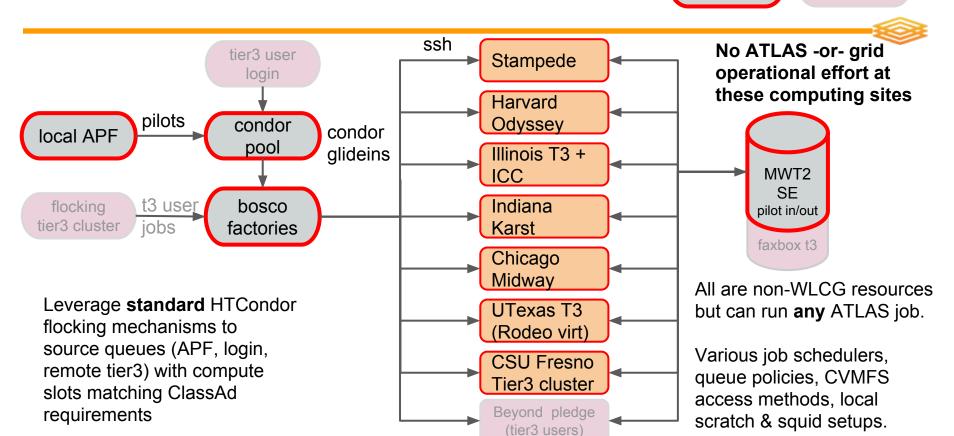
- T2_US_Nebraska 13.36% (6,340)
 T2_US_Purdue 7.35% (3,487)
- T2_US_Purdue 7.35% (3,487)
 T2_US_Caltech 1.54% (730.00)
 T3_US_Colorado 0.13% (61.00)
 T2_BR_SPRACE 0.00% (1.00)

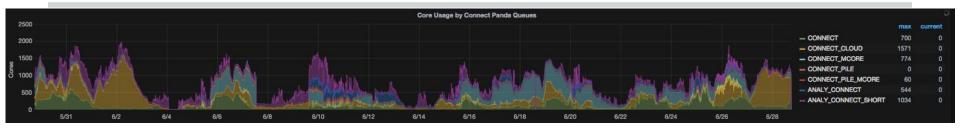
T2 US_UCSD - 13.01% (6.174) 13 US_PuertoRico - 3.29% (1.560) 12 US_Vanderbilt - 0.80% (378.00 13 US_UMiss - 0.01% (3.00)

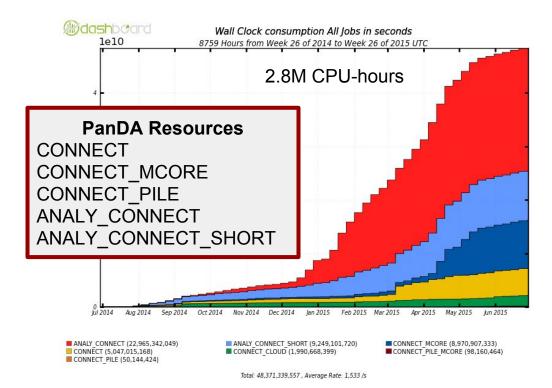
ATLAS Connect & Panda

Panda

tier3 users







Current scale:

~ 1/4 of typical Tier2

~2000 running jobs at peak

But at low operating cost

Only limited by available allocations

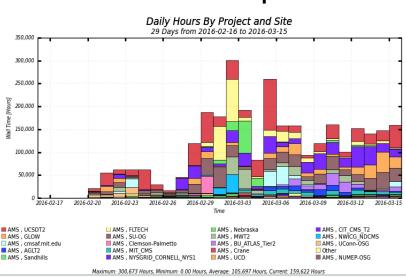
Easy to plug in additional resources or grow with new allocations

Present @ next US ATLAS Institution Board meeting to solicit interest from university research computing centers

MIT OSG Campus Infrastructure



- Supporting AMS space station experiment
- Up and running in hours 18k two days later
- Plans are to run Bosco to other campus
 - resources
- Eventually deploy HTCondor-CE



Campus Cyberinfrastructure futures

Leverage!



- Leverage investments from innovations and other NSF investment, e.g. from ACI DIBBS, CC-DNI, CC-*
- Push deployment of StashCache as primary delivery mechanism for campus Pls
- Hosted HTCondor-CE-Bosco
- Future projects e.g. "Ubiquitous CI substrate"

San Diego State University Stanford University Texas A&M University The Florida State University The University of California, Davis The University of Florida The University of North Carolina at Chapel Hill The University of Oregon The University of Southern Californi's Information Sciences Institute (ISI) University of Wisconsin-Madison Wayne State University **Auburn University** Case Western Reserve University Dartmouth College Lehiah University North Carolina State University Oregon State University Pittsburgh Supercomputing Center Stephen F. Austin State University Texas A&M University-Corpus Christi The Johns Hopkins University The University of California, Berkeley The University of California, Santa Cruz The University of Chicago The University of Connecticut The University of Connecticut Health Center The University of Dayton

The University of Houston

The University of Idaho The University of Illinois at Urbana-Champaign The University of Michigan The University of Montana The University of New Hampshire The University of Notre Dame The University of Pennsylvania The University of Puerto Rico, Río Piedras The University of Southern California The University of Utah The University of Virginia Wittenberg University Arizona State University Carleton College Earlham College Juniata College Keystone Initiative for Network Based Education and Research (KINBER) Northern Illinois University Northwest Indian College Princeton University Saint Anselm College South Dakota State Universit St. Olaf College **Texas State University** The Old Dominion University Research Foundation The University of Arkansa The University of California, Riverside

The University of Cincinnati

The University of Pittsburgh The University of Puerto Rico at Mayagüez The University of South Alabama The University of South Dakota The University of Texas at Arlington The US National Center for Atmospheric Research University of Louisiana at Lafavette University of Maryland, Baltimore Wabash College Washington State University West Virginia University Multiple Award Winners (2012-2014) Clemson University Colorado State University **Duke University** Florida International University Georgetown University Indiana University Kansas State University Louisiana State University and Agricultural and Mechanical College Renaissance Computing Institute (RENCI) The California Institute of Technology The Ohio State University The Pennsylvania State University The University of Central Florida The University of Colorado Boulder The University of Missouri The University of Nebraska-Lincoln The University of Oklahoma The University of Tennessee

The University of Colorado Boulder
The University of Missouri
The University of Nebraska-Lincoln
The University of Oklahoma
The University of Tennessee

120

NSF ACI CC-* DNI
SciDMZ Campuses

Tulane University University of Chicago University of California, San Diego University of Maryland University of Washington Vassar College Virginia Polytechnic Institute and State University Yale University Vanderbilt University The University of Hawai'i at Mānoa The University of New Mexico The University of Kentucky The University of Massachusetts Lowell Northwestern University Syracuse University The University of Wyoming The University of California, Irvine The University of Massachusetts Amherst The University of Alabama in Huntsville Cornell University The University of Michigan Washington University Boise State University Colorado State University - Pueblo Franklin and Marshall College Portland State University Univ of Minnesota Twin Cities Univ of Alabama Birmingham University of Missouri Kansas City University of Texas Dallas University of Alabama Tuscaloosa **UCLA** Marshall University Colorado School of Mines Malone University Northern New Mexico College University of Arkansas Pine Bluff Harrisburg Area Community College **Bucks County Community College** Utah Valley University Baylor College of Medicine

University of Arizona

Ubiquitous & Easy "CI Substrate"



- Pioneer a new phase of advanced cyberinfrastructure deployment, allowing sites to flexibly evolve and sustain both on-premise and commercial cloud-based infrastructure
- Hosted services, such as CEs, data caches, squid, etc., could be centrally deployed onto "CI substrates" within a trusted CI zones and remotely operated, upgraded, and optimized for performance
- Extend to shared, opportunistic university clusters and cloud resources

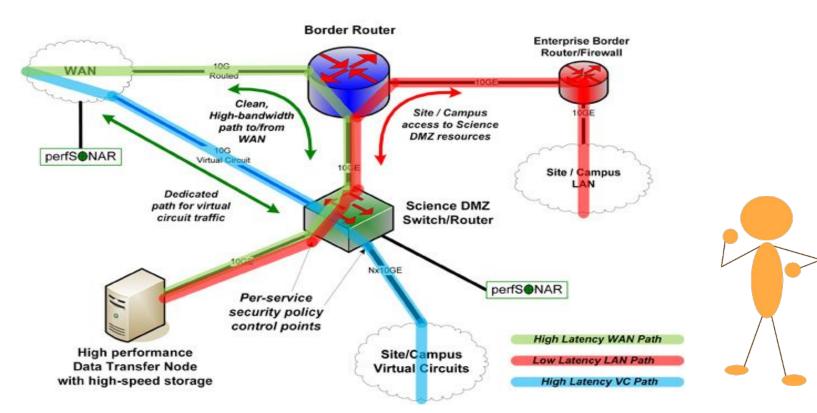
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Distributed Virtualized Data Centers



- Reduce IT footprint and ops burden
 - Centralize deployment & ops; reduce local admin cost
- Explore virtualized data center frameworks
 - E.g. container management over bare metal or VMs
- "Blue sky" goal
 - Establish a "trusted pattern" for a "CI substrate" on sites
 - Create distributed virtualized data center(s) overlaying the fabric substrate

SciDMZ



CI Connect central ops console: SuperDMZ \$ slate install osg-squid.3.3 --sites UAB Wellesley Wyo Enterprise Border Router/Firewall WAN Clean. Site / Campus High-bandwidth access to Science path to/from DMZ resources WAN perfS@NAR Site / Campus Dedicated path for virtual Science DMZ circuit traffic Switch/Router Let OSG do Edge container hosting zone on premise the work! perfS@NAR Stash squid CE **GUMS** cvmfs cache High Latency WAN Path Site/Campus Low Latency LAN Path Virtual Circuits Mesos High Latency VC Path node node node node 42

Example: Frontier Squid - Dockerfile



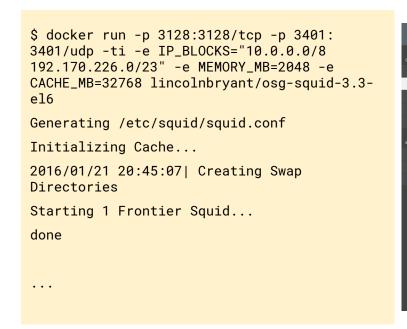
```
FROM lincolnbryant/osg-base-3.3-el6
MAINTAINER Lincoln Bryant <lincolnb@uchicago.edu>
# See https://twiki.grid.iu.edu/bin/view/Documentation/Release3/InstallFrontierSquid
RUN yum install -y frontier-squid initscripts
VOLUME ["/var/cache/squid"]
COPY customize.sh /etc/squid/customize.sh
RUN chown squid: /etc/squid/customize.sh && chmod +x /etc/squid/customize.sh
EXPOSE 3128 3401
```

CMD /sbin/runuser -s /bin/bash squid /usr/sbin/fn-local-squid.sh start && tail -f /var/log/squid/*.log

Example: Frontier Squid - Launching



 The container can be launched on another machine, or via Docker's remote API to a cloud resource

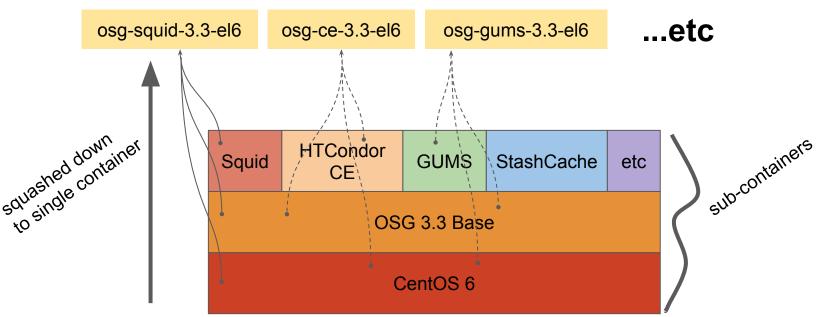




Goal: Containerize full OSG Stack



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Ease delivery of OSG services where they need to be

Summary of User Support, XD, Campus



- Lowering barries to entry
 - OSG as a Service for individual PI's
 - Training fundamentals of distributed high throughput
 - Cl Connect pattern for multi-campus collaborations
- Future: innovating ubiquitous CI substrate for small campuses



- user-support@opensciencegrid.org
- support.opensciencegrid.org
- www.opensciencegrid.org/links