# XSEDE and OSG

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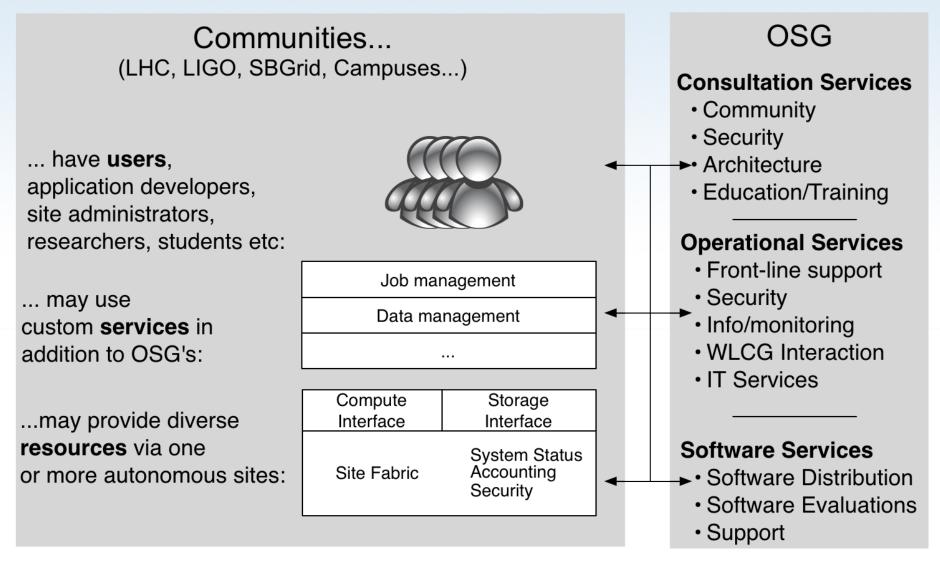
### What is OSG?

- A multi-disciplinary partnership to federate local, regional, community and national cyberinfrastructures to help share computing and storage resources of research and academic communities at all scales
- We provide common services and support for more than 100 resource providers and scientific institutions using a distributed fabric of high-throughput computational services
- We do not own computing resources but instead provide software and services to users and resource providers to enable the effective use and sharing of their resources based on the principles of Distributed High Throughput Computer (DHTC)





# OSG's Community Focus



There is a sharing of software, operational services, and knowledge between the communities and OSG in each of these areas.

## Where is OSG?





# How big is OSG?

From http://display.grid.iu.edu/

OSG delivered across 110 sites

#### In the last 24 Hours

439,000	Jobs
1,824,000	CPU Hours
2,344,000	Transfers
1,001	TB Transferred

#### In the last 30 Days

14,097,000	Jobs
61,271,000	CPU Hours
47,775,000	Transfers
27,242	TB Transferred

#### In the last Year

220,399,000	Jobs
649,521,000	CPU Hours
599,875,000	Transfers
274,284	TB Transferred





# How big is OSG? From http://display.grid.iu.edu/

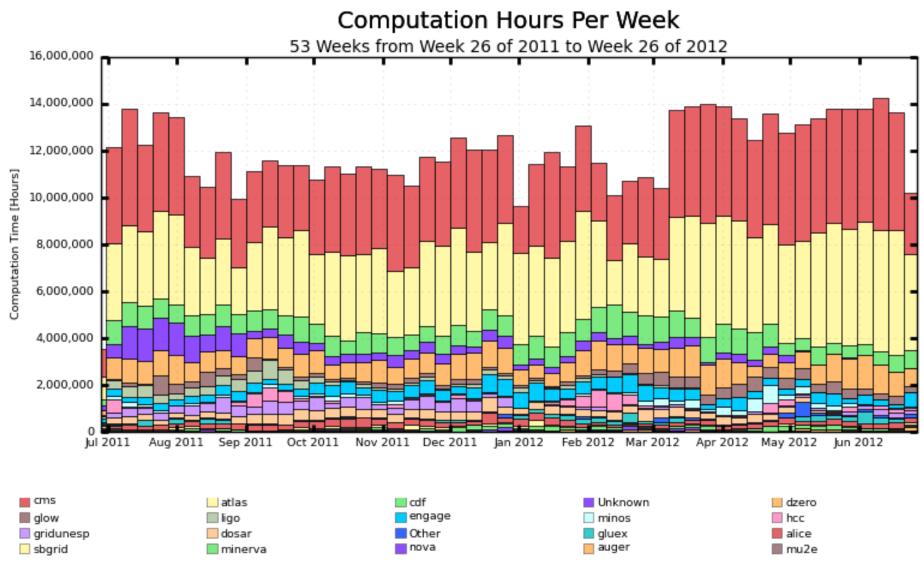


CPU hours spent on an OSG resource are reported to the central accounting system. The above graph shows the number of CPU hours per day. A total of 61,271,000 CPU hours were spent.



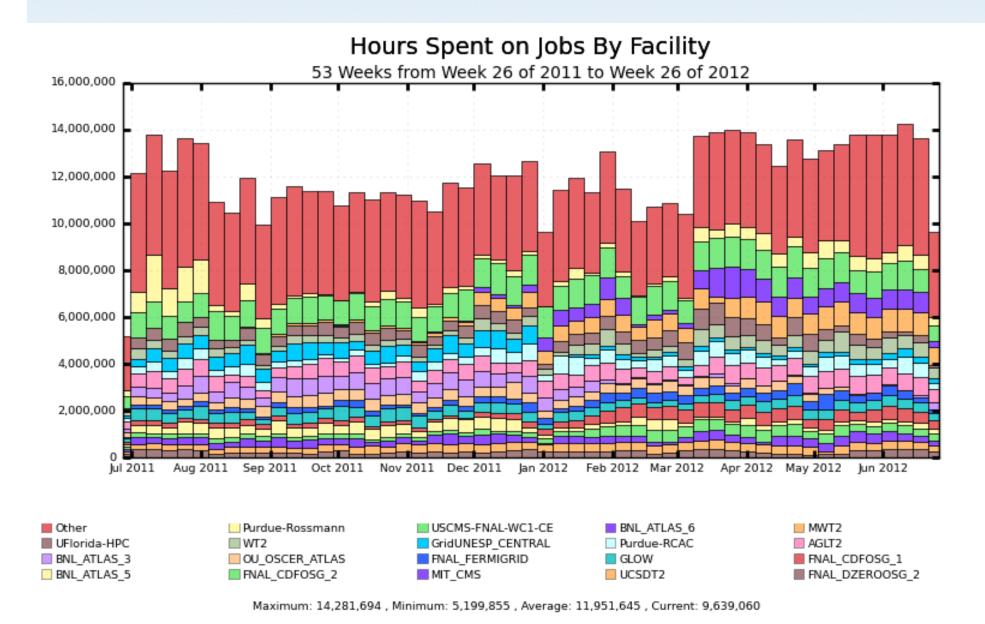


### Who uses OSG?



Maximum: 14,281,694 Hours, Minimum: 3,520,880 Hours, Average: 11,930,397 Hours, Current: 10,192,162 Hours

### Who contributes to OSG?



## How do you use OSG?

Step 1: Make sure you can use HTC

- Do you have a problem that needs HTC?
- Do you have local computing resources?
  - Use them first
  - You get local support
  - You gain experience with HTC
- When you need more resources, OSG is a good option to grow





## How do you use OSG?

Step 2: You must be in a Virtual Organization (VO)

- A VO is:
  - A collection of people and/or resources with a common purpose
  - Usually a scientific collaboration
     People + their computing & storage
- Which VO?
  - About 60 VOs in OSG: you might already be affiliated
  - Make your own for your collaboration
  - Join the "OSG" VO: miscellaneous





### How do you use OSG?

Step 3: Get access to glidein VO Frontend

- OSG runs a glidein factory, but you need a submission point (i.e. condor\_schedd)
   Called a VO Frontend (see Igor's talk)
- Larger VOs set up their own frontend
- Smaller VOs can use an OSG supplied frontend
  - We're in a transition period right now
  - This will probably be hosted at UCSD in the near future
- Sites need to authorize your VO





# How do you contribute to OSG?

- Usually contribution is based on VO needs
  - Scientific collaboration wants to share within the collaboration: OSG provides the tools
  - Other VOs can utilize unused capacity
- Some sites are simply generous and share
- Install and maintain the OSG software on:
  - Front end job submission computer
  - Storage interface computer (optional)
  - Authorization service (optional)

oen Science Grid

 Everyone is welcome, but it takes effort to do it (25% of a person's effort?)

# Autonomy

- OSG provides:
  - Software
  - Support
  - Central Services
- Sites and VOs are autonomous:
  - They make decisions about their sites
  - They decide when to install, upgrade
  - They make operational decisions
- This is HTC: if we mandate less, more people will join and we will have access to more





### What is XSEDE?

XSEDE is a comprehensive set of advanced, heterogeneous high-end digital services, integrated into a general-purpose infrastructure.



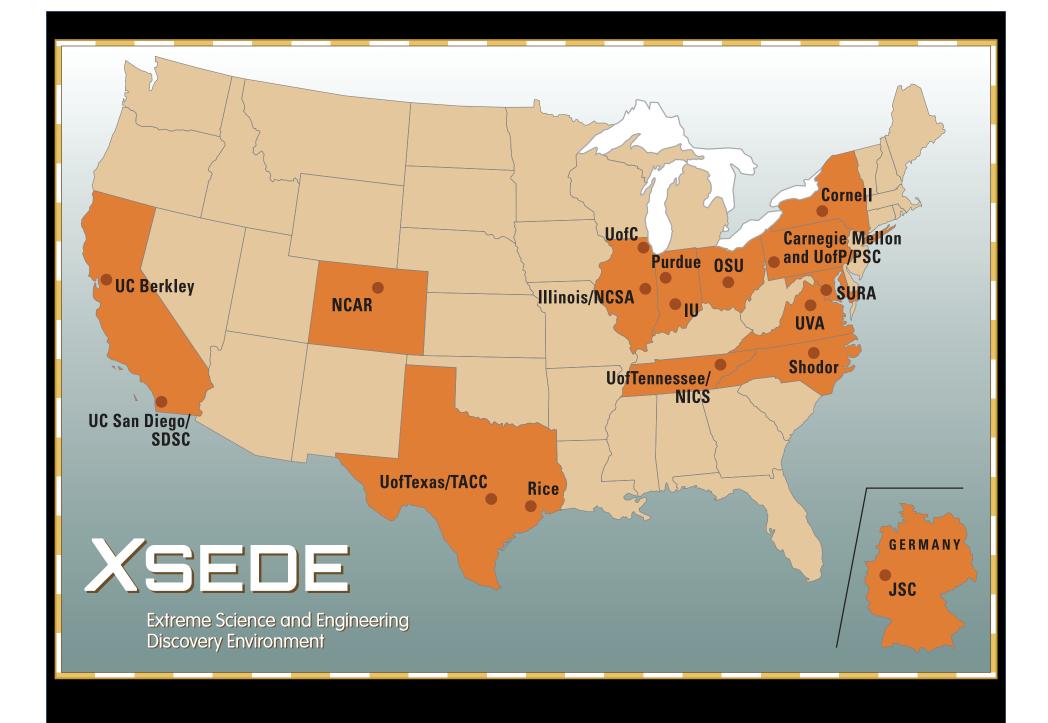


# NSF eXtreme Digital (XD) Program

- NSF's Transition from TeraGrid to XD
- High-Performance Computing and Storage Services
- High-Performance Remote Visualization and Data Analysis Services
- eXtreme Digital Resources for Science and Engineering (XSEDE)







#### org)

HP	C S	YST	ΈM

NAME

Kraken

Ranger

Gordon

Lonestar

Forge

Trestles

Steele

Queen

Bee

Blacklight |

Hostname	lonestar.tacc.teragrid.org

Manufacturer Dell

TACC Lonestar

Model PowerEdge M610

Operating System Linux 2.6.18 (hex-core)

Contact XSEDE Help Desk

Processor Cores 22656 Nodes 1880

Memory 45.00 TB

Peak Performance 302.00 TFlops

**Disk** 276.00 TB

**Description**: The Lonestar Linux Cluster consists of 1,888 nodes, with two 6-Core processors per node, for a total of 22,656 cores. It is configured with 44 TB of total memory and 276TB of local disk space. The peak performance is 302 TFLOPS. The system supports a 1PB global, parallel file storage, managed by the Lustre file system. Nodes are interconnected with InfiniBand technology in a fat-tree topology with a 40Gbit/sec point-to-point bandwidth. A 10 PB capacity archival system is available for long term storage and backups.

RUNNING

20

486

312

202

13

211

1655

95

60

3054





#### TACC Longhorn Hostname tg-login.longhorn.tacc.teragrid.org Manufacturer Dell/NVIDIA Model Intel Nehalem HPC SYSTEMS Operating System RedHat Enterprise Linux 5 XSEDE Help Desk Contact Processor Cores 2048 NAME INS Nodes 256 Longhorn TAC 13.50 TB Memory Peak Performance 20.70 TFlops NIC Nautilus 210 TB Disk TAC Spur

Description: Longhorn, the TACC Dell/NVIDIA Visualization and Data Analysis Cluster, consists of 256 dual-socket nodes, each with significant computing and graphics capability. Total system resources include 2048 compute cores (Nehalem quad-core), 512 GPUs (128 NVIDIA Quadro Plex S4s containing 4 NVIDIA FX 5800s), 13.5 TB of distributed memory and a 210 TB global file system. Two Dell R710 servers with 48GB of memory provide login/interactive support. Compute nodes include: 240 Dell R610 Servers with 48GB of memory and a 73GB 15K SAS local disk and 16 Dell R710 Servers, each with 144GB of memory and a 73GB 15K SAS local disk. Each of the 128 NVIDIA Quadro Plex S4 systems consists of 4 Quadro FX 5800 GPUs. Two GPUs from a Quadro Plex are connected to a single node, so that the GPU/CPU ratio is unity. The nodes are interconnected through an InfiniBand QDR switch. The IB network also supports a 210TB Lustre parallel file system, accessible to all nodes, and provides access to the Ranger Lustre file systems through a 10GigE





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q 4 NVIDIA

)IA Quadro

Us

# XSEDE Storage Systems

HPC SYSTEMS ADVANCED VIS SYSTEMS STORAGE SYSTEMS HTC SYSTEMS INSTITUTION OFFLINE STORAGE TB NAME SYSTEM ONLINE STORAGE TB Albedo Lustre-WAN PSC Lustre 1024 N/A IU Lustre 535 Data Capacitor N/A Data Replication Service TACC **iRODS** N/A 1024 **HPSS** NICS **HPSS** 12 6220 NCSA Tape Storage NCSA EMC DiskXtender 250 10000 Ranch Sun StorageTek Mass Storage Facility 110 40000 TACC Total: 1931 57244





#### Purdue Condor Pool

Hostname tg-condor.purdue.teragrid.org

Manufacturer Intel

Model

Operating System Unknown

XSEDE Help Desk Contact

N/A Processor Cores

Nodes N/A

Memory N/A Peak Performance

N/A

N/A Disk

Linux Cluster

ORY TBYTES

×

54.74

54.74

Description: The Purdue Condor pools consist of over 4500 CPU of computation: 1645 LINUX/X86\_64 CPUs, 1192 LINUX/INTEL (ia32) CPUs, and 1815 WINNT51/INTEL CPUs, as well as a small number of Itanium Linux, Solaris and MacOS X machines. Memory on compute nodes range from 512 MB to 16 GB, and most CPUs run at 3 GHz or better. With a total of approximately 150 TFLOPS available, the Purdue Condor pools can provide large numbers of cycles in a short amount of time. All shared areas and software packages available on Lear are available on Condor. Condor is designed for high-throughput computing, and is excellent for parameter sweeps, Monte Carlo simulation, or most any serial application. Also, some classes of parallel jobs (master-worker) may be run in Condor.



HPC SYSTEMS

Condor Pool

NAME

### **XSEDE Vision**

The eXtreme Science and Engineering Discovery Environment (XSEDE):

enhances the productivity of scientists and engineers by providing them with new and innovative capabilities.

#### Thus, XSEDE:

facilitates scientific discovery while enabling transformational science and engineering, and innovative educational programs.

XSEDE fulfills this vision by creating an advanced, capable, and robust cyberinfrastructure supported by the combined expertise of a distributed team of leading CI (cyberinfrastructure) professionals.





#### **XSEDE Characteristics:**

- XSEDE forms the foundation of a national cyberinfrastructure (CI) ecosystem
  - Its comprehensive suite of advanced digital services work with other high-end facilities and campusbased resources
- XSEDE integrates diverse digital resources
  - Its open architecture allows continued addition of new technology capabilities and services





# XSEDE is about . . .

- Increasing productivity
  - leading to more science
  - making the difference between a feasible project and an impractical one
- Transformative impact through
  - active, formal requirements gathering processes to
    - understand the needs of the community
  - new and expanded extended collaborative support that includes
    - external short-term contracting for expertise beyond the current team
    - Novel and Innovative Projects: supports novel science areas, demographic diversity, innovative technologies, science gateway development, data repositories, and campus bridging





### And...

- National Training and Education and Outreach programs with the scope and scale to:
  - increase diversity of topics, modes of delivery, and reach to new communities and audiences
  - broaden participation among under-represented communities
  - campus bridging for effective use of CI (cyberinfrastructure) resources
    - integrate with campuses through expanded Champions program and additional bridging activities
  - establish academic certificate and degree programs
    - institutional incorporation of CS&E curricula; professional development certificate
    - prepare undergraduates, graduates and future K-12 teachers





# **XSEDE Components**

- Coordination and Management Service
- Technology Audit and Insertion Service
- Extended Collaborative Support Service
- Training, Education and Outreach Service



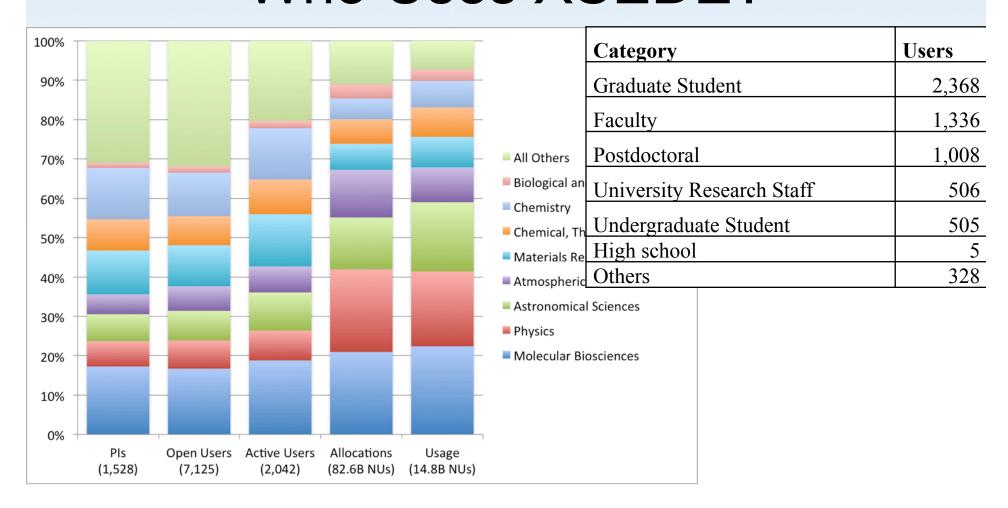


# Best of all you can use it for FREE!





# Who Uses XSEDE?

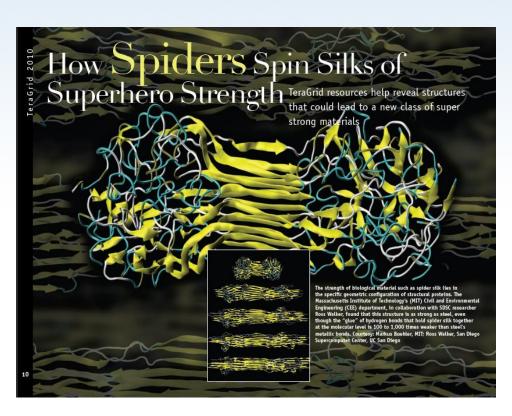






# Science Highlights 1:





PI: Markus Buehler

Institution: MIT

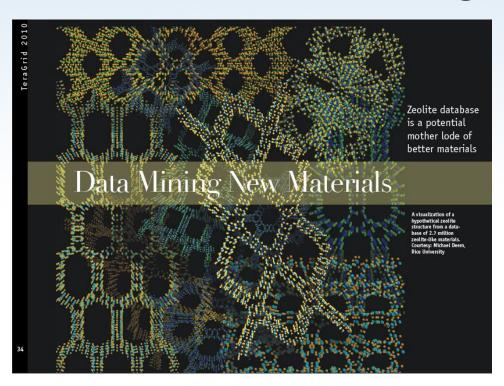
 "We found that the structure of spider silk at the nanoscale can explain why this material is as strong as steel, even though the "glue" of the hydrogen bonds holding spider silk together at the molecular level is 100 to 1,000 times weaker than steel's metallic bonds." says Buehler.





# Science Highlights 2:





- PI: Michael Deem, David Earl
- Institution: Rice University,
   University of Pittsburgh
- Identified millions of potentially new zeolites by searching computationally for properly configured, hypothetically stable structures.
- Zeolites are used to make everything from gasoline and asphalt to aquarium filters, laundry detergent and medical-grade oxygen.





# Science Highlights 3:





- PI: Sorin Matei, David Braun
- Institution: Purdue University
- Purdue researchers led by Sorin
   Adam Matei are analyzing the entire
   collection of articles produced in
   Wikipedia from 2001-2008, and all
   their revisions a computationally
   demanding task made possible by
   TeraGrid resources.
- "We looked at how article production is distributed across users' contributions relative to each other over time. The work includes visualizations of patterns to make them easier to discern," says Matei.





# How do you use XSEDE? Step 1: The basics

- Setup an XSEDE User Portal Account
  - https://portal.xsede.org/
  - You can do it right now: it's free and easy
- Review available resources and determine which will match the needs of your research
  - Resources -> Systems Monitor





# How do you use XSEDE? Step 2: Startup Allocation

- Submit a request (anytime)
- Easy to get—lightly reviewed
- Small: 200K hours
- Use to investigate the resources where your code will run
- Use to benchmarking your code to determine the best resource and how many SUs you will need to complete your research





# How do you use XSEDE? Step 3: Research Allocation

- Write and submit a full research allocation request
- Can be submitted quarterly
- Peer-reviewed
- Can be very large
- You should know exactly what resources you need





# How do you use XSEDE? Step 4: Use

- Log into individual resources
  - Can log in via User Portal (built in ssh + authentication)
  - Can download application to login (ssh + authentication)
  - Can request direct ssh access from individual sites
- When you run out:
  - You will be unable to submit more jobs
  - It is possible to request extensions to your allocation





### Differences between XSEDE and OSG

- Authentication
  - OSG: certificates obtained by user, member of VO
  - XSEDE: User has certificate but never sees it. Transparent access via MyProxy with name/password
- System Access:
  - OSG:
    - Access based on VO membership
    - Jobs submitted remotely (usually glideins)
  - XSEDE
    - Access based on allocations
    - Direct login to resource to submit jobs (via User Portal or gsissh or ssh)





# Differences (2)

#### Amount of Compute Cycles:

- OSG: only limited by excess cycles on available resources
- XSEDE: based on granted allocations (different amounts available for request based on allocation type with research allocation requests peer reviewed)

#### Job Types:

- OSG: serial or single-node parallel
- XSEDE: serial, shared memory, large parallel, large data

#### • Other:

- XSEDE: Can request an allocation of "people" resources (ECSS) to assist with technical aspects of project/code
- OSG: Can access all systems via a single submit host





# Questions? Comments?



