Open Science Grid

Advancing Open Science through distributed High Throughput Computing

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Goals for this Presentation

- Introduce OSG
- Explain how you can leverage OSG to meet the goals of the CC* solicitation
- Explain what else OSG can do for you and your scientists.

Advancing Open Science with OSG

Open Science Grid

Open Science

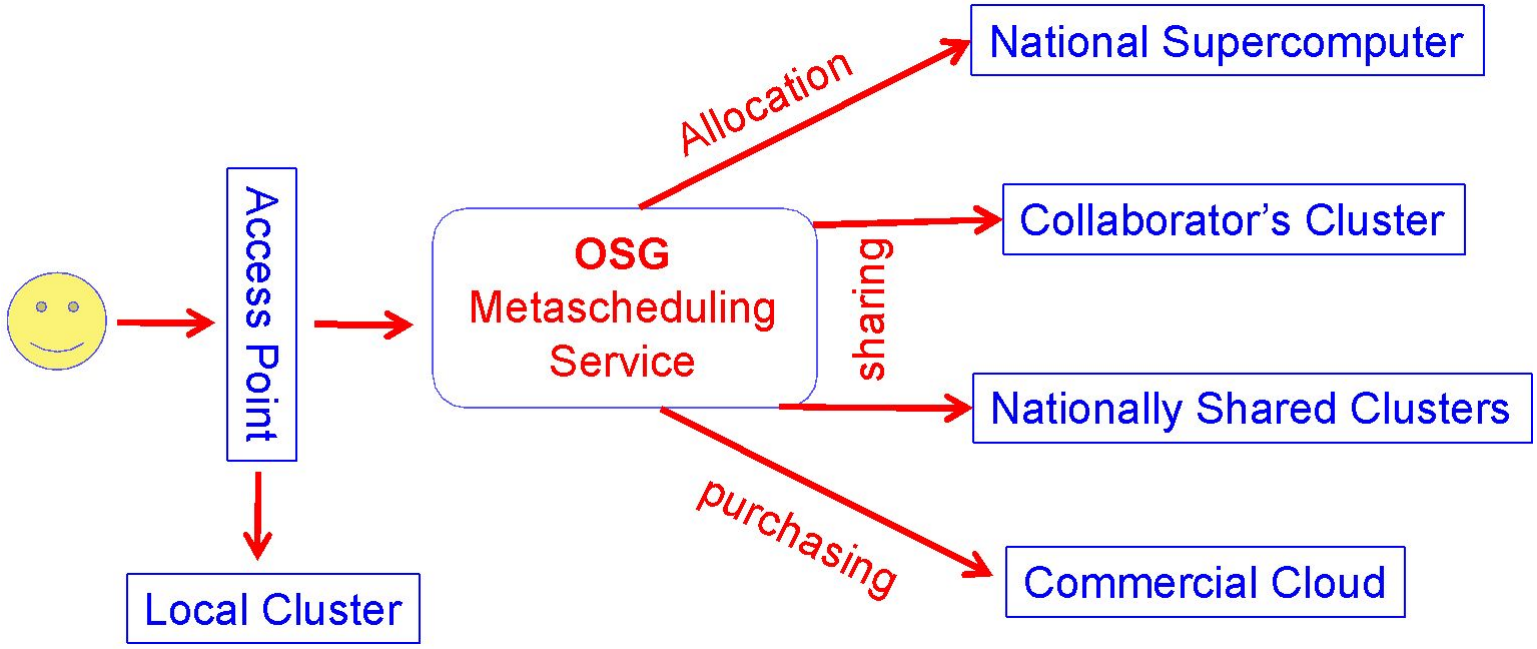
- All of open science irrespective of discipline
- Advance the maximum possible dynamic range of science, groups, and institutions
  - From individual undergraduates to international collaborations with thousands of members.
  - From small colleges, museums, zoos, to national scale centers of open science.
- Advancing this entire spectrum requires us to have a diversified portfolio of services

OSG serves 4 distinct groups

- The individual researchers and small groups on OSG-Connect
- The campus Research Support Organizations
  - Teach IT organizations & support services so they can integrate with OSG
  - Train the Trainers (to support their researchers)
- Multi-institutional Science Teams
  - XENON, GlueX, SPT, Simons, and many many more
  - Collaborations between multiple campuses
- The 4 "big science" projects:
  - US-ATLAS, US-CMS, LIGO, IceCube

Services OSG Operates (I)

- OSG-Connect, a submission host for individual researchers.
  - You get an account, and we teach you how to use OSG.
- A Compute Federation

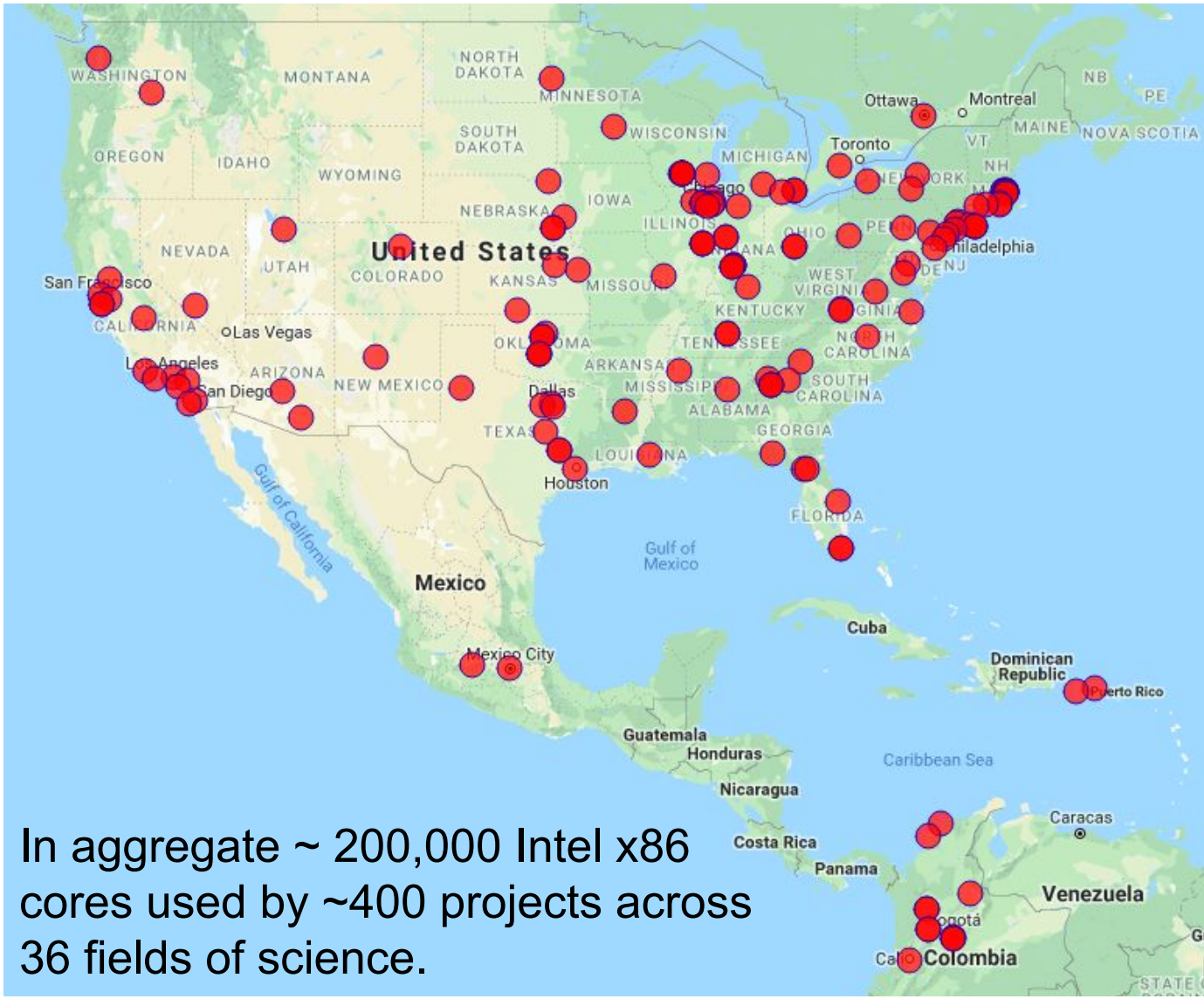


OSG Compute Federation

OSG federates ~100 clusters worldwide

Owners determine policy of use.

Many allow opportunistic use of spare capacity.



In aggregate ~ 200,000 Intel x86 cores used by ~400 projects across 36 fields of science.

Federation = distributed control

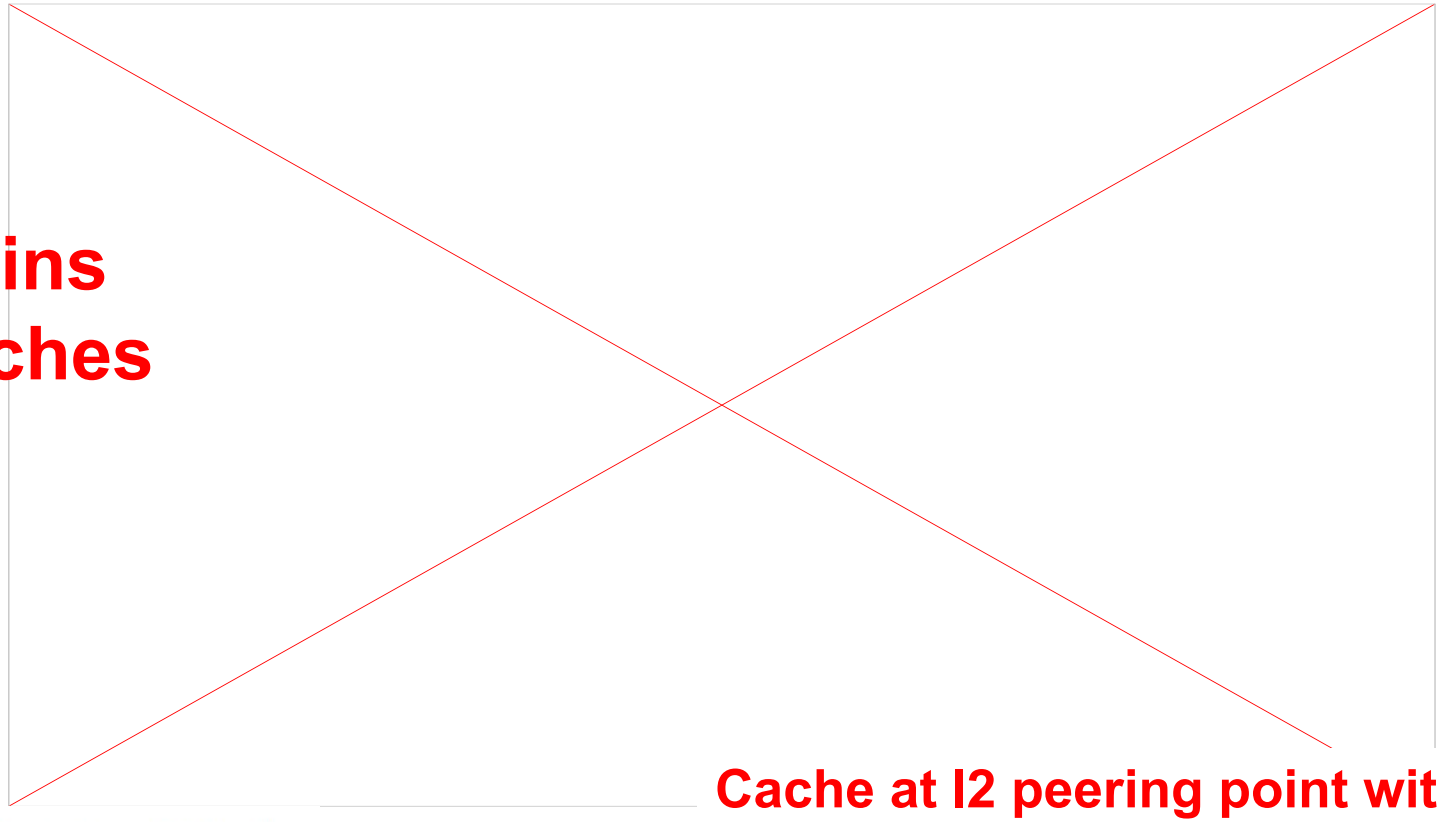
- OSG works on three simple principles:
  1. Resource Owners determine policy of use
     - This means that all policy of use is set locally by the clusters that join the federation.
  2. Resource Consumers specify the types of resources they are willing to use.
     - How much RAM? How many cores per node? …
  3. OSG submits it's *own* batch system as 'jobs' into local batch systems.
     - User jobs are submitted locally, queued centrally, and execute anywhere that matches requirements after resource becomes available.

OSG operates overlay system(s) as services for all of science

OSG Data Federation for "Big Data"

Open Science Grid

6 Data Origins
12 Data Caches



Cache at I2 peering point with Cloud providers in Chicago

Directory	Working Set	Total Read
/pnfs/fnal.gov/usr/dune	13.107GB	395.537TB
/pnfs/fnal.gov/usr/minerva	255.266GB	270.994TB
/gwdata/O1	169.585GB	258.341TB
/pnfs/fnal.gov/usr/des	193.57GB	120.993TB
/user/ligo	5.612TB	83.564TB
/pnfs/fnal.gov/usr/nova	162.632GB	18.841TB

30k
1k
15
100

Depending on community, files were read 10-30,000 times during 60 days.

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Data Federation Goals

- People come with their data on their local storage systems.
- OSG offers to operate a Data Origin Service to export your data into the OSG Data Federation.
  - We give you a globally unique prefix for your filesystem namespace, and then export your namespace behind it.
  - We allow you to decide who can access what.
- OSG then strives to guarantee ”uniform” performance across the nation by operating caches to:
  - Hide access latencies
  - Reduce unnecessary network traffic from data reuse (by many jobs)
  - **Protect the data origins from overloads**

OSG operates overlay system(s) as services to all of science

distributed High Throughput Computing (dHTC)

- The power of successful dHTC is two-fold:
  - Separate a big computing problem in many individually schedulable small problems.
  - Minimize requirements in order to maximize the raw capacity that can effectively be used.
- We teach researchers how to meet these challenges.
- We take the many small problems, and schedule their successful execution.
- We provide tools to curate & publish software & data and deliver them at runtime.

Ingenious Parallelism

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CC* Solicitation Context

20% for the Common Good

Proposals should commit to a minimum of 20% shared time on the cluster and describe their approach to making the cluster available as a shared resource external to the campus, with access and authorization according to local administrative policy. Conversely, the proposal should describe the approach to providing **on-demand** access to additional external computing resources to its targeted on-campus users and projects. One possible approach to implementing such a federated distributed computing solution is joining the Open Science Grid.

OSG offers to help you meet these goals from the solicitation by integrating your cluster into the OSG Compute Federation.

You remain in complete control over how much you provide (and when) to the national science community via OSG.

All control over sharing policy remains local, i.e. in your hands !!!

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Sharing does not imply "quid pro quo"

We are delighted to work with your campus to facilitate open science, in any form. Your researchers can utilize the OSG at any scale, regardless of how much computing you share with the community.

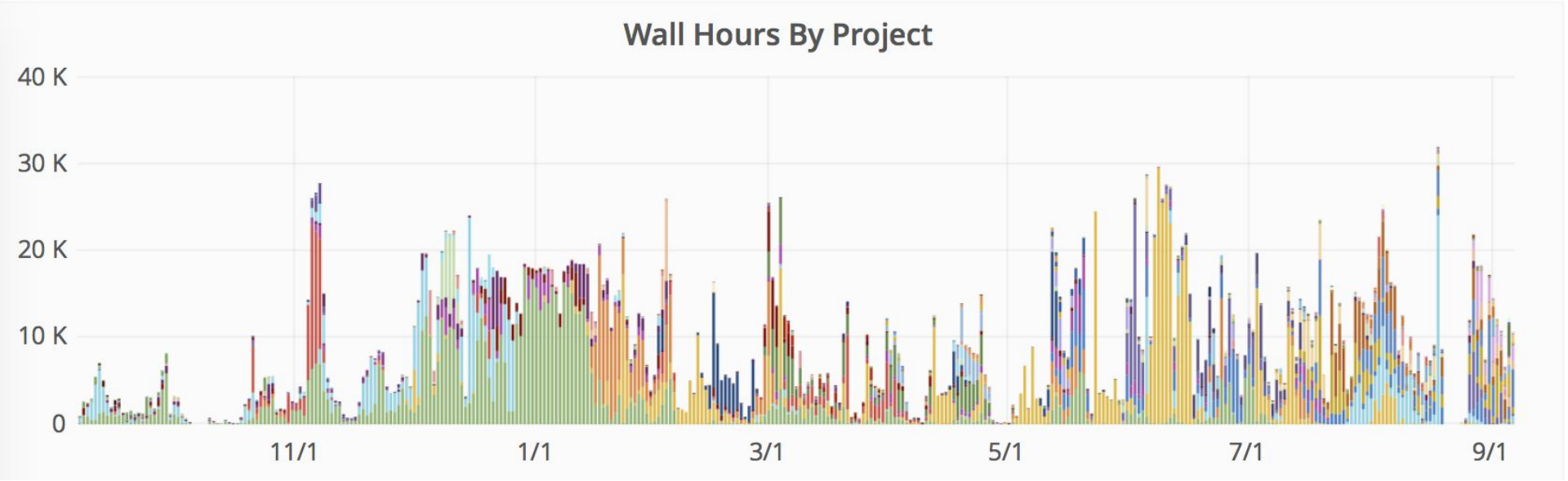
Shared Responsibilities

- **OSG provides:**
  - Scientific user communities to consume the 20% shared time.
    - We provide all the support to these scientists.
  - A mechanism for scientists to submit jobs to your cluster.
    - Your cluster becomes part of the OSG Compute Federation
  - A uniform runtime environment, incl. data access, for these scientists.
  - Accounting data for your annual report to the NSF to show who benefited from your cluster, when, and how much.

- **You provide:**
  - A set of ssh-key accessible accounts from which we can submit jobs to your cluster.
  - Access to the uniform runtime environment of OSG.

  (Technical details on both in Brian Bockelman's talk)
- **You decide:**
  - Which of the communities that OSG supports gets how much access to your cluster and when.

OSG Provides Accounting
Example: Last 1 Year at U.Connecticut



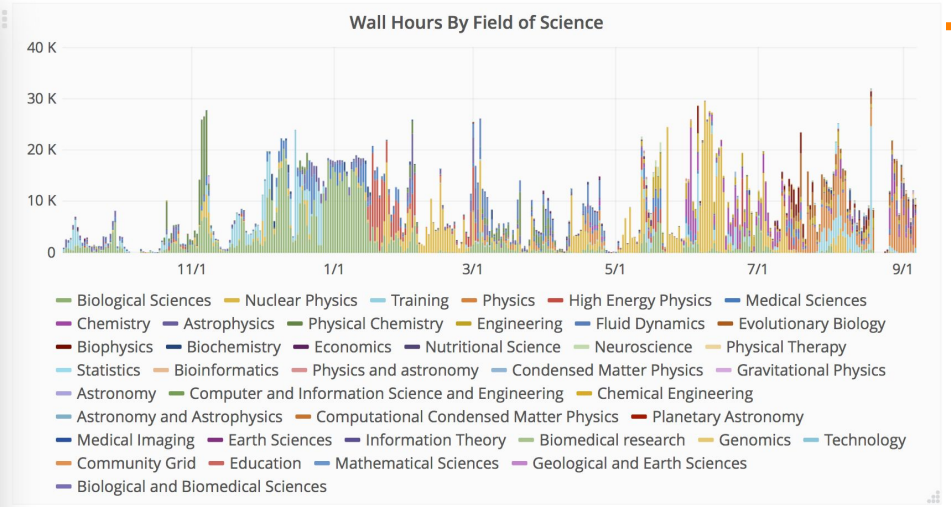
How much the cluster owner contributes when is completely left to to them.

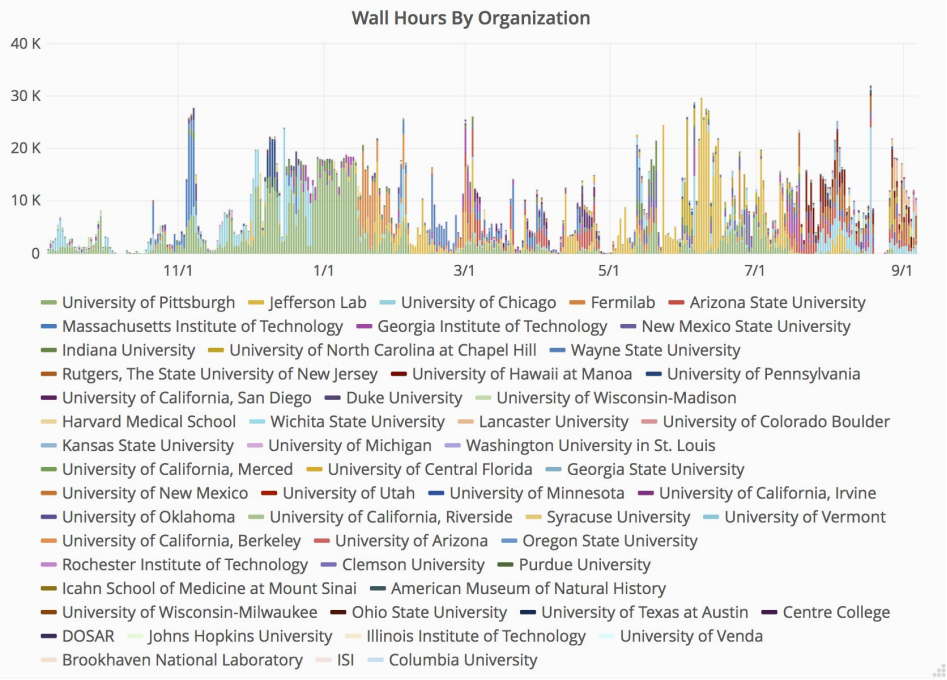
Large day by day fluctuations are completely ok.

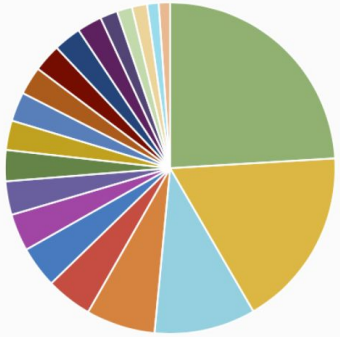
Ideally, we would help you meet the solicitation goals whenever your local users are leaving spare capacity behind.

The user community

By Field Of Science







	total
TG-IBN130001	747 K
GLUEX	545 K
ConnectTrain	308 K
REDTOP	210 K
CatalystHTVS	139.8 K
SourceCoding	125.6 K
SPLINTER	112.8 K
molcryst	101.6 K
ASU-CFD	94.2 K
DemoSims	89.1 K
PixleyLab	88.3 K
Hawaii_Doetinchem	85.4 K
VERITAS	84.3 K
TG-PHY180035	84.0 K
PainDrugs	75.3 K
chemml	53.1 K
EvolSims	46.4 K
bobbot	45.9 K
spt.all	35.1 K
Duke-QGP	34.6 K

We have short descriptions for each project online.

Example projects descriptions

```
Department: Particle Physics
Description: High intensity frontier experiment searching for physics beyond the Standard
  Model
FieldOfScience: High Energy Physics
ID: '346'
Name: REDTOP
Organization: Fermilab
PIName: Corrado Gatto
```

REDTOP

CatalystHTVS

```
Name: CatalystHTVS
Description: Using high throughput computing to screen molecular
  catalysts for energy fuel conversion based on experimental database or in-silico
  generated structures. In the next stage, the output from HTC calculations will
  be used to train machine learning models to allow faster and higher throughput
  molecular catalyst design.
Department: Chemical Engineering
FieldOfScience: Physical Chemistry
Organization: Massachusetts Institute of Technology
PIName: Heather J. Kulik
```

```
Department: Neurological Surgery
Description: 'The hope for magnetoencephalographic (MEG) measurements has been to
  produce functional brain mapping with high spatial (mm) and temporal (msec) resolution.
  Realizing this hope requires answers to these questions: (1) How many sources are
  active within the brain? (2) Where are they located. (3) What is their time course?
  MEG Virtual Recording (MVR) provides these while producing noninvasive measures
  of intracranial neuroelectric currents as if from 2,000,000+ directly implanted
  electrodes. It does so from single trial (unaveraged) data, has no free parameters,
  and provides very strong probabilistic measures to validate the existence of each
  identified source. We have demonstrated efficient implementation of MVR on the Open
  Sciences Grid. The measured computational load of 400 SU per second of MEG data
  makes supercomputing essential to practical implementation of MVR. We anticipate
  that MVR will enable identification of specific neurophysiological biomarkers of
  a variety of non-structural brain pathologies which have been refractory to date,
  e.g. concussion, post-traumatic stress disorder.'
FieldOfScience: Biological Sciences
ID: '33'
Name: TG-IBN130001
Organization: University of Pittsburgh
PIName: Donald Krieger
```

TG-IBN-13001

I picked the top 3 consumers at U. Connecticut via OSG.

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Other OSG Services

Open Science Grid

Overview

- OSG-operated and campus-operated submission points.
- Research Facilitation, training and workforce development.
- Software distribution and runtime environment.
- ”Content Delivery Network”

Submission Points

- We offer an integrated platform from which individual scientists can use the OSG.
  - Accounts via InCommon authentication
  - Interactive environment to test batch execution, and submit workflows from
  - Data areas that are fully integrated into the runtime environment.
  - ….
- Submission points may be OSG-operated (OSG Connect), campus-operated, or jointly-operated

Facilitation Services

Proactive, personalized guidance and support for:

- Institution-specific **submit points**
- **Sharing institutional resources** via OSG
- **Data federation** across OSG sites
- Individual researchers using **OSG Connect**
- **Local workshops**
- OSG-hosted education and training
- Learning from the OSG Facilitation Community

OSG USER SCHOOL 2019

Harness the power of distributed computing

More info + Financial support + Application (due 12 April 2019):
https://www.opensciencegrid.org/UserSchool

We are especially interested in "Training the Trainers"

Software Distribution & Runtime environment

- We help users with software portability solutions.
- We offer a standard “module environment” and are prepared to add new modules as needed by the community.
  - At present XX software modules are supported.
- We make extensive use of singularity containers, including YY curated containers to support a variety of application environments.
- We offer services that allow you to offer our environment for use by your local users on your local cluster.

Content Delivery Network

- We offer to export your data into our data federation, thus making it available to your scientific communities across all of OSG.
  - Facilitates inter-institutional sharing of data.
  - Facilitates elastic scale out of computing on your data, even in the cloud.
- We are expanding our network of caches nationally and globally in order to support access to your data anywhere.

Summary & Conclusion

- OSG's objective is to "Advance Open Science through distributed High Throughput Computing"
- OSG thinks of its science stakeholders in terms of 4 categories:
  - Individual Researchers
  - Campus Research Computing Organizations
  - Multi-campus Science Teams
  - "Big Science" Collaborations
- OSG offers a diversified portfolio of services to support these different science stakeholders.

Contact us at: help@opensciencegrid.org