



Open Science Grid



# The OSG Open Facility: A sharing ecosystem

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April 13, 2015





# The Open Science Grid

- Goal: **Advance science through open distributed high throughput computing (DHTC)** in the US
  - Operates as a partnership between **resource providers** (sites) and **stakeholders** (scientific communities of users)
  - OSG **project** provides middleware and R&D effort
  - Over 120 sites (computing and storage elements)
    - Mix of university and national labs; LHC experiment computing sites and campus clusters
  - Uses the **Virtual Organization (VO)** model
    - Most VOs correspond to large HEP experiments and university communities
- Funded by the **US Dept. of Energy** and **National Science Foundation**
  - Second 5 year period of support



# State of the OSG



In the last 24 Hours	
664,000	Jobs
1,633,000	CPU Hours
2,423,000	Transfers
330	TB Transfers
In the last 30 Days	
15,248,000	Jobs
69,955,000	CPU Hours
74,181,000	Transfers
13,151	TB Transfers
In the last 12 Months	
196,761,000	Jobs
808,076,000	CPU Hours
587,639,000	Transfers
157,000	TB Transfers

<http://display.grid.iu.edu>

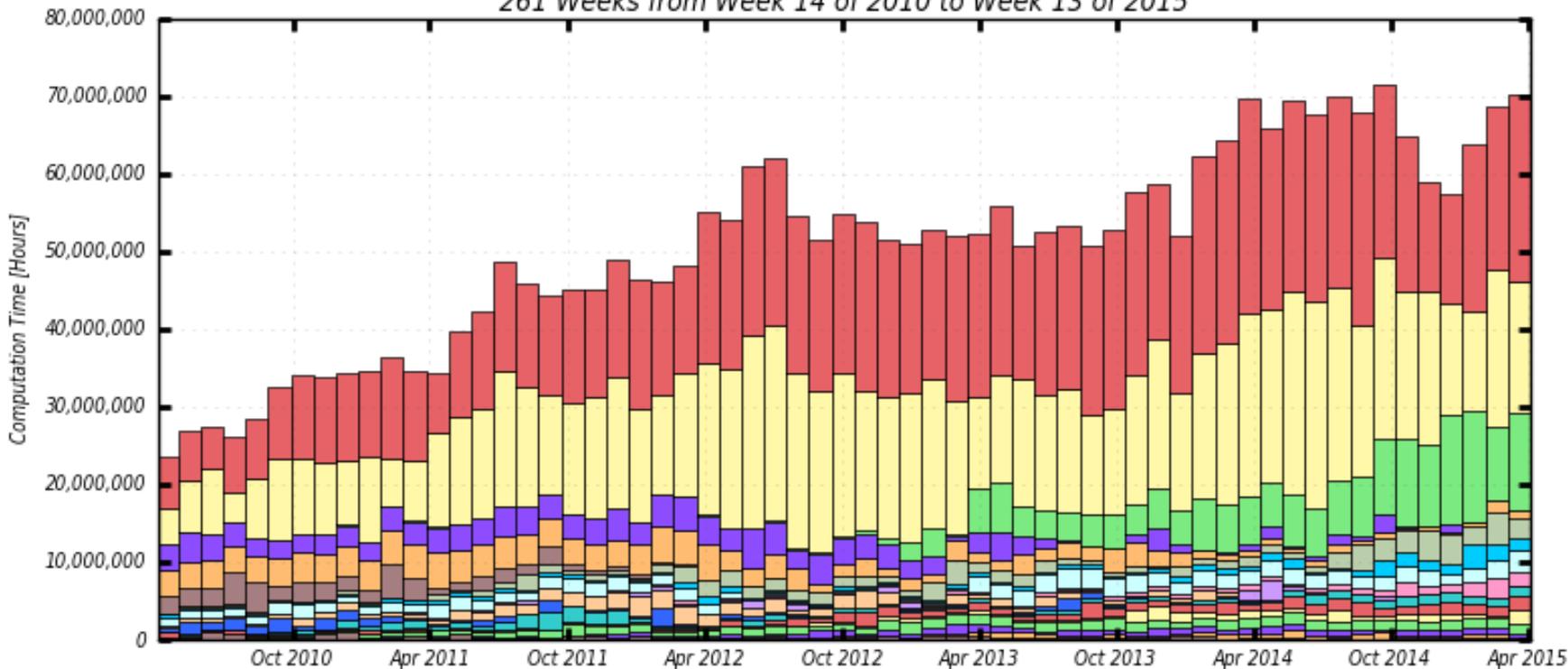


# Growth of the OSG

## Hours Spent on Jobs By VO

April 2010-April 2015

261 Weeks from Week 14 of 2010 to Week 13 of 2015



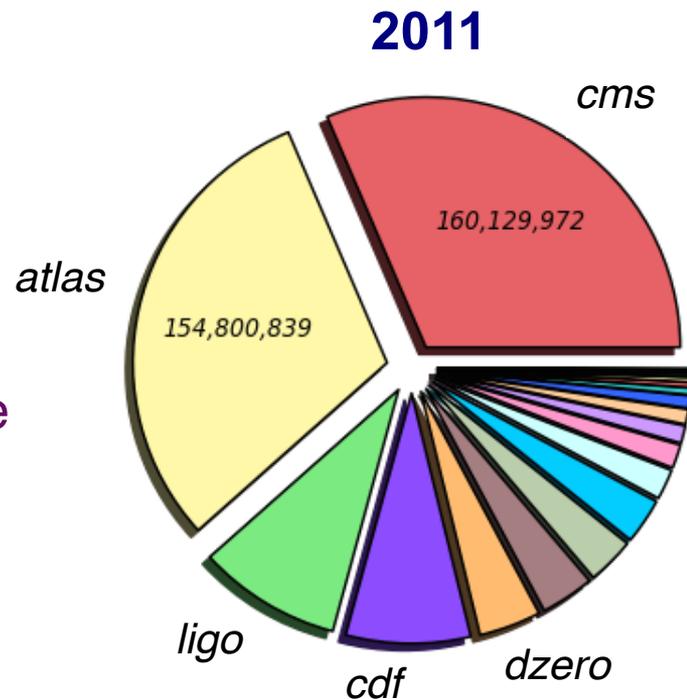
- atlas
- cms
- osg
- dzero
- cdf
- ligo
- glow
- minos
- dosar
- nova
- gluex
- engage
- hcc
- gridunesp
- Other
- mu2e
- alice
- minerva
- mars
- sbgrid

Maximum: 71,557,724 Hours, Minimum: 23,534,287 Hours, Average: 50,722,088 Hours, Current: 70,351,830 Hours



# Expanding usage of the OSG

- Most use of the OSG is by large physics experiments (e.g. ATLAS and CMS) and individual university communities
  - Primarily operate on their own sites
    - Utilization is high but not 100% 24/7
  - 85% of OSG hours in 2011 were from large HEP experiments
- Want to connect unused cycles with researchers who are not part of large VOs
- Reaching other sciences takes more work
  - Few have the organized computing efforts HEP experiments have
  - Not every research community can have their own VO (although many do)

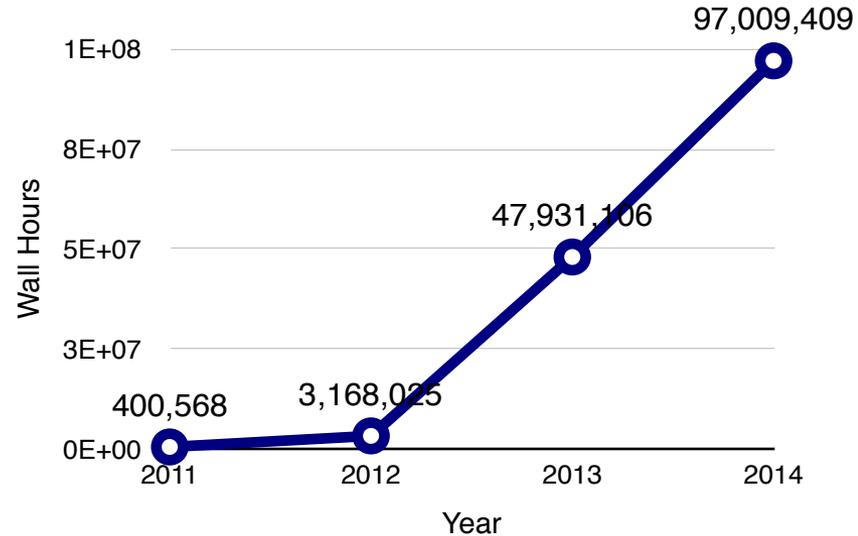




# The OSG open facility

- Implement **OSG VO** as a VO for individual researchers
  - Allow **any researcher** from US institutions
  - Resources accessed by the OSG VO are **entirely opportunistic**
  - All OSG sites encouraged to support OSG VO running
- An **XSEDE** service provider
  - Currently the only DHTC provider

OSG VO Growth 2011-2014



**Open Science Grid**  
User Guide



The Open Science Grid (OSG) advances science through open distributed computing. The OSG is a multi-disciplinary partnership to federate local, regional, community and national cyberinfrastructures to meet the researchers' high throughput computing needs.

**XSEDE**  
Extreme Science and Engineering  
Discovery Environment

HOME ABOUT USER SERVICES RESOURCES EDUCATION & OUTREACH TECHNOLOGY DATABASE GATEWAYS

## High Throughput Computing

While both High Performance Computing (HPC) and High Throughput Computing (HTC) jobs run parallel computations, HTC requires far less communication and synchronization between nodes. Parallel jobs commonly described as "embarrassingly parallel" or "pleasantly parallel" are a perfect fit for HTC resources.

The processes comprising an HTC parallel computation are loosely-coupled, typically communicating with each other very little or not at all. HTC jobs can therefore be executed on physically distributed resources using grid-enabled technologies, such as XSEDE's Open Science Grid (OSG) and the University of Wisconsin-Madison's HTCondor project.

Typical HTC applications include Monte Carlo simulations and other parameter sweep applications, where the same program is run with varying inputs, resulting in hundreds or thousands of executions of the same program overpites a typical HTC job. HTC jobs typically run on a much-longer timescale than HPC jobs.

### Available HTC resources

Open Science Grid  
User Guide

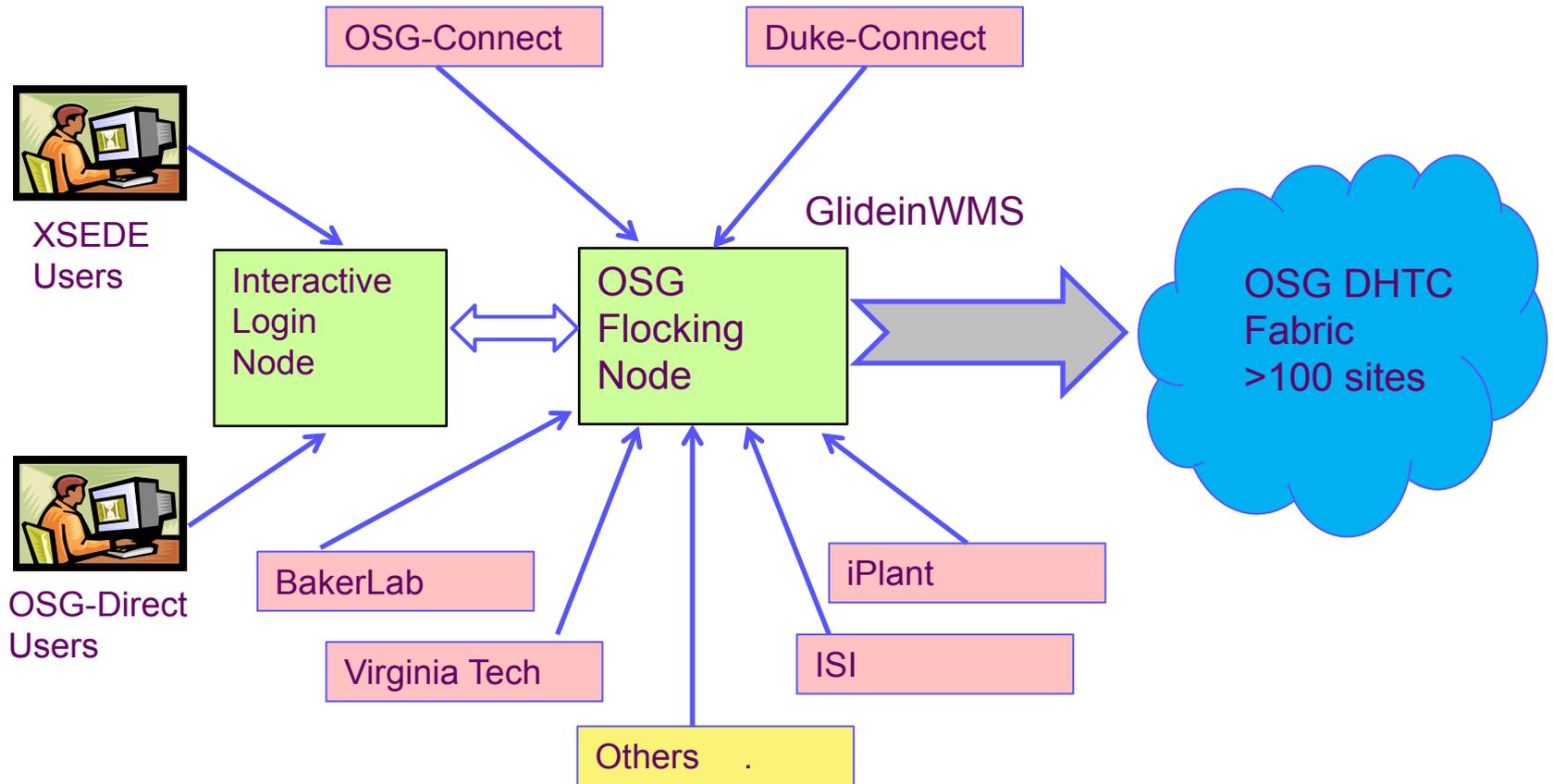
The Open Science Grid (OSG) advances science through open distributed computing. The OSG is a multi-disciplinary partnership to federate local, regional, community and national cyberinfrastructures to meet the researchers' high throughput computing needs.

Last update: January 20, 2015

Resources

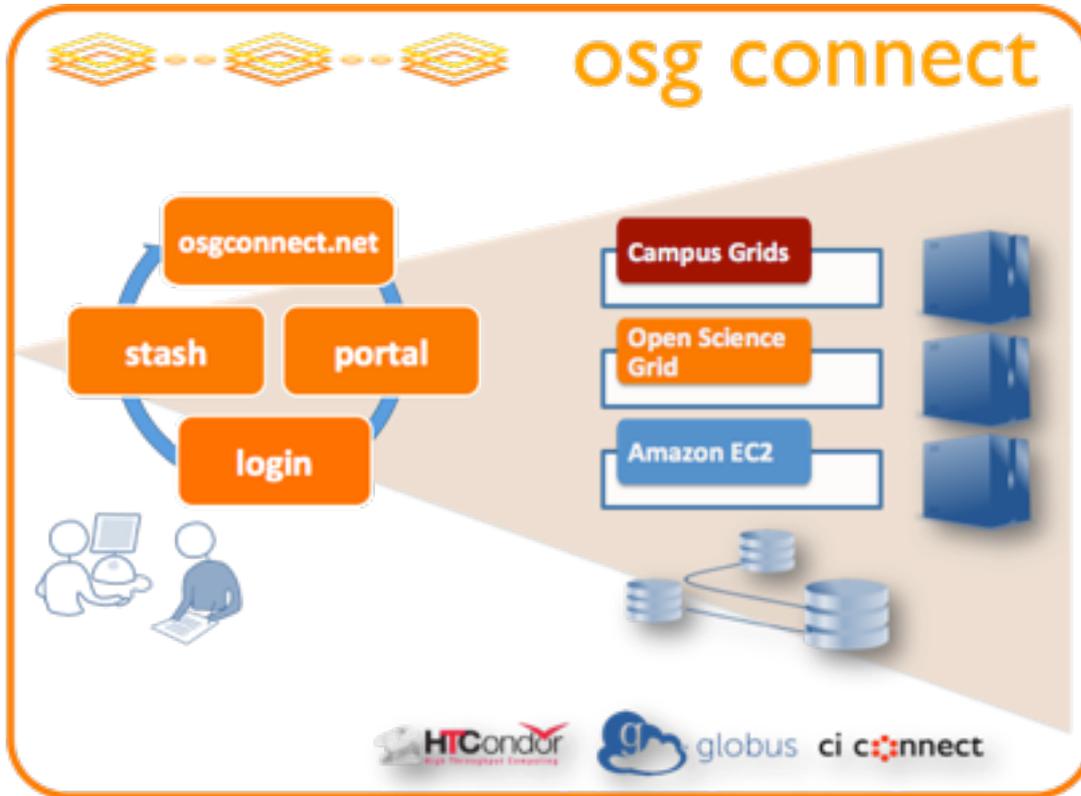
- Overview
- High Performance Computing
- High Throughput Computing
- Visualization
- Storage
- Testbeds
- Networking
- Software
- User Guides
- Metascheduling
- SU Converter

# On-ramp to the open facility





# OSG Connect



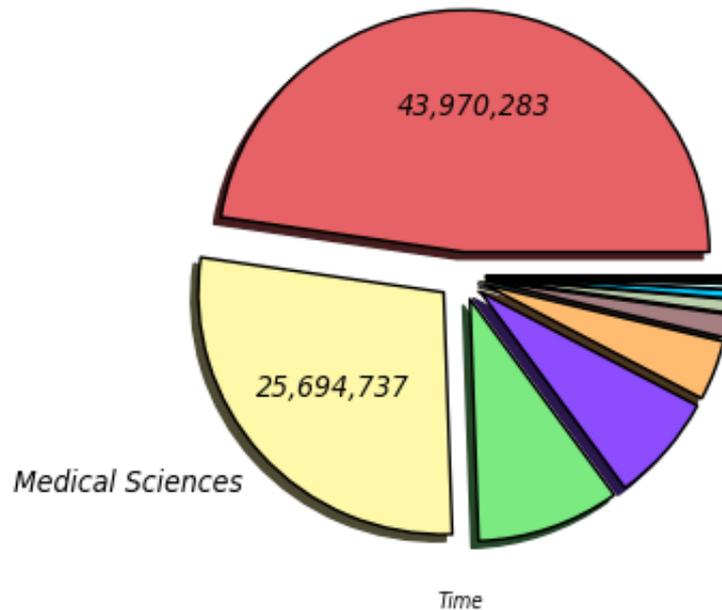
- Make OSG seem like a **virtual campus cluster**
  - Login host
  - Environmental modules
  - Job scheduling
  - Job data (including monitoring)
- Jobs run on the OSG as part of the OSG VO



# Science on the open facility

Wall Hours by Field of Science (Sum: 92,202,816 Hours)

365 Days from Week 00 of 2014 to Week 52 of 2014



30-40 unique projects use the Open Facility every month

**23 peer-reviewed publications in 2014**

- Biological Sciences (43,970,284)
- High Energy Physics (8,710,754)
- Computer and Information Science and Engineering (3,688,696)
- Materials Science (818,120)
- Physics and astronomy (332,932)
- Plant Biology (58,717)
- Molecular and Structural Biosciences (37,793)
- Information, Robotics, and Intelligent Systems (20,401)
- Medical Sciences (25,694,738)
- Nuclear Physics (6,661,506)
- Bioinformatics (1,409,715)
- Microbiology (508,368)
- Chemistry (204,194)
- Ocean Sciences (42,793)
- Multi-Science Community (24,328)
- Evolutionary Sciences (19,479)

# Projects using the open facility

## My Projects

You currently have no project that you are authorized to edit

➕ Add New Project

## 154 registered projects (39 XSEDE)

### Projects

- |  |                                   |                                    |                                |                                       |
|--|-----------------------------------|------------------------------------|--------------------------------|---------------------------------------|
| <a href="#">AIGDock</a>                | <a href="#">AMFORA</a>            | <a href="#">aprime</a>             | <a href="#">atlas-org-duke</a> | <a href="#">atlas-org-fresnostate</a> |
| <a href="#">atlas-org-illinois</a>     | <a href="#">atlas-org-indiana</a> | <a href="#">atlas-org-uchicago</a> | <a href="#">AtlasConnect</a>   | <a href="#">BioMolMach</a>            |
| <a href="#">BioStat</a>                | <a href="#">BNLPET</a>            | <a href="#">CometCloud</a>         | <a href="#">CompChem</a>       | <a href="#">compcomb</a>              |
| <a href="#">CompNeuro</a>              | <a href="#">ConnectTrain</a>      | <a href="#">CRCCanasta</a>         | <a href="#">CRCCanasta</a>     | <a href="#">DataAnalyze</a>           |
| <a href="#">duke-4fermion</a>          | <a href="#">duke-campus</a>       |                                    |                                |                                       |
| <a href="#">EIC</a>                    | <a href="#">EvoTheory</a>         |                                    |                                |                                       |
| <a href="#">GRASP</a>                  | <a href="#">gridsgenomes</a>      |                                    |                                |                                       |
| <a href="#">IU-GALAXY</a>              | <a href="#">KnowledgeLab</a>      |                                    |                                |                                       |
| <a href="#">NRELMatDB</a>              | <a href="#">NWChem</a>            |                                    |                                |                                       |
| <a href="#">OSGopsTrain</a>            | <a href="#">P0-LBNE</a>           |                                    |                                |                                       |
| <a href="#">Proteomics</a>             | <a href="#">ProtFolding</a>       |                                    |                                |                                       |
| <a href="#">SBGrid</a>                 | <a href="#">scicomp-analytics</a> |                                    |                                |                                       |
| <a href="#">SouthPoleTelescope</a>     | <a href="#">SoyKB</a>             |                                    |                                |                                       |
| <a href="#">Swift</a>                  | <a href="#">TG-ASC130043</a>      |                                    |                                |                                       |
| <a href="#">TG-CCR130001</a>           | <a href="#">TG-CDA080011</a>      |                                    |                                |                                       |
| <a href="#">TG-DEB140008</a>           | <a href="#">TG-DMR130036</a>      |                                    |                                |                                       |
| <a href="#">TG-MCB090163</a>           | <a href="#">TG-MCB090174</a>      |                                    |                                |                                       |
| <a href="#">TG-OCE130029</a>           | <a href="#">TG-PHY110015</a>      |                                    |                                |                                       |
| <a href="#">TG-TRA100004</a>           | <a href="#">TG-TRA120014</a>      |                                    |                                |                                       |
| <a href="#">UCSDPhysAstroExp</a>       | <a href="#">UCSDPhysAstroTheo</a> |                                    |                                |                                       |
| <a href="#">UNC-RESOLVE-photometry</a> | <a href="#">unicpass</a>          |                                    |                                |                                       |

Project / SouthPoleTelescope

### SouthPoleTelescope

<b>Name</b>	SouthPoleTelescope
<b>Description</b>	The South Pole Telescope (or SPT) is a new telescope deployed at the South Pole that is designed to study the Cosmic Microwave background. Constructed between November 2006 and February 2007, the SPT is the largest telescope ever deployed at the South Pole. This telescope provides astronomers a powerful new tool to explore dark energy, the mysterious phenomena that may be causing the universe to accelerate.
<b>Organization</b>	University of Chicago
<b>Department</b>	Kavil Institute for Cosmological Physics
<b>Sponsor Campus Grid</b>	OSG Connect
<b>Principal Investigator</b>	🇺🇸 John Carlstrom
<b>Field Of Science</b>	Astrophysics

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<https://oim.grid.iu.edu/oim/project>



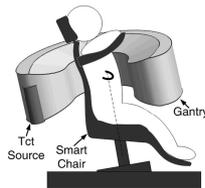
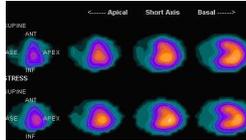
# Science on the open facility



## Detector Design

- Non-invasive diagnosis of coronary artery disease requires imaging of the myocardium
  - Predominantly with SPECT (single photon emission computed tomography)
  - Radio-pharmaceuticals+collimators and radiation detectors allow 3D imaging of the myocardium
  - Literally see areas not getting enough blood
- Design of new C-SPECT optimized for cardiac imaging (cheaper x2 and more sensitive x2-3)
  - Extensive Monte Carlo simulations utilized in design studies as well as in calibrating prototypes

John Strologas, Wei Chang  
Rush University



Bo Jayatilaka

March 25, 2015

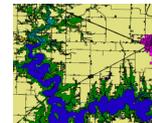
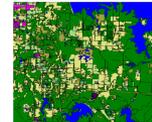
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## Agent-based modeling of disease transmission in white-tailed deer

- Chronic wasting disease (CWD) in white-tailed deer
  - Prion disease (like mad cow) causing fatal degeneration of the brain
  - Not much known about the disease and its long-term effects on deer population
- Simulate spread of CWD with an agent-based model (DeerLandscapeDisease)
  - Each deer modeled separately with its own behavioral rules (landscapes, empirically-based movement, deer behavior, disease)
  - OSG used for CPU
- DLD shows transmission may be a mix of direct (contact) and indirect (environmental) transmission
  - Potential for coexistence
  - Landscape and social structure play a major part in CWD transmission

Lene Jung Kjaer  
Southern Illinois University



Bo Jayatilaka

March 25, 2015

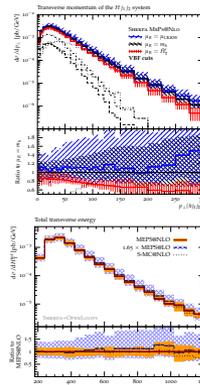
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## Collider phenomenology on the grid

- LHC final states are very complex and interesting signals are often in corners of phase space
- Precise theoretical prediction of known processes crucial in finding new physics
- OSG resources used for refining modeling of SM processes and reducing theory uncertainties
  - gluon fusion Higgs+jets production
  - top quark pairs+jets
  - Both cases  $\leq 2$  jets@NLO and 3 jets @LO
- Uses Sherpa+Rivet+MCFM+OpenLoops
- Each process used O(500k) hours over 1-2 weeks

Stefan Höche  
SLAC



Bo Jayatilaka

March 25, 2015

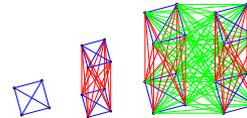
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## Enumeration of all $(C_5, C_5, C_5; n)$ Colorings

- A  $(G_1, G_2, \dots, G_k; n)$  coloring is a coloring of the edges of the complete graph on  $n$  vertices with  $k$  colors such that the  $i$ th color does not contain the graph  $G_i$
- $R_3(C_5) = 17$ . How many  $(C_5, C_5, C_5; 16)$  colorings are there?
- Start with smaller  $C_5$  colorings
  - Initial input of 140M  $n=12$  colorings
  - Iterated by adding one vertex at a time
- Result: 1,701,746,176 Ramsey 3-colorings avoiding  $C_5$ , the cycle of length 5, in all 3 colors

David Narváez,  
Stanislaw Radziszowski  
Rochester Institute of Technology



Bo Jayatilaka

March 25, 2015

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“Science on the OSG in 2014”

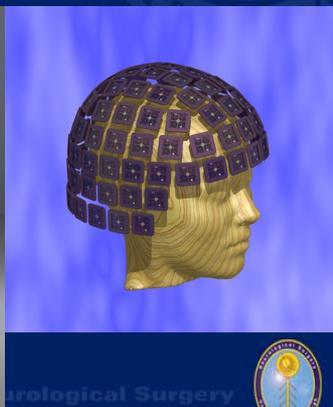
OSG AHM 3/25/15



# Science on the open facility

## The Measurement

Continuously record the extracranial magnetic field while the volunteer performs a cognitive task ...



Neurological Surgery  
at the University of Pittsburgh

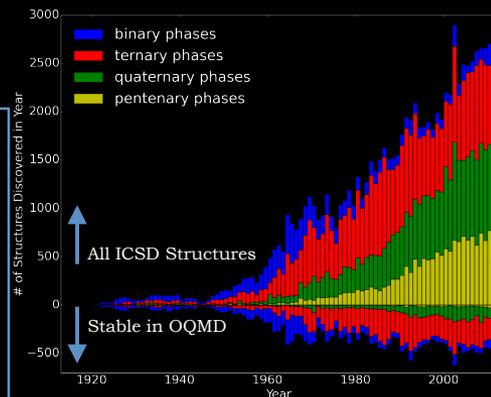


Combatting Concussions using  
“Virtual Recordings” (MEG)  
D. Krieger (Pittsburgh)

Building the Open Quantum  
Materials Database  
C. Wolverton (Northwestern)

## How many compounds in our database are stable?

- OQMD database:
- Total 297,099 compounds
  - 19,757 T=0K stable
  - 16,118 from ICSD
  - 3487 “prototype” structures



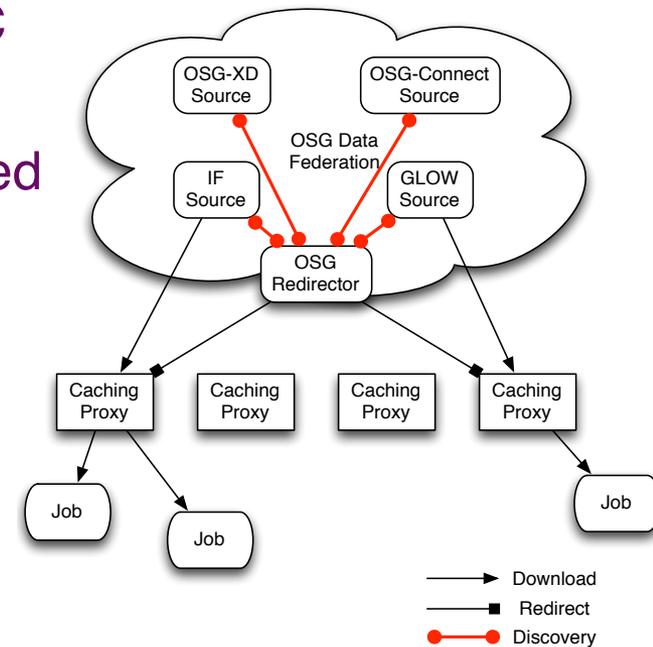
The rate of compound discovery (total and stable) within the ICSD by year.

Each of these cases represents a prediction of a system where new compounds should exist! Many gaps in our current knowledge of phase stability...

# Future growth and technologies

- Open Facility now provides more than 100M CPU hours per year
- Ongoing challenges
  - Understanding available resources after LHC Run 2 starts
  - Finding appropriate users to provide continued demand
- Developing auxiliary technologies useful for opportunistic users
  - **Data movement** is a key limitation
  - Currently inefficient beyond ~10GB/job
- Developing **XRootD**-based caching system “StashCache”
  - Increases effective data movement to ~1TB/job

## StashCache





# Conclusions

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- Opportunistic resources and their consumption continue to grow on the OSG
  - OSG Open Facility provides more than **100M CPU hours/year**
- A vibrant opportunistic user community co-exists with large (site-owning) VOs
  - A wide range of research is conducted (and published) using results obtained using OSG resources
- OSG Consortium committed to supporting these users in addition to large VOs
  - Principle of sharing is key to OSG vision and goals
  - Enshrined in by-laws: *Consortium members recognize that the OSG is a sharing eco-system and **strive to maximize the sharing of computing resources, software, and other assets to enable science.***



Open Science Grid

# Backup