Introduction to the Open Science Grid

HCC Kickstart

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Outline

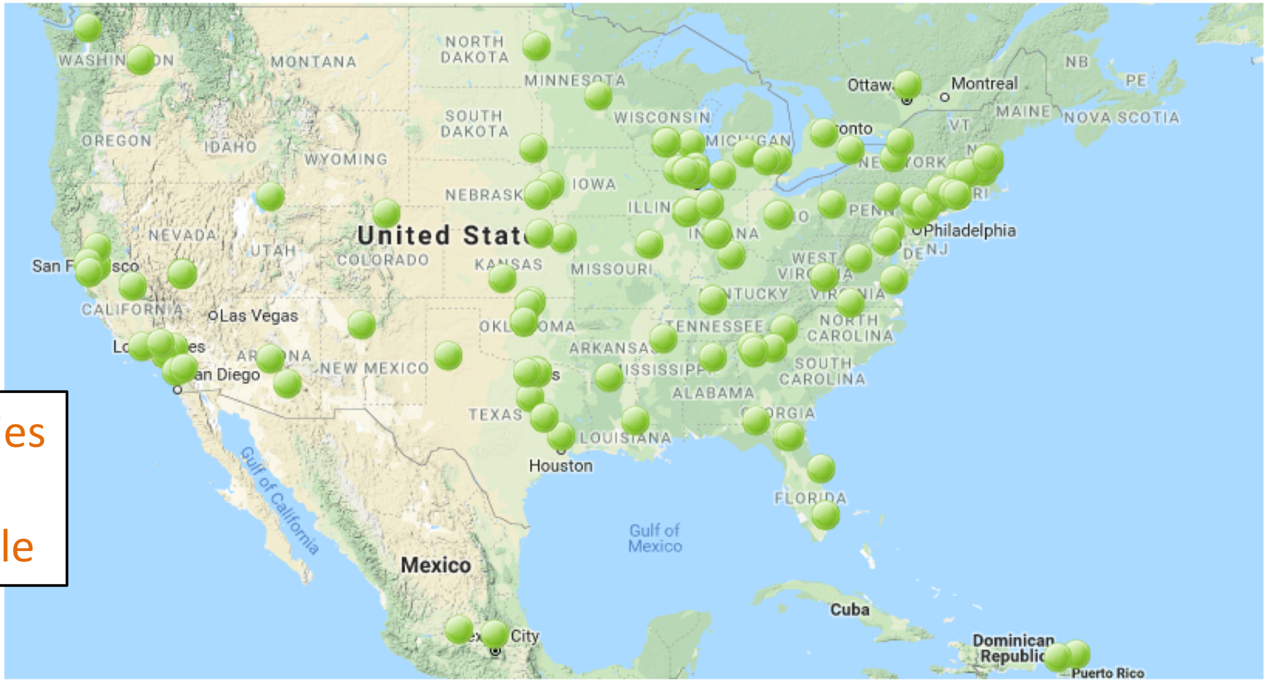
- What is the OSG?
- Who uses OSG?
- Owned vs. Opportunistic Use
- Characteristics of OSG-Friendly Jobs
- Is OSG Right for Me?
- Hands-on: How to submit jobs to the OSG from HCC clusters

The Open Science Grid

A **framework** **for large scale distributed resource sharing** addressing the technology, policy, and social requirements of sharing computing resources.

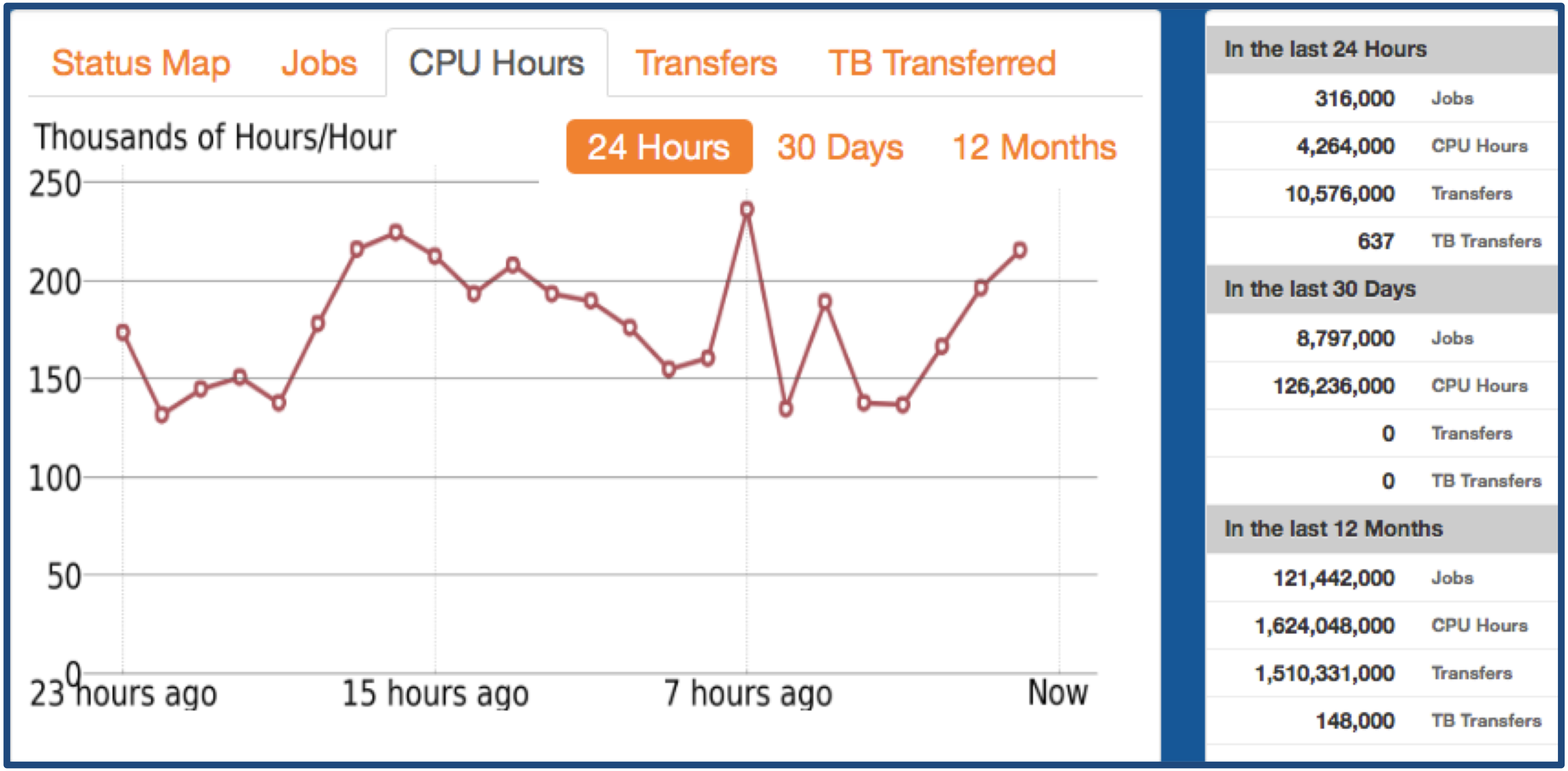
- The OSG is a consortium of software, service and resource providers and researchers, from universities, national laboratories and computing centers across the U.S., who together build and operate the OSG project.
- Funded by the NSF and DOE.

> 50 research communities
> 130 sites
> 100,000 cores accessible



The Open Science Grid

Over 1.6 billion CPU hours per year!!



In the last 24 Hours	
316,000	Jobs
4,264,000	CPU Hours
10,576,000	Transfers
637	TB Transfers
In the last 30 Days	
8,797,000	Jobs
126,236,000	CPU Hours
0	Transfers
0	TB Transfers
In the last 12 Months	
121,442,000	Jobs
1,624,048,000	CPU Hours
1,510,331,000	Transfers
148,000	TB Transfers

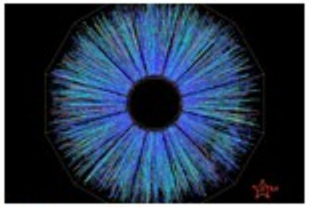
Who is Using the OSG?

- Astrophysics
- Biochemistry
- Bioinformatics
- Earthquake Engineering
- Genetics
- Gravitational-wave physics
- Mathematics
- Nanotechnology
- Nuclear and particle physics
- Text mining
- And more…

ATLAS Detector
Copyright CERN
Permission Information

SDSS Telescope
Image Credit Fermilab
Permission Information

CDMS photo
Image Credit Fermilab
Permission Information



STAR Collision
Image Credit Brookhaven National Laboratory/STAR Collaboration
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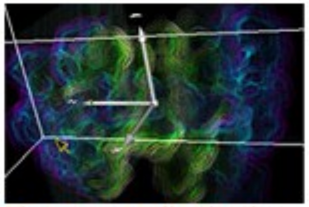

BioMOCA Application in nanoHUB
Image Credit Shawn Rice, Purdue University
Permission Information

CMS Detector
Copyright CERN
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Auger photo
Image Credit Pierre Auger Observatory
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MiniBooNE photo
Image Credit Fermilab
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DZero Detector
Image Credit Fermilab
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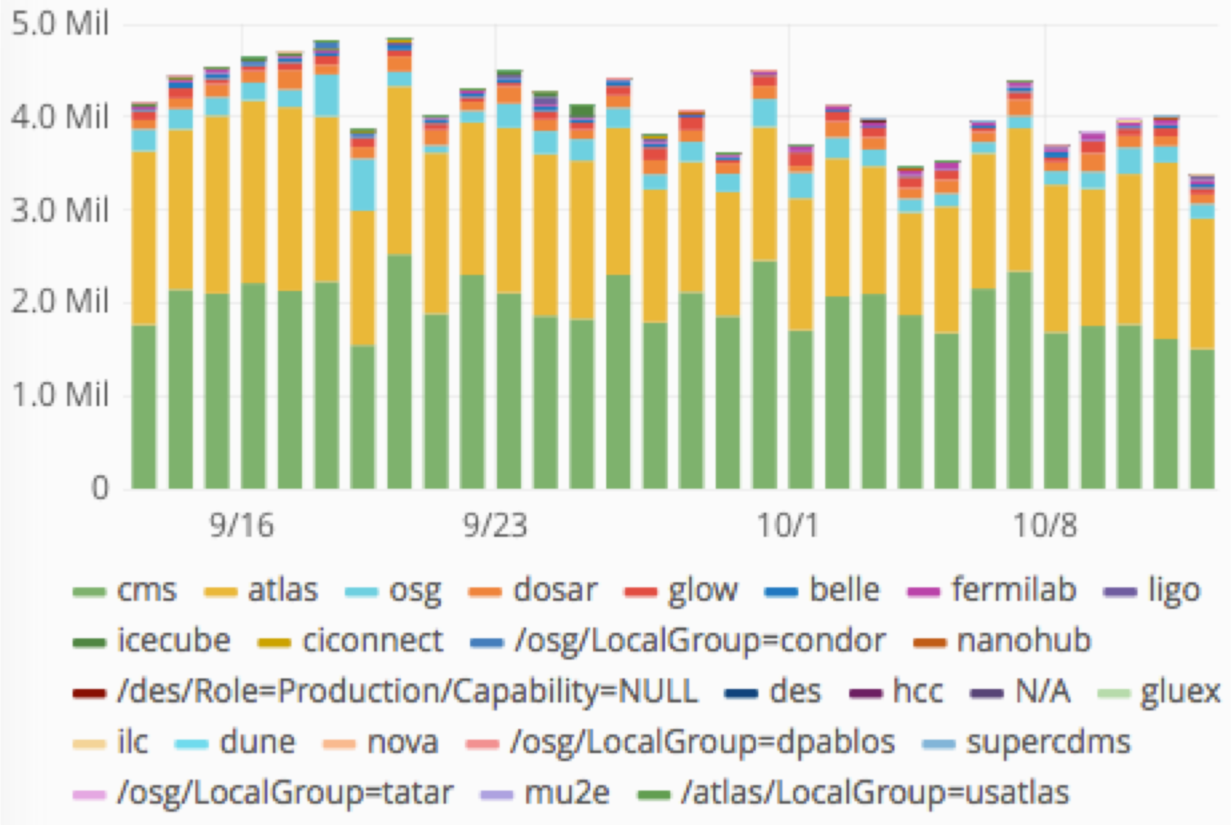
OSG Usage

Wall Hours by VO in past 30 days



- VO = Virtual Organization
- Most OSG use is on ***dedicated resources*** (used by resource owners) – 'atlas', 'cms'
- About ***8% is opportunistic*** use – 'osg', 'hcc', 'glow'

OSG Jobs

- **High Throughput Computing**
  - ➢ Sustained computing over long periods of time. Usually serial codes, or low number of cores threaded/MPI.

  vs. High Performance Computing
  - ➢ Great performance over relative short periods of time. Large scale MPI.

- ***Distributed* HTC**
  - ➢ No shared file system
  - ➢ Users ship input files and (some) software packages with their jobs.

- **Opportunistic Use**
  - ➢ Applications (esp. with long run times) can be *preempted* (or killed) by resource owner’s jobs.
  - ➢ Applications should be relatively short or support being restarted.

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OSG Jobs

- Run-time: 1-12 hours
- Single-core
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- Statically compiled executables (transferred with jobs)
- Non-proprietary software

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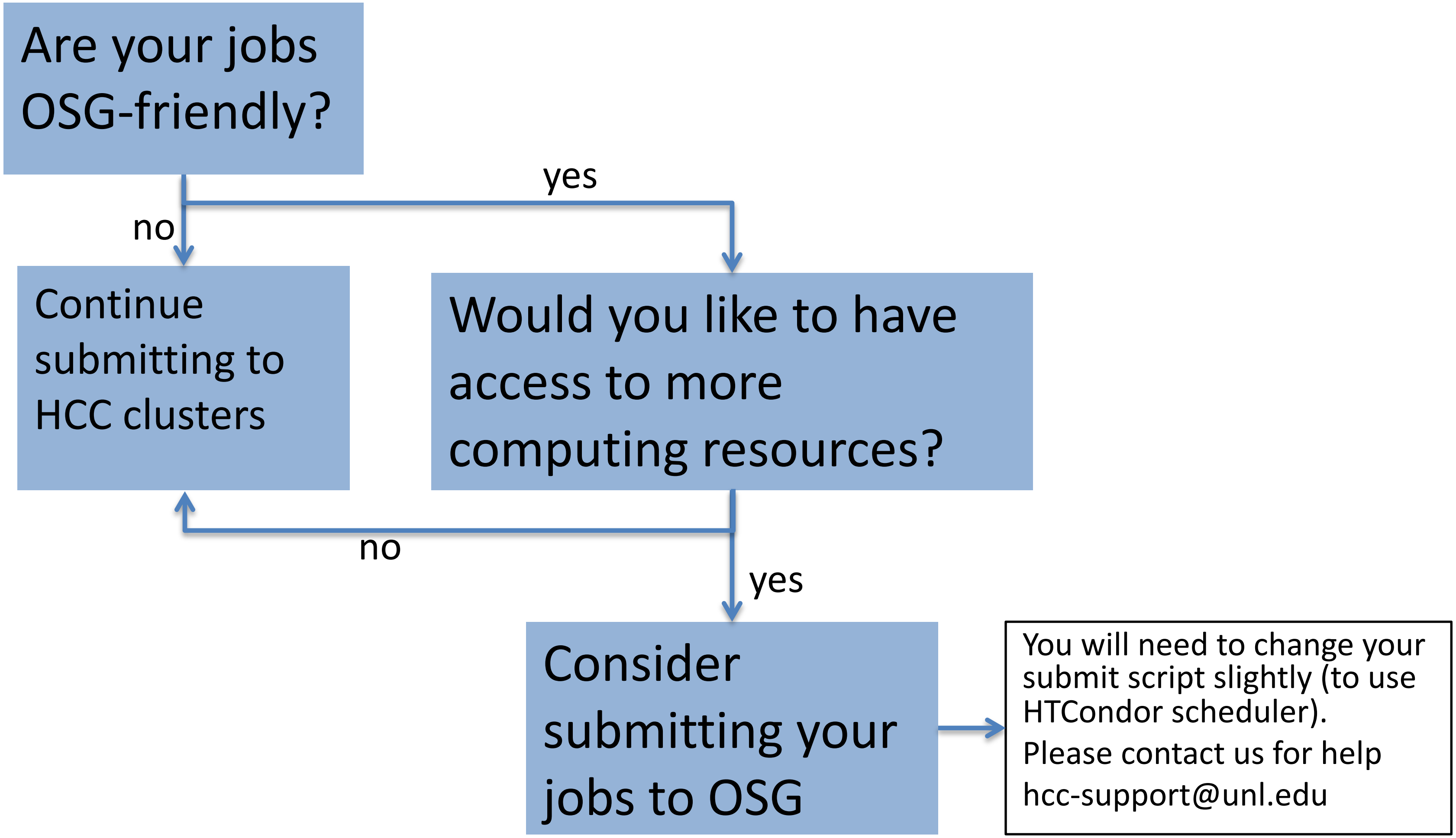
These are not hard limits!

- Checkpointing – for long jobs that are preempted
  - Many applications support built-in checkpointing
  - Job image is saved periodically so that it can be restarted on a new host after it is killed (without losing the progress that was made on the first host)
- Limited support for larger memory jobs
- "Partitionable" slots – for parallel applications using up to 8 cores
- Modules available – a collection of pre-installed software packages
- Can run compiled Matlab executables

Is OSG right for me?



Are your jobs OSG-friendly?

no

Continue submitting to HCC clusters

yes

Would you like to have access to more computing resources?

no

yes

Consider submitting your jobs to OSG

You will need to change your submit script slightly (to use HTCondor scheduler).

Please contact us for help

hcc-support@unl.edu

For more information on the Open Science Grid:

https://www.opensciencegrid.org/

For instructions on submitting jobs to OSG:

https://hcc-docs.unl.edu/display/HCCDOC/The+Open+Science+Grid

Quickstart Exercise

Submit a simple job to OSG from Crane

```
ssh <username>@crane.unl.edu
cd $WORK
git clone https://github.com/unlhcc/HCCWorkshops.git
cd $WORK/HCCWorkshops/OSG/quickstart
```

Exercise 1:

```
osg-template-job.submit       (HTCondor submit script)
short.sh                      (job executable)
```

Exercise 2:

```
osg-template-job-input-and-transfer.submit
short_with_input_output_transfer.sh
```

Quickstart Exercise

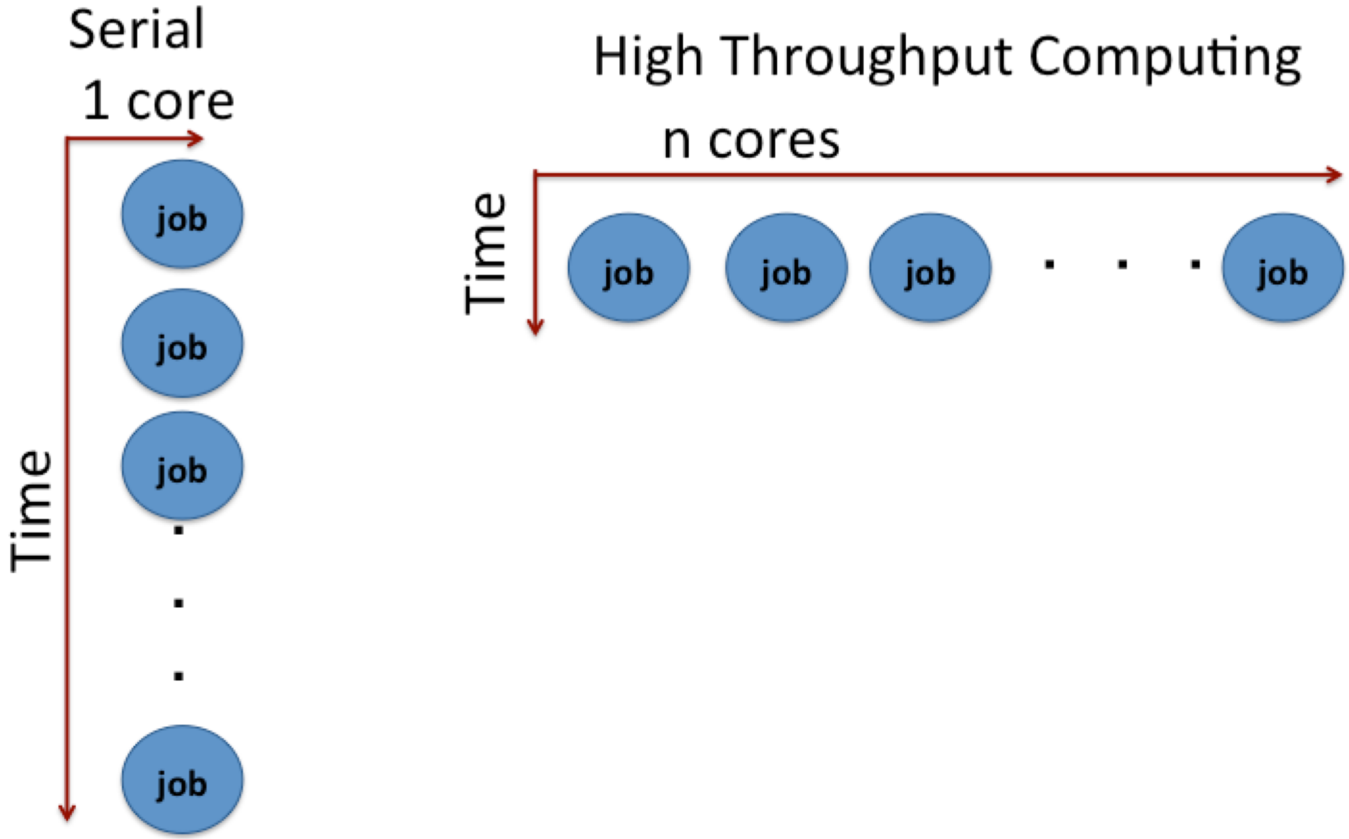
HTCondor Commands:

```
condor_submit <submit_script>    # submit a job to osg

condor_q <username>              # monitor your jobs

condor_rm <jobID>                # remove a job

condor_rm <username>             # remove all of your jobs
```

Everything you need to know and more about HTCondor submit scripts:
http://research.cs.wisc.edu/htcondor/manual/current/condor_submit.html

Scaling Up on OSG

Efficient approach to handle independent jobs



Serial

1 core

Time

job

job

job

. . .

job

High Throughput Computing

n cores

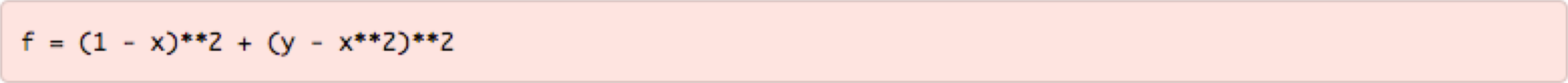
Time

job job job . . . job

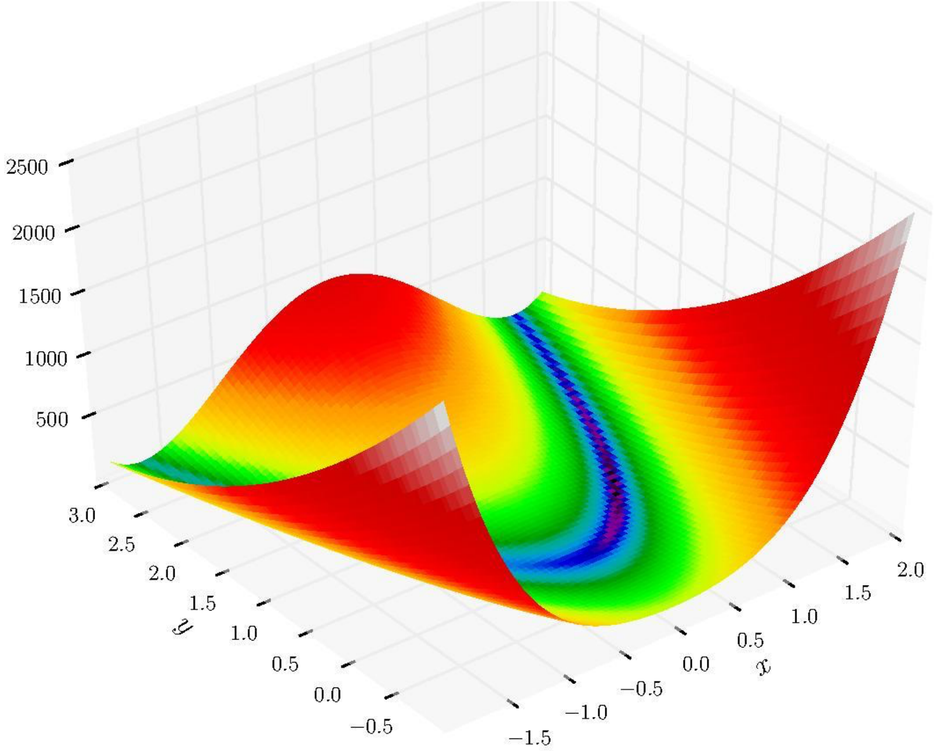
Scaling Up Exercise

```
cd $WORK/HCCWorkshops/OSG/ScalingUp-Python

scalingup-python-wrapper.sh   # job executable (wrapper)
rosen_brock_brute_opt.py      # Python script

Example1/ScalingUp-PythonCals.submit  # submit script 1
Example2/ScalingUp-PythonCals.submit  # submit script 2
Example3/ScalingUp-PythonCals.submit  # submit script 3
Example4/ScalingUp-PythonCals.submit  # submit script 4
```

Python Brute Force Optimization



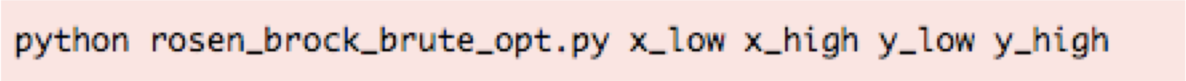
```
f = (1 - x)**2 + (y - x**2)**2
```



2-D Rosenbrock function
Used to test the robustness of an optimization method

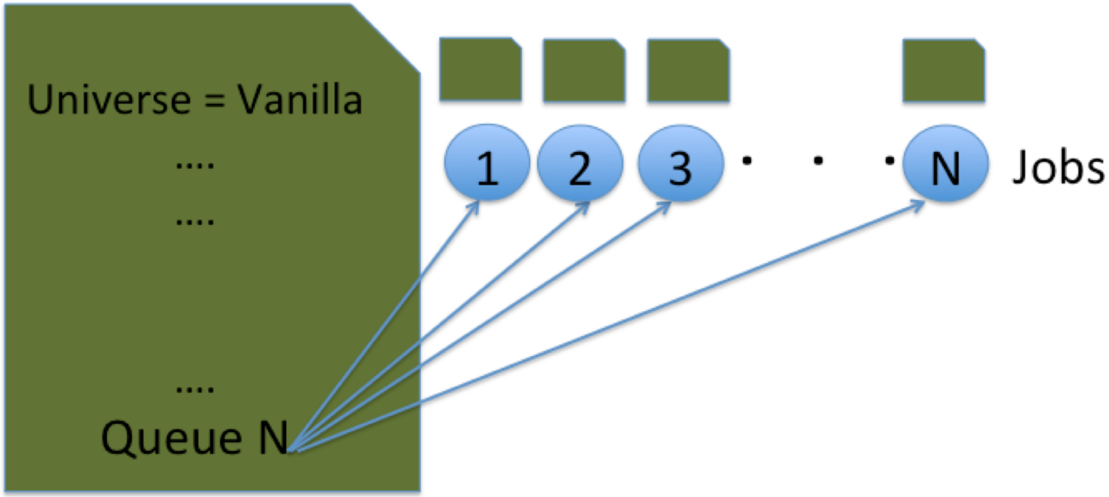
Python script `rosen_brock_brute_opt.py` finds the minimum of the function for a set of points (grid) between selected boundary values.

By default, Python script will randomly select the boundary values of the grid that the optimization procedure will scan over. These values can be overidden by user supplied values.



```
python rosen_brock_brute_opt.py x_low x_high y_low y_high
```

Python Brute Force Optimization



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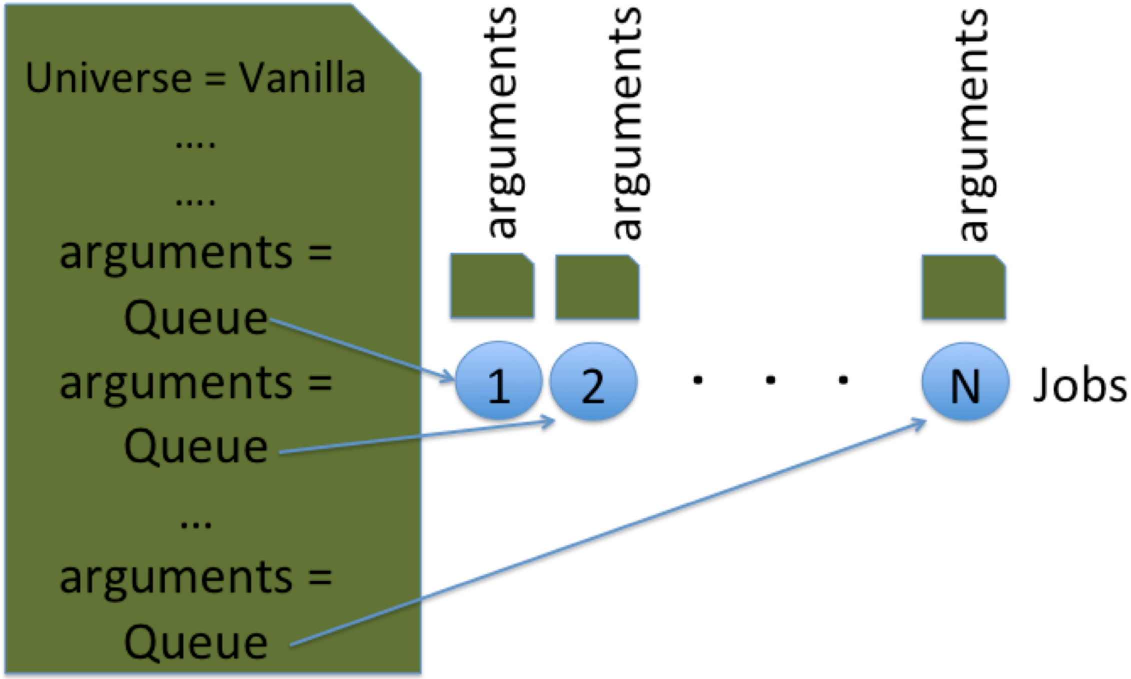


Universe = Vanilla

....

....

arguments =

Queue

arguments =

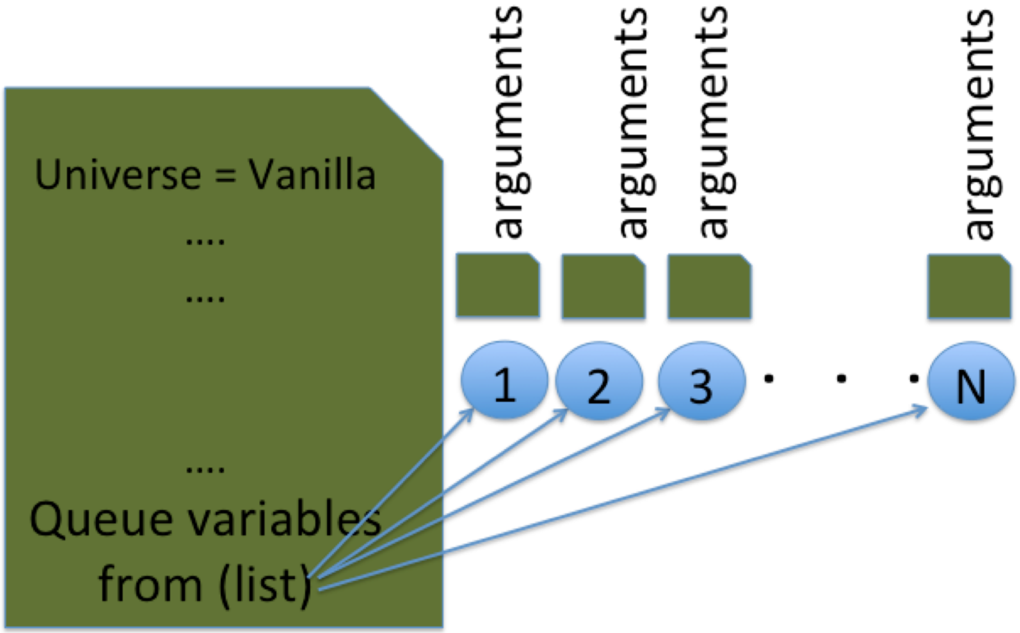
Queue

...

arguments =

Queue

Python Brute Force Optimization



Additional Slide(s)

To switch to OSG modules on Crane:

```
source osg_oasis_init
```

To analyze job matching:

```
condor_q -pool glidein.unl.edu -analyze <jobid>
```

To view hosts where previous jobs have run:

```
condor_history -long <username> | grep LastRemoteHost
```