



Intro to the Virtual School Pilot, HTC, and OSG

Monday, Aug 2

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Welcome to the **OSG Virtual School Pilot 2020!**

Why You Are Here

- You need large-scale, HTC-style computing – or you support researchers who do
- **Do not let computing block your research!**
 - Computing is cheap and plentiful
 - Push the limits of what you can do
 - If you run out of science to do, transcend the boundaries of your science
 - When computing becomes a barrier, push us to fix the problems
- Help & encourage others:
In your lab, in your department, in your field, friends, etc.
- Help us improve! **We** are here to support you.

Intro to HTC and OSG

Overview

- What is *high throughput computing (HTC)* ?
- What is the Open Science Grid (OSG)?
- How do you get the most out of the above?
 - School content organization

HTC: An Analogy



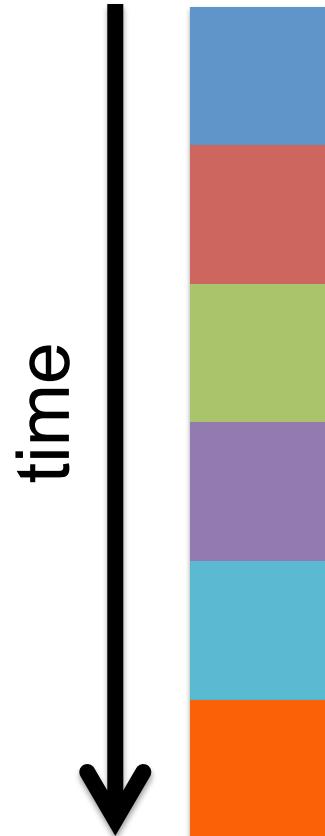
HTC: An Analogy



Serial Computing

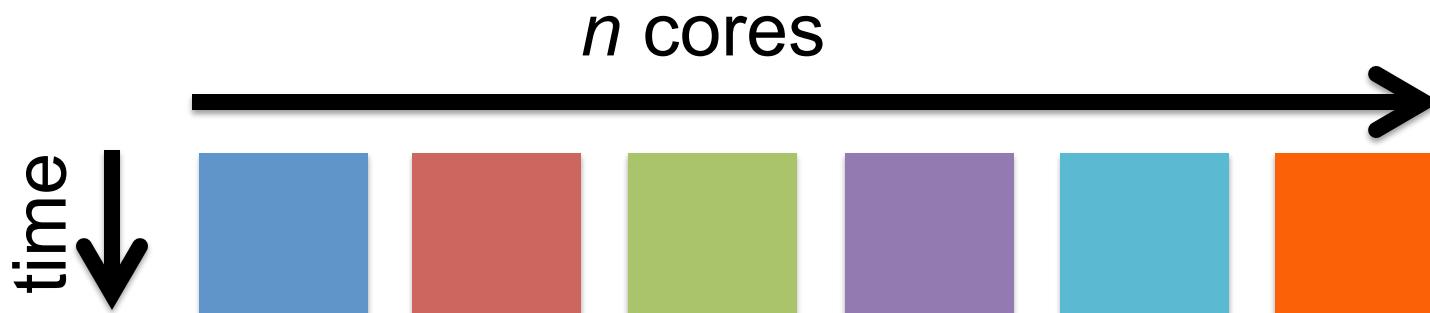
What many programs look like:

- *Serial execution*, running one task at a time
- Overall compute time grows significantly as individual tasks get more complicated (long) or if the number of tasks increases
- ***How can you speed things up?***



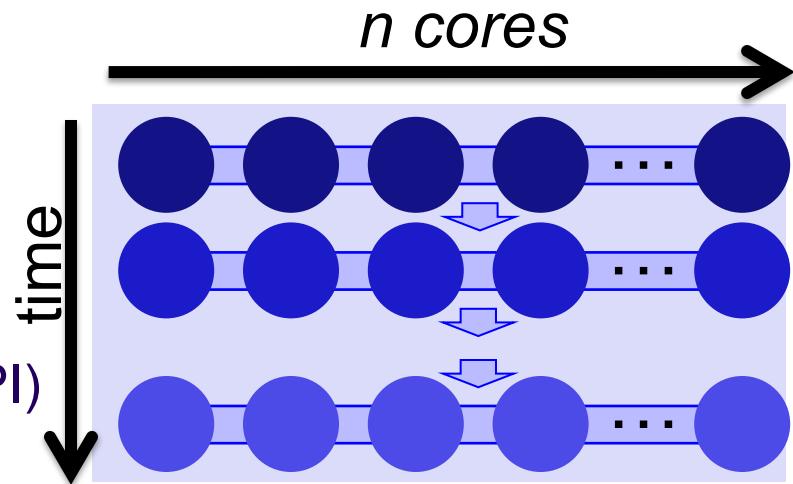
High Throughput Computing (HTC)

- Parallelize!
- Independent tasks run on different cores

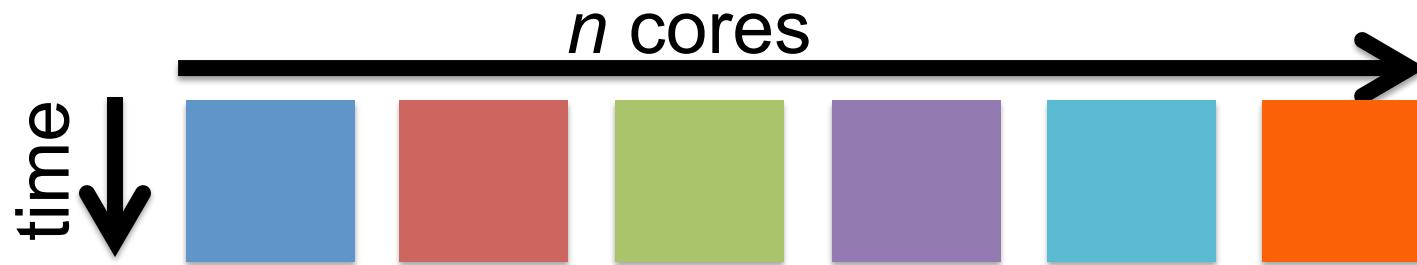


High Performance Computing (HPC)

- Benefits greatly from:
 - CPU speed + homogeneity
 - shared filesystems
 - fast, expensive networking (e.g. Infiniband) and servers co-located
- Requires special programming (MP/MPI)
- Scheduling: **Must wait until all processors are available, at the same time and for the full duration**
- ***What happens if one core or server fails or runs slower than the others?***



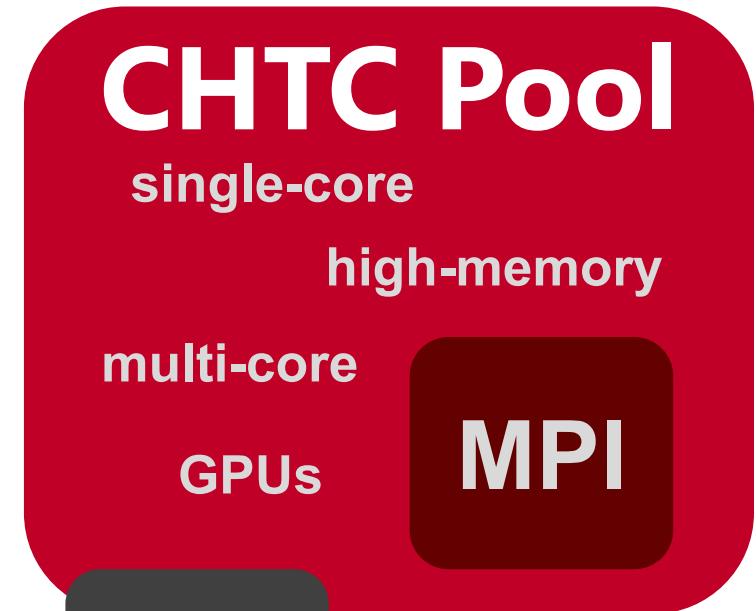
High Throughput Computing (HTC)



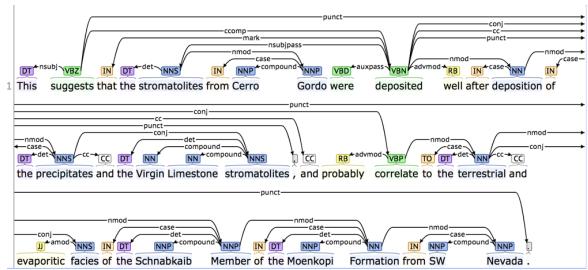
- Scheduling: only need **1 CPU core for each** (shorter wait)
- Easier recovery from failure
- No special programming required
- Number of concurrently running jobs is *more* important
- CPU speed and homogeneity are *less* important

Example Local Cluster

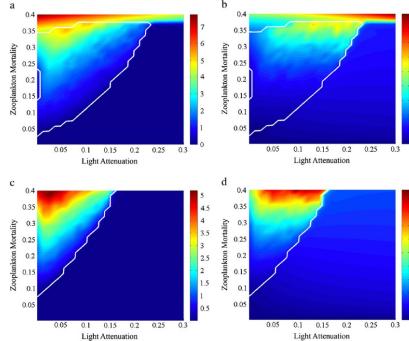
- UW-Madison's **Center for High Throughput Computing (CHTC)**
- Recent CPU hours:
 - ~120 million hrs/year (~15k cores)
 - Up to 15,000 per user, per day (~600 cores in use)



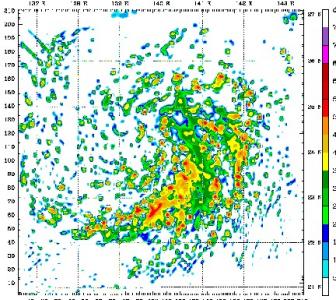
HTC Examples



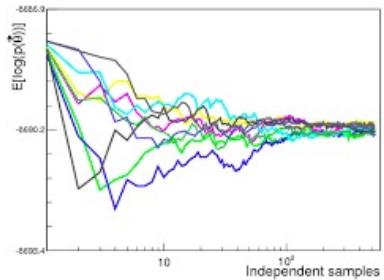
text analysis (most genomics ...)



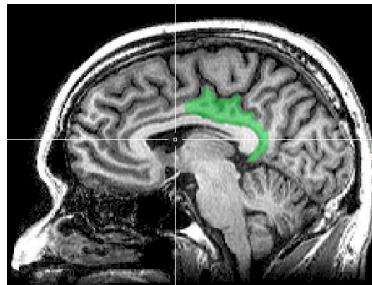
parameter sweeps



multi-start simulations



statistical model optimization
(MCMC, numerical methods, etc.)

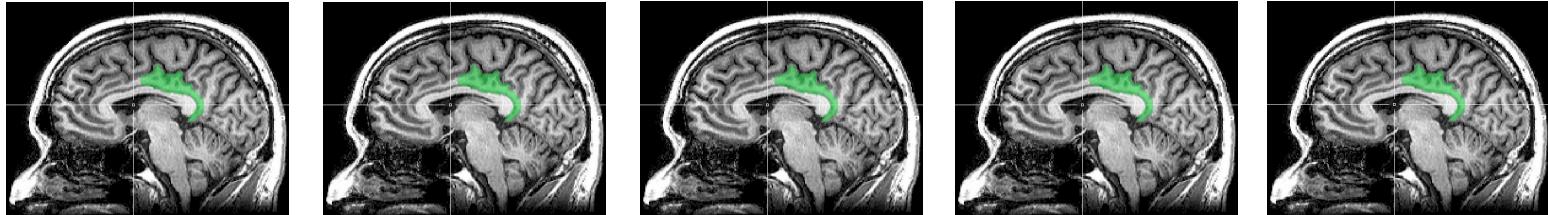


multi-image and
multi-sample analysis

Signs of HTC-able work

- Any mention of numerous samples, images, models, parameters, etc.
- Nearly anything written by the primary user (e.g. c/fortran, Python, R)
 - Break out of loops!
 - Common internal parallelism could really be HTC (e.g. Matlab's 'parfor', 'distributed server', etc.)
- Some community softwares that use multi-threading or multiprocessing (e.g. OpenMP)
 - many are simply looping over data portions or independent tasks
 - HTC-able: break up input (or 'parameter' space), turn off multi-threading, combine results
- Long-running jobs (especially if non-MPI); see above explanations

Example Challenge



You need to process 64 brain images for each of 168 patients. **Each image takes ~1 hour of compute time.**

168 patients x 64 images = ~8000 tasks = ~8000 hrs

Conference is next week.

Distributed Computing

- Use many computers, each running one instance of our program
- Example:
 - **1 laptop (1 core) => 12,000 hrs = ~1.5 years**
 - **1 server (~40 cores) => 750 hrs = ~2 weeks**
 - **1 MPI job (400 cores) => 30 hrs = ~1 days**
 - **A whole cluster (12,000 cores) = ~1 hour**

What computing resources are available?

- A server?
- A local cluster?
 - Consider: Queue wait time? Can you program MP/MPI? Typical clusters tuned for HPC (large MPI) jobs may not be best for HTC workflows! Could you use even more than that?
- OSG?
- Other
 - EGI (European)
 - Other national and regional grids
 - Commercial cloud systems (e.g. HTCondor on AWS)

- (d)HTC for Open Science
 - ~100 contributors
 - **Past year:**
 - >1.6 billion CPU hours
 - >200 petabytes transferred



- Can submit jobs locally, they backfill across the country
 - *interrupted at any time (but not too frequent)*
- <https://www.opensciencegrid.org/>



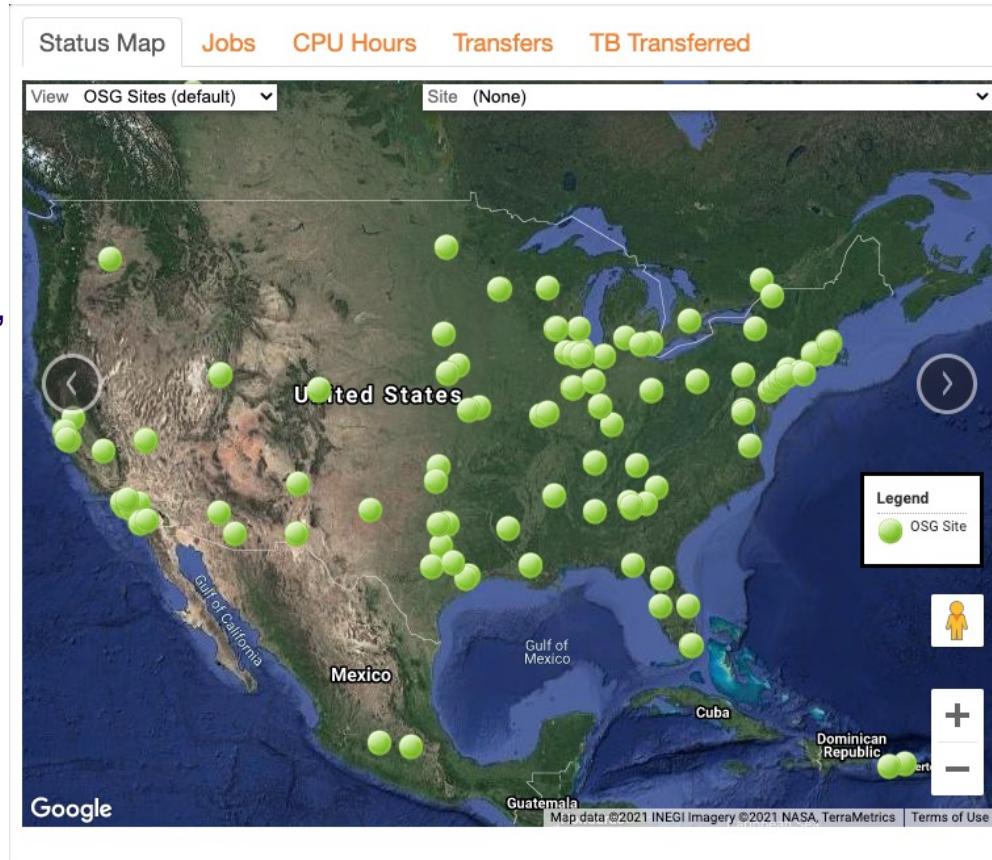
What is the OSG?

a consortium of researchers and institutions who share compute and data resources for ***distributed*** high-throughput computing (**dHTC**) in support of open science

Who Participates?

- Researchers
- Science Gateways
- Multi-Institution Collaborations
 - Atlas/CMS (Higg Boson), IceCube, South Pole Telescope, and others
- Academic Institutions and National Laboratories that support the above

Campuses are critical to OSG's ability to advance research.



Total Core Hours per Month

200 Mil

total ▾

Research Communities (Pools) in the OSG

("virtual organizations")

>2 billion hrs in the last year

150 Mil

100 Mil

50 Mil

0

2006

2008

2010

2012

2014

2016

2018

2020

cms	4.9676 Bil
atlas	4.4322 Bil
osg	1.0743 Bil
dosar	316.0 Mil
fermilab	295.2 Mil
cdf	259.4 Mil
glow	255.7 Mil
dzero	225.4 Mil
ligo	114.5 Mil
alice	113.3 Mil
mu2e	94.4 Mil
gridunesp	80.1 Mil
nova	76.2 Mil
engage	64.5 Mil
minos	62.9 Mil
hcc	57.8 Mil



HOW IS CMS SEARCHING FOR THE HIGGS BOSON?



[Previous](#)

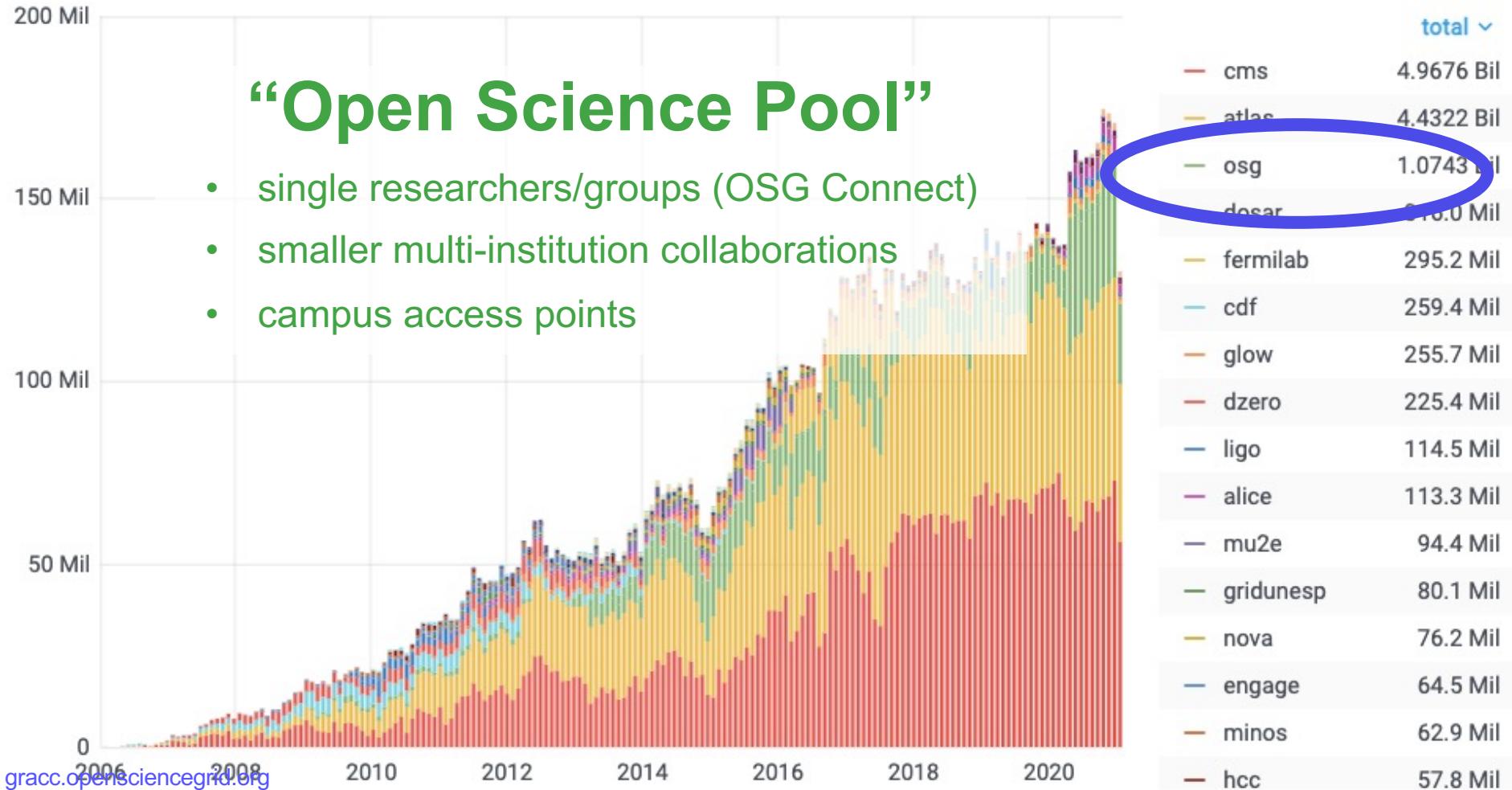
[Next](#)

OSG Supports Multi-Messenger Astronomy.

OSG integrates global computing to support detection of colliding neutron stars by LIGO, VIRGO, and DECam.

[Read more](#)

Total Core Hours per Month



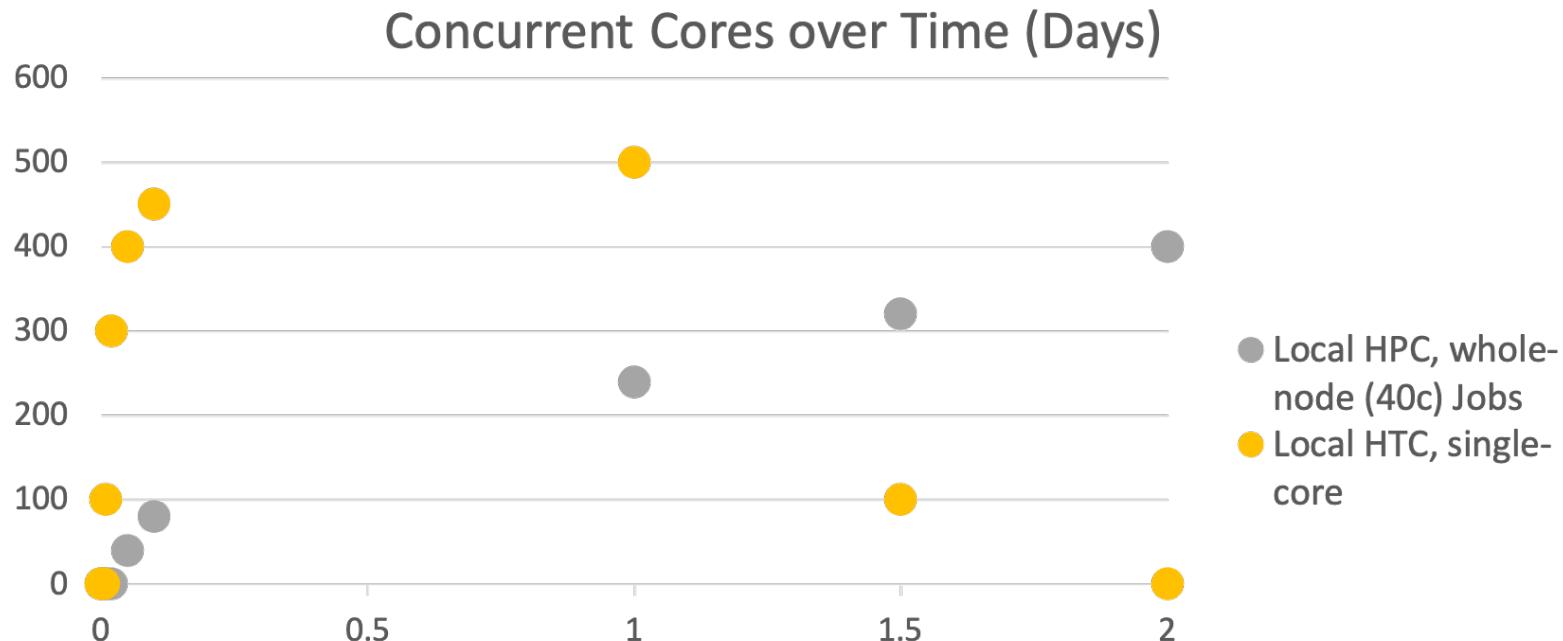
“Open Science Pool”

- single researchers/groups (OSG Connect)
- smaller multi-institution collaborations
- campus access points

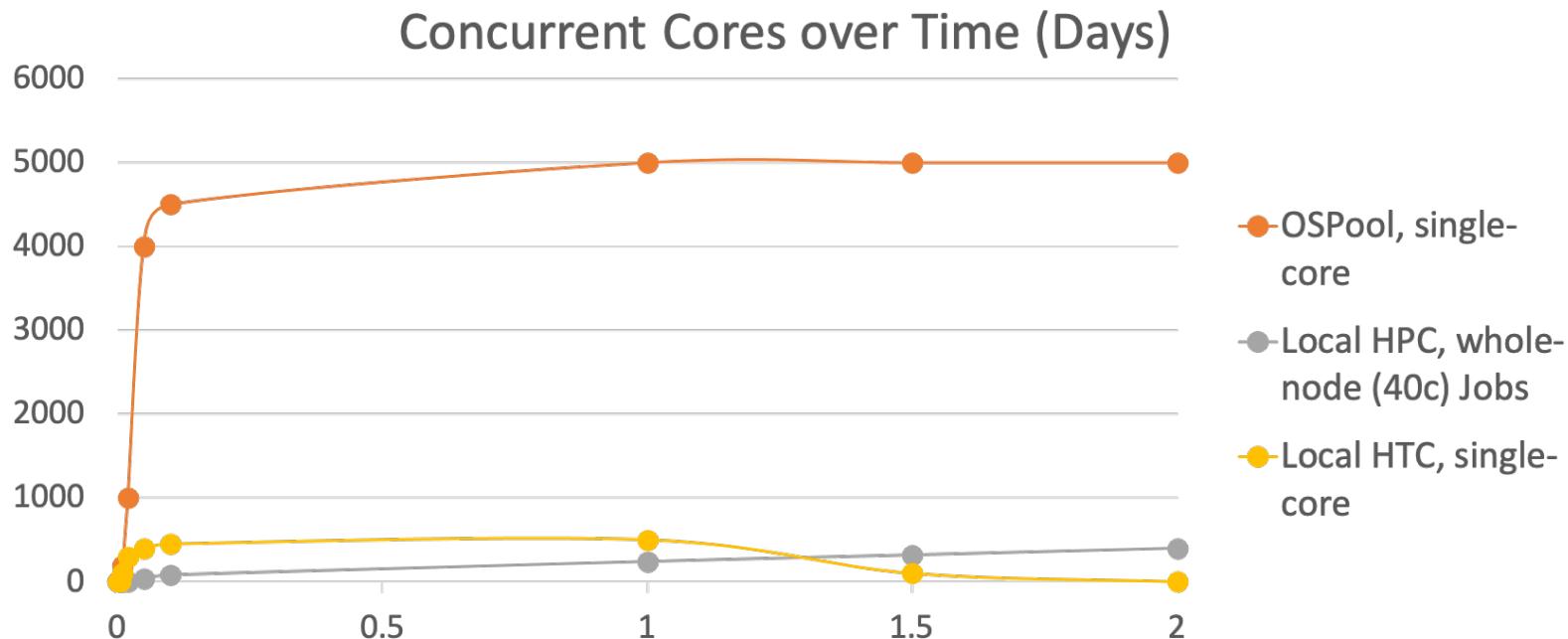
Can the OSPool Help?

Per-Job Resources	Ideal Jobs! (up to 10,000 cores, per user!)	Still Very Advantageous!	Probably not...
cores (GPUs)	1 (1; non-specific)	<8 (1; specific GPU type)	>8 (or MPI) (multiple)
Walltime (per job)	<10 hrs* *or checkpointable	<20 hrs* *or checkpointable	>20 hrs
RAM (per job)	<few GB	<10 GB	>10 GB
Input (per job)	<500 MB	<10 GB	>10 GB
Output (per job)	<1 GB	<10 GB	>10 GB
Software	'portable' (pre-compiled binaries, transferable, containerizable, etc.)	most other than →→→	licensed software; non-Linux

Hypothetical Throughput, 10k core hours



Hypothetical Throughput, 10k core hours





For Researchers and Campuses

Proactive, personalized facilitation and support for:

- Individual researchers via **OSG Connect**
- Institutions and large collaborations
 - Share local resources via the OSG
 - Locally-supported submit points
 - data and identity federation
 - integration of cloud capacity
 - Local HTC Capacity
 - Learn from OSG's **Research Computing Facilitators**
- **Presentations/Training** in OSG compute execution, HTC Facilitation, and local HTC systems administration



OSG Virtual School Content

- **Lectures:** Tue-Fri, 10am CT & 2:30pm* CT
 - HTC via **HTCondor**
 - (d)HTC on the **OSG**
 - **Software Portability** for HTC
 - **Data Portability** for HTC
- **Bonus topics** (2nd Mon-Tue): optional
- **Showcase** (2nd Wed): science transformed by HTC
- **Lightning Talks+Close** (2nd Fri): chance to show work

**presented ‘publicly’, via registration; all others for selected participants*