Intro to the Virtual School, HTC, and OSG

Monday, Aug 2
Tim Cartwright, Lauren Michael

This work was supported by NSF grants MPS-1148698, OAC-1836650, and OAC-2030508
Welcome to the OSG Virtual School 2021!
Why We 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.
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 co-located servers

• 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)
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 72 brain images for each of 168 patients. Each image takes ~1 hour of compute time.

168 patients x 72 images = ~12000 tasks = ~12000 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 (10,000 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 Grid Infrastructure)
  - Other national and regional grids
  - Commercial cloud systems (e.g. HTCondor on AWS)
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 (Higgs 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.
Research Communities (Pools) in the OSG
("virtual organizations")
>2 billion hrs in the last year
How is CMS searching for the Higgs Boson?
OSG Supports Multi-Messenger Astronomy.

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

Read more
“Open Science Pool”

- single researchers/groups (OSG Connect)
- smaller multi-institution collaborations
- campus access points
## Can the OSPool Help?

<table>
<thead>
<tr>
<th><strong>Per-Job Resources</strong></th>
<th><strong>Ideal Jobs! (up to 10,000 cores, per user!)</strong></th>
<th><strong>Still Very Advantageous!</strong></th>
<th><strong>Probably not...</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>cores (GPUs)</strong></td>
<td>1 (1; non-specific)</td>
<td>&lt;8 (1; specific GPU type)</td>
<td>&gt;8 (or MPI) (multiple)</td>
</tr>
<tr>
<td><strong>Walltime (per job)</strong></td>
<td>&lt;10 hrs* *or checkpointable</td>
<td>&lt;20 hrs* *or checkpointable</td>
<td>&gt;20 hrs</td>
</tr>
<tr>
<td><strong>RAM (per job)</strong></td>
<td>&lt;few GB</td>
<td>&lt;10 GB</td>
<td>&gt;10 GB</td>
</tr>
<tr>
<td><strong>Input (per job)</strong></td>
<td>&lt;500 MB</td>
<td>&lt;10 GB</td>
<td>&gt;10 GB</td>
</tr>
<tr>
<td><strong>Output (per job)</strong></td>
<td>&lt;1 GB</td>
<td>&lt;10 GB</td>
<td>&gt;10 GB</td>
</tr>
<tr>
<td><strong>Software</strong></td>
<td>‘portable’ (pre-compiled binaries, transferable, containerizable, etc.)</td>
<td>most other than →→→ licensed software; non-Linux</td>
<td></td>
</tr>
</tbody>
</table>
Hypothetical Throughput, 12k core hours

Concurrent Cores over Time (Days)

- Gray dots: Local HPC, whole-node (40c) Jobs
- Yellow dots: Local HTC, single-core

0 0.5 1 1.5 2
0 100 200 300 400 500 600
Hypothetical Throughput, 12k core hours

Concurrent Cores over Time (Days)
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
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 access 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