The Practice of High Performance Computing

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Thank you

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Information Technology Services
Information Technology Services
Information Technology Services
Information Technology Services
Information Technology Services
Information Technology Services
Purdue University

and

National Science Foundation
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Great Lakes Consortium for Petascale Computing
Outline

• Remote Computing at National Supercomputing Centers

• Data Management

• Code Management

• Scientific Validation and Benchmarking

• Managing a Computational Research Program

• Applying for a Computing Allocation
National Supercomputing Centers

- Most Supercomputing Centers require running in **Batch mode** using PBS (Portable Batch System) and a scheduler (like **Helium**)
  - Usually your job will wait around in a queue for a while (sometimes days, or even weeks) before running
  - It is important to get used to this method of remote computing

- To best take advantage of the computer, **learn the queue rules** for that computer:
  - Often, if you modify how you run slightly (i.e., number of processors or total wallclock time), you can achieve much higher **throughput** of runs
  - Many people pay no attention, and consequently have poor throughput
Queue Rules (Scheduling Policy)

The way you run jobs will differ dramatically depending on the queue rules.

#1 Jaguar Cray XT5 ORNL (DOE)

#3 Kraken Cray XT5 NICS (NSF)

### Priority/Limits Based on Job Size

<table>
<thead>
<tr>
<th>Bin</th>
<th>Min</th>
<th>Max</th>
<th>XT5 Partition</th>
<th>Maximum Wall-Time (Hours)</th>
<th>Aging Boost (Days)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>120,000</td>
<td>24.0</td>
<td>15</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>80,004</td>
<td>119,999</td>
<td>24.0</td>
<td>10</td>
<td></td>
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<tr>
<td>3</td>
<td>40,008</td>
<td>80,003</td>
<td>24.0</td>
<td>5</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>5,004</td>
<td>40,007</td>
<td>12.0</td>
<td>0</td>
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<tr>
<td>5</td>
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<td>5,003</td>
<td>6.0</td>
<td>0</td>
<td></td>
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<tr>
<td>6</td>
<td>1</td>
<td>2,003</td>
<td>2.0</td>
<td>0</td>
<td></td>
</tr>
</tbody>
</table>

### Queue Limits

<table>
<thead>
<tr>
<th>Queue</th>
<th>Min Size</th>
<th>Max Size</th>
<th>Max Wall Clock Limit</th>
</tr>
</thead>
<tbody>
<tr>
<td>small</td>
<td>0</td>
<td>512</td>
<td>24:00:00</td>
</tr>
<tr>
<td>*longsmall</td>
<td>0</td>
<td>256</td>
<td>60:00:00</td>
</tr>
<tr>
<td>medium</td>
<td>513</td>
<td>8192</td>
<td>24:00:00</td>
</tr>
<tr>
<td>large</td>
<td>8193</td>
<td>49536</td>
<td>24:00:00</td>
</tr>
<tr>
<td>capability</td>
<td>32769</td>
<td>99072</td>
<td>24:00:00</td>
</tr>
</tbody>
</table>
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Data Management

• Standard Procedure for Supercomputing Centers:
  - **HOME** directory is for source code and small files
  - **SCRATCH** directory is where your code will produce output
    - Usually this directory has faster access to the compute nodes
    - This directory is not backed up
  - **ARCHIVAL STORAGE** is where you will store your large data sets

• Transferring Files to/from Offsite:
  - Moving TB of data is a very slow process
  - You can use secure parallel file copy facilities such as **bbcp**
  - You’ll often want to work with support staff to figure out the best way

• Compressed, Portable, Self-Describing data formats are highly recommended
  - **NetCDF** (Network Common Data Form)
  - **HDF** (Hierarchical Data Format) also has parallel I/O capability
  - You can link your code using these widely used, standardized libraries

• National Science Foundation now requires all funding proposals to include an explicit Data Management Plan
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If you are developing a code that may be widely used, here is some advice:

- Use the **standard language**, not specialized extensions of a specific compiler
- **Comments, Comments, Comments!**
- Software tools for team development
  - Other older packages: CVS (Concurrent Versions System), RCS, PRCS
- Packaging code so that it is easy to transport and compile
  - tar archives are useful to allow unpack the entire directory structure
  - Makefiles make compiling easy
  - HYDRO gives an example of how to do this
- Porting
  - If many people use your code, porting to different computers is important
- Documentation
  - Also important is to write up clear documentation on how to use code
- Making a Code Publicly Available
  - Sourceforge ([http://sourceforge.net/](http://sourceforge.net/)) will host open source software that is to be shared with the community
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Scientific Validation and Benchmarking

- Scientific codes need to be validated before most will accept the results
  - Publish results of validation tests in peer-reviewed scientific journals (i.e. *Journal of Computational Physics*, etc.)
  - Often you can find standard test problems in the literature

- When packaging up code for distribution:
  - Include input files for the suite of test runs that you used for validation
  - A benchmark run is helpful
    - The benchmark is a relatively short run that test the full capability of the code and will only yield the correct answer if the code works correctly
    - This is good to verify proper compilation and installation and can be used to compare code performance on different computers
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Managing a Computational Research Program

- Organization of simulation runs is fundamentally important
  - You need to keep good records of runs performed in the past
    - What were the parameters, where is the data, etc.
  - I keep a notebook with all of my large-scale runs logged into it.

- Think hard about the research questions you want to answer
  - What are the critical runs that will enable you to answer those questions?

- Allocation Management:
  - It is always better to use up your allocation before the end of the award period than to have some left over
  - Often when this happens, they will give you a little more if you need it
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Applying for a Computing Allocation

• National Supercomputing Resources:
  - NSF TeraGrid
    https://www.teragrid.org/
  - DOE Office of Advanced Scientific Computing Research
    http://science.energy.gov/ascr/
  - NASA Advanced Supercomputing Division
    http://www.nasa.gov/
  - NIH Center for Information Technology
    http://www.nih.gov/scene.html

• Computing Proposal:
  - Describe the scientific problem you want to solve
  - Describe your code (algorithm, parallelization strategy, etc.)
  - Provide parallel performance results (strong and/or weak scaling)
Applying through NSF TeraGrid

Startup Allocation
• The application procedure for a startup allocation is rather simple
• Cannot apply as a graduate student, but can as a postdoc
  - But you can apply with your advisor as PI and then your advisor can set you up with an account
• Can apply for up to 200,000 SUs (valid for 1 year)
  NOTE: 8760 hours/year, thus 200,000 cpu-h is like 23 cores for a year!
• Application requires only:
  - Estimate of computing time needed
  - Short abstract of computational project
  - CV for the PI
• Review of your proposal will be returned within 1 week

Research Allocation
• Requires a 10-15 page proposal (depending on size of request)
• Requires supporting code performance and scaling information
• Reviewed quarterly with multiple reviewers
Local Resources at the University of Iowa

Research Services of ITS

- Supports computational research at the University
  - Ben Rogers, Director of Research Services, ben-rogers@uiowa.edu

- Helium
  - Shared resource funded by University and 12 faculty research groups
  - Open to all University researchers (using all.q)
  - 1600 cores, helium.hpc.uiowa.edu
  - Glenn Johnson administers this clusters, glenn-johnson@uiowa.edu
  - Documentation
    https://www.icts.uiowa.edu/confluence/display/ICTSit/User+Documentation
    - Plans to double size of the machine beginning this summer

- New Research Services GPU System (coming online soon)
  - NVIDIA GeForce GTX 580 (512 cores, 1536 MB RAM)
  - Host: Intel Core i7 (4 core), 12 GB RAM, 2 TB storage