The Practice of High Performance Computing

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Iowa High Performance Computing Summer School
University of Iowa
Iowa City, Iowa
6-8 June 2012
Thank you

Ben Rogers  Information Technology Services
Glenn Johnson Information Technology Services
Mary Grabe Information Technology Services
Amir Bozorgzadeh Information Technology Services
Preston Smith Purdue University

and

National Science Foundation
Rosen Center for Advanced Computing, Purdue University
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>Cores Min</th>
<th>Cores 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>
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<td>24.0</td>
<td>15</td>
<td></td>
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<tr>
<td>2</td>
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<td>80,003</td>
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<td></td>
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<td>1</td>
<td>2,003</td>
<td>2.0</td>
<td>0</td>
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</table>

<table>
<thead>
<tr>
<th>Queue</th>
<th>Min Size</th>
<th>Max Size</th>
<th>Max Wall Clock Limit</th>
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</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>
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<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 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 XSEDE (Extreme Science and Engineering Discovery Environment)
    [https://www.xsede.org/](https://www.xsede.org/)
  - DOE Office of Advanced Scientific Computing Research
    [http://science.energy.gov/ascr/](http://science.energy.gov/ascr/)
  - NASA Advanced Supercomputing Division
    [http://www.nasa.gov/](http://www.nasa.gov/)
  - NIH Center for Information Technology

• 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 XSEDE

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)
  - 3500 cores, helium.hpc.uiowa.edu
  - Glenn Johnson administers this cluster, glenn-johnson@uiowa.edu
  - Documentation
    https://www.icts.uiowa.edu/confluence/display/ICTSit/User+Documentation

• Research Services GPU System (clustered with Helium)
  - NVIDIA GeForce GTX 580 (512 cores, 1536 MB RAM)
  - Host: Intel Core i7 (4 core), 12 GB RAM, 2 TB storage