The Practice of High Performance Computing

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Thank you

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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

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- 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)

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

#1 Jaguar Cray XT5 ORNL (DOE)

Priority/Limits Based on Job Size

	XT5 Partition			
Bin	Cores		Maximum Wall-Time (Hours)	Aging Boost (Days)
	Min	Max		
1	120,000		24.0	15
2	80,004	119,999	24.0	10
3	40,008	80,003	24.0	5
4	5,004	40,007	12.0	0
5	2,004	5,003	6.0	0
6	1	2,003	2.0	0

#3 Kraken Cray XT5 NICS (NSF)

Queue	Min Size	Max Size	Max Wall Clock Limit
small	0	512	24:00:00
*longsmall	0	256	60:00:00
medium	513	8192	24:00:00
large	8193	49536	24:00:00
capability	32769	99072	24:00:00

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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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Code Management

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
  - Subversion `http://subversion.apache.org/`
  - 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/`) will host open source software that is to be shared with the community

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Scientific Validation and Benchmarking

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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

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- 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.nas.nasa.gov/
  - NIH Center for Information Technology
    http://www.cit.nih.gov/science.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

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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

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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