

# The Practice of High Performance Computing

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Iowa City, Iowa  
20-22 May 2013



# Thank you



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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

Bin	Cores		XT5 Partition	
	Min	Max	Maximum Wall-Time (Hours)	Aging Boost (Days)
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

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

- 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/>
  - **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 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](mailto: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](http://helium.hpc.uiowa.edu)
  - Glenn Johnson administers this cluster, [glenn-johnson@uiowa.edu](mailto: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