



Institute for Cyber-Enabled Research

Dr. Dirk Colbry

Director, High Performance
Computing Center

<http://contact.icer.msu.edu>

Research Resource

iCER is a research unit at MSU. We provide:

- Advanced computing hardware
- Software-as-a-service
- Training
- Consulting
- Proposal writing support

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Funding From ...

- The Vice President office for Research and Graduate Studies (VPRGS)
- Engineering College, College of Natural Science and College of Social Science
- This allows us to provide services and resources for **FREE!**

Advanced Architectures

- Anything more advanced than your desktop
- Local resources
 - Lab, Department, Institution (HPCC)
- National resources
 - NSF (XSEDE), DOE (Titan) , Others
- Commercial Resources (cloud computing)
 - Amazon, Azure, Liquid Web, Others

Advanced Architectures (II)

- Science takes too long
- Computation runs out of memory
- Needs licensed software
- Needs advanced interface (visualization/
database)
- Lots of file i/o

Bigger & Better ?

- The goal of iCER is NOT:
 - Kflops / second
- Instead, the goal of iCER IS:
 - KSciences / second
- Doing More Science, Faster
 - Reducing the “Mean time to Science”
- iCER is designed to help researchers do their science and when appropriate scale them up to national resources



Accounts (Access)

- Pis can request accounts (for each group member) at
<http://contact.icer.msu.edu/account>
- Each account has access to:
 - 50 GB of replicated file spaces
 - 520 processing cores
 - 360 TB of high-speed scratch space
- Also available: shared group folders

Hardware Highlights

- > 600 nodes, 7600 computing cores, 50 TB RAM
 - Large Memory Nodes (up to 6TB!)
 - GPU clusters (K20, M1060)
 - Xeon PHI cluster (5110p)
 - + 8000-core condor cluster
- High-speed file servers
 - 360TB parallel scratch file space
 - 1PB replicated home/research file servers
- High-speed network (FDR,QDR,SDR,10g)
- Evaluation nodes

Shared System

- Queueing system
 - Submit jobs to the queue
 - Jobs will run as resources become available
 - Up to one-week walltime
 - Up to 520 processing cores per user at any time
 - The larger the job, the longer/harder it is to schedule
- Priority access available!
 - You purchase the nodes, we manage them + provide cyber-infrastructure
 - When you are not using your nodes, we will run short jobs on them.

Buy-In Bonanza (2014)

- 20 cores, 64 Gb, \$3,806*
- 20 cores, 256 Gb, \$5339*
- 20 cores, 128 Gb, 2 Nvidia K20, \$7899*
- 20 cores, 128 Gb, 2 Intel 5115P, \$9043*
- 48 cores, 1 Tb, \$29,979
- 48 cores, 1.5 Tb, \$34,989
- 48 cores, 3 Tb, \$60,995
- 96 cores, 6 Tb, \$142,772
- Replicated storage: \$175/TB per year

Software Stack

- All nodes run Red Hat Linux 6.3
- Almost 2000 software titles installed!
 - Includes several commercial software titles such as MATLAB, ANSYS, Comsol, Stata
 - Many open-source titles
 - Full list: <http://wiki.hpcc.msu.edu>
 - Users can install software in their own directories
- If you have windows software / complicated workflows, we may have solutions ...

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Training Timeline

Date	Event
9/30 - 10/1	Software Carpentry
10/7	OpenMP Parallelism
10/23	<ul style="list-style-type: none">• Intro to HPCC• Intro to Python• Intro to Matlab
11/5 – 11/6	MPI Parallelism
11/?	Intro to Bioinformatics
12/4	OpenACC Parallelism

Training Timeline (II)

- MSU Seminars in Research and Instructional Technology
- In December (date TBD)
- Two days, free seminars
 - Morning sessions, 8:30 – 11:30
 - Afternoon sessions, 1:30 – 4:30
 - Lunch provided, guest speakers
- Sessions will include:
 - Introduction to HPC
 - Advanced HPC

Training Timeline (III)

Anticipated Spring Workshops

- Software Carpentry / Unix Basics
- Data Carpentry
- Intro to R
- Intro to Python
- Bioinformatics Workshop
- Molecular Modeling Workshop
- + many more ...
- See <http://wiki.hpcc.msu.edu>

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- **Proposal writing support**

Specialist Support



Dr. Yongjun Choi
Computational Physics

Specialist Support



Dr. Dirk Colbry
Computer Science

HPCC
High Performance Computing Center

Specialist Support



Dr. Benjamin Ong
Applied Mathematics

Specialist Support



Dr. Matthew Scholz
Bioinformatics



Computing Consultations

- Open office hours, Mondays 1 – 2pm
Biomedical and Physical Science (BPS 1440)
- 1-on-1 consultation sessions
<http://contact.icer.msu.edu>
- Guest lectures @ group or department meeting
- iCER cream Thursdays (monthly)
- Support (via email):
<http://contact.icer.msu.edu>
<http://rt.hpcc.msu.edu>

Proposal Preparation

- Personalized letters of support
 - HPC facilities statement
 - Data Management suggestions
 - Computing equipment consultations
- <http://icer.msu.edu/proposal-writing>

Miscellaneous Musings

iCER provides many other services:

- Data sharing (Globus Online Subscriptions)
- Visualization Servers
- Virtual Computing Lab
- Specialized bioinformatics support (BICEP)
- Support for scaling to XSEDE resources
- + ... ?

CYBERINFRASTRUCTURE DAYS 2014

OCTOBER 23 & 24

- Learn how cyberinfrastructure can benefit scholarly pursuits
- Networking opportunities
- Resource fair
- Poster session showcasing CI-enabled research

<http://vprgs.msu.edu/CI-Days/>

We are here to help

<http://contact.icer.msu.edu>

- Questions
- Schedule consultations
- Code reviews
- Programming help
- Hardware purchasing
- Grant writing support