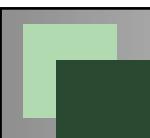


Introduction to iCER and the HPCC

Dr. Dirk Colbry
Research Specialist, CI Campus Champion
Institute for Cyber-Enabled Research

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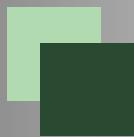


What is Advanced Computing Hardware?

- 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

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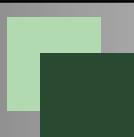


Why use Advanced Computing Hardware?

- Science takes too long
- Computation runs out of memory
- Need licensed software
- Need advanced interface (visualization)

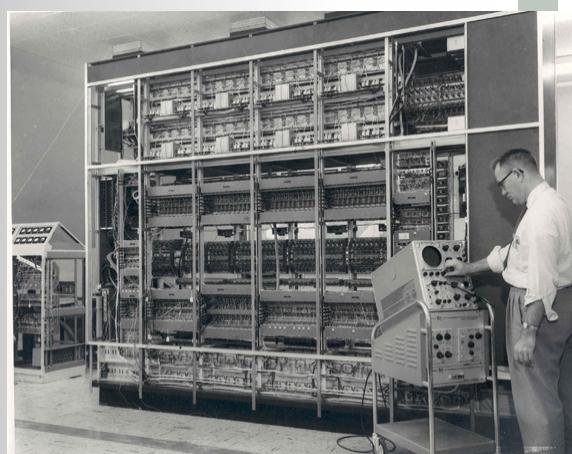


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1957 MISTIC Mainframe

- MSU's first mainframe
- Hand built by grad students
 - Dick Reid
 - Glen Keeney



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After MISTIC

- 1957 MISTIC
- 1963-1973 CDC 3600
- 1967 Computer Science Department
- 1968 CDC 6500
- 1971 MERIT
- 1978 Cyber 750
- **2005 High Performance Computing Center**
- **2009 Institute for Cyber-Enabled Research**

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2005 MSU HPCC

- Provide a level of performance beyond what you could get and reasonably maintain as a small group.
- Provide a variety of technology, hardware and software, that would allow for innovation not easily found.

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2009 iCER

- Institute for Cyber-Enabled Research
 - Established in 2009 to encourage and support the application of advanced computing resources and techniques by MSU researchers.
 - Goal is to maintain and enhance the university's national and international standing in computational disciplines and research thrusts.

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Bigger Science

- 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 one of the national labs


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Accounts

- Each user has 50Gigs of backed-up personal hard drive space.
 - /mnt/home/username/
- Users have access to more than 363TB of high speed parallel scratch space.
 - /mnt/scratch/username/
- Shared group space is also available upon request.

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ICER

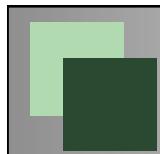
Hardware

The timeline diagram illustrates the evolution of the cluster over six years:

- 2005:** General Purpose Graphics Cluster featuring NVIDIA CUDA. A note specifies: "512 core, 128 node cluster installed in 2005. Each node contains four 2.2 GHz AMD Opteron cores, 8 GB of RAM, and 146 GB of local disk."
- 2010:** High speed network interconnect (InfiniBand) and Large Capacity "FAT" Nodes. The InfiniBand connection is highlighted with a callout. The FAT nodes are described as having up to 2TB of RAM and 64 cores.
- 2011:** Common OS Image (RHEL6.3) and 64-bit architecture. A note specifies: "1 612GB - 2TB RAM nodes -64 core 2.66 GHZ Xeon processors."

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ICER

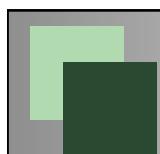


HPC Systems

FREE*

- Large Memory Nodes (up to 2TB!)
- GPU Accelerated cluster (K20, M1060)
- PHI Accelerated cluster (5110p)
- Over 540 nodes, 10000 computing cores
- Access to high throughput condor cluster
- 363TB high speed parallel scratch file space
- 50GB replicated file spaces
- Access to large open-source software stack and specialized bioinformatics VMs





Available Software

- Center Supported Development Software
 - Intel compilers, openmp, openmpi, mvapich, totalview, mkl, pathscale, gnu...
- Center Supported Research Software
 - MATLAB, R, fluent, abaqus, HEEDS, amber, blast, ls-dyna, starp...
- Customer Software
 - gromacs, cmake, cuda, imagemagick, java, openmm, siesta...
 - For a more up to date list, see the documentation wiki:
 - <http://wiki.hpc.msu.edu/>






VIRTUAL COMPUTING LAB
powered by Apache VCL

- Coming soon...
 - Uses HPC Resources to run Virtual Machines through simple browser interfaces.
 - Enables advanced workflows not typically available in standard HPC environments.
 - Enables improved science reproducibility and sharing.
 - Unique environment to facilitate specialized software in a classroom setting.

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Buy-In Opportunities

- Every 6 months to a year
- We will maintain your computers for you
- Researchers get exclusive use of their nodes within 4 hours of submitting a job
- Buy-in jobs will automatically overflow into the general resources.

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2013 Buy-in

- MSU researchers
- In progress now!
 - \$X,XXX* - General purpose base nodes
 - 20 cores, 64 gb
 - \$X,XXX* - 256gb nodes
 - \$X,XXX* - 256gb and 2xK20 GPU nodes
 - \$X,XXX* - 256gb and 2xPhi Card nodes

* Estimate only, other costs may apply. Please talk to me if you would like more details

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<https://wiki.hpcc.msu.edu/x/dwH3>

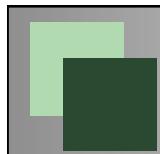


More than Just Hardware

- Consulting
 - Education
 - Grant Writing / Support
 - Advancing Computational Science

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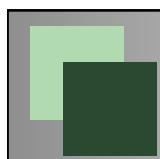
iCER Research Specialist

Ben Ong and Me

- Research Consulting
- HPCC Programming
- Proposal Writing
- Training and Education
- Outreach




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User Training, Education and Support

- Local Workshops
 - Software carpentry
 - Introduction to Linux and HPCC
 - Advanced HPCC
- Remote Training
 - VSCSE – Virtual School for Computer Science Education
 - XSEDE training Workshops



software carpentry



XSEDE
Extreme Science and Engineering
Discovery Environment

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Grant Writing / Support

- Buy-in opportunities
- ½ time post-doc support
- Part time HPCC Programmer Support
- Support finding research collaborations
- News about funding opportunities
- Technical Expertise

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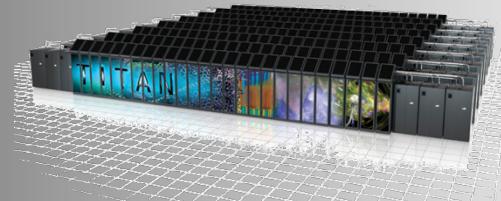
What if I want more?

XSEDE

Extreme Science and Engineering
Discovery Environment



Open Science Grid



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BLUE WATERS
SUSTAINED PETASCALE COMPUTING



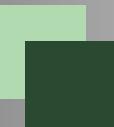


Advancing Computational Science

- One-on-one consulting
- iCER Research Seminars
- Workshop Sponsoring
- Research/Study groups. Ex:
 - GPGPU Group
 - Parallel Programming Group
- News about research opportunities
- Job and Resume Postings and Support



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2013 CYBER INFRASTRUCTURE DAYS



OCTOBER 24-25
Save The Date!



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



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MSU Seminars in Research and Instructional Technology

Dec TBD, 2013

- Two days of no-cost seminars to faculty and graduate students on technology topics.
 - Morning sessions run from 8:30 to 11:30 am.
 - Afternoon sessions run from 1:30 to 4:30 pm.
 - Lunch is provided that will feature guest speakers on instructional technology.
 - Introduction to HPC
 - Advanced HPC

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<http://train.msu.edu/faculty/seminars/>




We are here to help

- www.hpcc.msu.edu/contact
 - Questions
 - Schedule Consultations
 - Code Reviews
 - Programming help
 - Hardware Purchasing
 - Help with Grants
 - Support for Grants

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