

**Introduction to iCER  
and the HPCC**

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HPC Programmer      Research Specialist  
Institute for Cyber-Enabled Research

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**Agenda**

- Introduction to HPCC/iCER
- Bioinformatics Support at iCER
- Doing more faster - Pleasantly Parallel

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**Science and Computation**

- Pillars of Science:
  - Theory
  - Experimentation
  - Simulation
  - (Big) Data

The End of Science?



The quest for knowledge used to begin with grand theories. Now it begins with massive amounts of data. Welcome to the Petabyte Age.

Wired Magazine, 2009

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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, Blue Waters), DOE (Jaguar) , 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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 Types of problems

- CPU bound
  - Lots of computing (think simulation)
- Memory bound
  - Requires lots of memory (think genomics)
- I/O bound
  - Requires lots of data (think astronomy)

\*\* Many problems fall in more than one category





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## Types of Systems

## Local Resources

- Special Use Systems
    - SMP – Symmetric Multiprocessor (fat node)
    - GPGPU (General Purpose Graphics Processing Unit)
  - Typical HPC cluster
    - Commodity computers
    - High speed backbone
    - High speed network storage

## National and Commercial

- Advanced HPC
    - Specialty hardware
    - High speed backbone
    - High speed storage
  - Grid
    - Many HPC systems linked together by high speed network
  - Cloud
    - Lots of definitions
    - Typically refers to computing as a service using highly flexible virtual machines



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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
  - 2004 HPCC
  - 2009 ICER



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2004 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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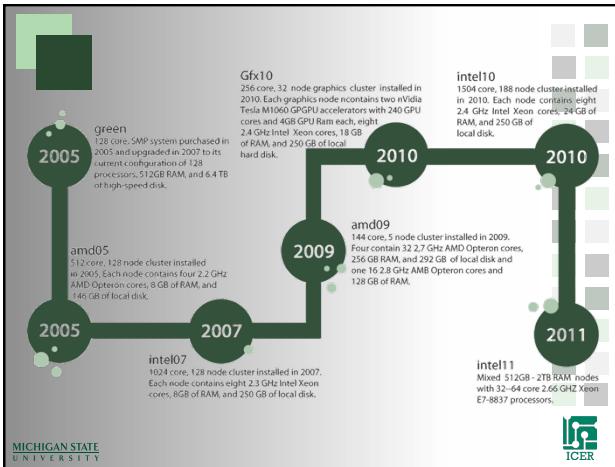


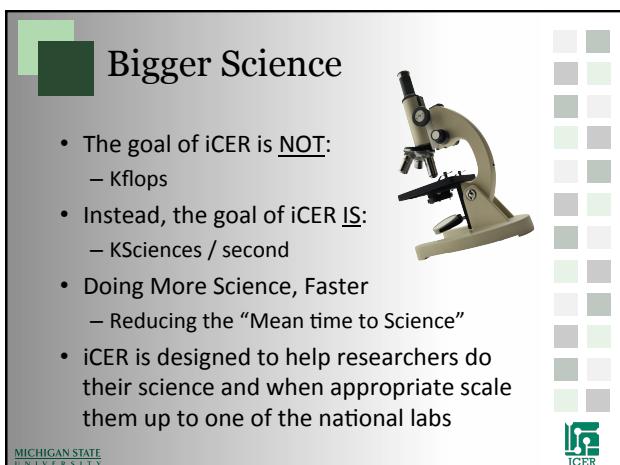
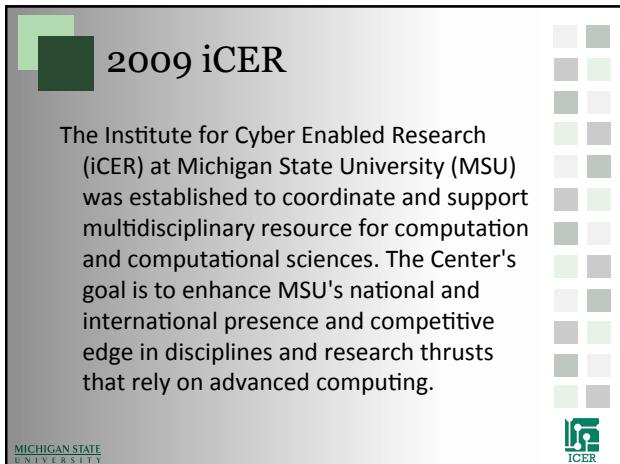
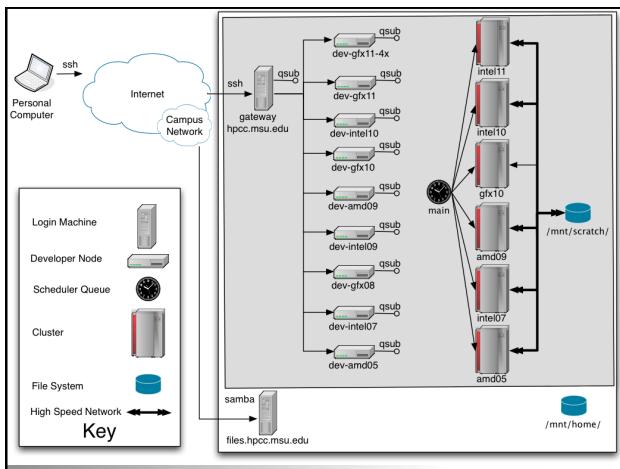
## HPCC Hardware

- Over 3110 Nodes
  - Over 23072 CPU cores
  - Over 33 TB of scratch memory space
  - GPGPU cluster with 64 Tesla Nodes
  - 2 TB Shared memory machines
  - 50GB backed up home directory space



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# 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.hpcg.msu.edu/>



# Accounts

- Each user has 50Gigs of backed-up personal hard drive space.
  - /mnt/home/username/
- Users have access to more than 33TB of high speed parallel scratch space.
  - /mnt/scratch/username/
- Shared group space is also available upon request.



# Buy-In Opportunities

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

 Beyond Local Resources

- National resources
  - NSF (XSEDE, Blue Waters)
  - DOE (Jaguar)
  - Others
- Commercial Resources (cloud computing)
  - Amazon
  - Azure
  - Liquid web
  - Others

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 More than Just Hardware

- Education
- Grant Writing / Support
- Advancing Computational Science

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 VSCSE

- **Science Cloud:** July 30-August 3
- **Many-core Programming:** August 13-17

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CI-Days, Save the Date!!!

- October 25-26
  - CI Days is an opportunity for the MSU research community to share information about cyberinfrastructure resources and their use in research.
  - All events will be held on campus in the Biomedical and Physical Sciences (BPS) building.

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

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People

- iCER Director
  - Dr. Wolfgang Bauer
- HPCC Director
  - Dr. Bill Punch
- Administrative Assistant
  - Kelly Osborn





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HPC Administrators

- Andrew Keen
- Jim Leikert
- Gregory Mason





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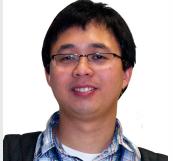
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 **iCER Research Specialist**

Ben Ong and Me

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







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 **HPC Programmers**

- John Johnson
  - 50% Biology
  - 50% iCER
  - Primary liaison to Biology





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 **iCER Bioinformatics Support**

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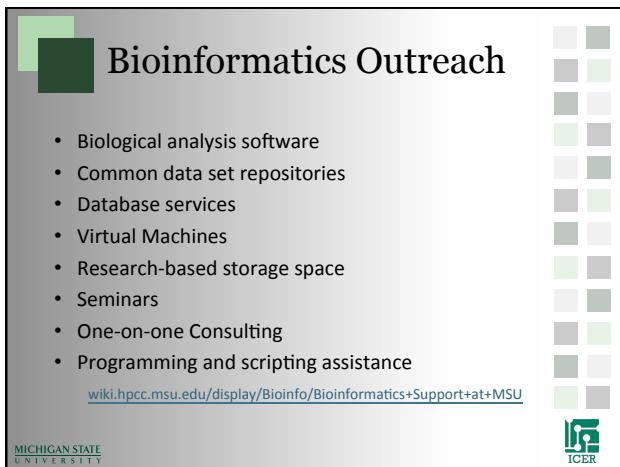
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## Bioinformatics Outreach

- Biological analysis software
- Common data set repositories
- Database services
- Virtual Machines
- Research-based storage space
- Seminars
- One-on-one Consulting
- Programming and scripting assistance

[wiki.hpc.msu.edu/display/BioInfo/Bioinformatics+Support+at+MSU](http://wiki.hpc.msu.edu/display/BioInfo/Bioinformatics+Support+at+MSU)

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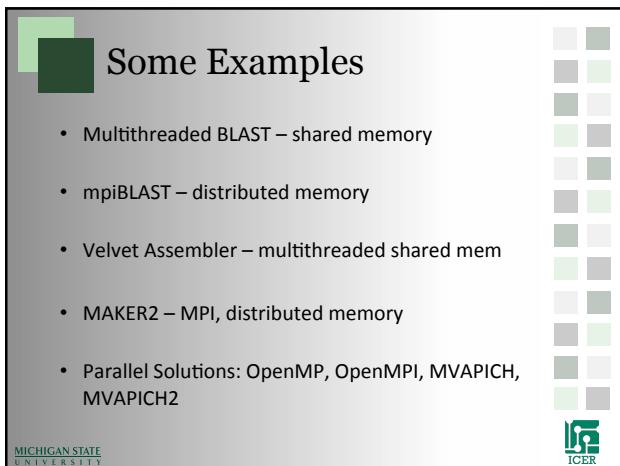
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## Some Examples

- Multithreaded BLAST – shared memory
- mpiBLAST – distributed memory
- Velvet Assembler – multithreaded shared mem
- MAKER2 – MPI, distributed memory
- Parallel Solutions: OpenMP, OpenMPI, MVAPICH, MVAPICH2

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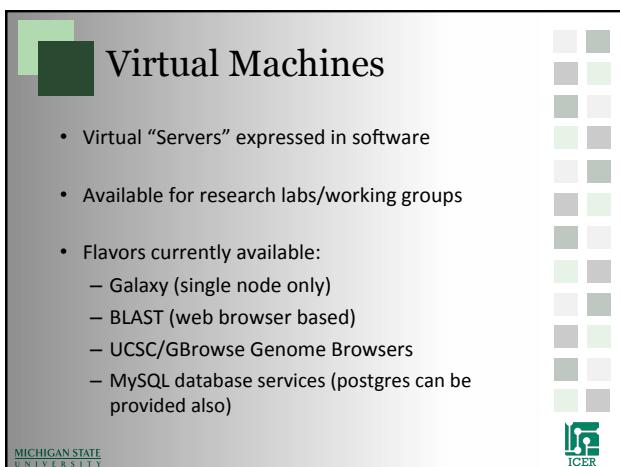
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## Virtual Machines

- Virtual “Servers” expressed in software
- Available for research labs/working groups
- Flavors currently available:
  - Galaxy (single node only)
  - BLAST (web browser based)
  - UCSC/GBrowse Genome Browsers
  - MySQL database services (postgres can be provided also)

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## Tutorials

- Titus Brown's ANGUS-NGS tutorials, converted for using examples on HPC instead of Amazon
- Using UCSC for certain tasks
- mpiBLAST
- Velvet and Oases
- Others being developed...

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## Bioinformatics Contact

- John Johnston, HPC Programmer
  - M-W, 1449 BPS, 884-2572
  - Th-F, 505 BMB, 432-7177
  - [johnj@msu.edu](mailto:johnj@msu.edu)
- Ticket requests:
  - <https://rt.hpc.msu.edu/index.html>
  - Please include "Bioinformatics Help" in the subject to more quickly route your request.

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## Doing more faster

Pleasantly Parallel Techniques

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## How much Communication?

- Pleasantly parallel
  - No communication required
- Loosely coupled
  - Typically sync at regular intervals
- Tightly coupled
  - Constant communication

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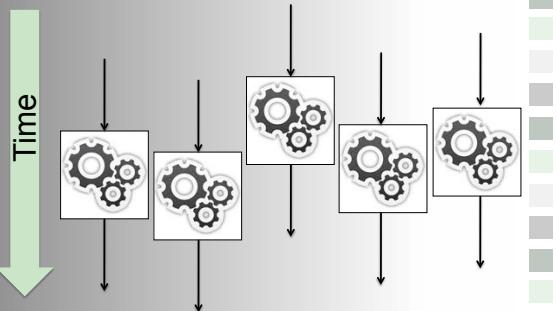


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## Pleasantly Parallel

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## How fast can we go?

- T - How long does each operation take?
- N - How many operations do you need to run?
- CPUs – Number of Cores job will run on.
- Single CPU time estimate:
  - $T \times N$
- Best possible Pleasantly parallel time:
  - $(T \times N) * \text{overhead/CPUs}$

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## Who are you? -- Biometrics

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## Pairwise-All Problem

- Database of faces
- Compare everything to everything else
- Calculate a Matching score to use for identification <http://tech.msu.edu/CI-Days/>

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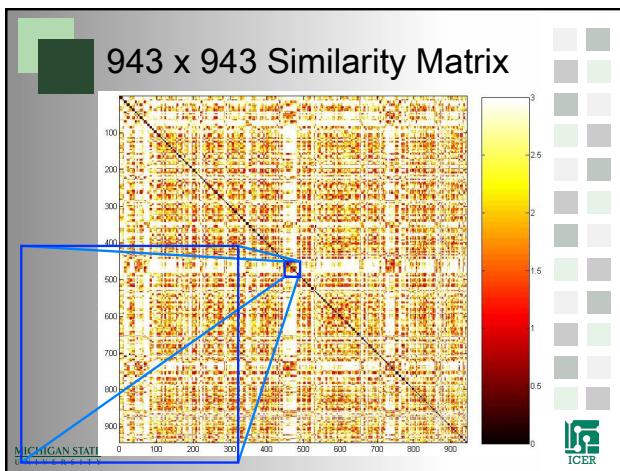
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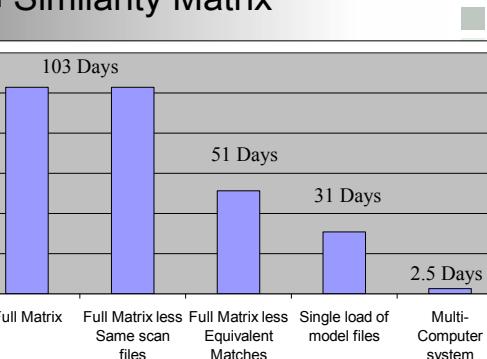
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## Estimated Calculation Times

- Preprocessing
    - $943 * 12$  (seconds)  $\approx 189$  Minutes
  - Matching
    - $943 * 943 * 5$  (seconds)  $\approx 103$  Days
  - Scans matched to themselves always result in 0 mm
    - $(943 * 943 - 943) * 5$  (seconds)  $\approx 103$  Days
  - The Proposed Alignment Algorithm is symmetric.
    - $(943 * 943 - 943)/2 * 5$  (seconds)  $\approx 51.5$  Days
  - We also load models once per row instead of every time
    - $(943*943-943)/2 * 3$  (seconds) +  $943 * 2$  (seconds)  $\approx 31$  Days

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## How do we go even bigger?

- 5000 scans.
    - 1.5 years on a single processor computer
    - 13 days on our ad-hoc cluster.
    - 1.5 days on the HPCC

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## Step to Pleasantly Parallel

- Figure out command line
- Estimate single job time:
  - Should be > 5 minutes
  - Should be < 1 week
  - Best if < 4 hours
- Make a submissions script
- Submit Job

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## Example

- Folder full of input files:

1.in	5.in	9.in	13.in	17.in
2.in	6.in	10.in	14.in	18.in
3.in	7.in	11.in	15.in	19.in
4.in	8.in	12.in	16.in	

- Want folder full of output files:

1.out	5.out	9.out	13.out	17.out
2.out	6.out	10.out	14.out	18.out
3.out	7.out	11.out	15.out	19.out
4.out	8.out	12.out	16.out	

- Command Syntax:
  - ./myprogram inputfile > outputfile

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## PBS Job Arrays

- One submission script copied many times
- Uses the PBS –t option
  - Ranges: 1-10
  - Lists: 2,4,100,3
  - Combination: 1-10,20,50,100
- Distinguish between jobs by using the PBS\_ARRAYID environment variable

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## Simple Job Array





`#!/bin/bash -login  
#PBS -l walltime=00:05:00,mem=2gb  
#PBS -l nodes=1:ppn=1,feature=gbe  
#PBS -t 1-100  
  
cd ${PBS_O_WORKDIR}  
  
.myprogram ${PBS_ARRAYID}.in > ${PBS_ARRAYID}.out  
  
qstat -f ${PBS_JOBID}`

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## Example: Job Arrays





- Get the bleder\_farm example:  
`>module load powertools  
>getexample blender_farm  
>cd ./blender_farm`
- Look at the qsub file, using “less” command  
`>less blender_farm.qsub`
- Submit the job  
`>qsub blender_farm.qsub`

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## HPCC Job array limitations





- Can not have more than 144 cores running
- Can not submit more than 256 jobs at once
- Lots of ways to work around this problem.

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## Job array numbers

- All numbers in a job array have the same base number
  - 7478210
- Each PBS\_ARRAYID is show in square brackets
  - 7478210[1]
  - 7478210[2]
- Delete all jobs using one command
  - qdel 7478210[]

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**Condor**  
High Throughput Computing

- Job submission system
- Runs like a screen saver
- Steals CPU Cycles from computers on campus



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