Making Your Research Go Faster: Advanced HPCC
CI-Days
October 23, 2014

https://wiki.hpcc.msu.edu/x/5AJZAQ

Dirk Colbry
colbrydi@msu.edu
Director, High Performance Computing Center
Institute for Cyber-Enabled Research

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Agenda

• Overview
• Advanced System Description
• Powertools
• Doing more faster
  – Pleasantly Parallel, Shared Memory, Shared Network, Accelerators, Standard Libraries
• Tricks and tips
Assumptions

- You have logged in and used the HPCC or similar system
- You are familiar with the Linux command line
- You have some programming / scripting experience
- You are here to learn how to leverage HPCC resources better
How this workshop works

• I think you work best from doing. So we will do a lot of hands on examples.
• When you get tired of listening to me talk, skip ahead to an exercise and give it a try.
• Exercises are denoted by the following icon in your notes:
Red and Green Flags

• Use the provided sticky notes to communicate without raised hands:
  – **NO Sticky** = I am working
  – **Green** = I am done and ready to move on
  – **Red** = I am stuck and need more time and/or I could use some help
Submission Scripts

• Design Goals
  – One script does everything
  – Easy to read
  – Easily given to others
  – Easily moved to different directories
Agenda

• Overview

• Advanced System Description

• Powertools

• Doing more faster
  – Pleasantly Parallel, Shared Memory, Shared Network, Accelerators, Standard Libraries

• Tricks and tips
What problems are we solving?

• Simulations
• Data Analysis
• Search

Images from, “Understanding the H₂ Emission from the Crab Nebula”, C.T. Richardson, J.A. Baldwin, G.J. Ferland, E.D. Loh, Charles A. Huehn, A.C. Fabian, P. Salomé

Image Provided by Dr. Mantha Phanikumar, MSU
Simulations

- Typically System of PDE (Partial Differential equations)
  - Fluid dynamics
  - Finite element analysis
  - Molecular dynamics
  - Weather
  - Etc.

- Mathematically equivalent to inverse of a matrix

Premixed mixture of H2-air auto igniting and flame propagation at supersonic flow
Provided by Dr Jabari and Mani (Abolfazl) Irannejad
Data Analysis

- Computer vision tasks
- Some Bioinformatics
- Astrophysics
- Etc.

Video Provided by Dr. Fred Dyer
Search

- Genome sequencing
- Analytics
- Optimization
- Etc.

Evolution of an artificial organism that can move and forage for food, Dr. Nicolas Chaumont
HPC Systems

- Large Memory Nodes (up to 6TB!)
- GPU Accelerated cluster (K20, M1060)
- PHI Accelerated cluster (5110p)
- Over 600 nodes, 7000 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
Free Access to software

- Compiled open-source software stack
  - Close to 2000 titles!
- Optimized Math/Communications libraries
- Some commercial software available
  - E.g. Ansys, MATLAB (+many toolboxes), Stata, Gauss, SAS

Full list: http://wiki.hpcc.msu.edu
General Purpose Clusters
Commodity Cluster

- Cores
- Processors / Sockets
- Nodes
- Chassis
- Rack
- High Speed Network
Buy-In Opportunities

• 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.
Current Buy-In options (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

* Some grant/funding agencies require a chassis for an additional $1216 (8 slots).
Large Shared Memory Systems (Fat Nodes)
Shared Memory Communication

- Fast!
- Cores on a system share the same memory
- OpenMP
- Fat nodes
  - 96 cores
  - 6TB of memory
Accelerated Systems
**GPU**

- Cards used to render graphics on a computer
- Hundreds of cores
- Not very smart cores
- But, if you can make your research look like graphics rendering you may be able to run really fast!
Intel Xeon Phi

- Cross between CPU and GPU
- About 61 Pentium III cores
  - Less cores/slower than GPU
  - Easier to use than GPU
High Throughput HTCondor Cluster
MSU HTCondor Cluster

• Runs like a screen saver and Scavenges CPU cycles:
  – Approximately 400+ nodes
  – Approximately 7000 cores
  – Windows 7
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  – Pleasantly Parallel, Shared Memory Parallelization, Shared Network, Accelerators, Standard Libraries
• Tricks and tips
What are Powertools

• Powertools are scripts and programs to make interfacing with the HPCC simpler
• The tools are written mostly by HPCC staff and users.
• Think of most of these as “Beta” software.
How to Access Powertools

• When you are logged on to gateway or the developer nodes, load the powertools module file:
  
  >module load powertools

• To list the currently available tools type “powertools” after loading the powertools module
  
  >powertools
Common Powertools

• Any developer node shortcut
  
  > dev

• Developer node shortcuts
  (intel07, gfx08, intel09, gfx10, gfx11, intel14)

• Two commands in one:
  – Automatically ssh directly to the developer node
  – Then automatically cd to the current directory from the previous node
More Common Powertools

- **powertools** – list powertools and common commands not standard on linux systems
- **sj** – show jobs in the queue for the current user
- **starttime** – show estimated start times for a job
- **mailme** – E-mail yourself a file
- **clusterstate** – show a summary of the current state of the nodes in the cluster
Even More Powertools

- **getexample** – provides a copy of examples for various tasks written by iCER staff
- **quota** – list your home directory disk usage
- **priority_status** – Shows the status of an individuals buy-in nodes.
- **poweruser** – Set up your account to load powertools by default
How to turn on powertools as default?

• Edit your .bashrc
  > nano ~/.bashrc

• add the following line:
  module load powertools

Note: You can also just use the “poweruser” powertool

• Note: this is required if you want to use the developer node shortcuts and hop between different nodes
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What is the Bottleneck

• Not enough Memory
  – Solution: use a bigger node (6tb 96 cores)
• Slow File I/O
  – Solution: use scratch
  – Solution: use a ram disk
• Too many calculations
  – Solution: run your code in parallel
Steps to parallel code

Note: Every application is different

1. Analyze your code
   - Profilers (gprof, vtune, map, perfreport, tau)
   - Debuggers / memory trackers (gdb, ddt, totalview)

1. Optimize calculations
   - Trade memory for time (i.e., never do the same calculation twice)

1. Find ways to parallelize
   - Look for loops
   - Find iterations independent from each other
   - Determine how much information needs to be transferred
Single Thread Jobs

One CPU can only run one thing at a time. (sort of)
Pleasantly Parallel
Loosely Coupled
Tightly Coupled
Communication

- Shared Memory
- Shared Network
- Distributed Network
- Dedicated Accelerators
- Hybrid Systems
Pleasantly Parallel
Pleasantly Parallel
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:
  – TxN
• Best possible Pleasantly parallel time:
  – (TxN)*overhead/CPUs
Who are you? -- Biometrics
Pairwise-All Problem

- Database of faces
- Compare everything to everything else
- Calculate a Matching score to use for identification
943 x 943 Similarity Matrix
Estimated Calculation Times

- **Preprocessing**
  - $943 \times 12$ (seconds) $\approx 189$ Minutes

- **Matching**
  - $943 \times 943 \times 5$ (seconds) $\approx 103$ Days

- Scans matched to themselves always result in 0 mm
  - $(943 \times 943 - 943) \times 5$ (seconds) $\approx 103$ Days

- The Proposed Alignment Algorithm is symmetric.
  - $(943 \times 943 - 943)/2 \times 5$ (seconds) $\approx 51.5$ Days

- We also load models once per row instead of every time
  - $(943\times943-943)/2 \times 3$ (seconds) + $943 \times 2$ (seconds) $\approx 31$ Days
Calculation Time for Full Similarity Matrix

- Full Matrix: 103 Days
- Full Matrix less Same scan files: 51 Days
- Full Matrix less Equivalent Matches: 31 Days
- Single load of model files: 2.5 Days
- Multi-Computer system: 0 Days
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 a commodity cluster at MSU
Steps 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
Pleasantly Parallel 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
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
#!/bin/bash -login
#PBS -l walltime=00:05:00,mem=2gb
#PBS -l nodes=1:ppn=1,feature=gbe
#PBS -t 1-19

cd ${PBS_O_WORKDIR}

mkdir ${PBS_ARRAYID}
Cd ${PBS_ARRAYID}

../myprogram ../${PBS_ARRAYID}.in > ${PBS_ARRAYID}.out

qstat -f ${PBS_JOBID}
Example: Job Arrays

• Get the bleder_farm example:
  > getexample
  > 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
HPCC Job array limitations

• Can not have more than 520 cores running at once
• Can not submit more than 1000 jobs at once
• Each job can not run longer than one week

• Lots of ways to work around these limitations
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[]
Unrolling Loops

• Your program has independent loops
  – Each iteration of the loop does not depend on the other iterations
  – Loop can be executed in any order
  – 5 Minutes < Iteration Time < 1 week
  – Output of each iteration must be easy to save and recombine for next step of workflow

• Rewrite your program to accept an iteration number as an input
  – ./myprogram IterationNumber

• Rewrite your program to save output and use an additional program for post processing
#!/bin/bash -login
#PBS -l walltime=00:05:00
#PBS -l nodes=1:ppn=1,feature=gbe
#PBS -t 1-100

cd ${PBS_O_WORKDIR}

./myprogram ${PBS_ARRAYID}

qstat -f ${PBS_JOBID}
Task Queue

- A list of tasks (also called treatments, inputs, ...) that distinguish what needs to be done.
- Each pleasantly parallel process (worker) checks the list and picks work not yet completed.
- The trick is to not have two workers do the same task.
List of Commands

- Commands.txt

./myprogram -a 100 -z 3023
./myprogram dosomething different
./myprogram
./myprogram -s 100
./myprogram -s 200
./myprogram -s 300
./myprogram -w 400
./myotherporgram
./mythirdprogram
#!/bin/bash -login

#PBS -l walltime=00:05:00
#PBS -l nodes=1:ppn=1,feature=gbe
#PBS -t 1-100

cd ${PBS_O_WORKID}

cmd=`tail -n ${PBS_ARRAYID} commands.txt | head -n 1`

echo ${cmd}

${cmd}

qstat -f ${PBS_JOBID}
Files as Semaphores (FAS)

• Use a list of input files as your task list
• Use a list of output files (or flag files) as your in-progress/complete list
• Rely on the file system to ensure that no two jobs are selected at the same time (not a great assumption but it works)
#!/bin/bash -login
#PBS -l walltime=00:05:00
#PBS -l nodes=1:ppn=1,feature=gbe
#PBS -t 1-100

cd ${PBS_O_WORKID}
sleep $(( ${RANDOM} % 100 ))

for file in *.in; do
  output="./${file%.*}.out"
  if [ ! -f ${output} ]; then
    touch ${output}
    ./myprogram ${file} > ${output}
    qsub -t 0 -N ${PBS_JOBNAME} ${0}
    exit 0
  fi
done
Loosely Coupled
Tightly Coupled
Shared Memory Parallelization
Shared Memory

- Different threads (cores, processes) communicate though pointers to the same memory location
- Problems can occur if different threads write the same memory at the same time
- Flags (also called locks and/or semaphores) are used to allow only one thread to access memory at the same time
Shared Memory Communication

- Cores on a processor share the same memory
- OpenMP
- Fat nodes
  - 96 cores
  - 6TB of memory
Intel®

- 8 cores
- 24 GB memory
Large Memory Example

- 32 cores
- 256 GB memory

- We also have nodes with up to 64 cores and 2TB of memory
Shared memory submission scripts

- Typically one node with multiple processors per node (ppn)
  - `#PBS -l nodes=1:ppn=8`

- Different programs use different methods to tell them how many processors to use
  - Command line arguments
  - Environment variables
Example: shared memory Script

- Bowtie uses shared memory parallelization
- Get the bowtie example
  ```
  > getexample bowtie
  ```
- Change to the bowtie directory
  ```
  > cd ./bowtie
  ```
- Look at the submission script
  ```
  > less ./bowtie.qsub
  ```
- Run the job
  ```
  > qsub bowtie.qsub
  ```
OpenMP

- Common Shared Memory parallelization
- Single program runs in many threads
- Really easy to pick loops that are parallel and split them into multi threads
- Minor modifications to code that can be written not to affect single
OpenMP is easy

```c
#include <omp.h>

...  
#pragma omp parallel for
for (i=0;i<100;++i) {
    A(I) = A(I) + B
}
...  
```
Compile OpenMP Jobs

• Use compiler option fopenmpi.
  –fopenmp

• Example:

  gcc –fopenmp mycode.cc –o mycode
simpleOMP.qsub example

#!/bin/bash -login
#PBS -l walltime=00:01:00
#PBS -l nodes=1:ppn=5,feature=gbe

cd ${PBS_O_WORKDIR}
export OMP_NUM_THREADS=${PBS_NUM_PPN}

./simpleOMP

qstat -f ${PBS_JOBID}
Try another getexample

getexample helloOpenMP
getexample OpenMP_profiling
Shared Network
Parallelization
MPI on HPCC

• Two Flavors of MPI
• Switching flavors and compiling
• Running in a script
• Running on the developer nodes
MPI program (1 of 4)

/* Needed for printf'ing */
#include <stdio.h>
#include <stdlib.h>

/* Get the MPI header file */
#include <mpi.h>

/* Max number of nodes to test */
#define max_nodes 264

/* Largest hostname string hostnames */
#define str_length 50
int main(int argc, char **argv)
{
    /* Declare variables */
    int proc, rank, size, namelen;
    int ids[max_nodes];
    char hostname[str_length][max_nodes];
    char p_name[str_length];

    MPI_Status status;
    MPI_Init(&argc, &argv);
    MPI_Comm_rank(MPI_COMM_WORLD, &rank);
    MPI_Comm_size(MPI_COMM_WORLD, &size);
    MPI_Get_processor_name(p_name,&namelen);
if (rank==0) {
    printf("Hello From: %s I am the receiving processor %d of %d\n", p_name, rank+1, size);
    for (proc=1;proc<size;proc++) {
        MPI_Recv(&hostname[0][proc], str_length, MPI_INT, proc, 1, MPI_COMM_WORLD, &status);
        MPI_Recv(&ids[proc], str_length, MPI_INT, proc, 2, MPI_COMM_WORLD, &status);
        printf("Hello From: %20s I am processor %d of %d\n", &hostname[0][proc], ids[proc]+1, size);
    }
}
} else { // NOT Rank 0
    srand(rank);
    int t = rand()%10+1;
    sleep(t);
    MPI_Send(&p_name,str_length, \n        MPI_INT,0,1,MPI_COMM_WORLD);
    MPI_Send(&rank,str_length, \n        MPI_INT,0,2,MPI_COMM_WORLD);
}

MPI_Finalize();

return(0);
Two Flavors of MPI

• mvapich vs openmpi (default)
• Historically mvapich was much faster than openmpi
• The newest version of openmpi is just as fast as mvapich
• I feel that openmpi is much easier to use, but either will work on HPCC
Switching Flavors

- Use the “module” command to switch between the two versions of mpi
- **Openmpi** module is loaded by default
- To switch to mvapich you first need to unload **openmpi**:
  
  > module unload OpenMPI
- Then you need to load **mvapich**:
  
  > module load MVAPICH
- You can do both commands in one step by using swap:
  
  > module swap OpenMPI MVAPICH
MPI Submission Scripts

openmpi

#!/bin/bash -login
#PBS -l nodes=10:ppn=1
cd ${PBS_O_WORKDIR}
mpirun <program_name>

mvapich

#!/bin/bash -login
#PBS -l nodes=10:ppn=1
cd ${PBS_O_WORKDIR}
module swap OpenMPI MVAPICH
mpiexec <program_name>
1. Log on to one of the developer nodes
2. Load the powertools module:
   > module load powertools
1. Run the getexample program. This will create a folder called helloMPI:
   > getexample helloMPI
1. Change to the helloMPI directory and read the readme files
2. Or just type the following on the command line:
   > ./README
Testing MPI jobs on dev node

• Use mpirun instead of mpiexec

• Need a hostfile

  > echo $HOST >> ./hostfile
  > echo $HOST >> ./hostfile
  > echo $HOST >> ./hostfile
  > echo $HOST >> ./hostfile

• MPIRUN example:

  > mpirun –np 4 –hostfile ./hostfile helloMPI
Running on the Command Line

• The scheduler automatically knows how many and where to run MPI processes.
• However, on the command line, you need to specify the nodes and processors.
• openmpi and mvapich are a little different.
Command Line Differences

- **Openmpi**
  - `mpirun`
  - Default assumes one process on the current host.
  - You do not even need the `mpirun` command to run the default.
  - Optionally you can use the `–n` and `–hostfile` options to change the default

- **mvapich**
  - `mpirun`
  - Requires both the `–np` and `–machinefile` flag to run.
Command line

• mvapich

```sh
mpirun -np 4 -machinefile machinefile machinefile <program_name>
```

• openmpi

```sh
mpirun -n 4 -hostfile machinefile machinefile <program_name>
```

• NOTE: I did a check and either MPI implementation will work with either notation.
Which MPI command do you use?

<table>
<thead>
<tr>
<th>Command</th>
<th>Command Line</th>
<th>Job Script</th>
</tr>
</thead>
<tbody>
<tr>
<td>openmpi</td>
<td>mpirun</td>
<td>mpirun</td>
</tr>
<tr>
<td>mvapich</td>
<td>mpirun</td>
<td>mpiexec</td>
</tr>
</tbody>
</table>
Accelerator Cards
GPU

- Cards used to render graphics on a computer
- Hundreds of cores
- Not very smart cores
- But, if you can make your research look like graphics rendering you may be able to run really fast!
Running on the GPU

• Program Starts on the CPU
  – Copy data to GPU (slow-ish)
  – Run kernel threads on GPU (very fast)
  – Copy results back to CPU (slow-ish)

• There are a lot of clever ways to fully utilize both the GPU and CPU.
Pros and Cons

• Benefits
  – Lots of processing cores.
  – Works with the CPU as a co-processor
  – Very fast local memory bandwidth
  – Large online community of developers

• Drawbacks
  – Can be difficult to program.
  – Memory Transfers between GPU and CPU are costly (time).
  – Cores typically run the same code.
  – Errors are not detected (on older cards)
  – Double precision calculations are slow (On older cards)
CUDA program (1 of 5)

#include "cuda.h"
#include <iostream>

using namespace std;

void printGrid(float an_array[16][16]) {
    for (int i = 0; i < 16; i++){
        for (int j = 0; j < 16; j++) {
            cout << an_array[i][j];
        }
        cout << endl;
    }
}
CUDA program (2 of 5)

```c
__global__ void theKernel(float * our_array)
{
    // This is array flattening,
    // (Array Width * Y Index + X Index)
    our_array[(gridDim.x * blockDim.x) * \n        (blockIdx.y * blockDim.y + threadIdx.y) + \n        (blockIdx.x * blockDim.x + threadIdx.x)] = \n    = 5;
}
```
int main()
{
    float our_array[16][16];

    for (int i = 0; i < 16; i++) {
        for (int j = 0; j < 16; j++) {
            our_array[i][j] = 0;
        }
    }
}
CUDA program (4 of 5)

//STEP 1: ALLOCATE
float * our_array_d;
int size = sizeof(float)*256;
cudaMalloc((void **) &our_array_d, size);

//STEP 2: TRANSFER
cudaMemcpy(our_array_d, our_array, size, cudaMemcpyHostToDevice);
CUDA program (5 of 5)

```cpp
//STEP 3: SET UP
dim3 blockSize(8,8,1);
dim3 gridSize(2,2,1);

//STEP 4: RUN
theKernel<<<gridSize, blockSize>>>(our_array_d);

//STEP 5: TRANSFER
printGrid(our_array);
cudaMemcpy(our_array, our_array_d, size, cudaMemcpyDeviceToHost);
cout << "------------------------" << endl;
printGrid(our_array);
```

```
Compile CUDA Jobs

• Just like MPI, to compile an cuda program you need to use the cuda compiler wrappers:
  – nvcc simple.cu -o simple_cuda
Try a cuda getexample

getexample cuda
getexample cuda_clock
getexample cuda_hybrid
getexample NAMD_CUDA_example
Intel Xeon Phi

- Cross between CPU and GPU
- About 61 Pentium III cores
  - Less cores/slower than GPU
  - Easier to use than GPU

- MPI
- OPenMP
Try a Phi Card example

getexample MIC_examples
getexample MKLMic
Standard Libraries
Standard Libraries

• When possible take advantage of parallel libraries
  – Easy to use
  – Saves time
  – Takes care of the parallel coding for you
  – Tested and vetted by the community
Math Kernel Library

- getexample MKL_benchmark
- getexample MKL_c_eigenvalues
- getexample MKL_Example
- getexample MKL_mic
- getexample MKL_parallel
Other Libraries

- Fftw
- BLAS
- ACML
- BLAS (Basic Linear Algebra)
- Lapak
- trilinos
- petci
- Magma
- Cudatools
- Mumps
Which approach is the best?

- Depends on what you are doing?
- Depends on how much communication you need.
- Depends on what hardware you have.
- Depends on how much time you have.
My Recommendations

• Pleasantly Parallel
• Standard Libraries
• OpenMP
• OpenACC
• OpenMP on Phi
• MPI
• MPI on Phi?
• GPGPU
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• Tricks and tips
Tips and Tricks
Going beyond system Limits
• Going beyond system Limits
  – More than 520 jobs
  – Jobs longer than 1 week
  – Taking advantage of more nodes
Finding more Nodes

- Owners are guaranteed access to their buy-in node within 4 hours. If they are not using the node, others can use it:
  - `#PBS -l walltime=04:00:00`

- Some of the nodes do not have Infiniband. If you are not using scratch and do not need between node communication you can access these nodes:
  - `#PBS feature=gbe`
Checkpoint / Restart

• What?
  – Save the state of your program
  – Restart your program from the saved point

• How?
  – Design into your program
  – BLCR (Berkley Lab Checkpoint Restart)
  – Condor Checkpoint Restart
  – Others

• Why?
  – Robust jobs
    • As HPC scales … hardware failures are guaranteed
  – Longer jobs
  – Better science
Getting Help

• Documentation and User Manual – wiki.hpcc.msu.edu
• Contact HPCC and iCER Staff for:
  – Reporting System Problems
  – HPC Program writing/debugging Consultation
  – Help with HPC grant writing
  – System Requests
  – Other General Questions
• Primary form of contact - http://contact.icer.msu.edu/
• HPCC Request tracking system – rt.hpcc.msu.edu
• HPCC Phone – (517) 353-9309
• HPCC Office – 1400 PBS
• Open Office Hours – 1pm Monday (BPS 1440)