Making Your Research Go Faster: Advanced HPCC
CI-Days
December 16, 2014

https://wiki.hpcc.msu.edu/x/JwJiAQ

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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 the 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 H$_2$ 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

Image Provided by Dr. Warren F. Beck, 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
• 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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Evaluation Gateway

• Same as regular gateway just a different URL:
  – eval.hpcc.msu.edu

• Also slightly different splash screen.

• Great “back door” if there is a problem on the gateway VM.
Evaluation Nodes

- Intended for Testing and Evaluation of different hardware.
- Just special development nodes.
- No corresponding hardware in the cluster.

<table>
<thead>
<tr>
<th>Name</th>
<th>Cores</th>
<th>Memory</th>
<th>Accelerators</th>
<th>Notes</th>
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</thead>
<tbody>
<tr>
<td>eval-amd09</td>
<td>8</td>
<td>8GB</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>eval-k10</td>
<td>4</td>
<td>8GB</td>
<td>1 Nvidia k10</td>
<td>Nvidia Graphics Node</td>
</tr>
<tr>
<td>eval-atom13</td>
<td>8</td>
<td>24GB</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>eval-k40</td>
<td>20</td>
<td>128GB</td>
<td>1 Nvidia K40</td>
<td>Nvidia Graphics Node</td>
</tr>
</tbody>
</table>
Exercise: Connect to eval gateway

- Step 1: Log into eval.hpcc.msu.edu
- Step 2: ssh into an eval node (evaluation node)
  
  > ssh eval-k40

- Step 3: do something
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

• 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

• Modifying your bashrc is required if you want to use the developer node shortcuts and hop between different nodes without constantly typing “module load powertools”

  You can also just use the “poweruser” powertool
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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:
  - $T \times N$
- Best possible Pleasantly parallel time:
  - $(T \times N) \times \text{overhead}/\text{CPUs}$
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**
  - $(943 \times 943 - 943)/2 \times 3$ (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**: 2.5 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

#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_WORKID}

./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 *.*; 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 through pointers to the same memory location
- Problems can occur if different threads write to 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 10

- 2 sockets
- 8 cores
- 24 GB memory

Figure generated using hwloc
Intel14 – basic node

- 2 sockets, 20 cores, 64 GB memory
Large Memory Example

- eval-amd09
- 8 sockets, 32 cores, 256 GB RAM
Intel14-xl

- 8 sockets
- 96 cores
- 6TB of RAM

Figure generated using hwloc
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

#include <omp.h>

...  

#pragma omp parallel for  
for (i=0;i<100;++i) {  
  A(i) = A(i) + B  
}

...
Compile OpenMP Jobs

• Use compiler option fopenmp.
  –fopenmp
• Example:

  gcc –fopenmp mycode.cc –o mycode
#!/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], \n                 str_length,MPI_INT,proc, \n                 1,MPI_COMM_WORLD,&status);
        MPI_Recv(&ids[proc], \n                 str_length,MPI_INT,proc, \n                 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, MPI_INT,0,1,MPI_COMM_WORLD);
    MPI_Send(&rank,str_length, 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**

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

**mvapich**

```bash
#!/bin/bash -login
#PBS -l nodes=10:ppn=1
cd ${PBS_O_WORKDIR}
module swap OpenMPI MVAPICH
mpiexec <program_name>
```
Trying out an example

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 $HOSTNAME >> ./hostfile
  > echo $HOSTNAME >> ./hostfile
  > echo $HOSTNAME >> ./hostfile
  > echo $HOSTNAME >> ./hostfile

• M PiRUN 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**

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

- **openmpi**

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

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

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<tr>
<th>Open MPI</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)

```c++
#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)

//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 GP

- MPI
- OPenMP
Try a Phi Card example

getexample MIC_examples
getexample MKL_mic
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 MKLMic
- getexample MKL_parallel
Other Libraries

- fftw
- BLAS
- ACML
- BLAS (Basic Linear Algebra)
- Lapak
- trilinos
- petsc
- 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
Agenda

• Overview
• Advanced System Description
• Powertools
• Doing more faster
  – Pleasantly Parallel, Shared Memory, Shared Network, Accelerators, Standard Libraries
• Tricks and tips
Tips and Tricks
Going beyond system Limits
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)