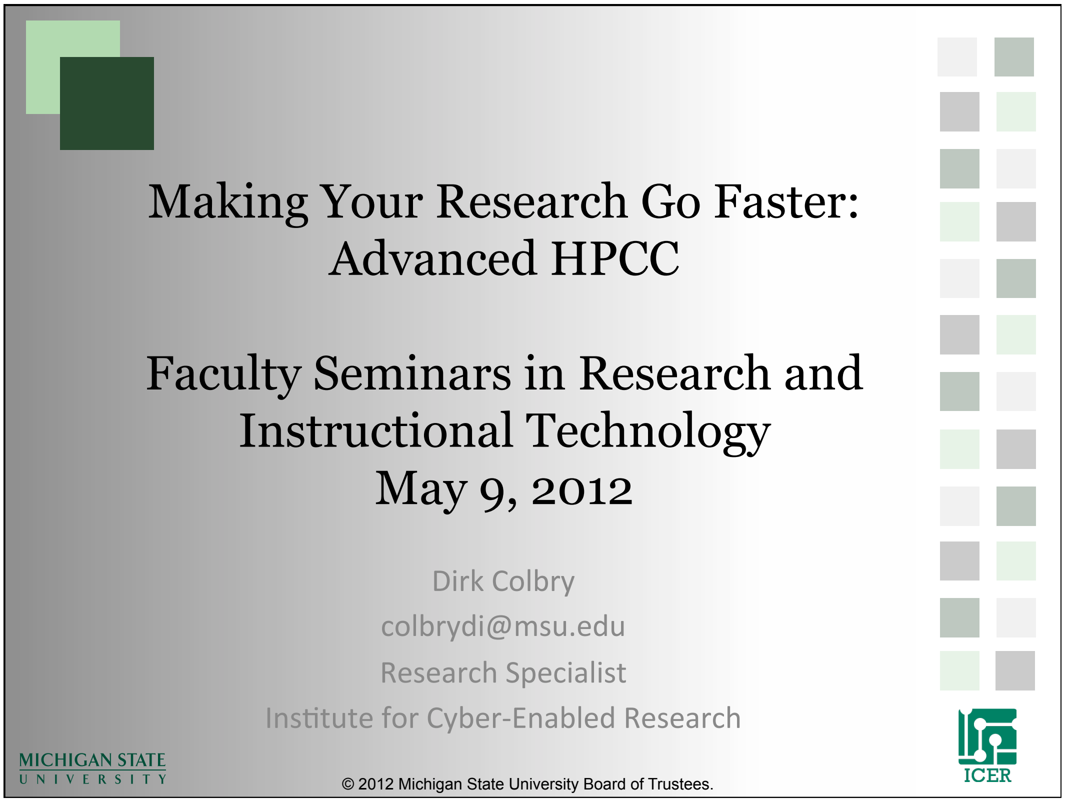

Making Your Research Go Faster: Advanced HPCC

Faculty Seminars in Research and Instructional Technology
May 9, 2012

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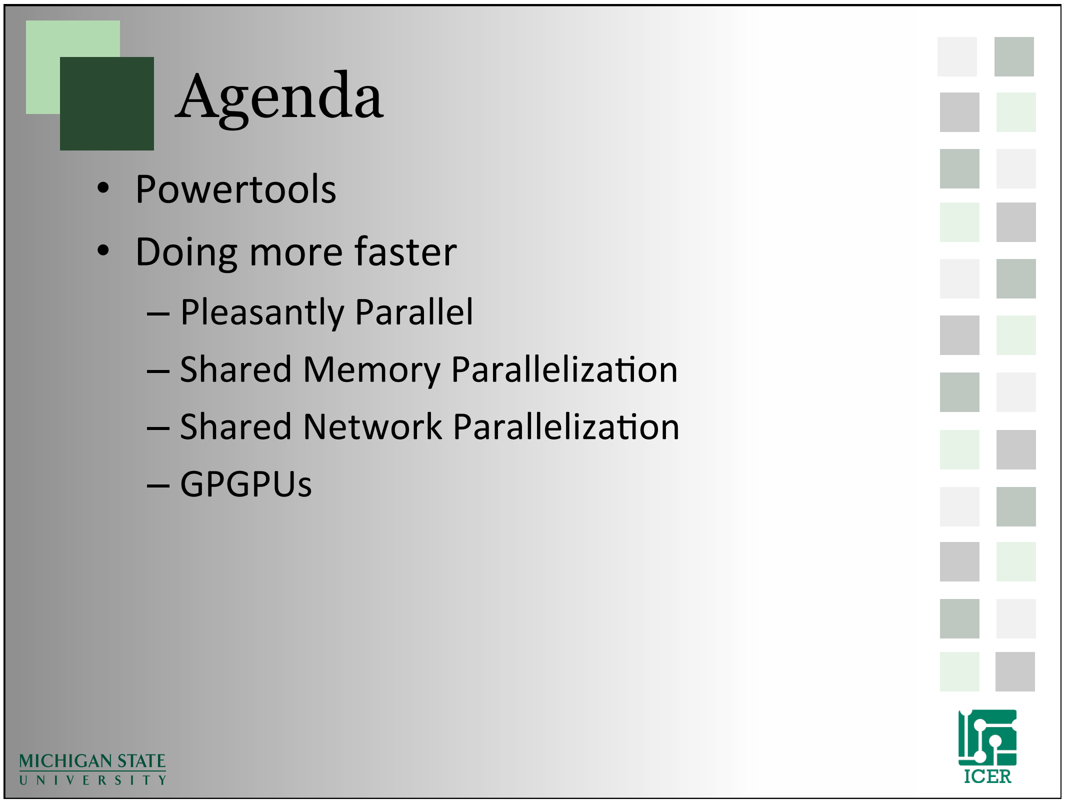

Agenda

- Powertools
- Doing more faster
  - Pleasantly Parallel
  - Shared Memory Parallelization
  - Shared Network Parallelization
  - GPGPUs

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Submission Scripts

- Design Goals
  - One script does everything
  - Easy to read
  - Easily given to others
  - Easily moved to different directories

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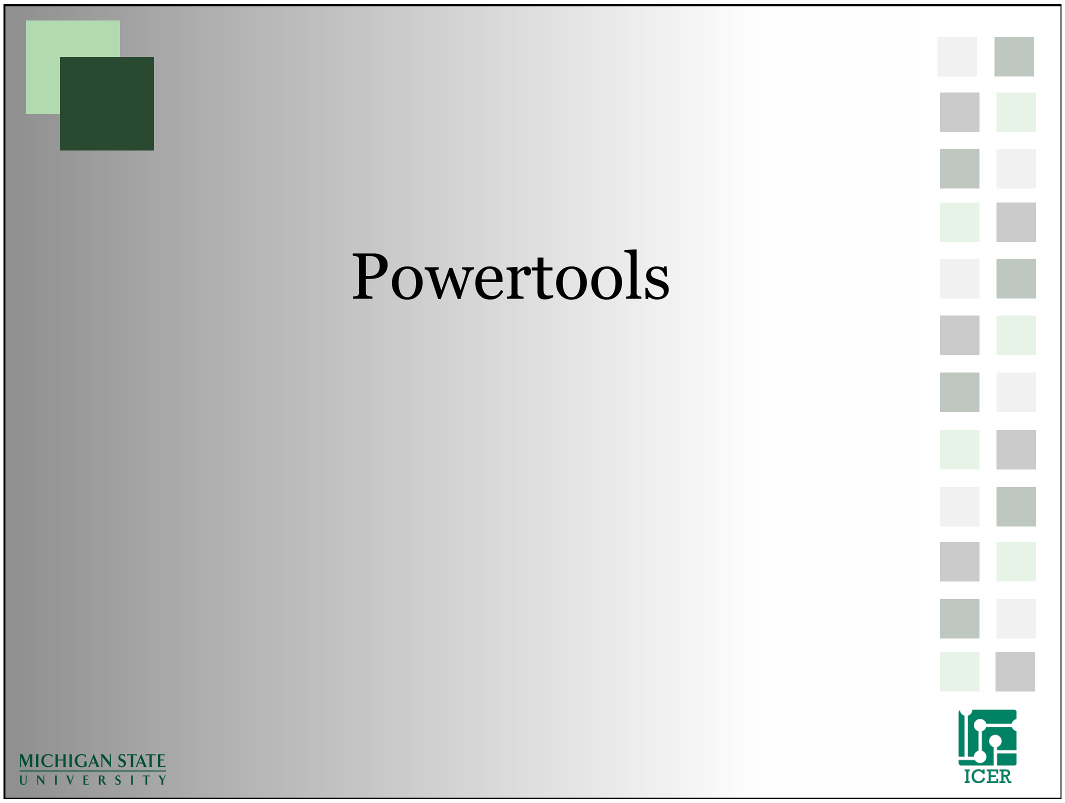

Powertools

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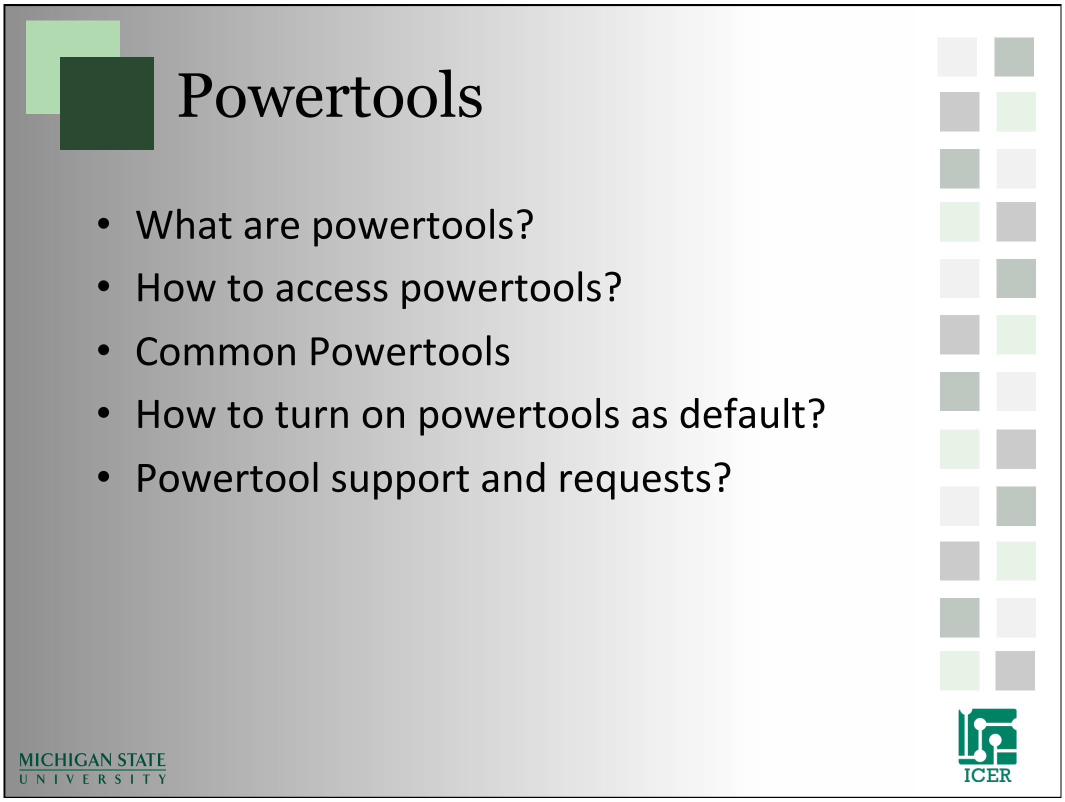

Powertools

- What are powertools?
- How to access powertools?
- Common Powertools
- How to turn on powertools as default?
- Powertool support and requests?

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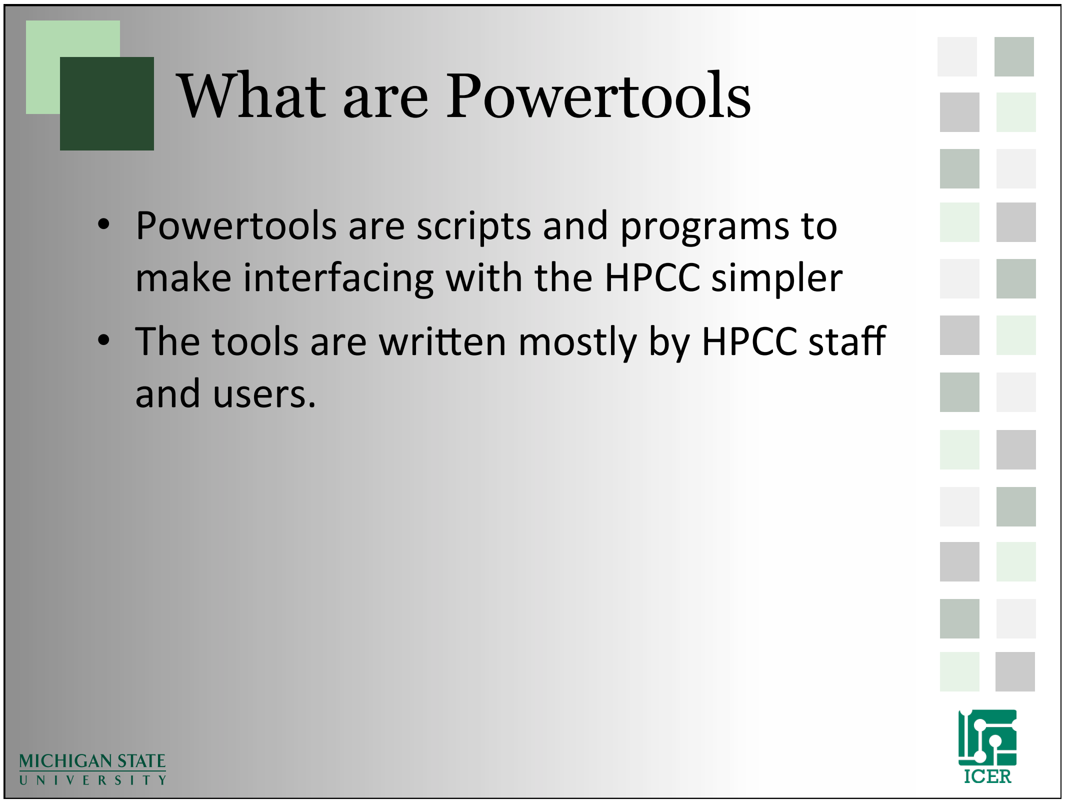

What are Powertools

- Powertools are scripts and programs to make interfacing with the HPCC simpler
- The tools are written mostly by HPCC staff and users.

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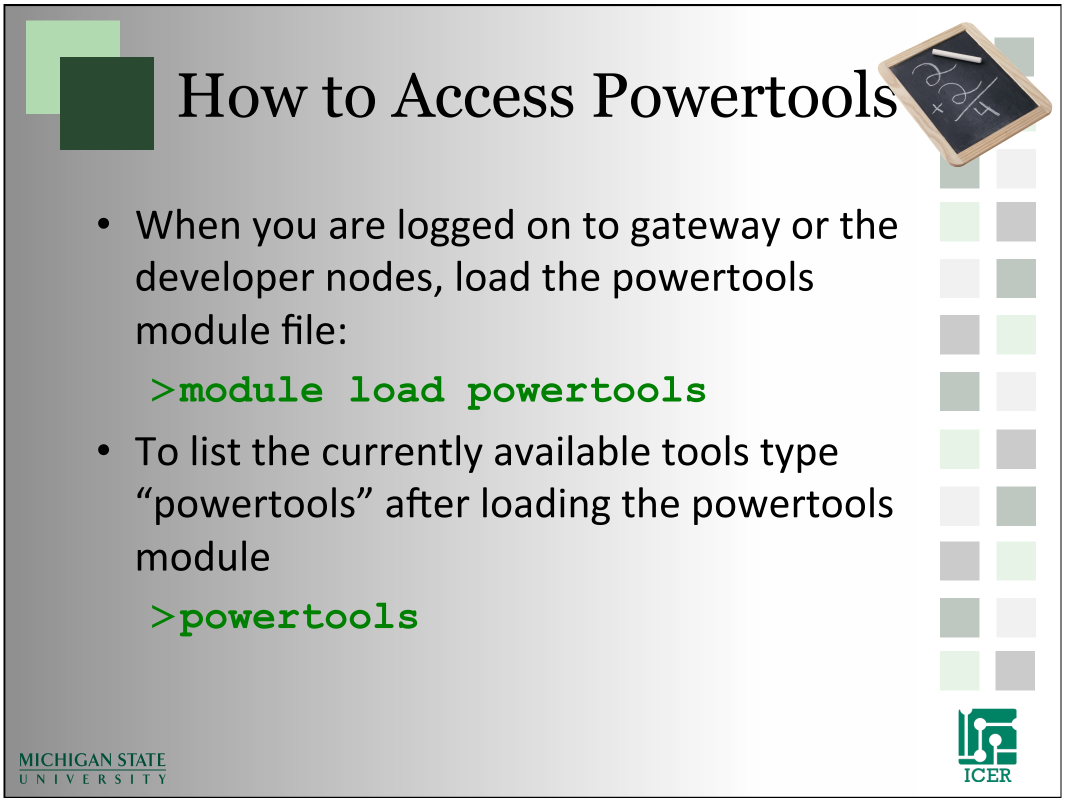


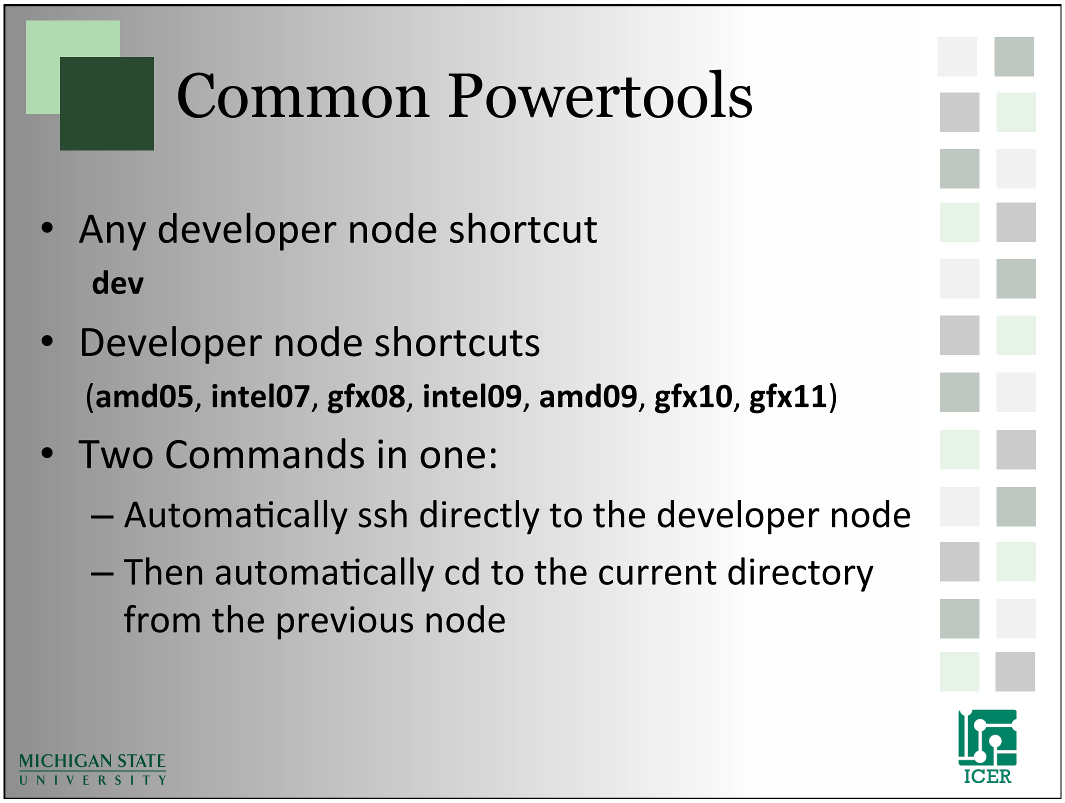
How to Access Powertools

- 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

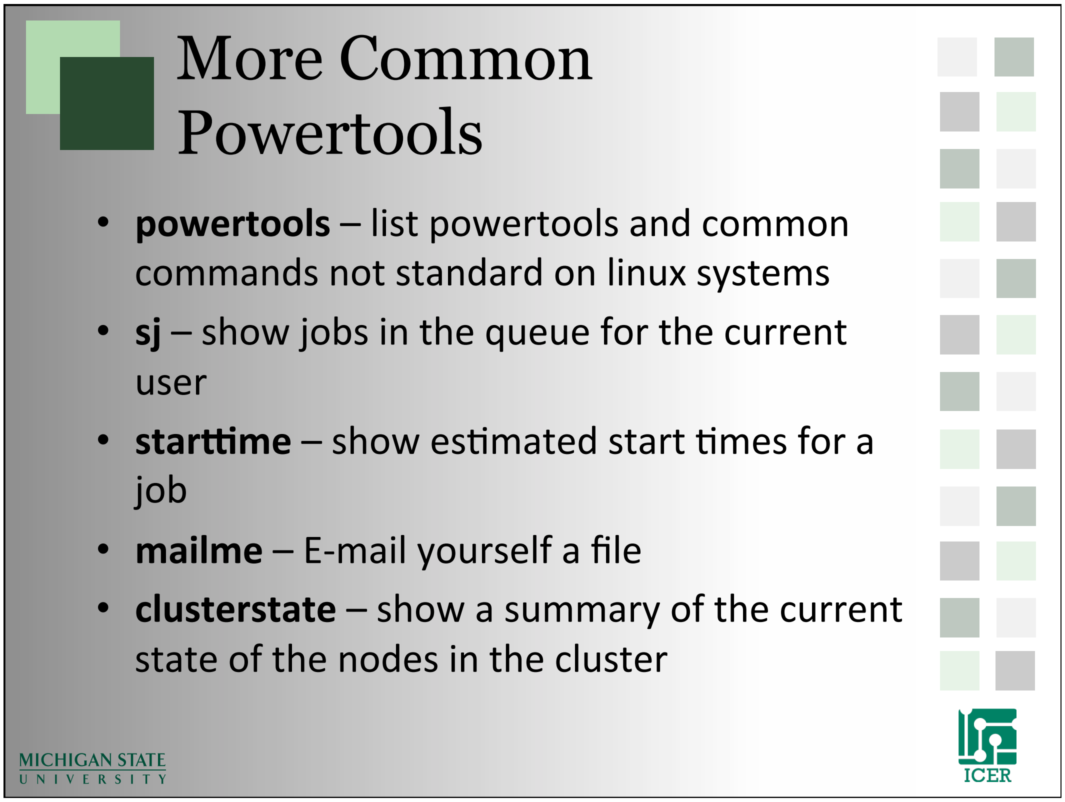
- Any developer node shortcut

  dev

- Developer node shortcuts

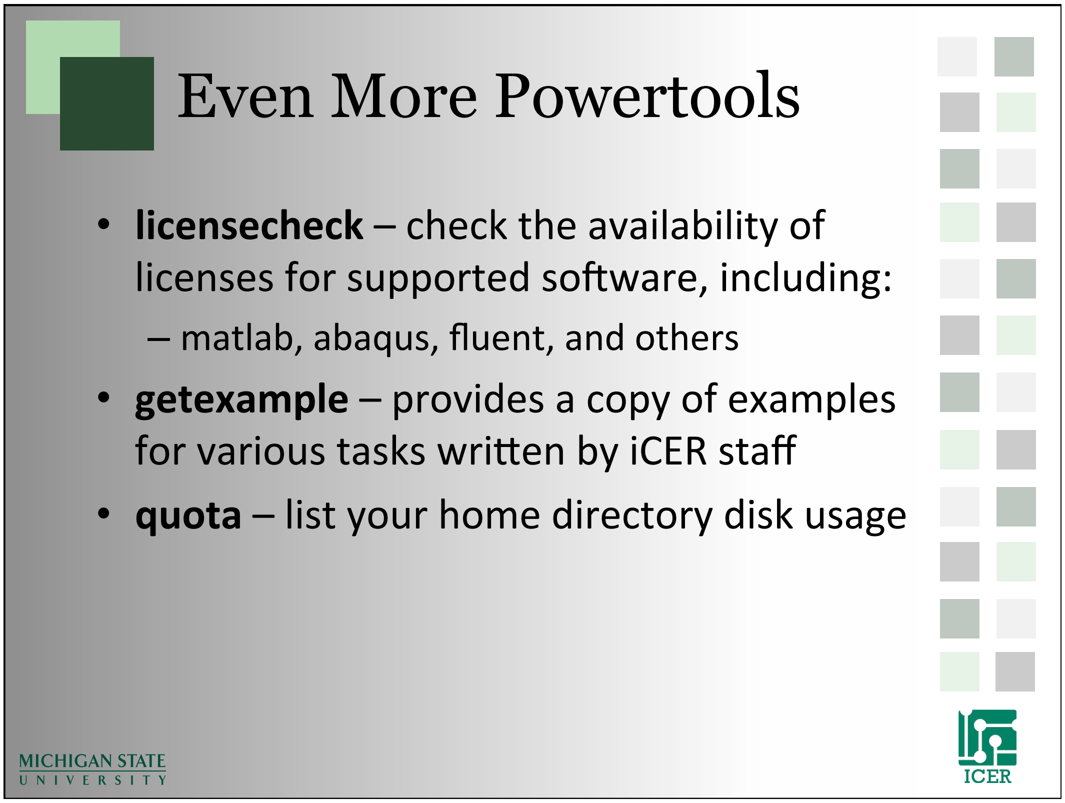
  (**amd05**, **intel07**, **gfx08**, **intel09**, **amd09**, **gfx10**, **gfx11**)

- Two Commands in one:
  - Automatically ssh directly to the developer node
  - Then automatically cd to the current directory from the previous node



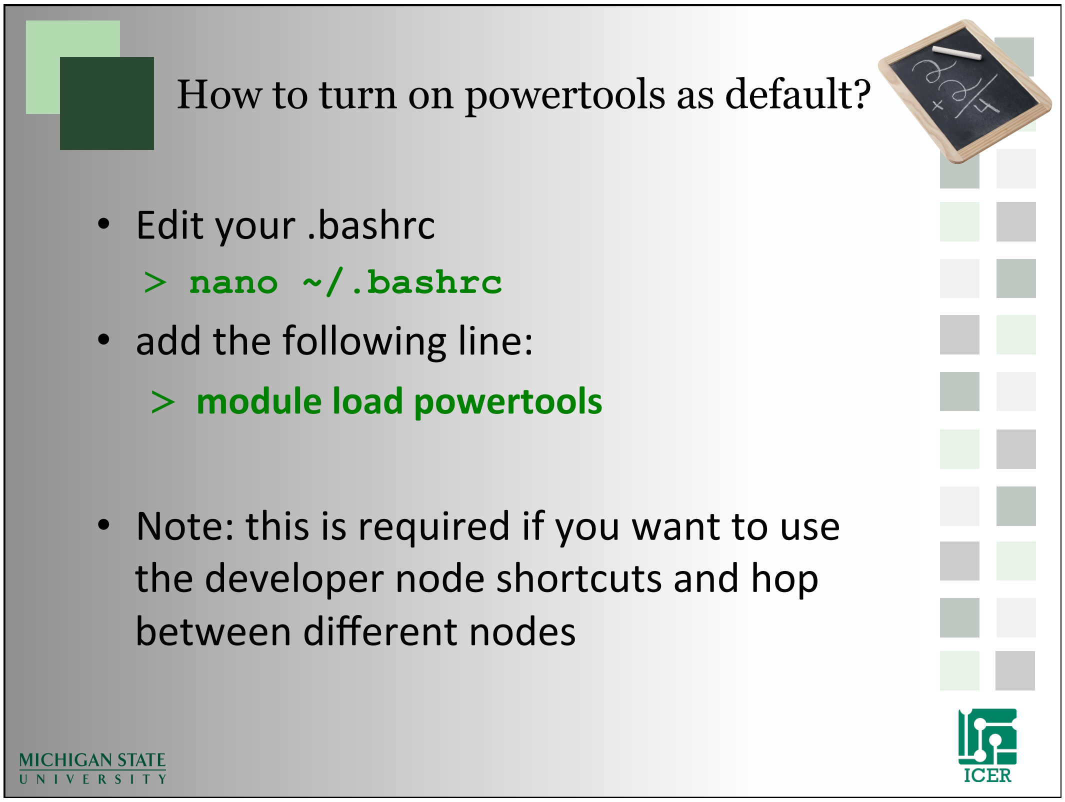
More Common Powertools

- **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

- **licensecheck** – check the availability of licenses for supported software, including:
  - matlab, abaqus, fluent, and others
- **getexample** – provides a copy of examples for various tasks written by iCER staff
- **quota** – list your home directory disk usage



How to turn on powertools as default?

- Edit your .bashrc

```
> nano ~/.bashrc
```

- add the following line:

```
> module load powertools
```

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

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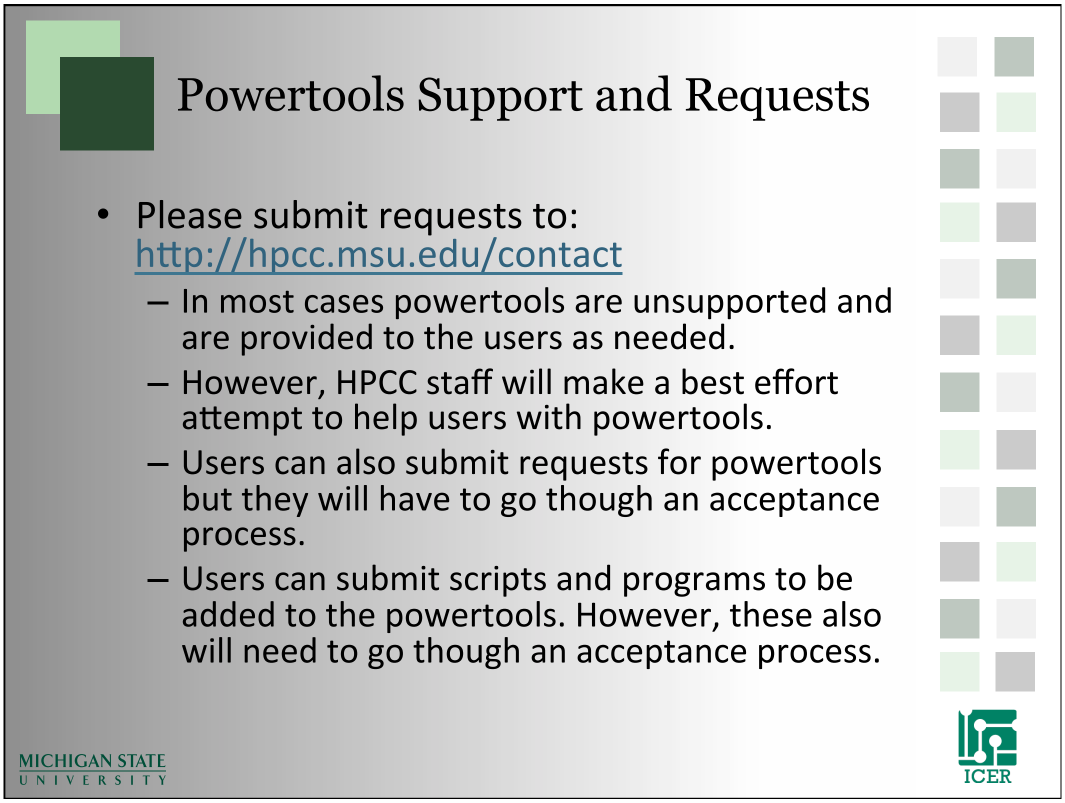

Powertools Support and Requests

- Please submit requests to: http://hpcc.msu.edu/contact
  - In most cases powertools are unsupported and are provided to the users as needed.
  - However, HPCC staff will make a best effort attempt to help users with powertools.
  - Users can also submit requests for powertools but they will have to go though an acceptance process.
  - Users can submit scripts and programs to be added to the powertools. However, these also will need to go though an acceptance process.

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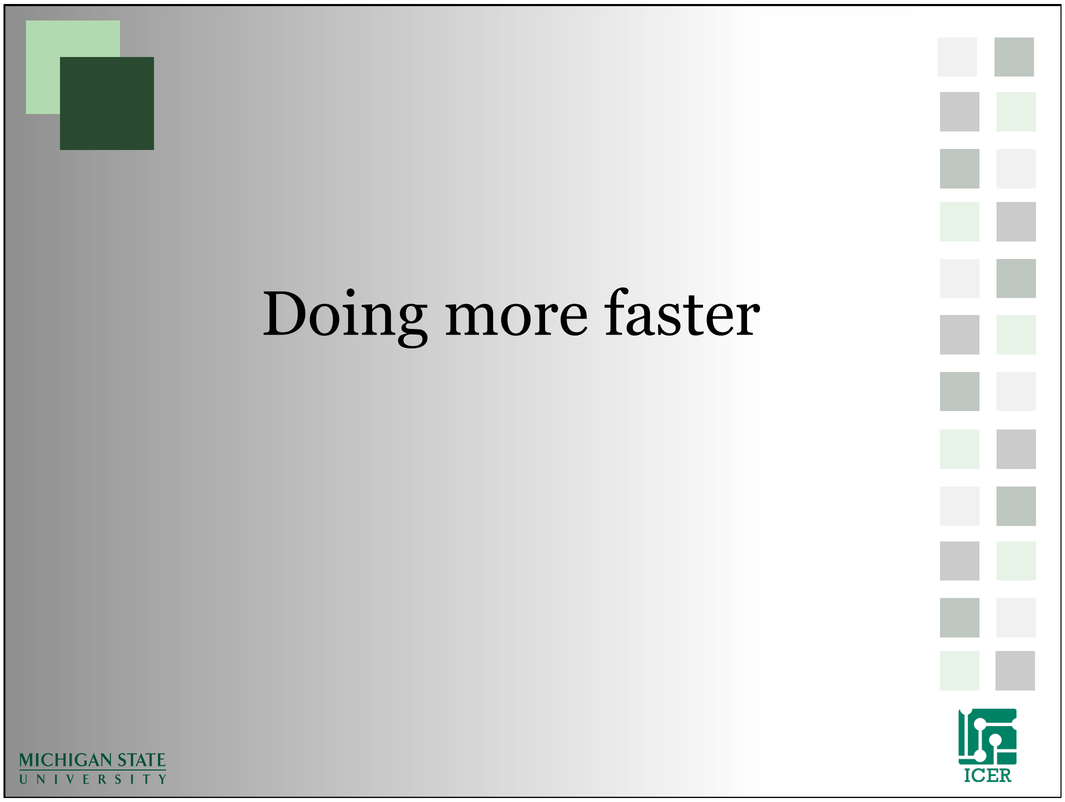

Doing more faster

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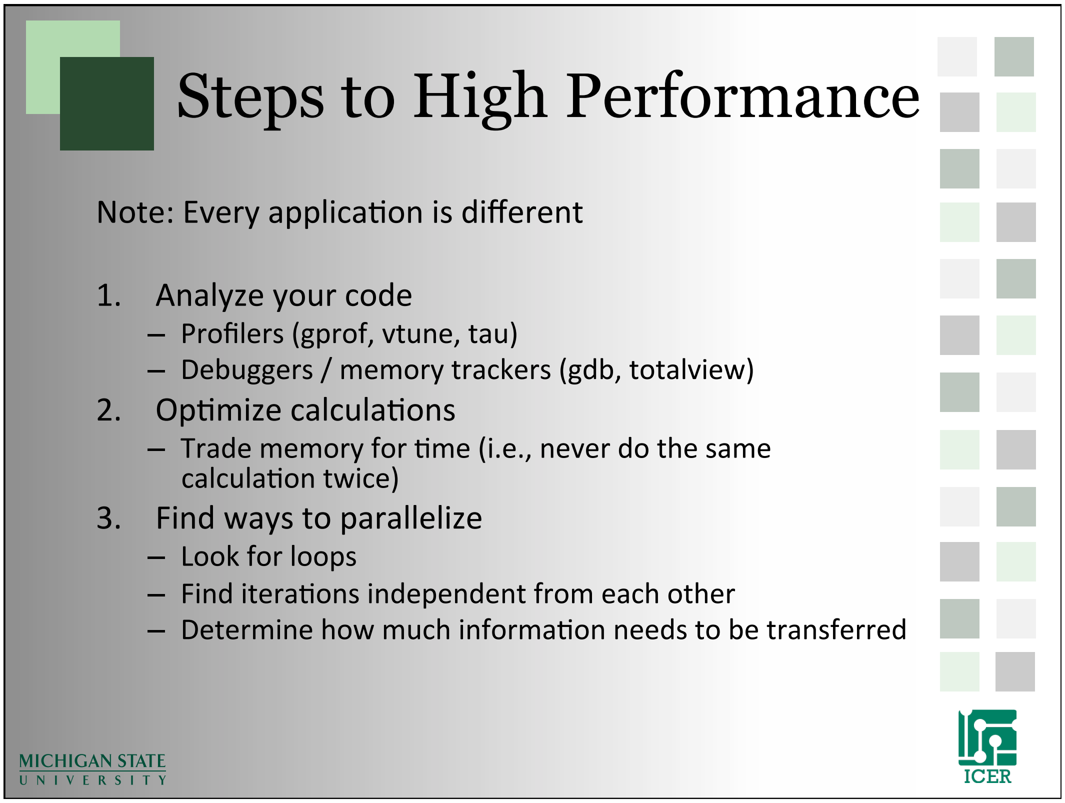

Steps to High Performance

Note: Every application is different

1. Analyze your code
   - Profilers (gprof, vtune, tau)
   - Debuggers / memory trackers (gdb, totalview)
2. Optimize calculations
   - Trade memory for time (i.e., never do the same calculation twice)
3. Find ways to parallelize
   - Look for loops
   - Find iterations independent from each other
   - Determine how much information needs to be transferred

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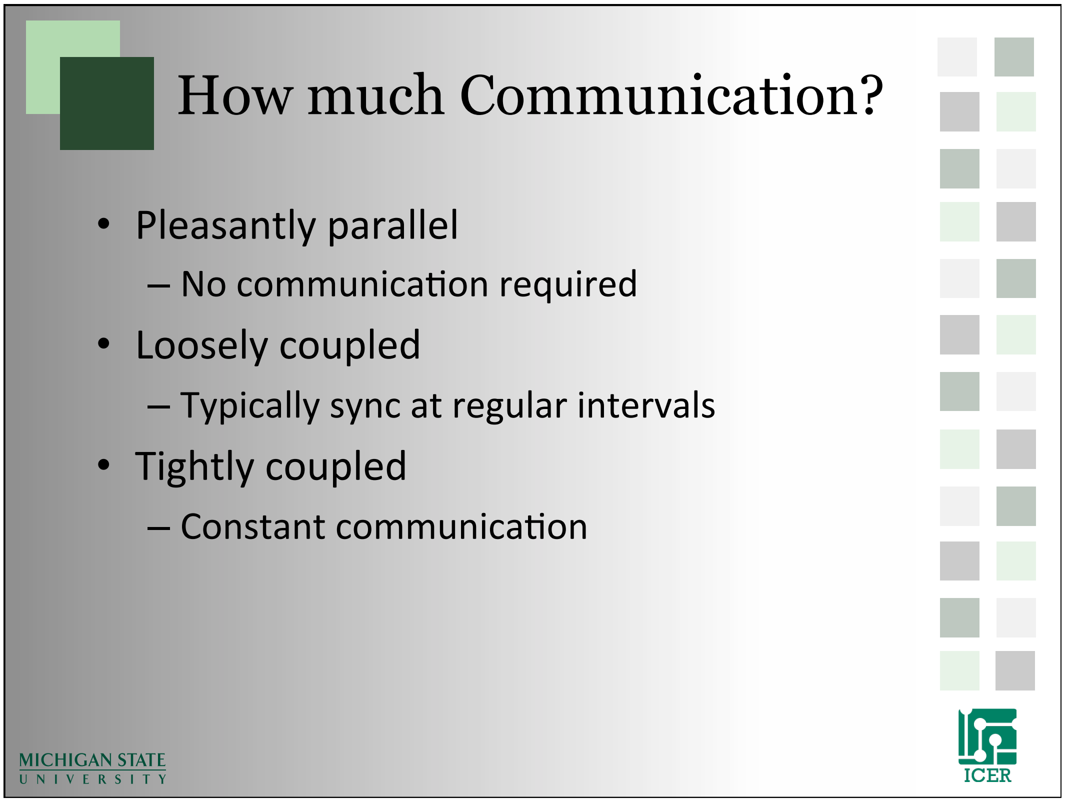
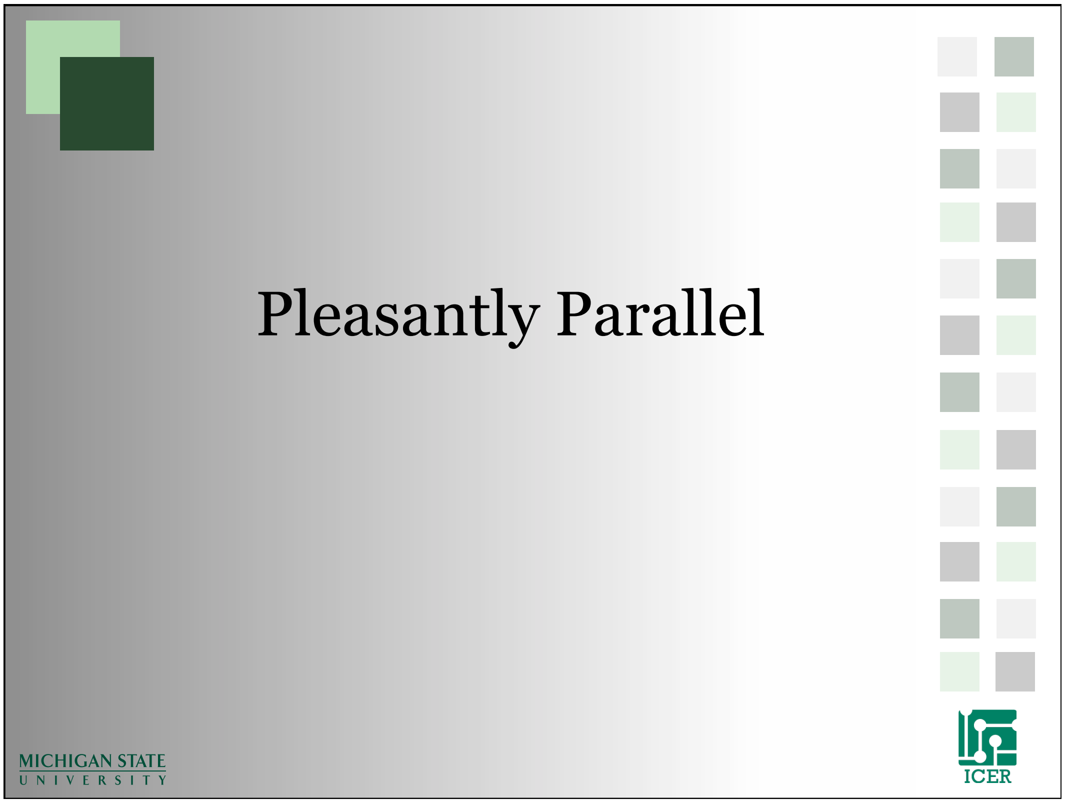
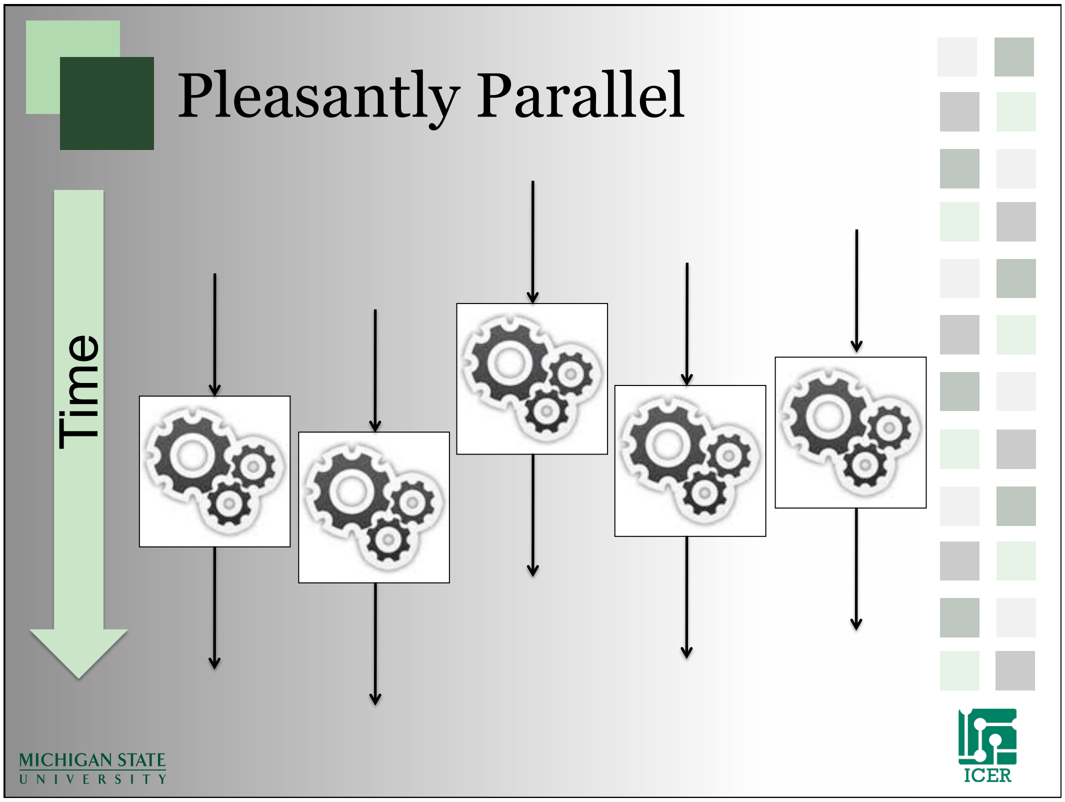


How much Communication?

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



Pleasantly Parallel



Pleasantly Parallel

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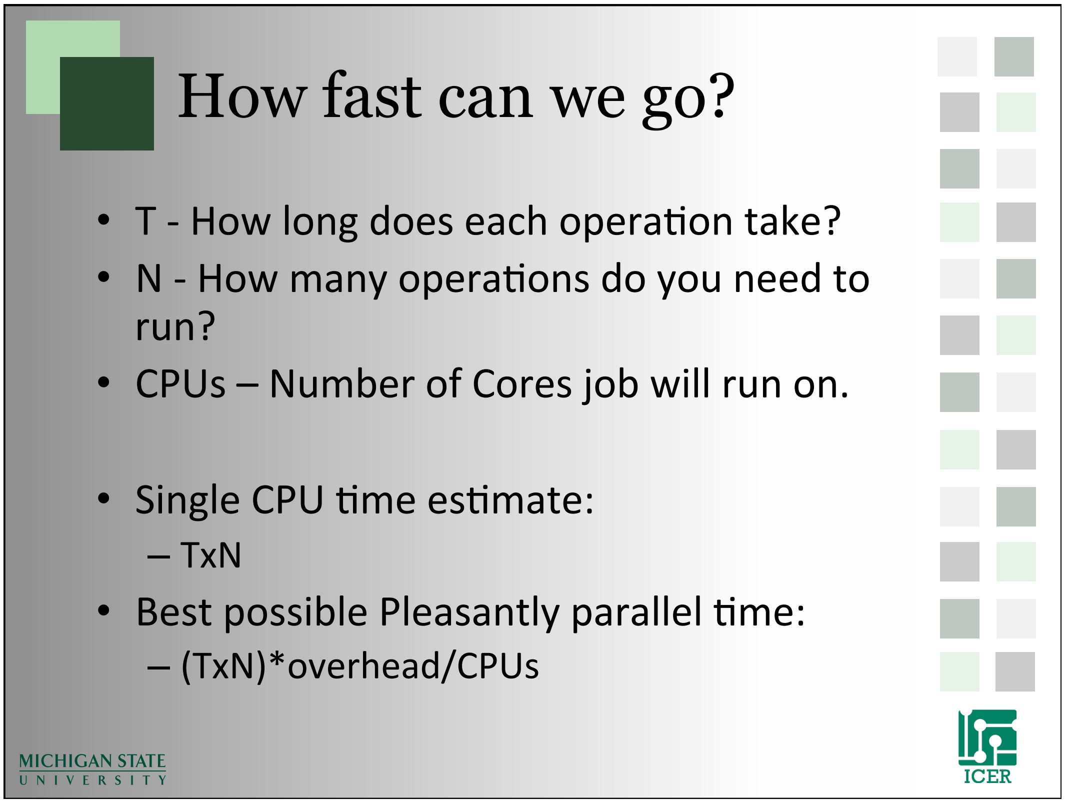

How fast can we go?

- 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:
  - TxN
- Best possible Pleasantly parallel time:
  - (TxN)*overhead/CPUs

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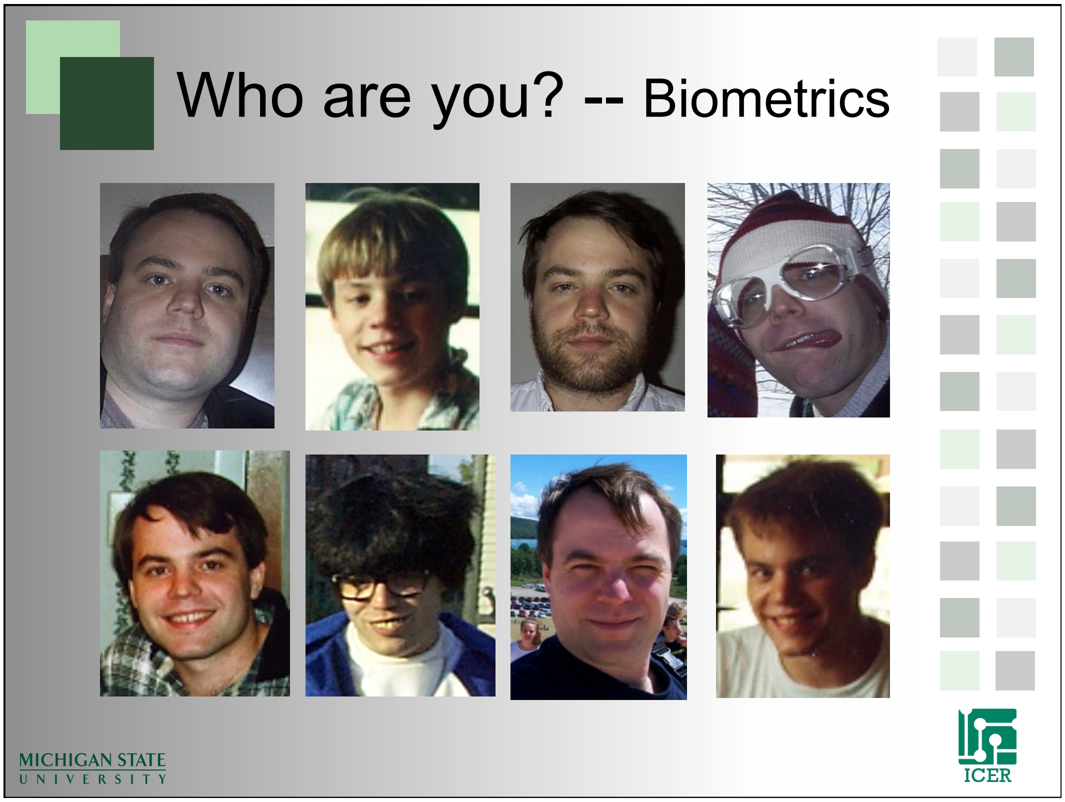

Who are you? -- Biometrics

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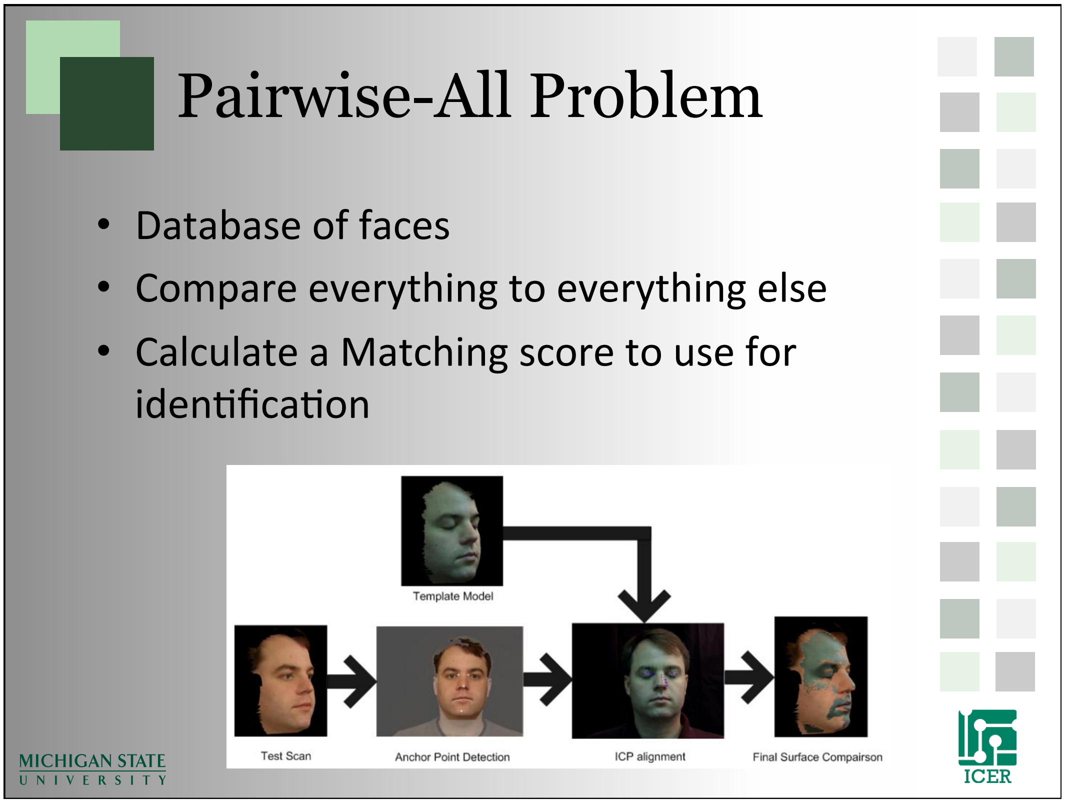

Pairwise-All Problem

- Database of faces
- Compare everything to everything else
- Calculate a Matching score to use for identification

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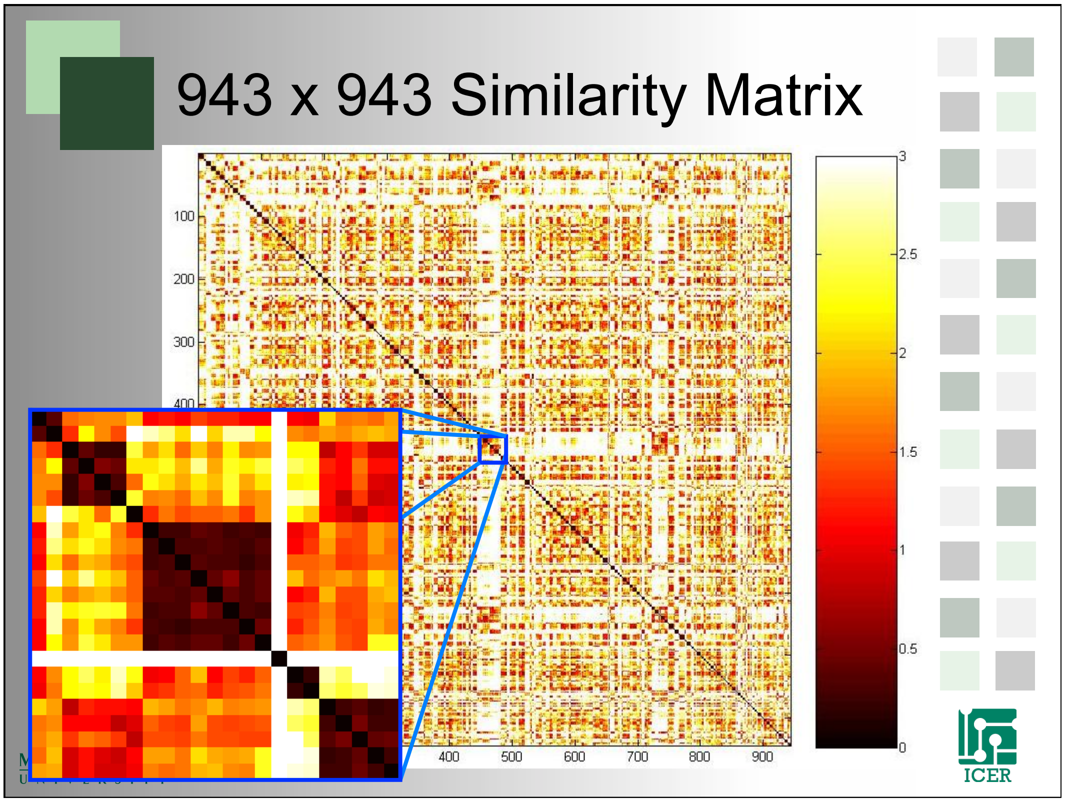

943 x 943 Similarity Matrix

Estimated Calculation Times

- Preprocessing
  - 943 * 12 (seconds) ≈ 189 Minutes
- Matching
  - 943 * 943 * 5 (seconds) ≈ 103 Days
- Scans matched to themselves always result in 0 mm
  - (943 * 943 – 943) * 5 (seconds) ≈ 103 Days
- The Proposed Alignment Algorithm is symmetric.
  - (943 * 943 – 943)/2 * 5 (seconds) ≈ 51.5 Days

- We also load models once per row instead of every time
  - (943*943-943)/2 * 3 (seconds) + 943 * 2 (seconds) ≈ 31 Days

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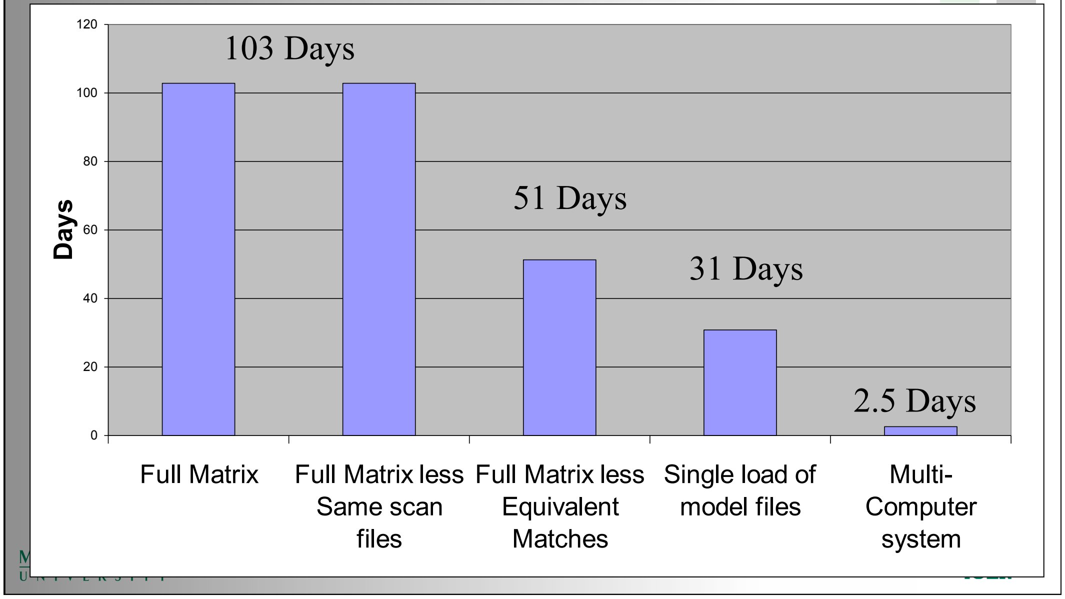
Calculation Time for Full Similarity Matrix



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

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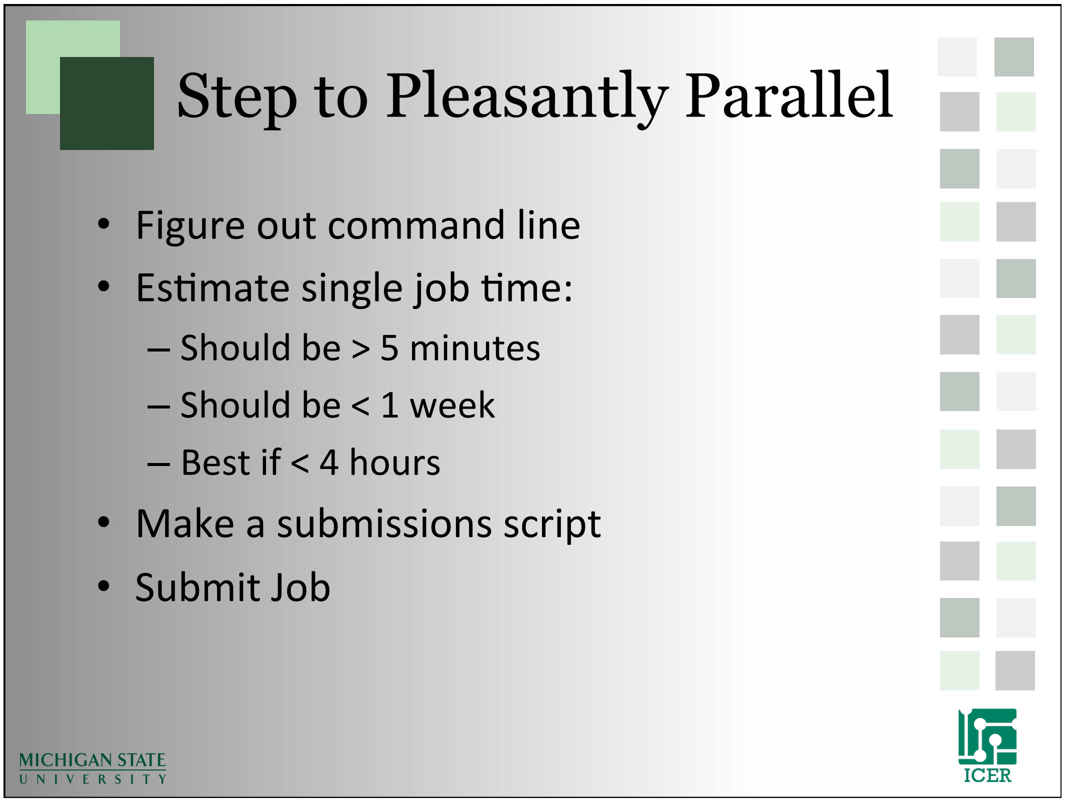

Step to Pleasantly Parallel

- 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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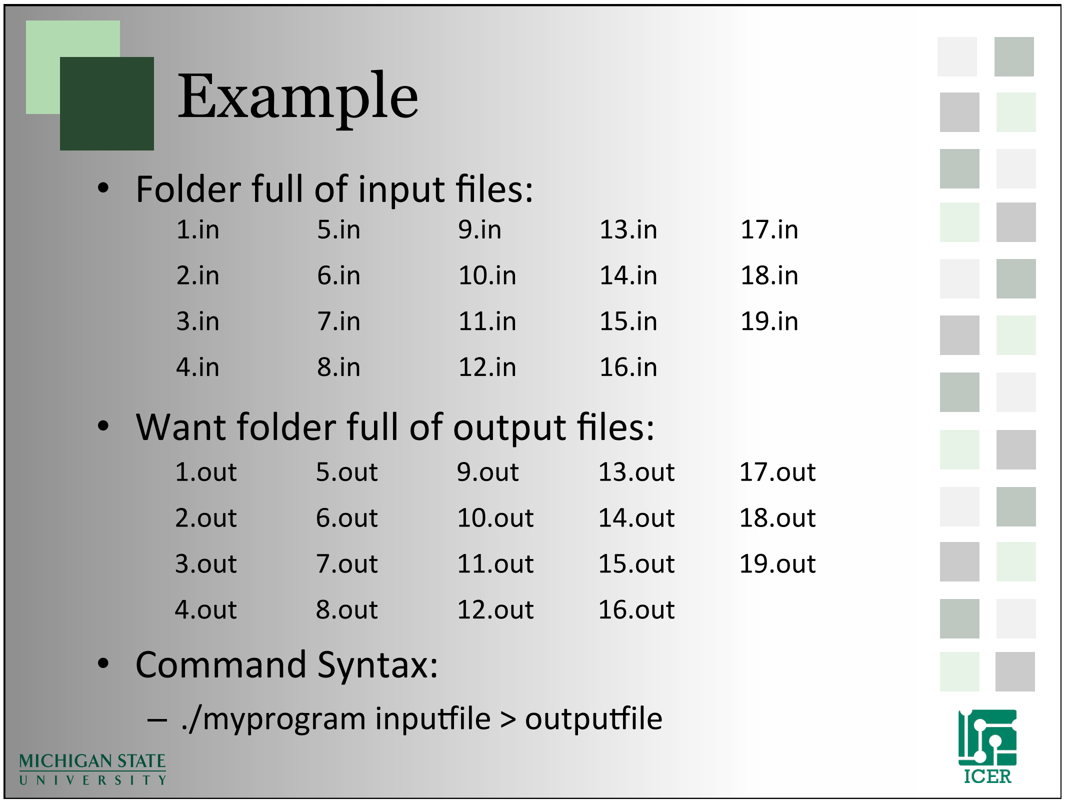

Example

- Folder full of input files:

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

- Want folder full of output files:

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

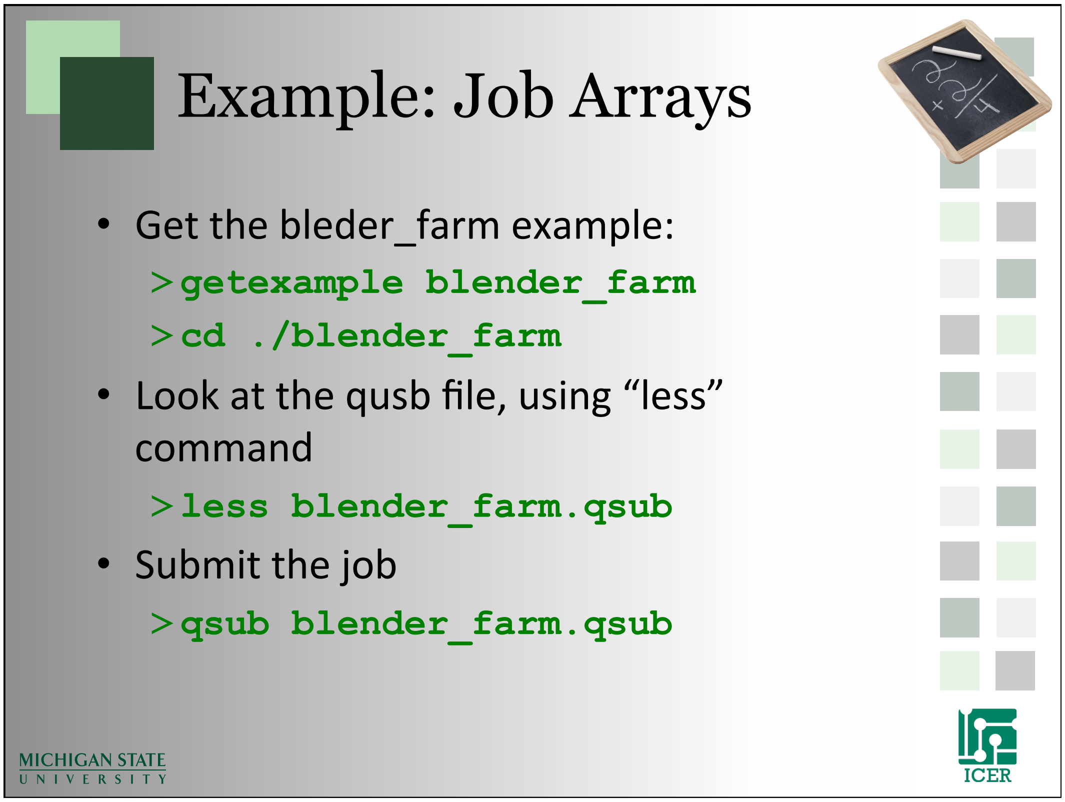
Simple Job Array

```
#!/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_WORKID}

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

qstat -f ${PBS_JOBID}
```



Example: Job Arrays

- Get the bleder_farm example:

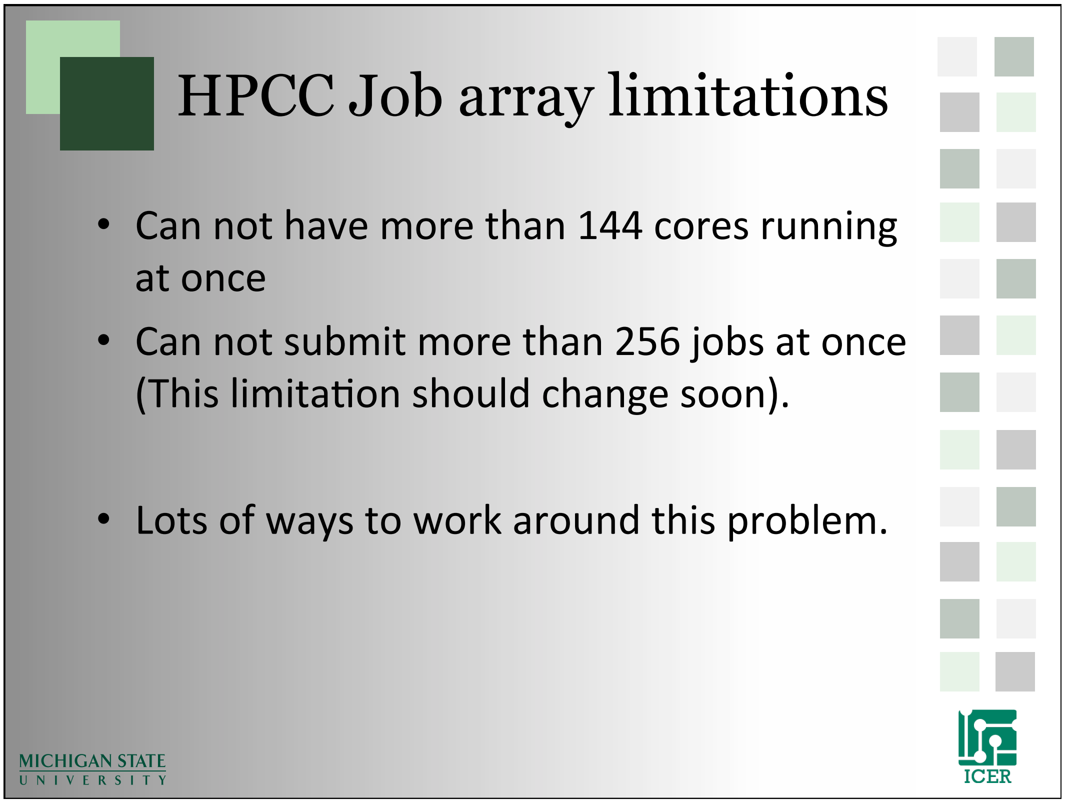
```
>getexample blender_farm
>cd ./blender_farm
```

- Look at the qusb file, using “less” command

```
>less blender_farm.qsub
```

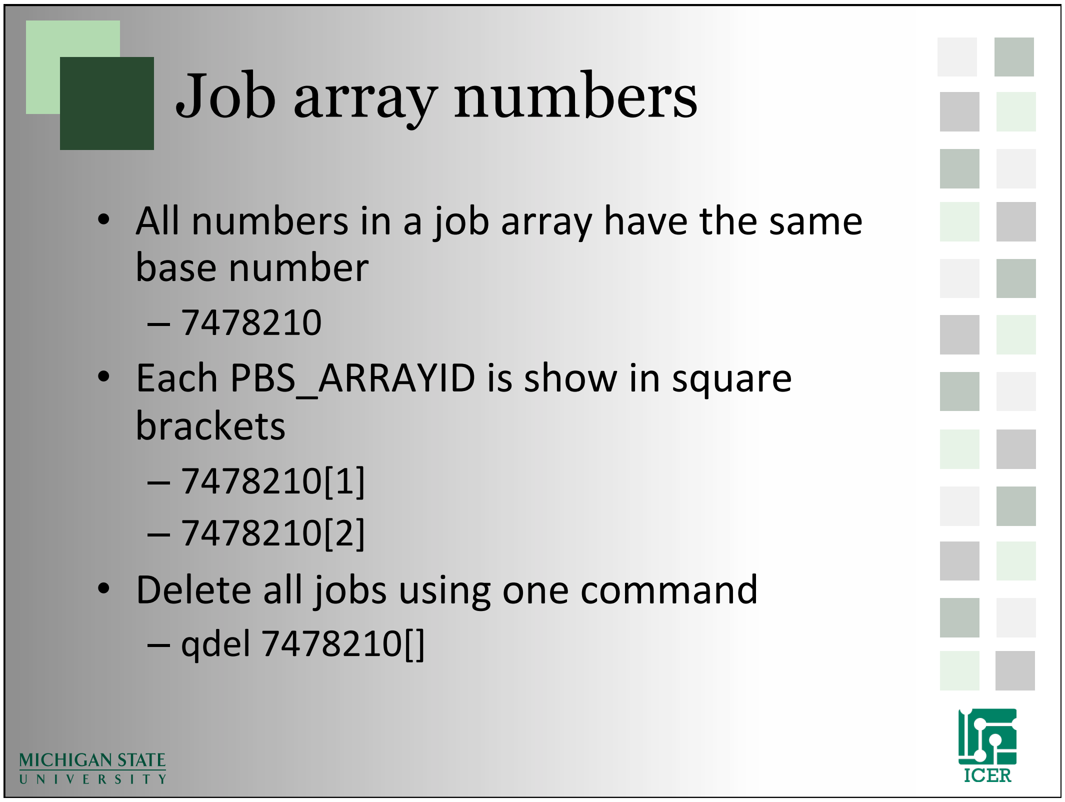
- Submit the job

```
>qsub blender_farm.qsub
```



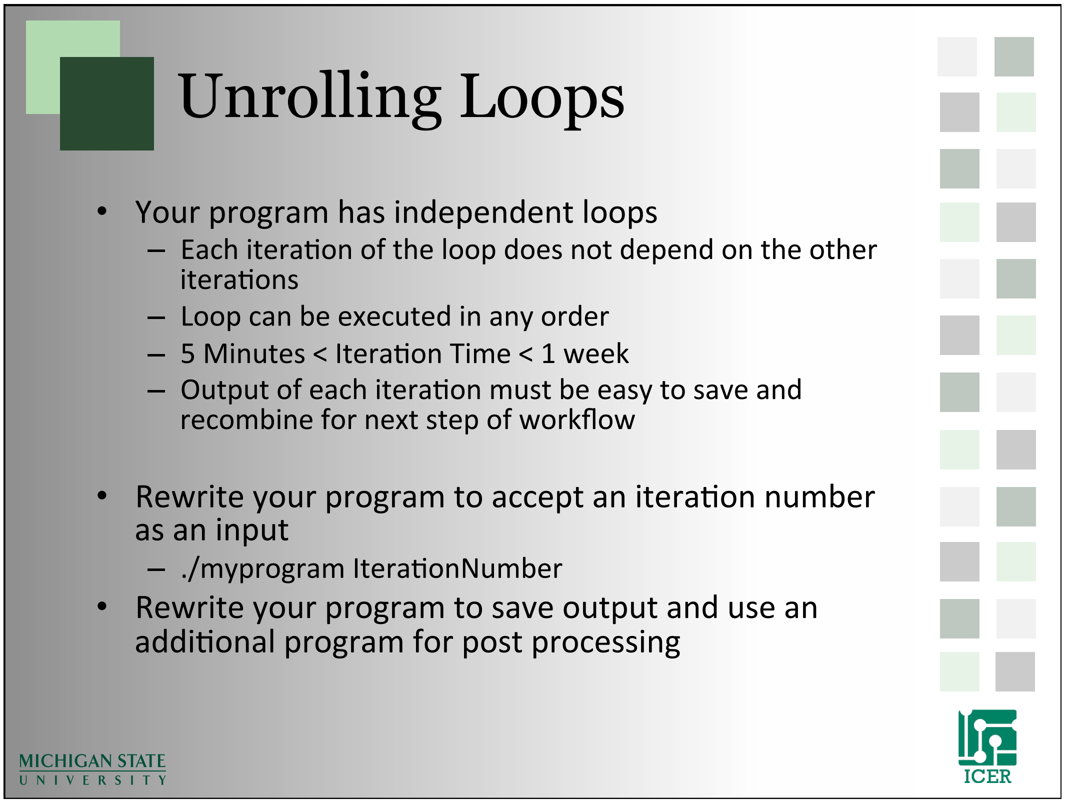
HPCC Job array limitations

- Can not have more than 144 cores running at once
- Can not submit more than 256 jobs at once (This limitation should change soon).
- Lots of ways to work around this problem.



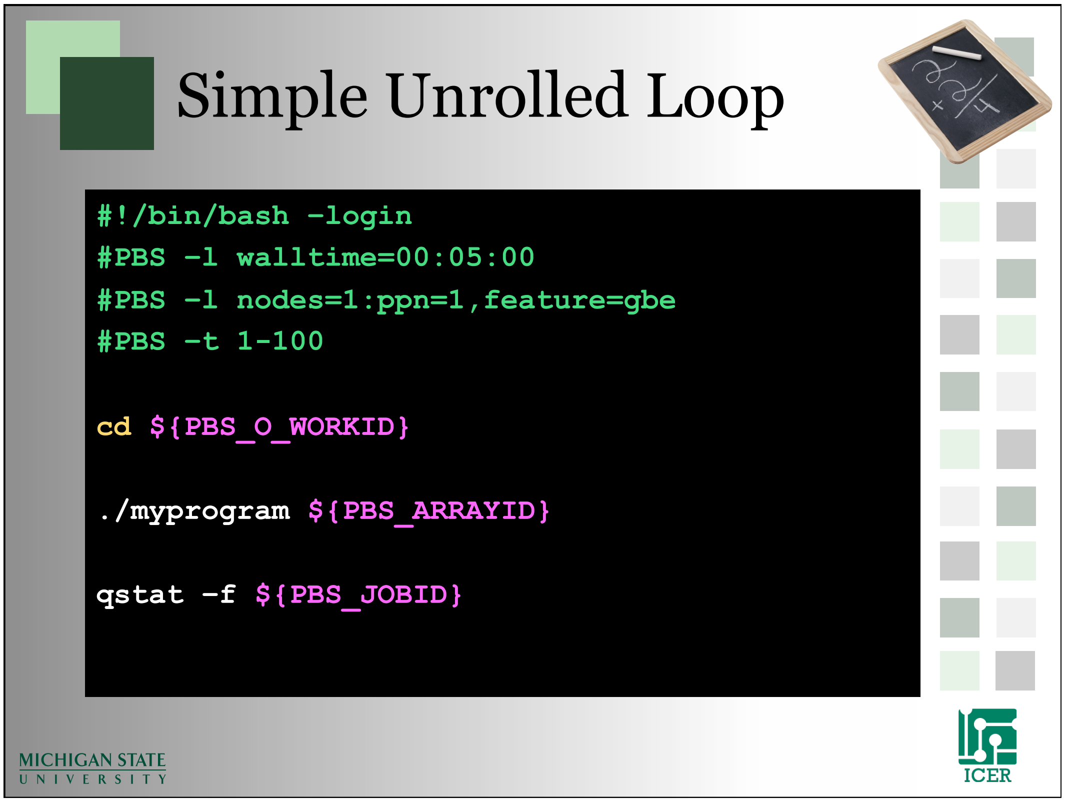
Job array numbers

- 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



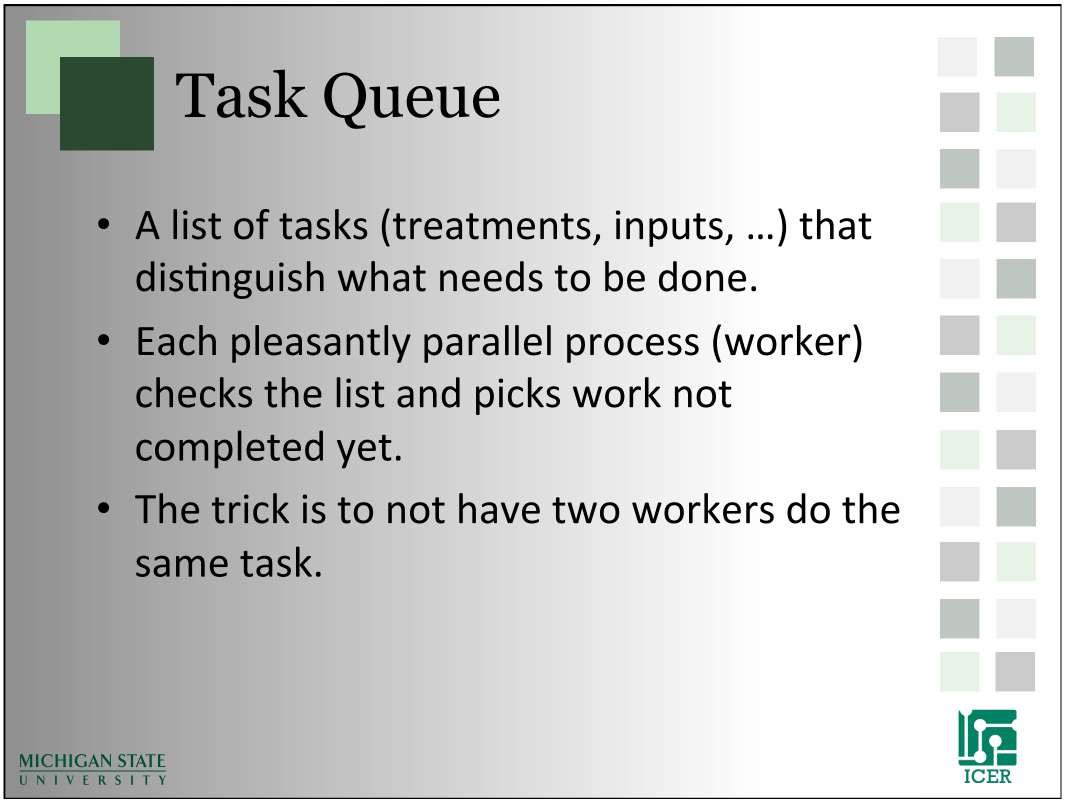
Simple Unrolled Loop

```
#!/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 (treatments, inputs, …) that distinguish what needs to be done.
- Each pleasantly parallel process (worker) checks the list and picks work not completed yet.
- The trick is to not have two workers do the same task.

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)

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Simple FAS

```
#!/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
```

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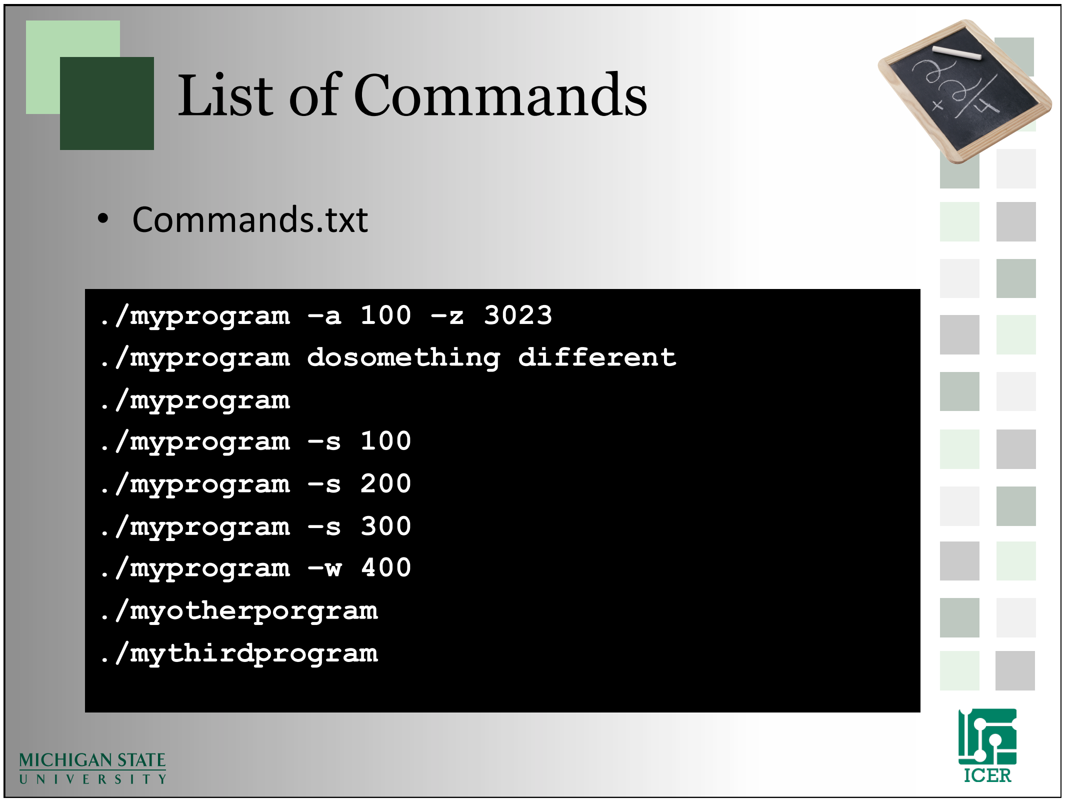
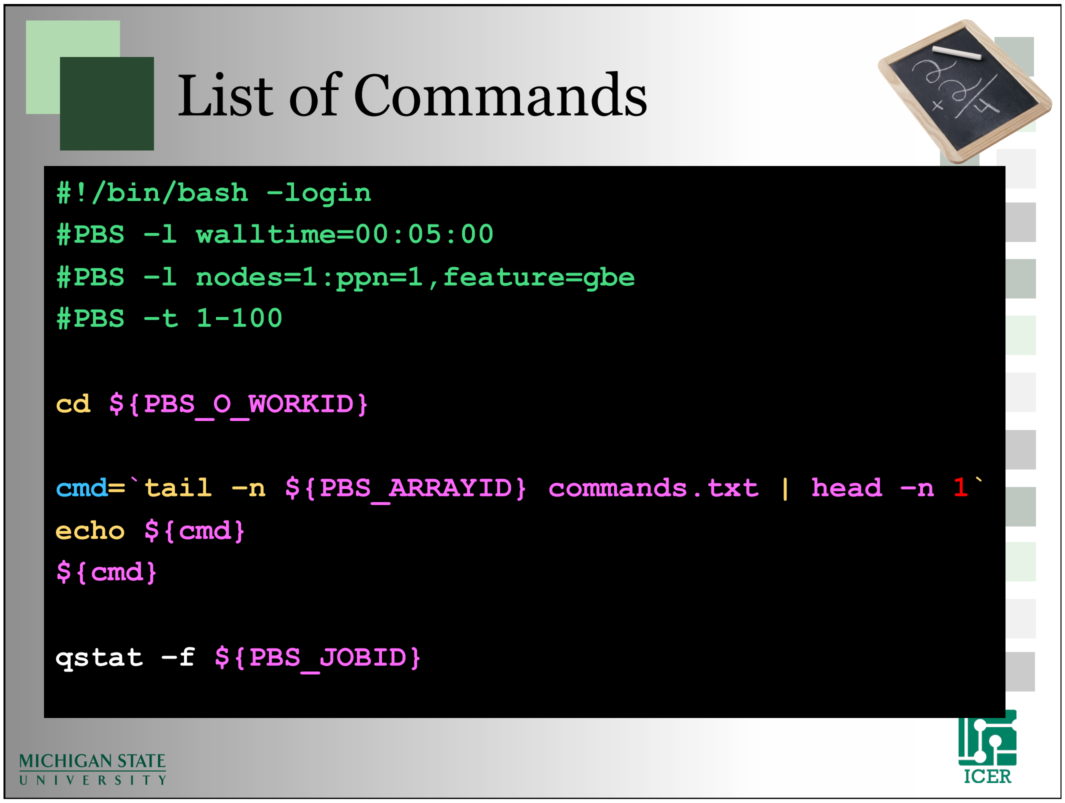


List of Commands

- 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
```

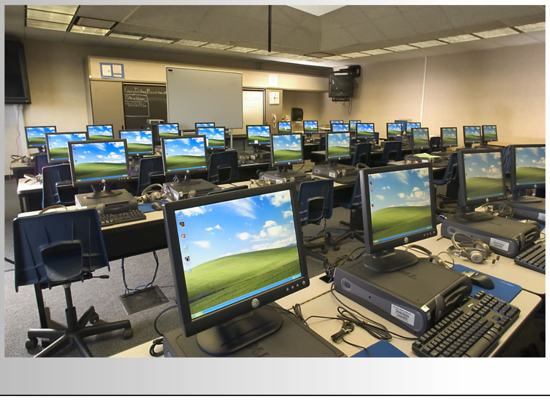


List of Commands

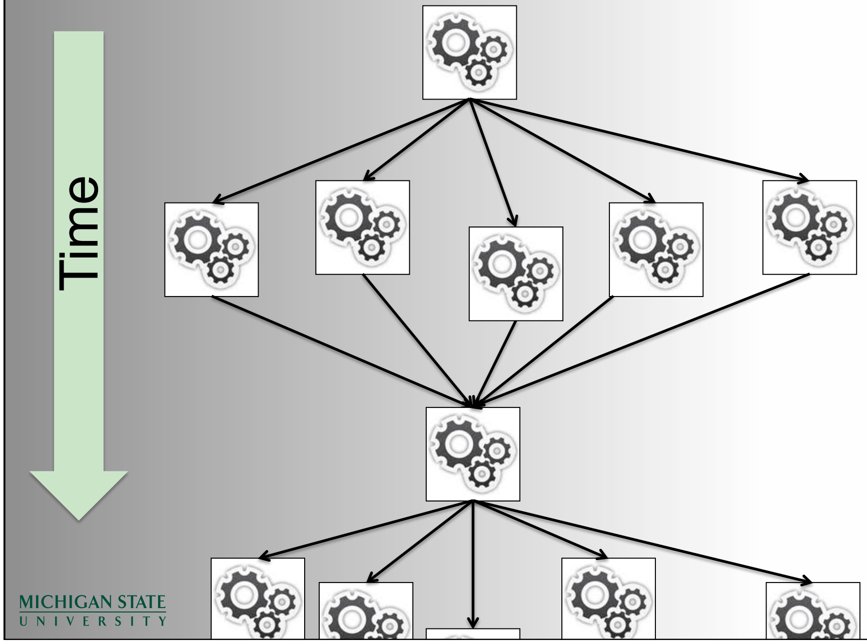
```
#!/bin/bash -login
#PBS -l walltime=00:05:00
#PBS -l nodes=1:ppn=1,feature=gbe
#PBS -t 1-100

cd ${PBS_O_WORKID}

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

qstat -f ${PBS_JOBID}
```

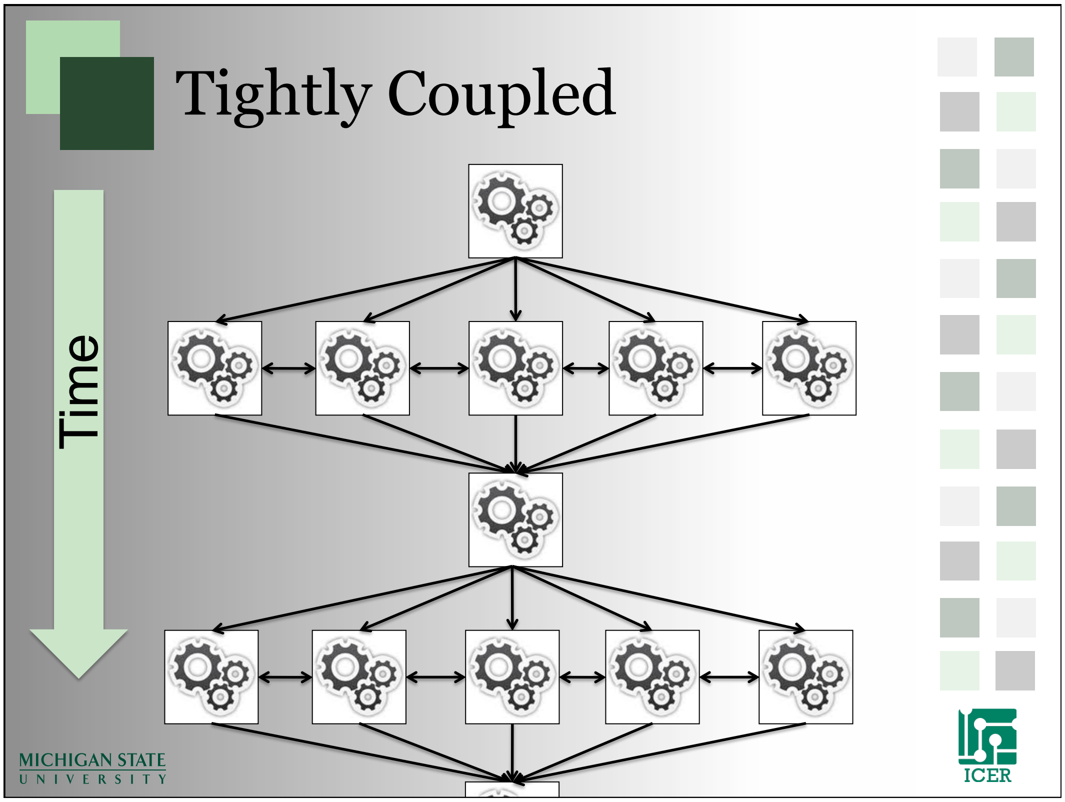
Condor High Throughput Computing

- Job submission system
- Runs like a screen saver
- Steals CPU Cycles

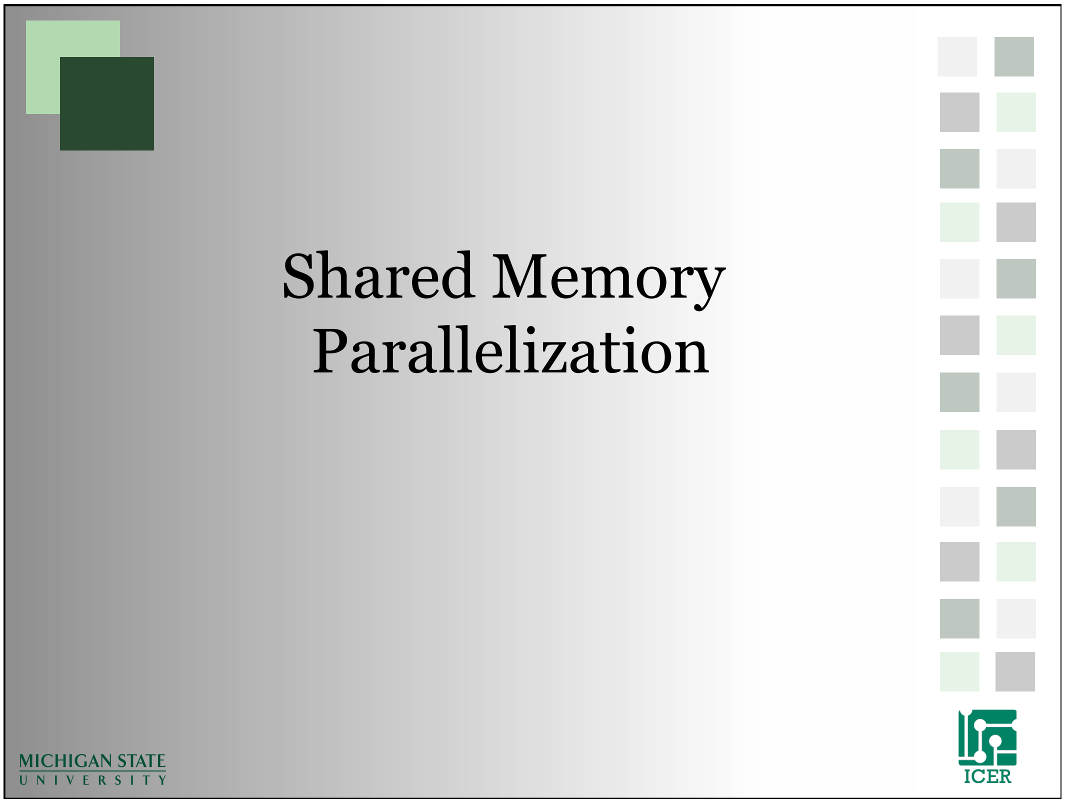


Loosely Coupled

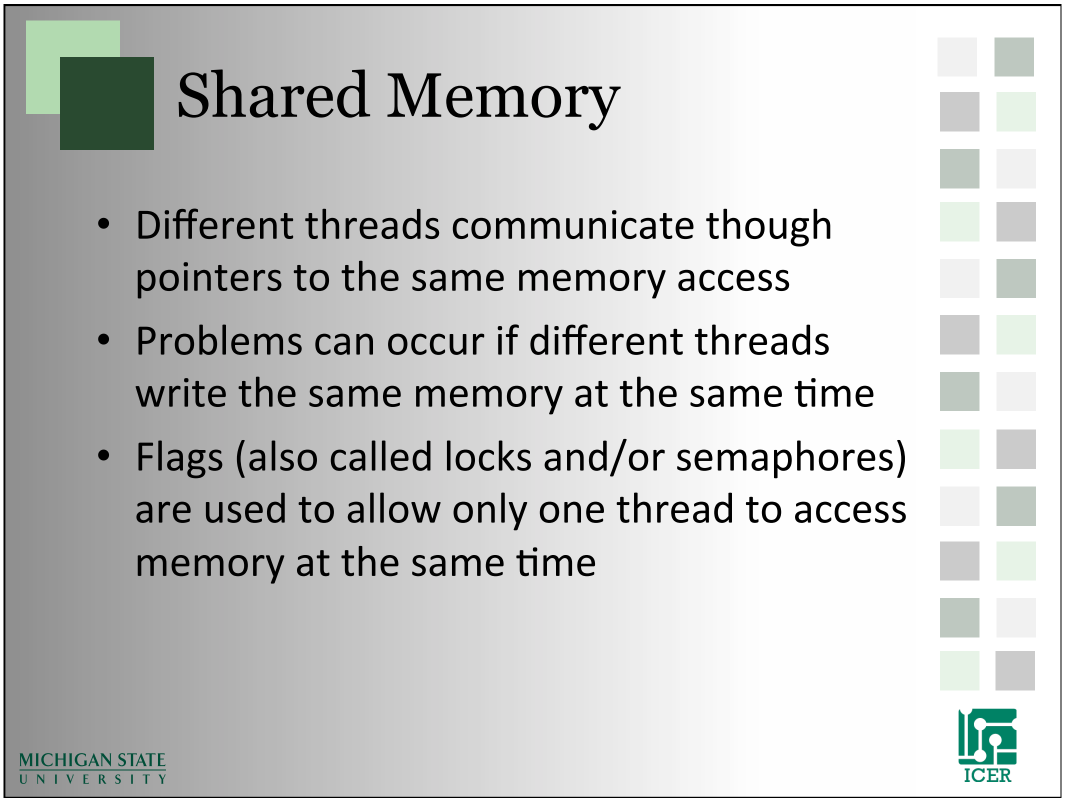




Tightly Coupled



Shared Memory Parallelization



Shared Memory

- Different threads communicate though pointers to the same memory access
- 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

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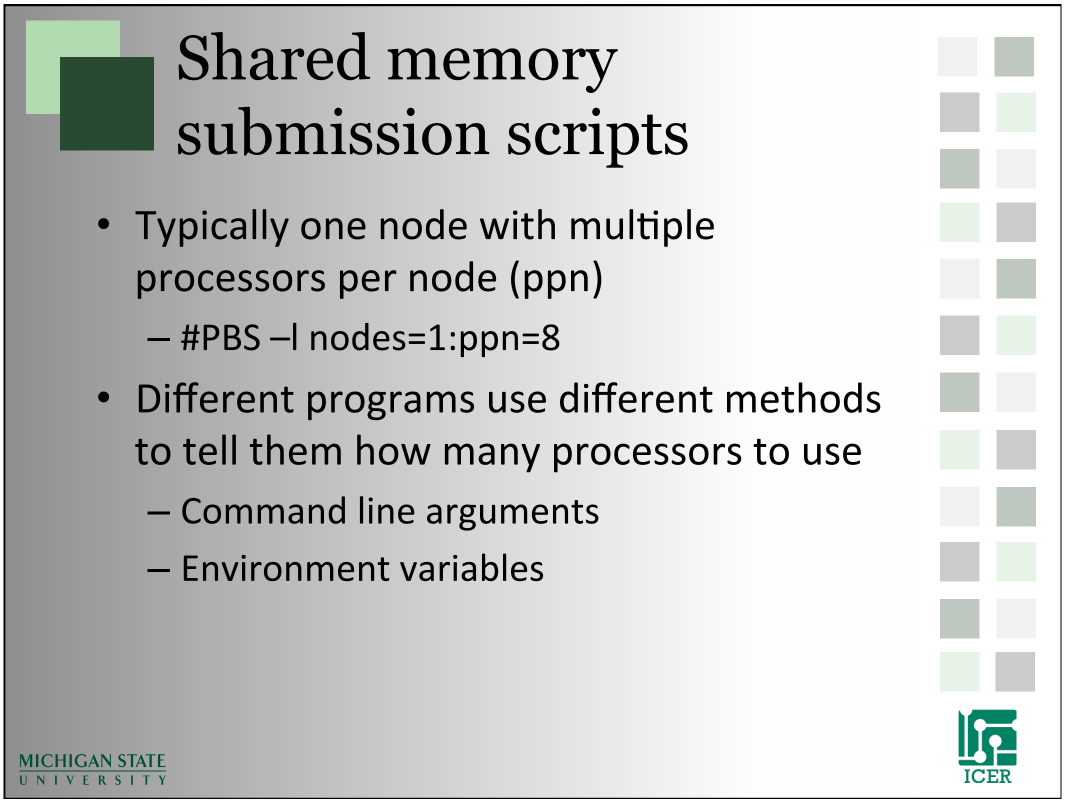

Shared memory submission scripts

- 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

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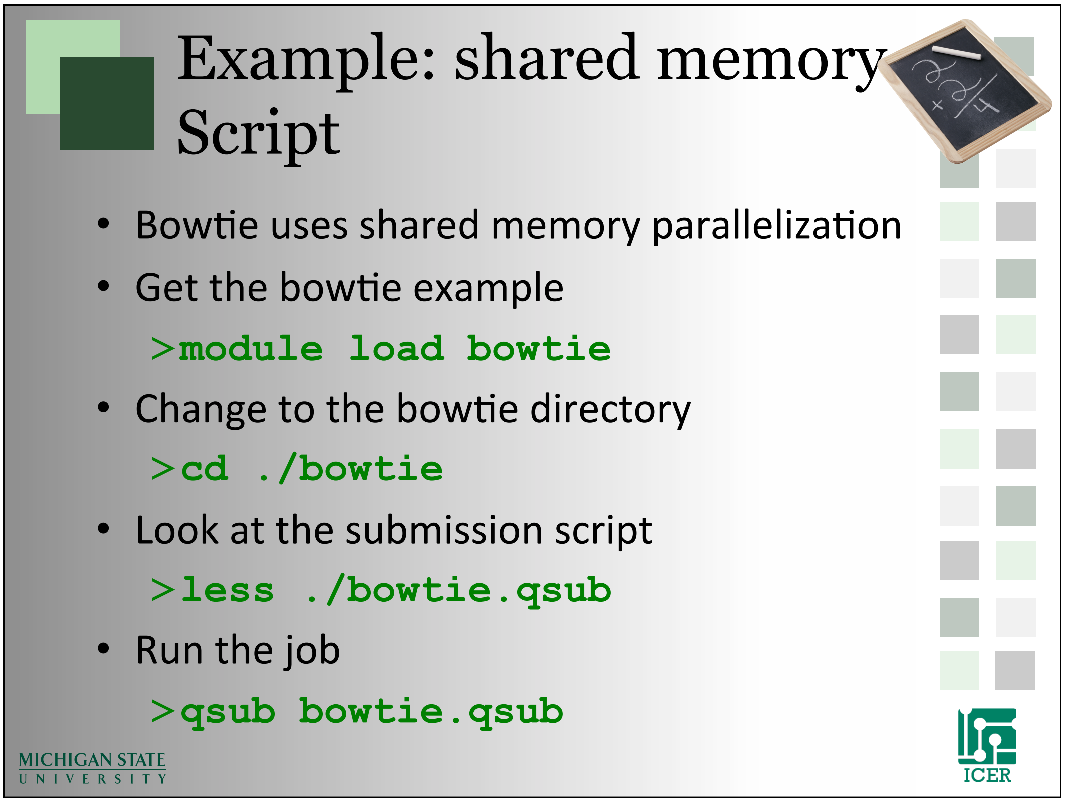


Example: shared memory Script

- Bowtie uses shared memory parallelization
- Get the bowtie example

```
>module load bowtie
```

- Change to the bowtie directory

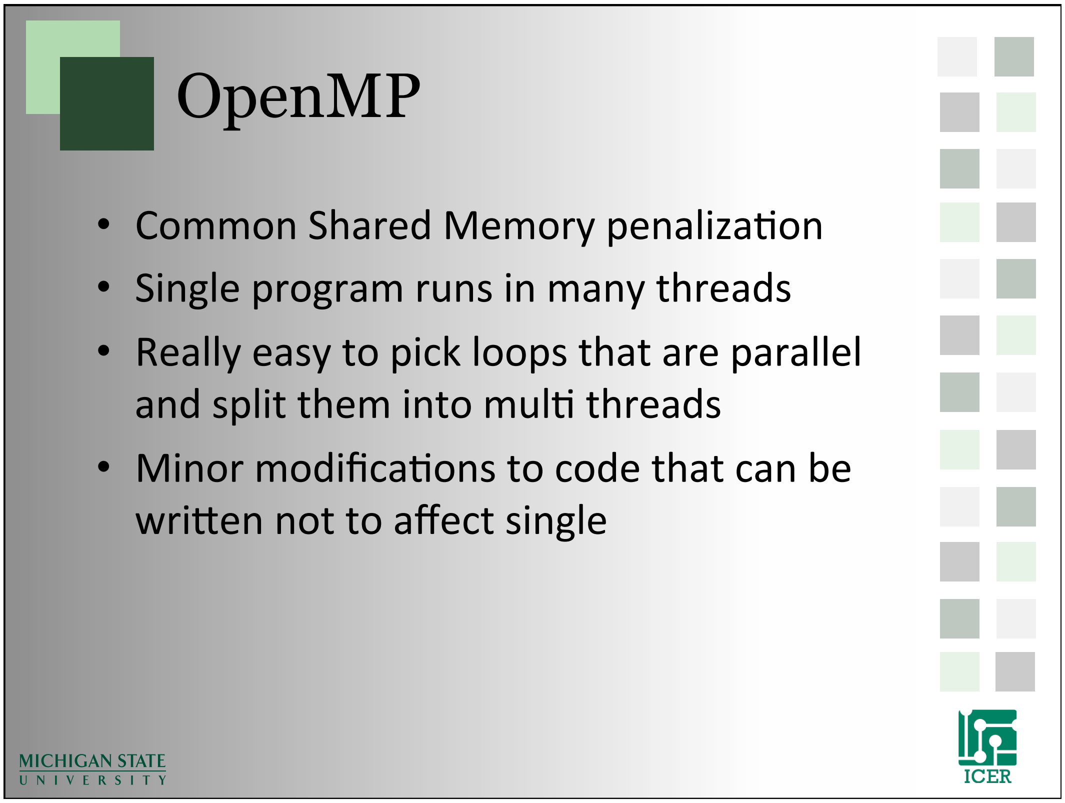
```
>cd ./bowtie
```

- Look at the submission script

```
>less ./bowtie.qsub
```

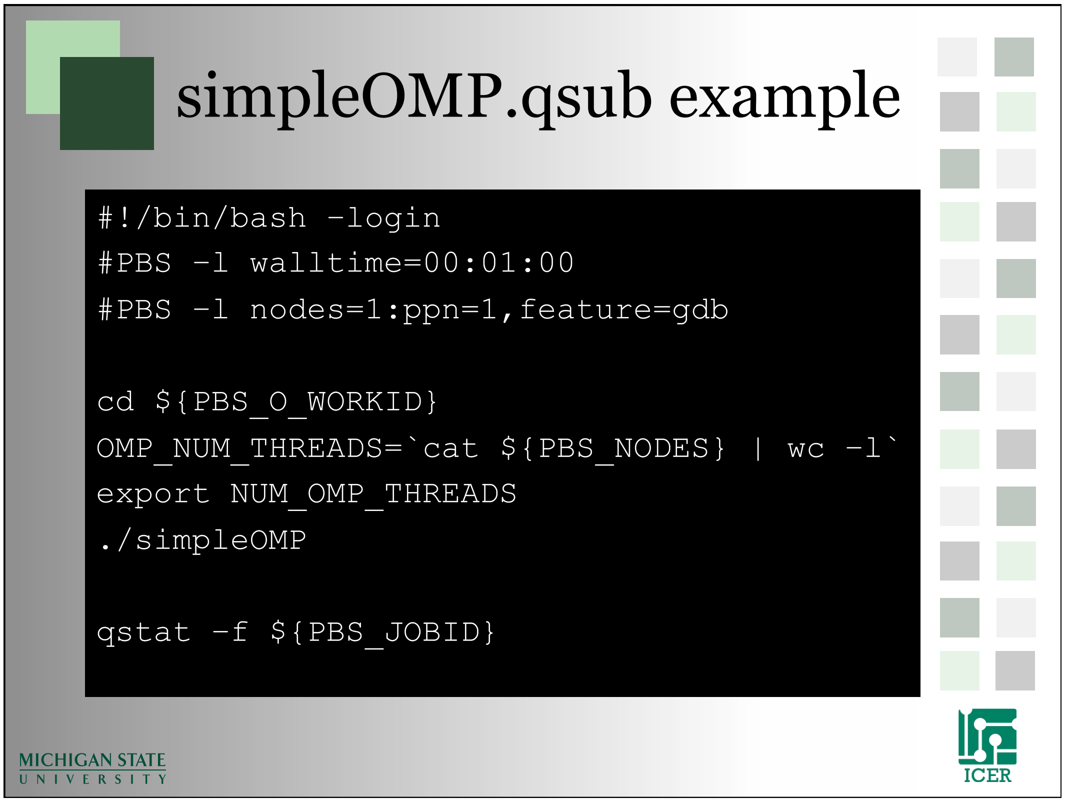
- Run the job

```
>qsub bowtie.qsub
```



OpenMP

- Common Shared Memory penalization
- 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

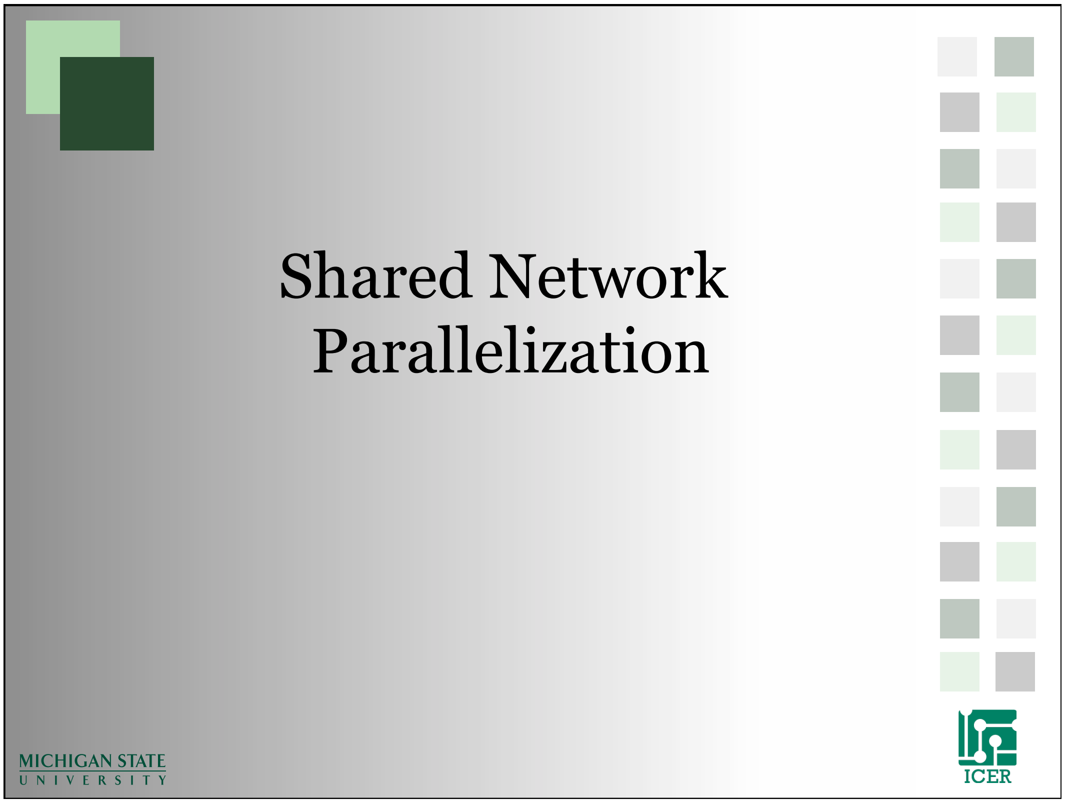


simpleOMP.qsub example

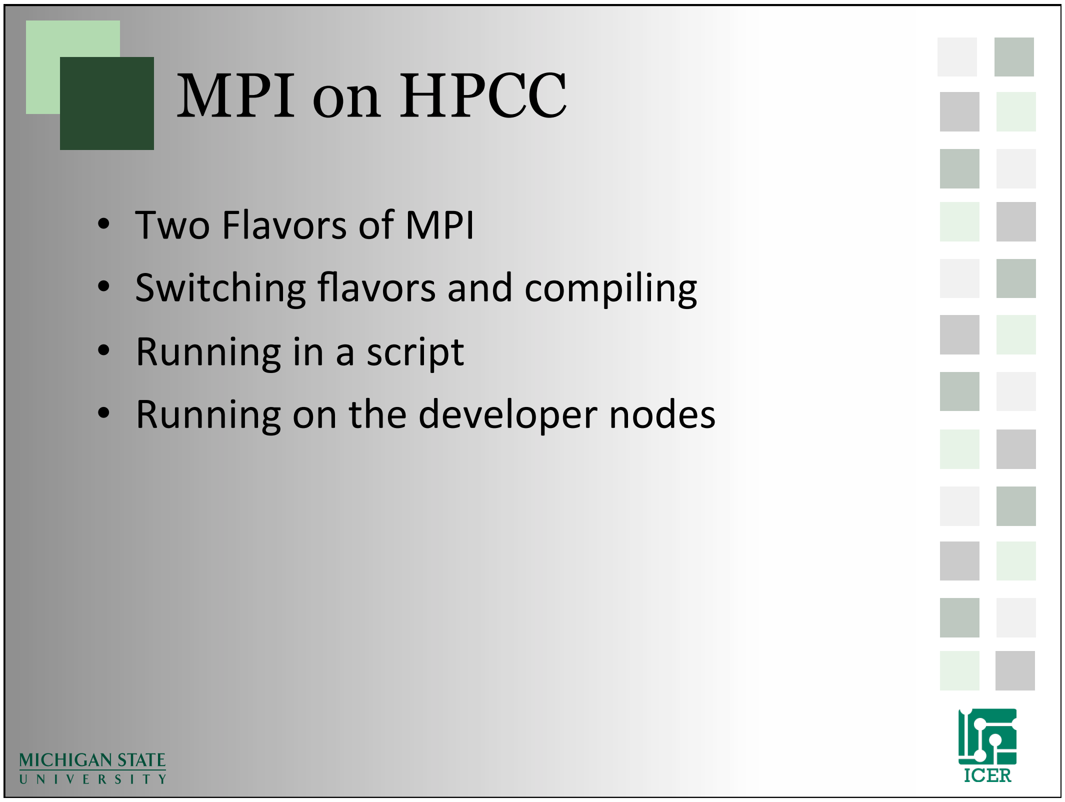
```
#!/bin/bash -login
#PBS -l walltime=00:01:00
#PBS -l nodes=1:ppn=1,feature=gdb

cd ${PBS_O_WORKID}
OMP_NUM_THREADS=`cat ${PBS_NODES} | wc -l`
export NUM_OMP_THREADS
./simpleOMP

qstat -f ${PBS_JOBID}
```

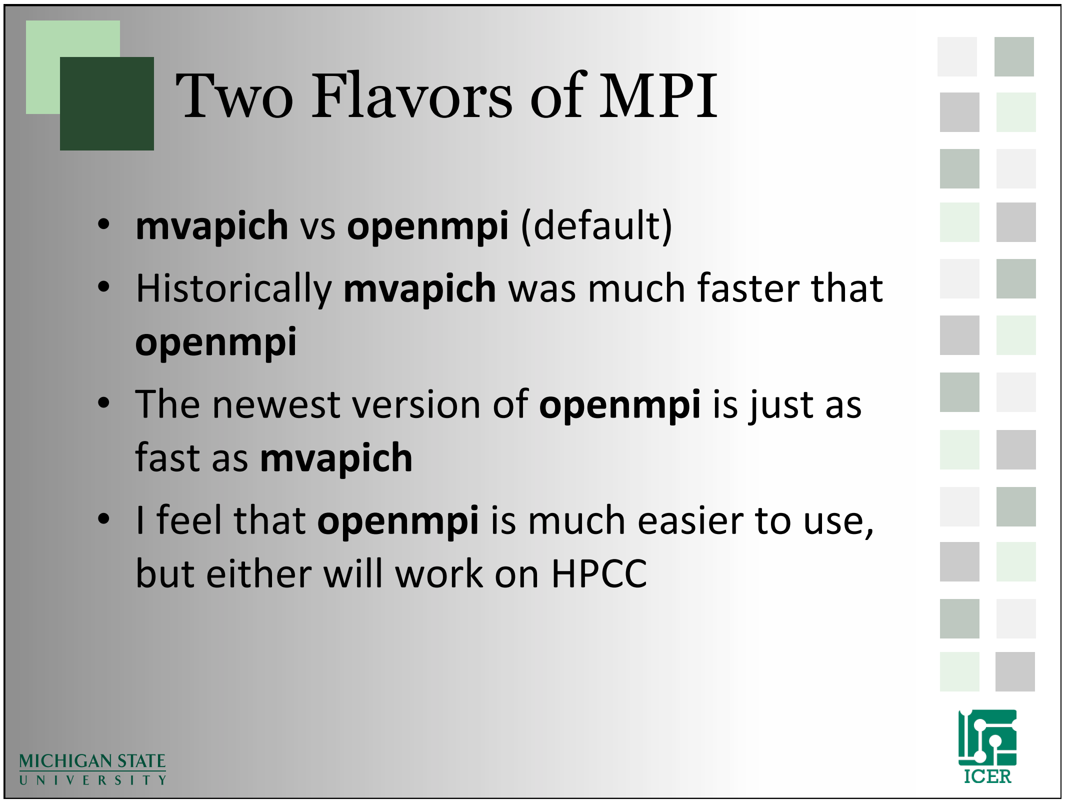


Shared Network Parallelization



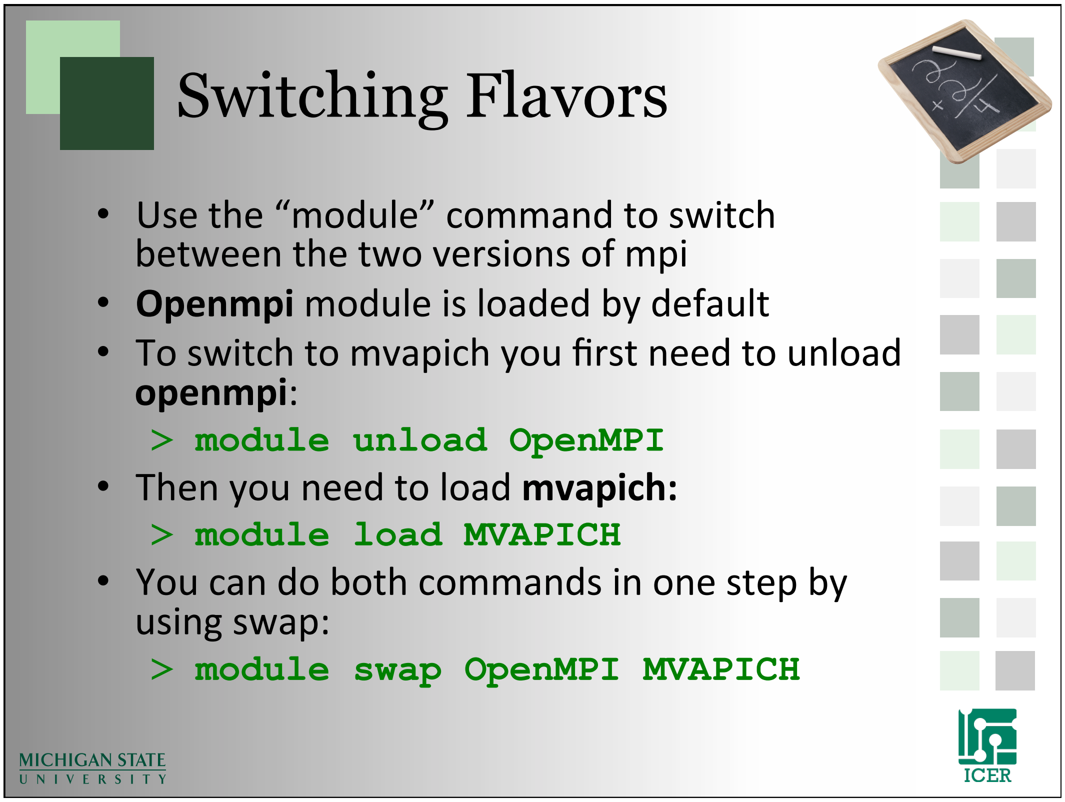
MPI on HPCC

- Two Flavors of MPI
- Switching flavors and compiling
- Running in a script
- Running on the developer nodes



Two Flavors of MPI

- **mvapich** vs **openmpi** (default)
- Historically **mvapich** was much faster that **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
```

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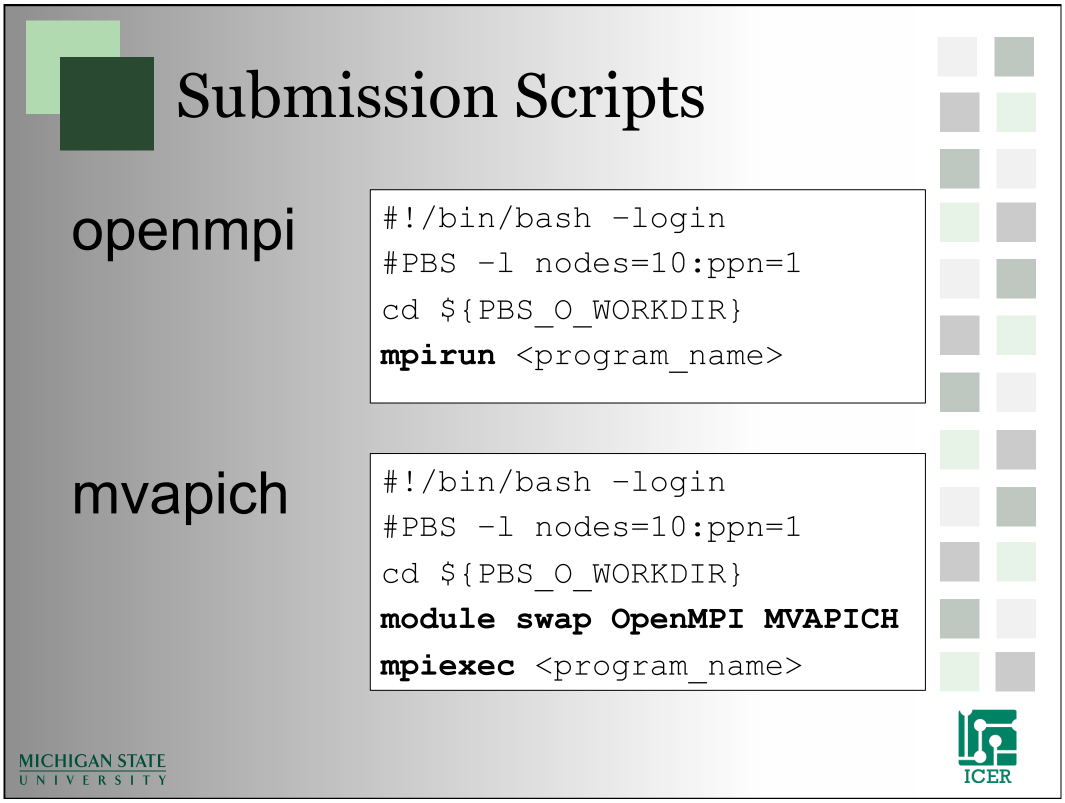

Submission Scripts

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>
```

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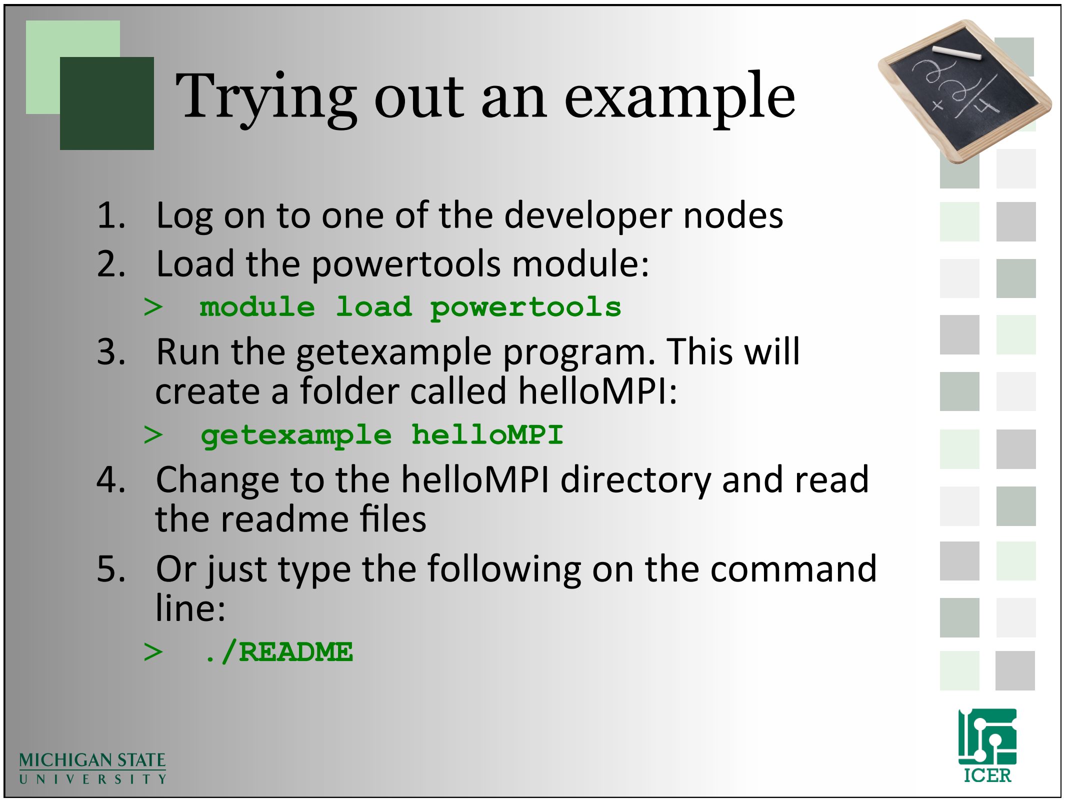

Trying out an example

1. Log on to one of the developer nodes
2. Load the powertools module:

```
> module load powertools
```

3. Run the getexample program. This will create a folder called helloMPI:

```
> getexample helloMPI
```

4. Change to the helloMPI directory and read the readme files
5. Or just type the following on the command line:

```
> ./README
```

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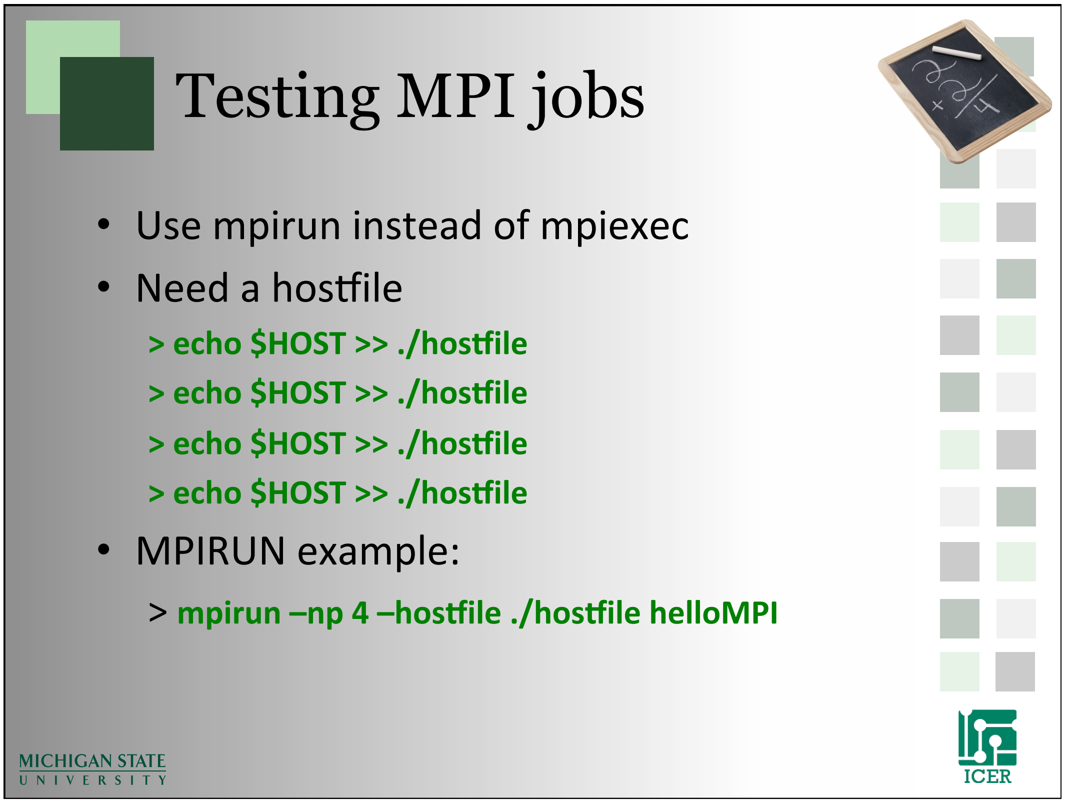

Testing MPI jobs

- 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
```

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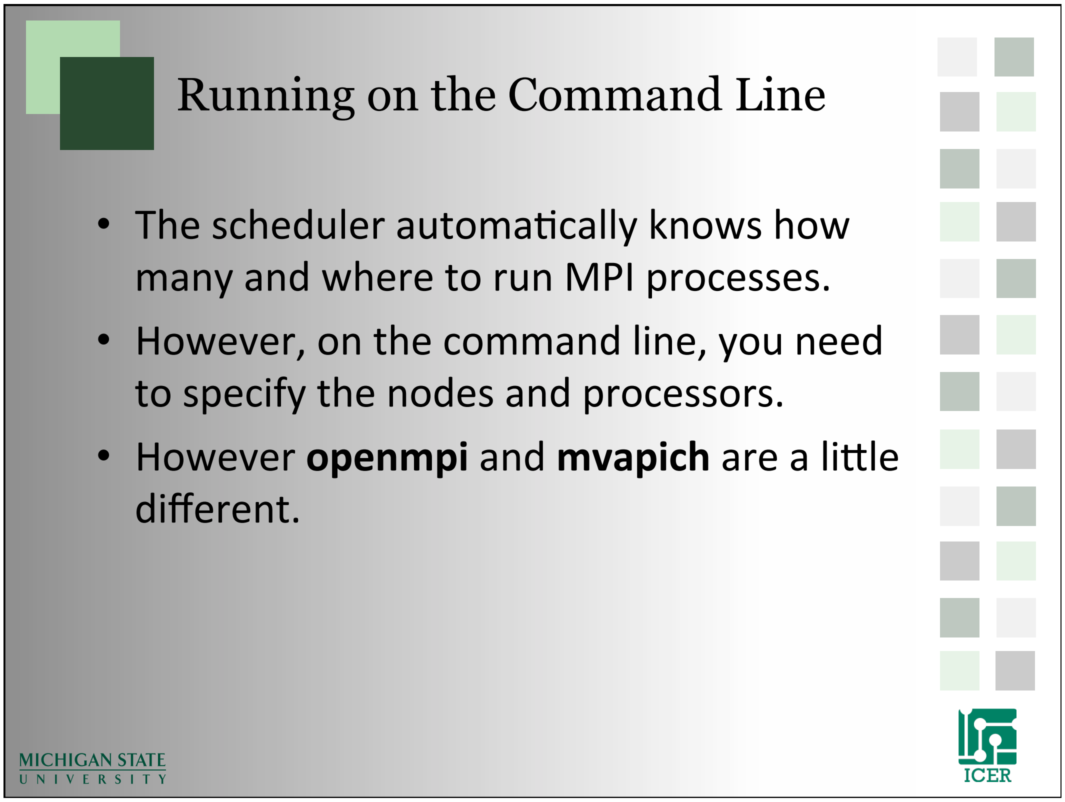

Running on the Command Line

- 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.
- However **openmpi** and **mvapich** are a little different.

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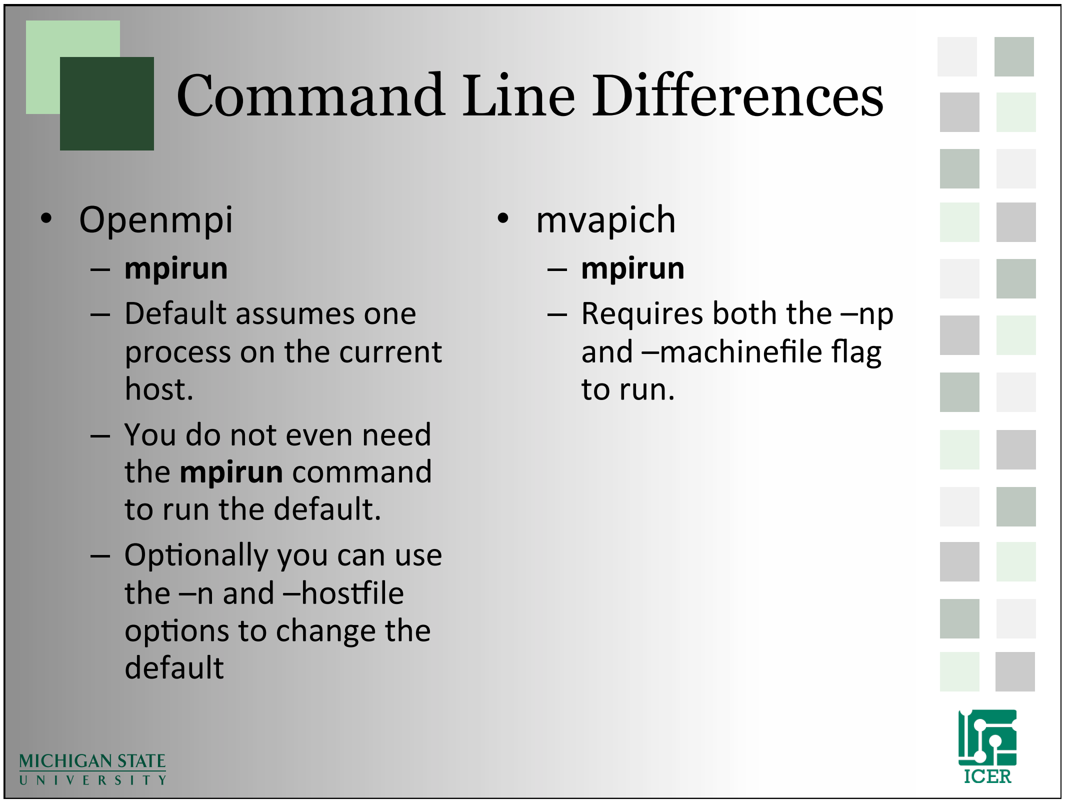

Command Line Differences

- 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.

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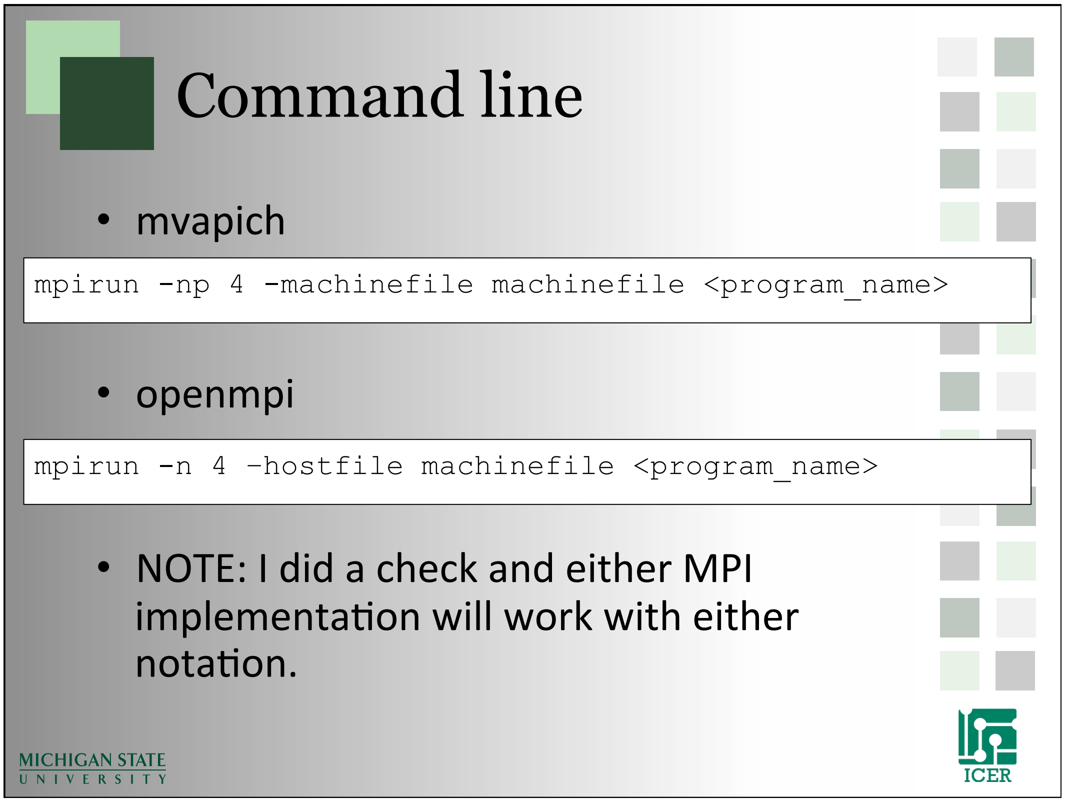

Command line

- mvapich

```
mpirun -np 4 -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.

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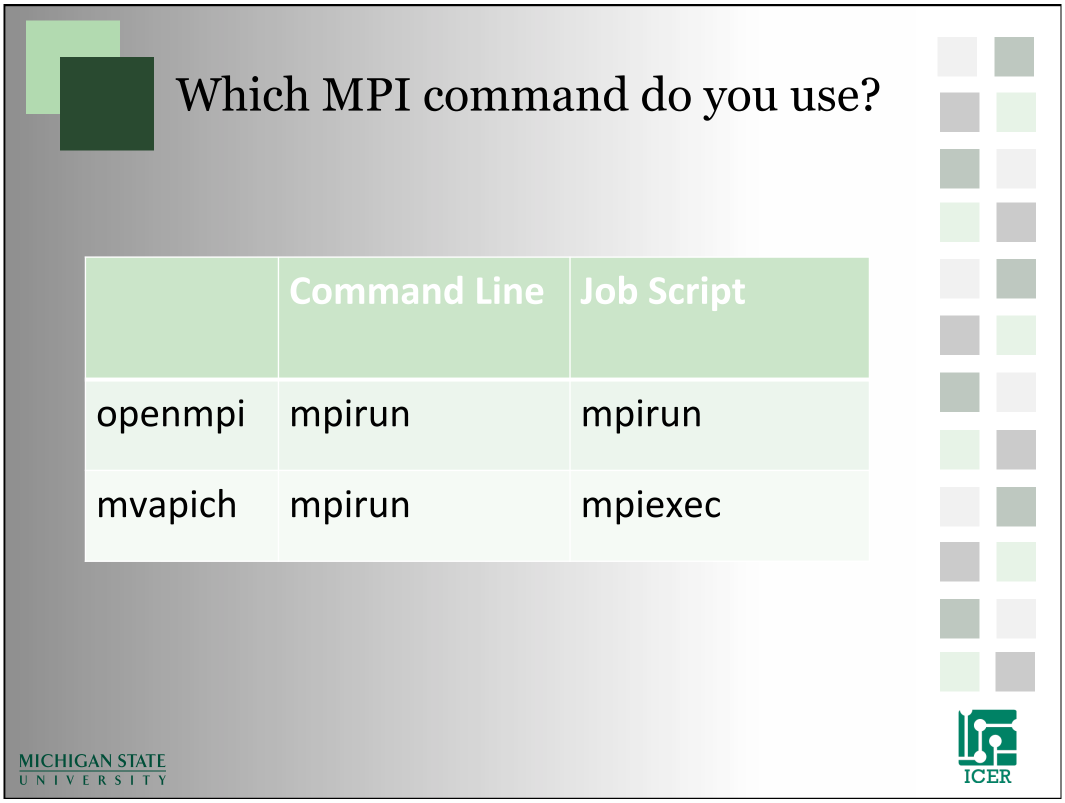

Which MPI command do you use?

	Command Line	Job Script
openmpi	mpirun	mpirun
mvapich	mpirun	mpiexec

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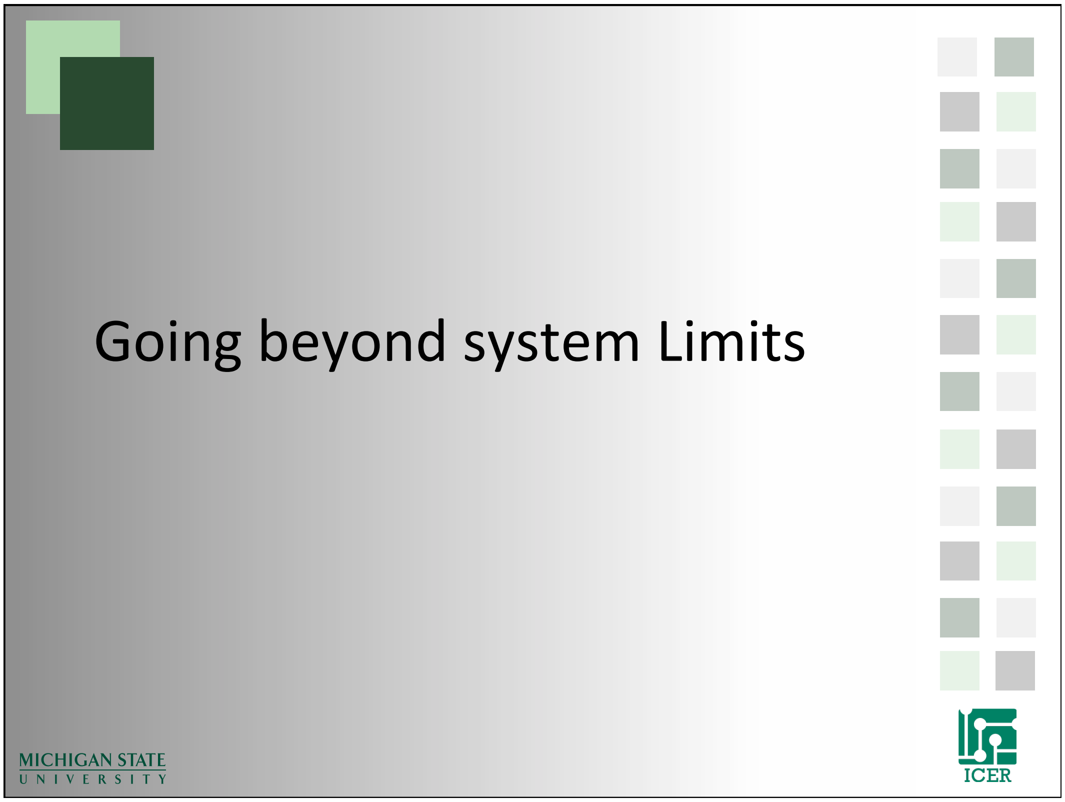

Going beyond system Limits

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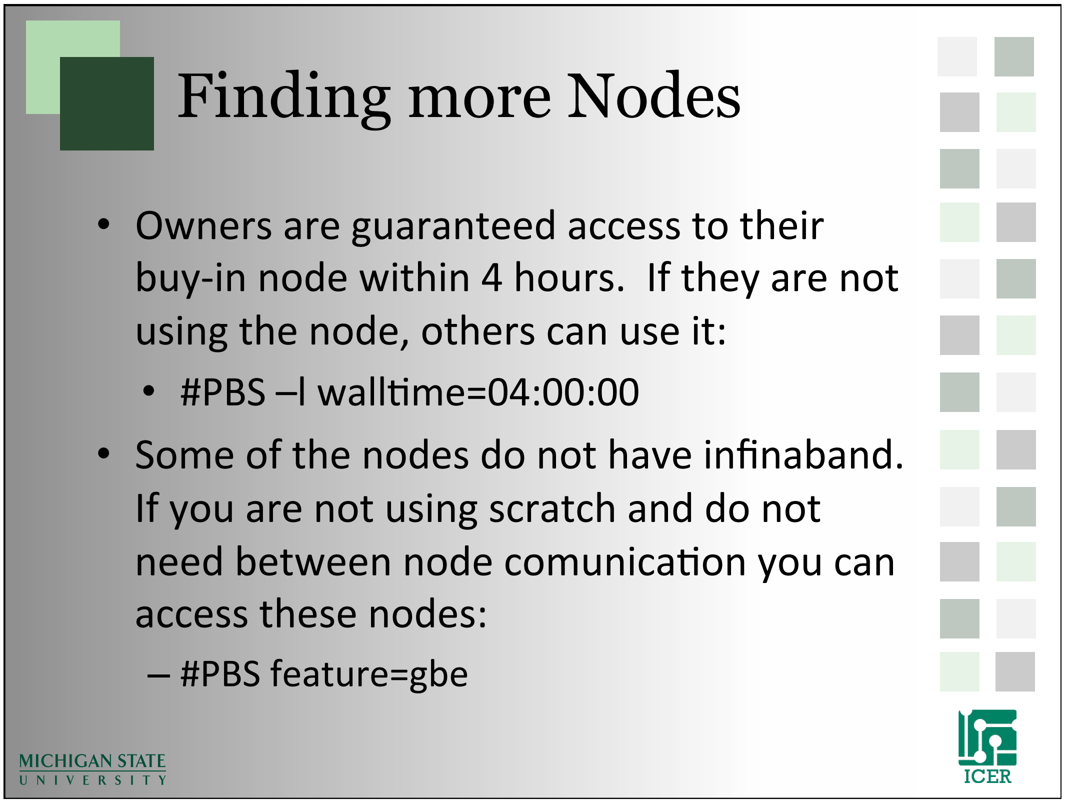

Finding more Nodes

- 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 infinaband. If you are not using scratch and do not need between node comunication you can access these nodes:
  - #PBS feature=gbe

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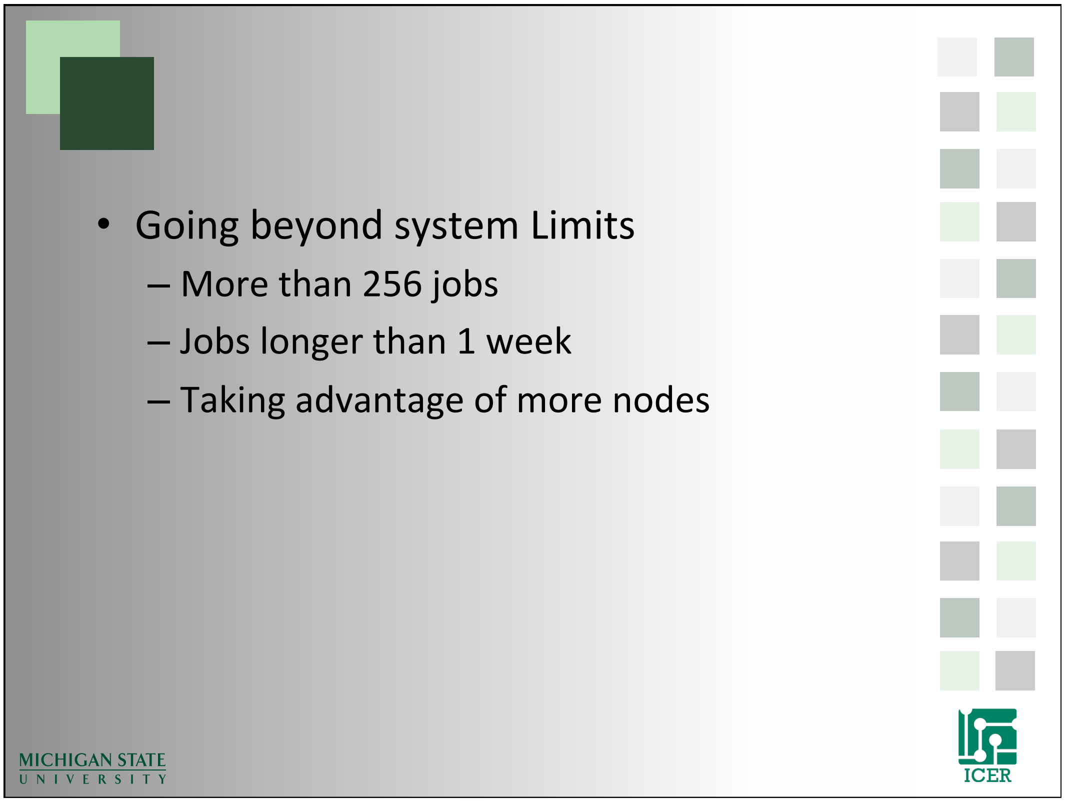
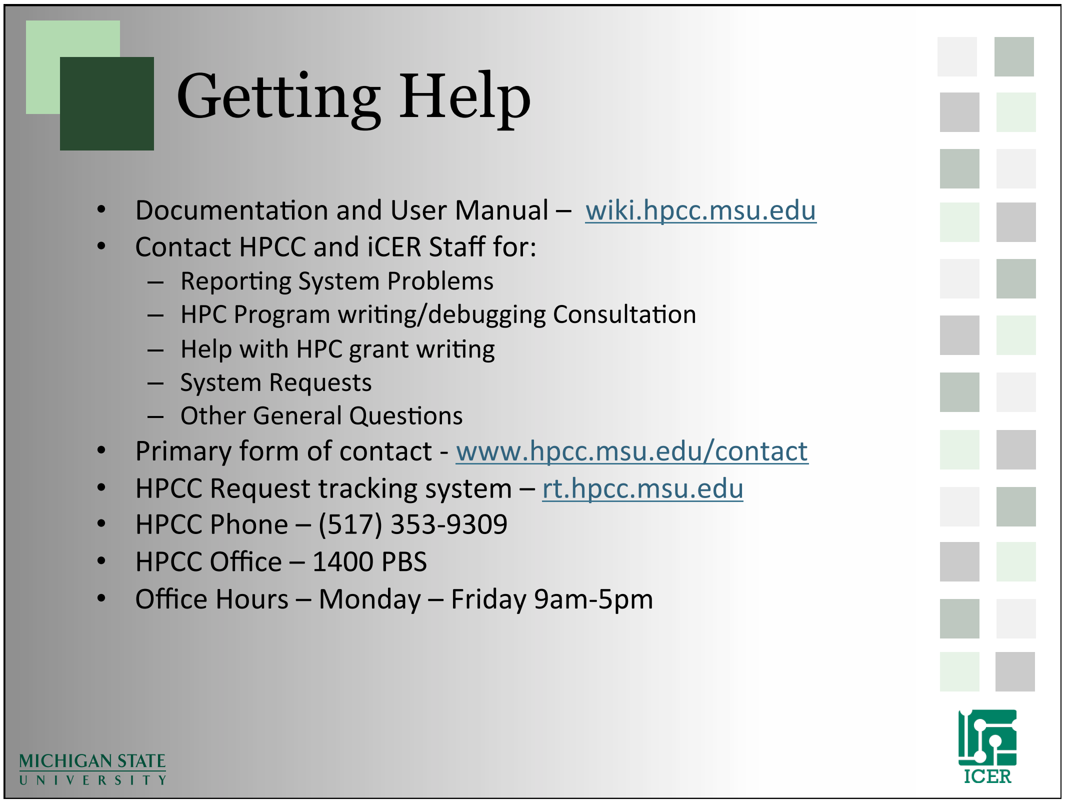


- Going beyond system Limits
  - More than 256 jobs
  - Jobs longer than 1 week
  - Taking advantage of more nodes



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 - www.hpcc.msu.edu/contact
- HPCC Request tracking system – rt.hpcc.msu.edu
- HPCC Phone – (517) 353-9309
- HPCC Office – 1400 PBS
- Office Hours – Monday – Friday 9am-5pm