# Making Your Research Go Faster: Advanced HPCC
May 8, 2013

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## XSEDE Multi-Site Workshop

XSEDE
Extreme Science and Engineering Discovery Environment

- **MPI Multi Site Workshop**: June 18-19

http://wiki.hpcc.msu.edu/

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# VSCSE – Summer Workshops

VIRTUAL SCHOOL OF COMPUTATIONAL SCIENCE AND ENGINEERING

MPI Multi Site Workshop

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- **Data Intensive Summer School**: July 8-10
- **Proven Algorithmic Techniques for Many-core processors**: July 29 - August 2

http://wiki.hpcc.msu.edu/

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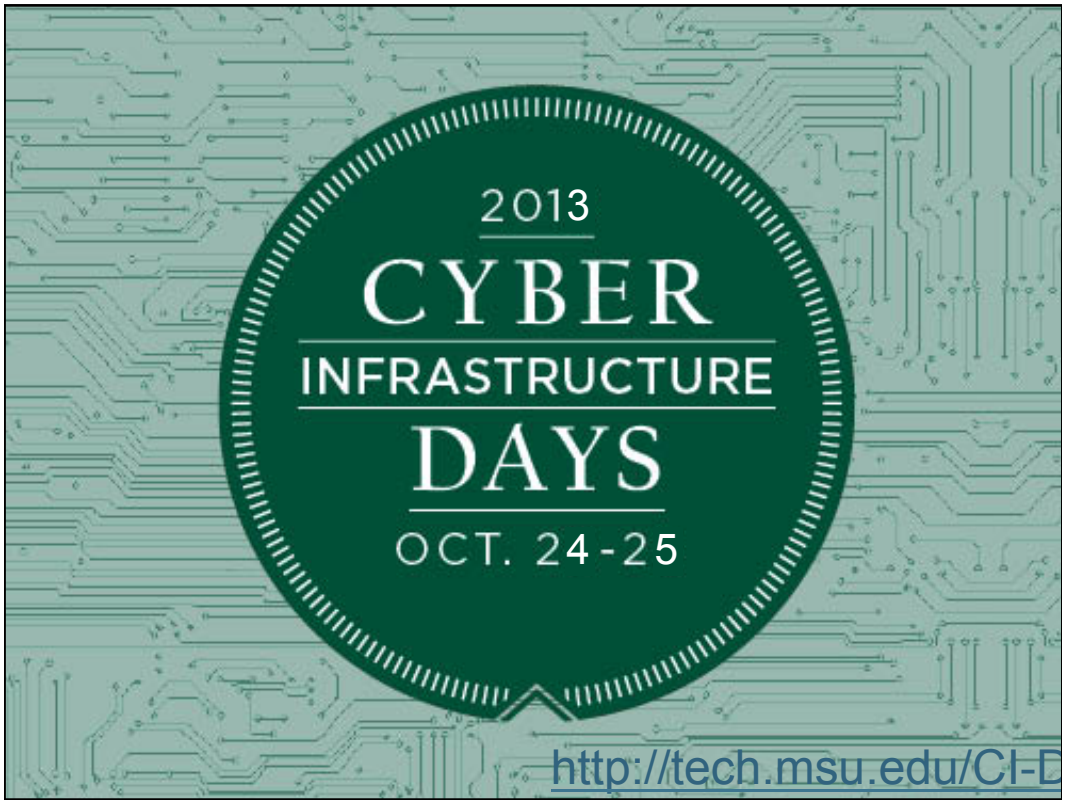

# Agenda

- **Overview**
- Advanced System Description
- Powertools
- Doing more faster
  - Pleasantly Parallel
  - Shared Memory Parallelization
  - Shared Network Parallelization
  - Accelerators

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# How this workshop works

- We are going to cover some basics. Lots 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:

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# Red and Green Flags

- Use the provided sticky notes to help me help you.
  - **Green** = I am doing fine.
  - **Red** = I am stuck and need more time and/or I could use some help.

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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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# What problems are we solving?

- Boundary Simulations
- Data Analysis
- Search

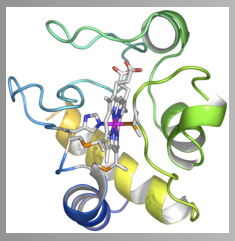
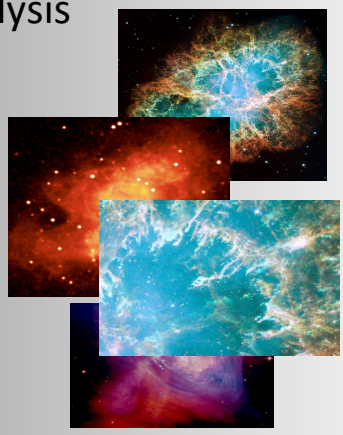


Image Provided by Dr. Warren F. Beck, MSU



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

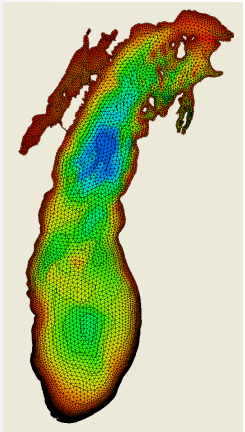


Image Provided by Dr. Mantha Phanikumar, MSU

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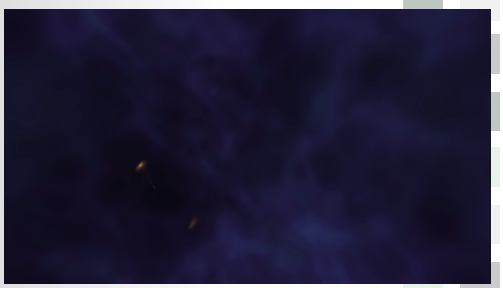
# Boundary Simulations

- Fluid dynamics
- Finite element analysis
- Molecular dynamics
- Weather
- Etc.



Formation of a spiral Galaxy
ENZO Simulation, Drs. O'Shea and Smith

- System of PDE (Partial Differential equations)
- Mathematically equivalent to inverse of a matrix

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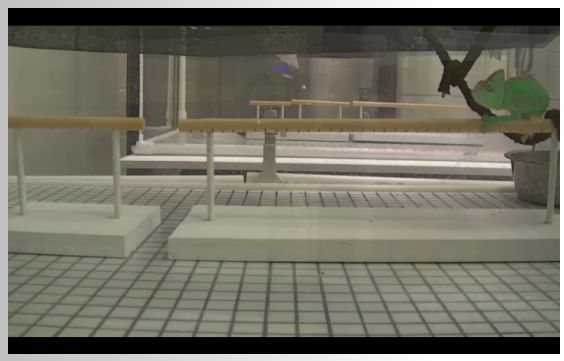
# Data Analysis

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



Video Provided by Dr. Fred Dyer

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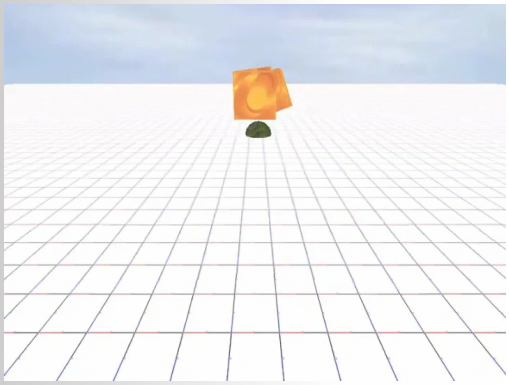
# Search

- Genome sequencing
- Analytics
- Optimization
- Etc.



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

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# Hardware Summary

FREE*

- Approximately 800 Nodes
- Approximately 4000 CPU cores
- Approximately 350TB of scratch space
- 2TB Shared memory machines
- 50GB backed up home directory space
- GPGPU cluster with 64 Tesla Nodes
- High Throughput condor cluster
- Specialized Bioinformatics VMs

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# General Purpose Clusters


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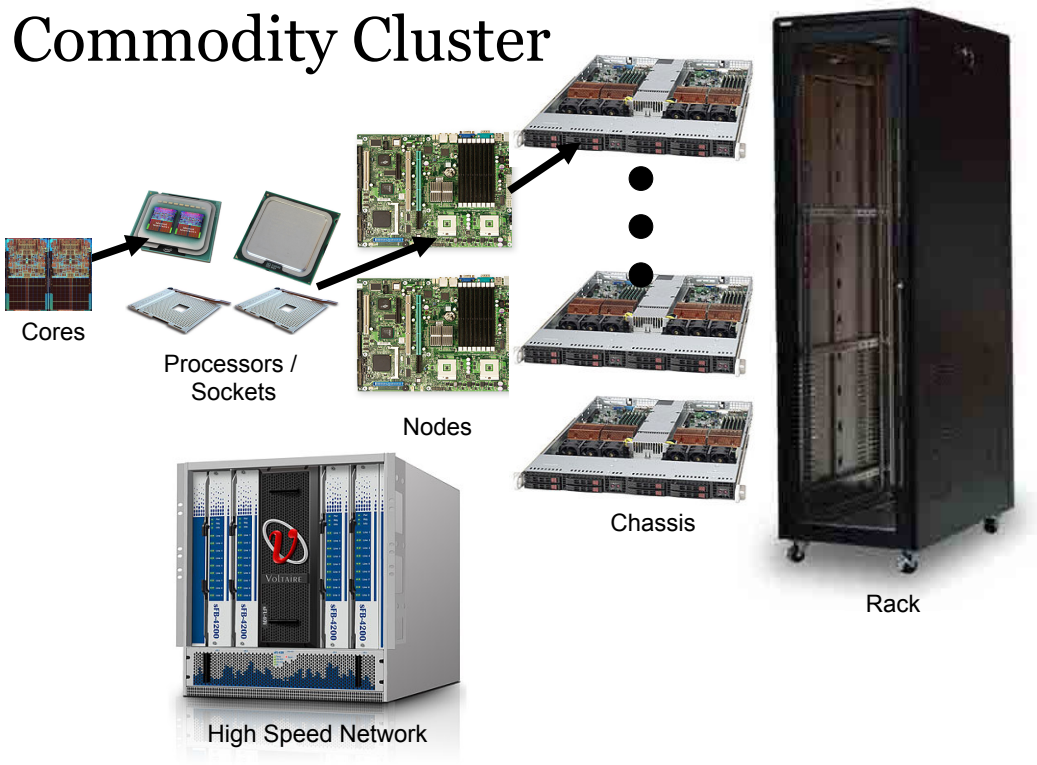
# Commodity Cluster



# 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

- In progress now!
  - General purpose cluster
  - Probably around $X,XXX per node or $XX,XXX per chassis
  - Possible large memory (256gb) option
  - Possible Accelerator Options
    - GPGPU
    - MIC / PHI
  - Please talk to me if you are interested or if you would like more details

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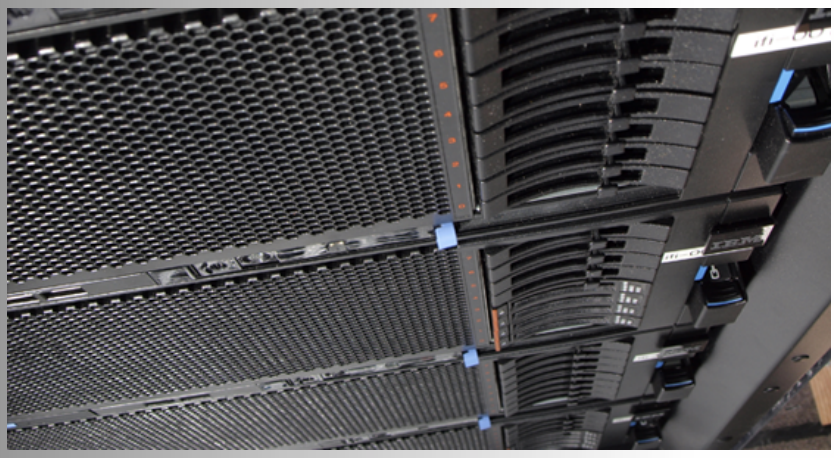
# Large Shared Memory Systems (Fat Nodes)



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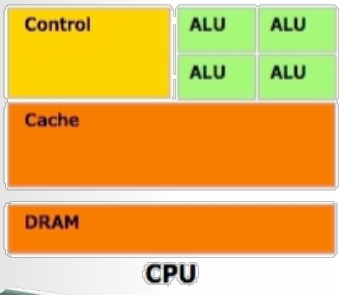
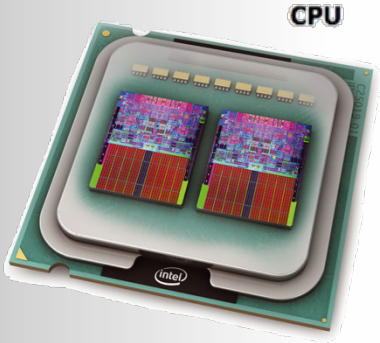
# Shared Memory Communication

- Cores on a processor share the same memory
- OpenMP
- Fat nodes
  - 64 cores
  - 2TB of memory



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# General Purpose GPU Accelerated Systems


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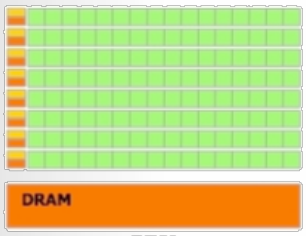
# GPUs

- 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!





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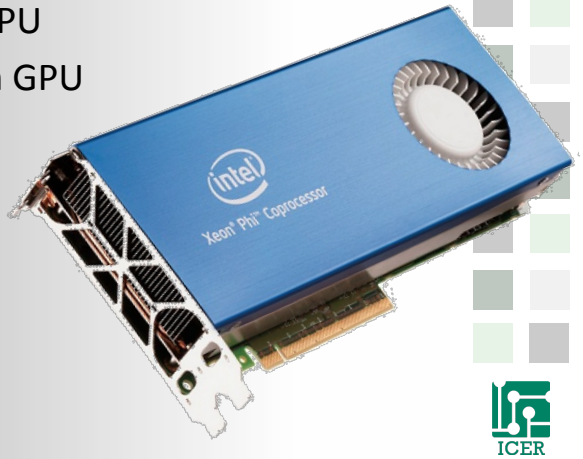
# Intel Xeon Phi

- Cross between CPU and GPU
- About 60 Pentium I cores
  - Less cores than GPU
  - Easier to use than GPU
    - OpenMP
    - MPI
- Very new
  - January 2013

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# High Throughput HTCondor Cluster

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# MSU HTCondor Cluster

- Runs like a screen saver and Scavenges CPU cycles:
  - Approximately 400 nodes
  - Approximately 800 cores
  - WindowsXP


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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
```

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# 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

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# 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

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# Even More Powertools

- **getexample** – provides a copy of examples for various tasks written by iCER staff
- **quota** – list your home directory disk usage

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## 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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# 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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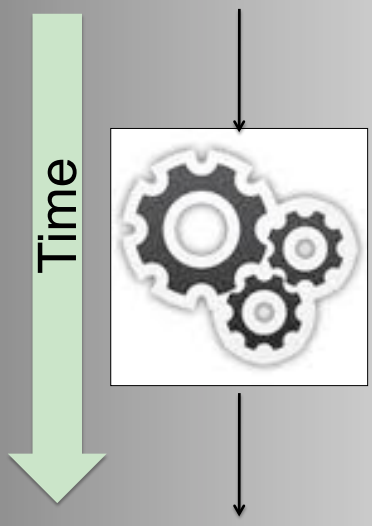
# Single Thread Jobs




One CPU can only run one thing at a time. (sort of)

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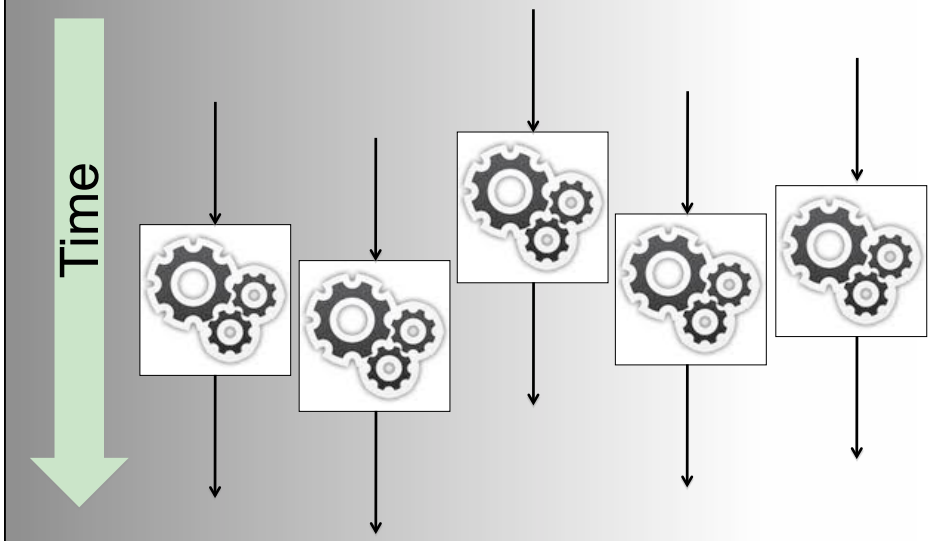
# Pleasantly Parallel

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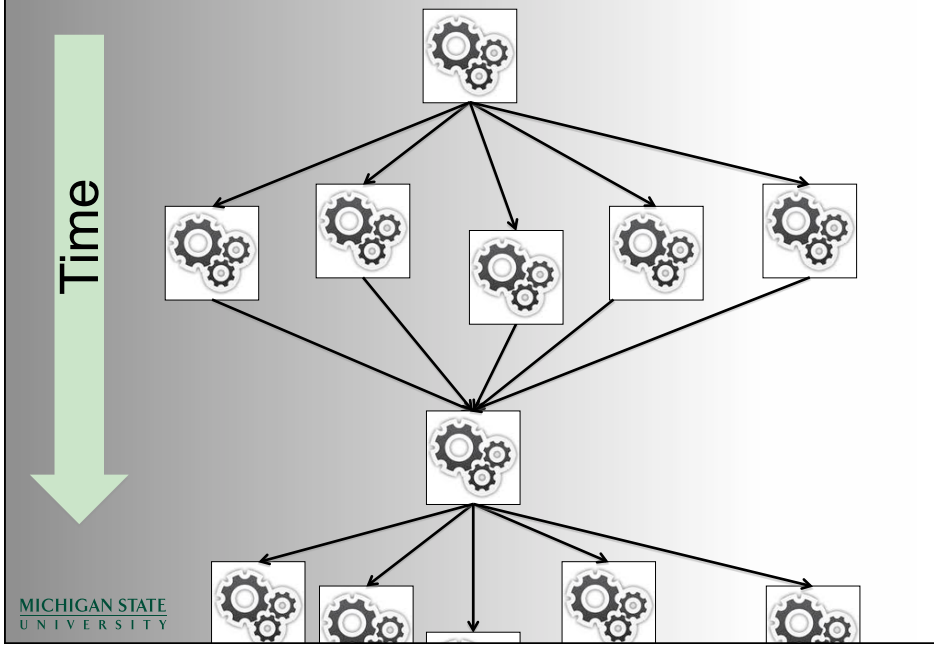
# Loosely Coupled

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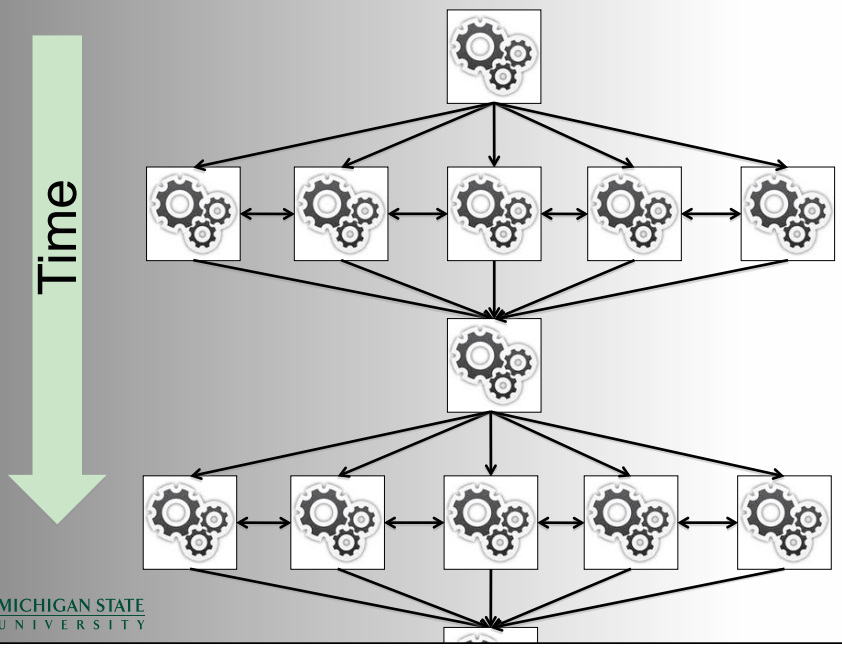
# Tightly Coupled

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# Communication

- Shared Memory
- Shared Network
- Distributed Network
- Dedicated Accelerators
- Hybrid Systems

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# Pleasantly Parallel

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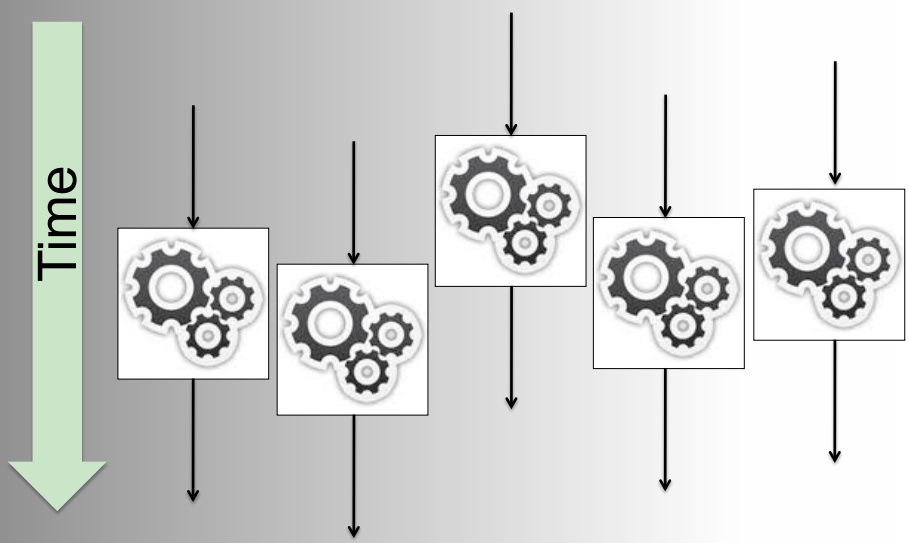
# Pleasantly Parallel

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

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# Who are you? -- Biometrics

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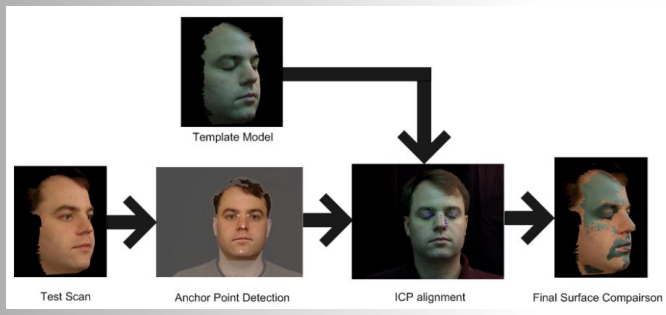
# Pairwise-All Problem

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

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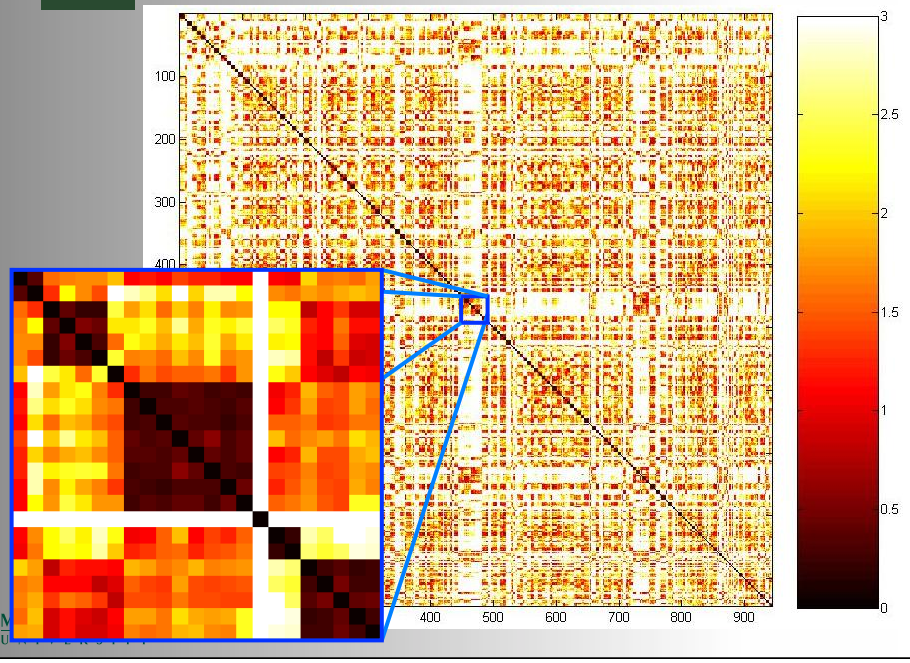
# 943 x 943 Similarity Matrix

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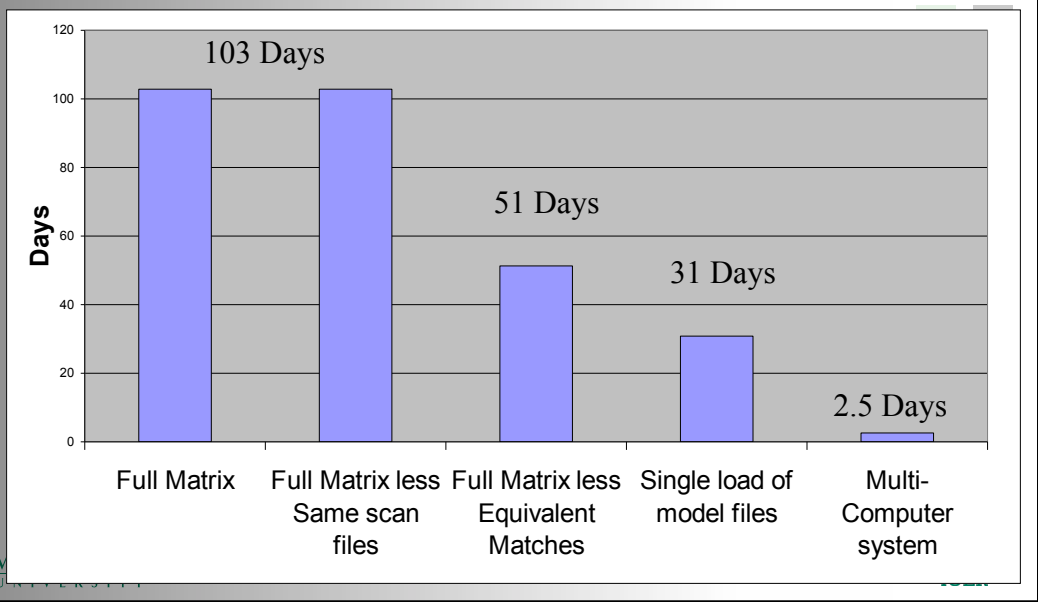
# Estimated Calculation Times

- 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



# 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



# 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

# 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 1-19

cd ${PBS_O_WORKDIR}

mkdir ${PBS_ARRAYID}
Cd ${PBS_ARRAYID}


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

qstat -f ${PBS_JOBID}
```

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# Example: Job Arrays

- Get the bleder_farm example:
  - `>getexample`
  - `>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`

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# HPCC Job array limitations

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

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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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# 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

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# 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}
```

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# 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 completed yet.
- 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
```

# 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}
```

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# 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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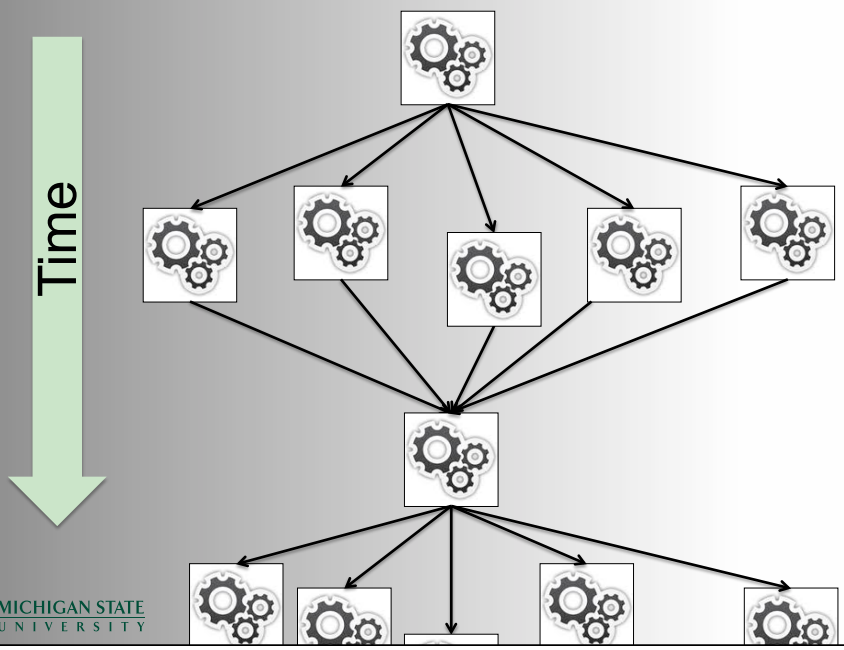
# Loosely Coupled

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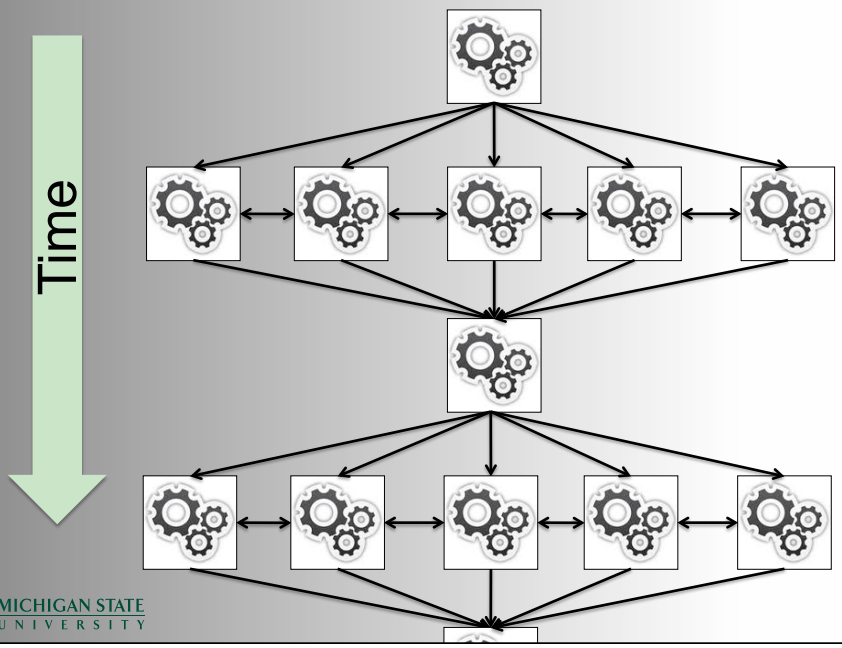
# Tightly Coupled

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# Shared Memory Parallelization

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# 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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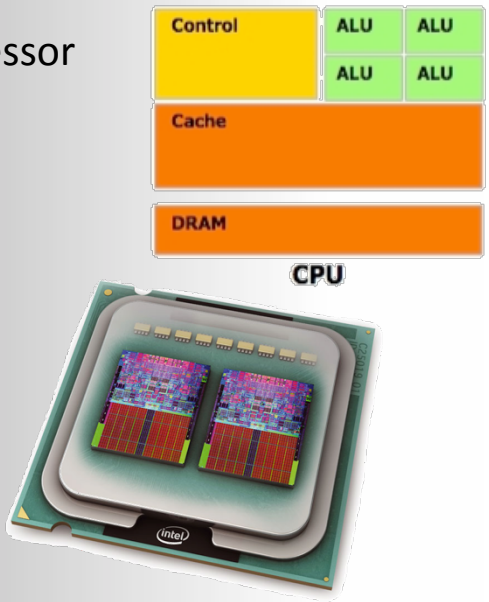
# Shared Memory Communication

- Cores on a processor share the same memory
- OpenMP
- Fat nodes
  - 64 cores
  - 2TB of memory

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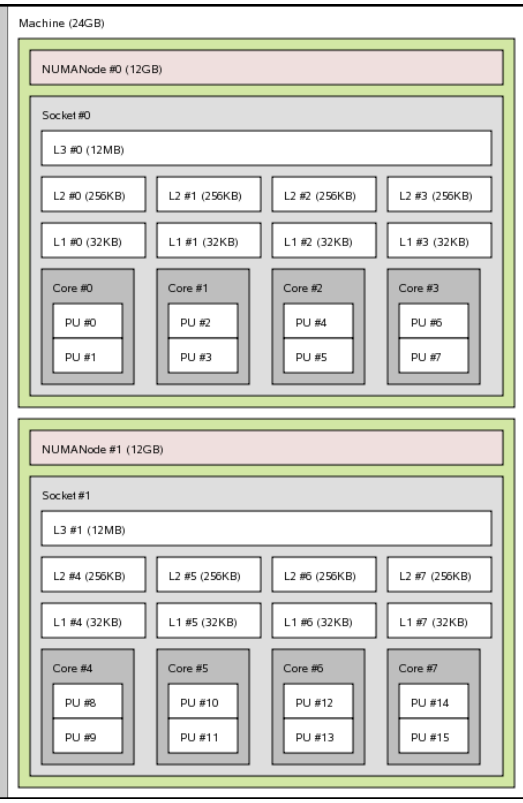
# Intel10

- 8 cores
- 24 GB memory

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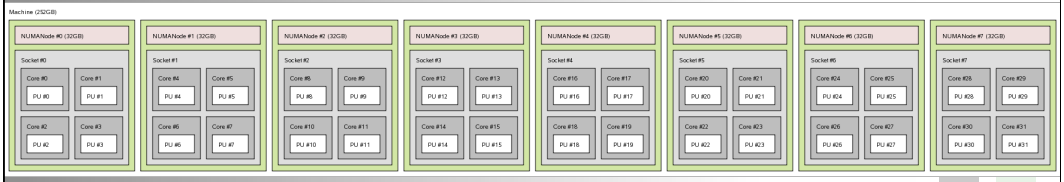
# amd09

- 32 cores
- 256 GB memory



- We have nodes with 64 cores and 2TB of memory

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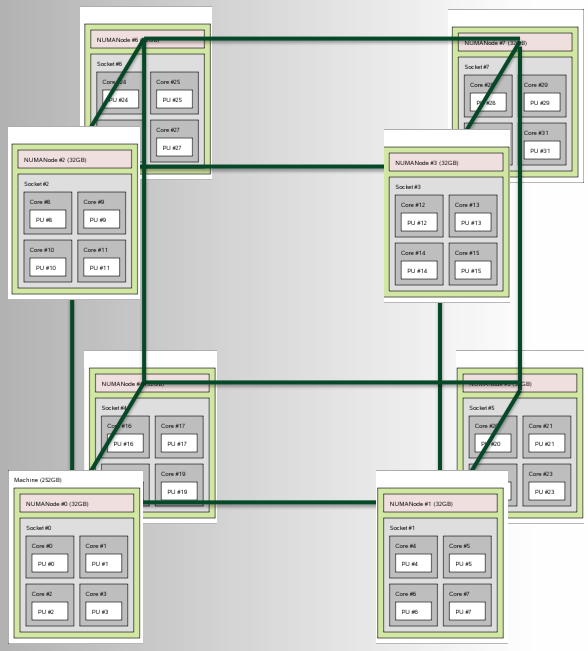
# NUMA



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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

```
>getexample bowtie
```

- Change to the bowtie directory

```
>cd ./bowtie
```

- Look at the submission script

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

- Run the job

```
>qsub bowtie.qsub
```

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# OpenMP

- Common Shared Memory parallelizaiton
- 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

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# OpenMP is easy

```
#include <omp.h>
...
  #pragma omp parallel for
  for (i=0;i<100;++i) {
    A(I) = A(I) + B
  }
...
```

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# Compile OpenMP Jobs

- Use compiler option openmpi.
  - –fopenmp
- Example:

gcc –fopenmp mycode.cc –o mycode

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# 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}
```

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# Shared Network Parallelization

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# 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
```

# MPI program (2 of 4)

```
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);
```

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# MPI program (3 of 4)

```
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);
   }
```

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# MPI program (4 of 4)

```
} 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);
}
```

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# 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

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# 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.
- **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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# Accelerator Cards

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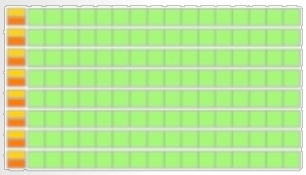
# GPUs

- 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!





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# 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.

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# 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)

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# 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;
    }
}
```

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# CUDA program (2 of 5)

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

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# CUDA program (3 of 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);


}
```

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# 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

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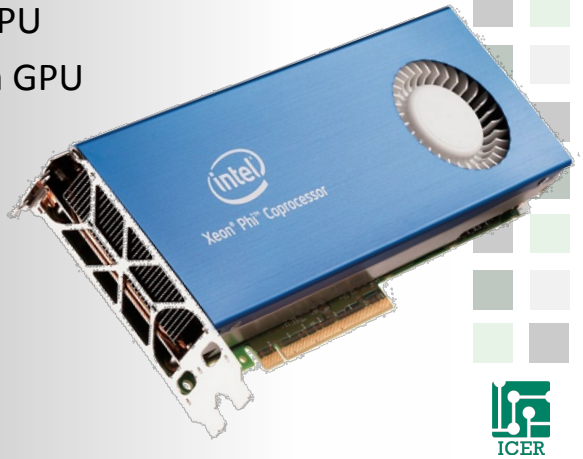
# Intel Xeon Phi

- Cross between CPU and GPU
- About 60 Pentium I cores
  - Less cores than GPU
  - Easier to use than GPU
    - OpenMP
    - MPI
- Very new
  - January 2013

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# 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.

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# My Recommendations

- Plesently Parallel
- OpenMP
- OpenMP on Phi
- MPI
- MPI on Phi?
- GPGPU


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# Going beyond system Limits

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

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

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# 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

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# myqusb

- Powertool that allows you to submit as many jobs as you want.
- Stores jobs in a local FIFO queue.
- Use “myqsub next” at the end of each job script to submit the next job.
- Type“myqsub manual” for more information

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# 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

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