Parallel Paradigms

Dirk Colbry, Research Specialist
Institute for Cyber-Enabled Research

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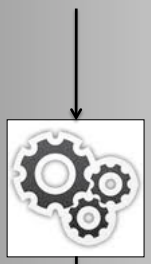
Scientific Programming

Time



Inputs (Data)

Computation

Outputs (Results)

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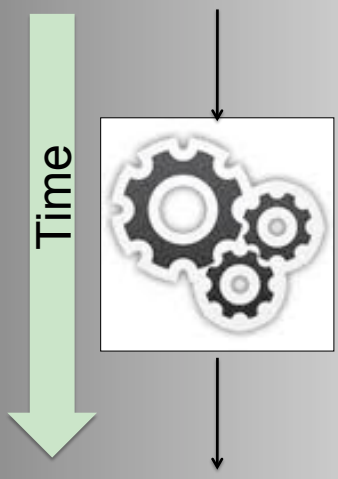
Single Thread Jobs



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

Goal: Use more than one CPU at a time to get more work done

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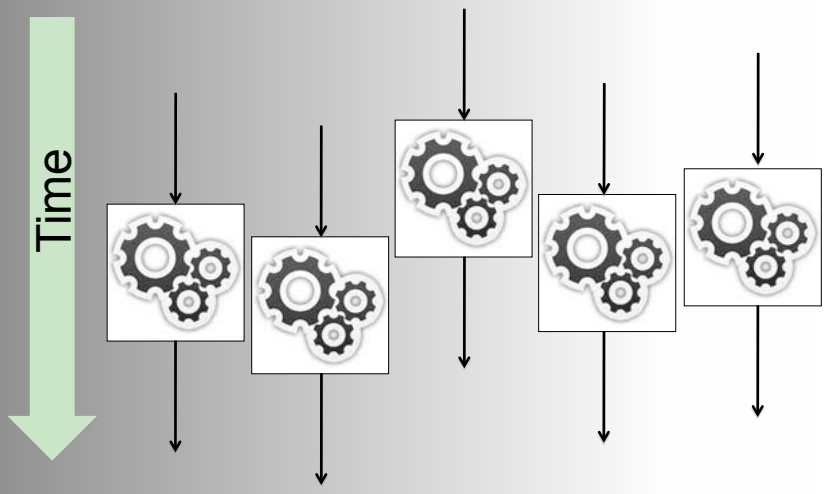
Pleasantly Parallel



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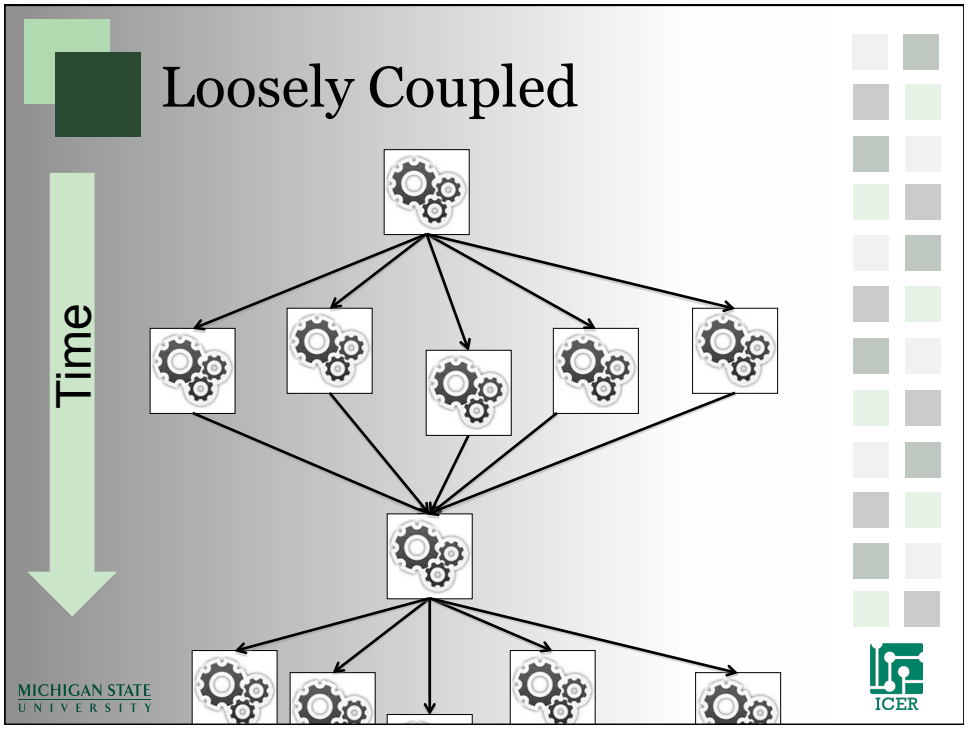
Loosely Coupled
Time
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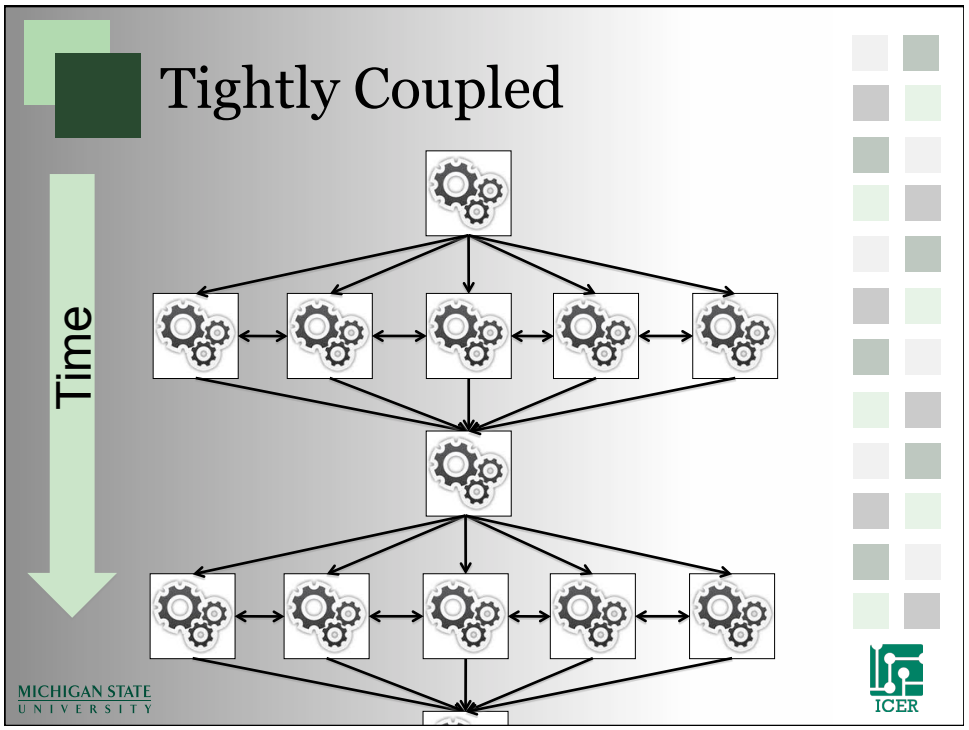
Tightly Coupled
Time
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Agenda

- Introduction to High Performance Computing
- Job Schedulers
- Example Computational Research Problems
- Running Code in Parallel

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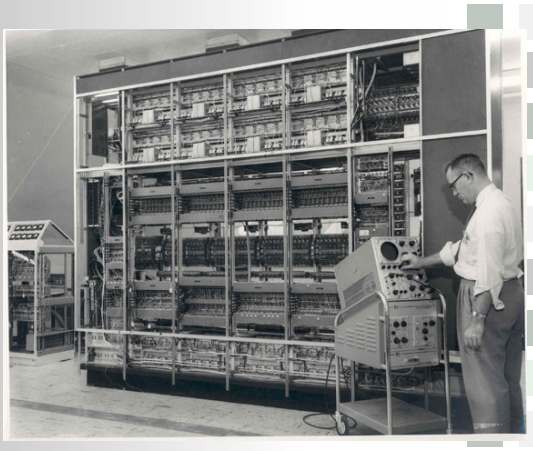
1957 MISTIC Mainframe

- MSU's first mainframe
- Hand built by grad students
  - Dick Reid
  - Glen Keeney



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After MISTIC

- 1957 MISTIC
- 1963-1973 CDC 3600
- 1967 Computer Science Department
- 1968 CDC 6500
- 1971 MERIT
- 1978 Cyber 750
- **2004 HPCC**
- **2009 ICER**

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2004 MSU HPCC

- Provide a level of performance beyond what you could get and reasonably maintain as a small group
- Provide a variety of technology, hardware and software, that would allow for innovation not easily found

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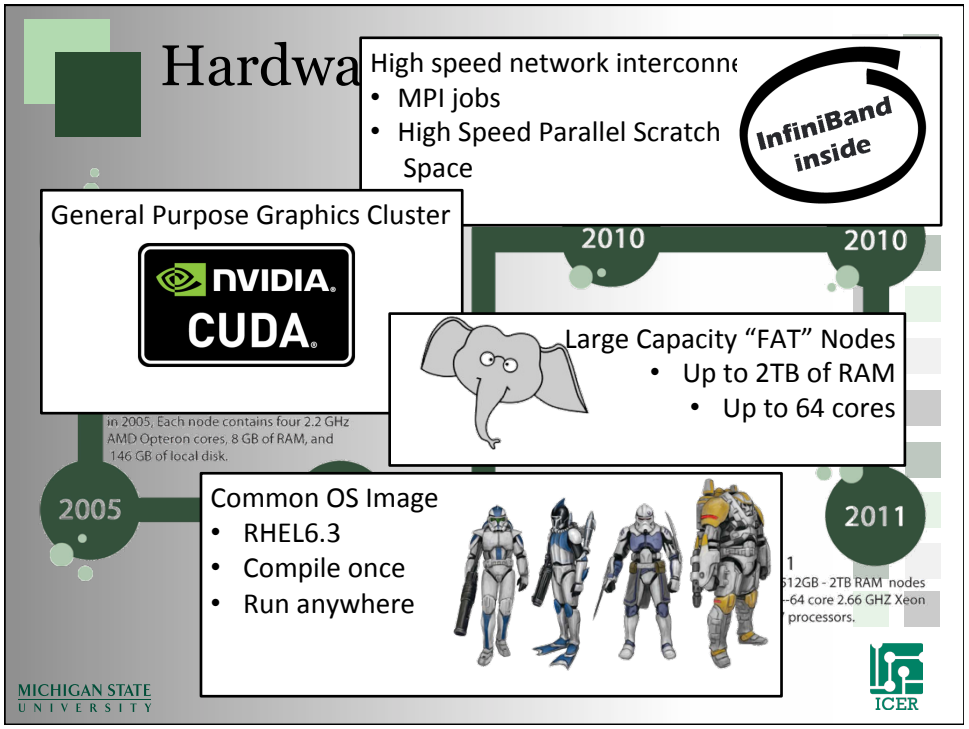
Hardwa
High speed network interconne
• MPI jobs
• High Speed Parallel Scratch Space
InfiniBand inside
General Purpose Graphics Cluster
NVIDIA CUDA
2010
2010
Large Capacity "FAT" Nodes
• Up to 2TB of RAM
• Up to 64 cores
in 2005, Each node contains four 2.2 GHz AMD Opteron cores, 8 GB of RAM, and 146 GB of local disk.
2005
Common OS Image
• RHEL6.3
• Compile once
• Run anywhere
2011
512GB - 2TB RAM nodes
-64 core 2.66 GHZ Xeon
processors.
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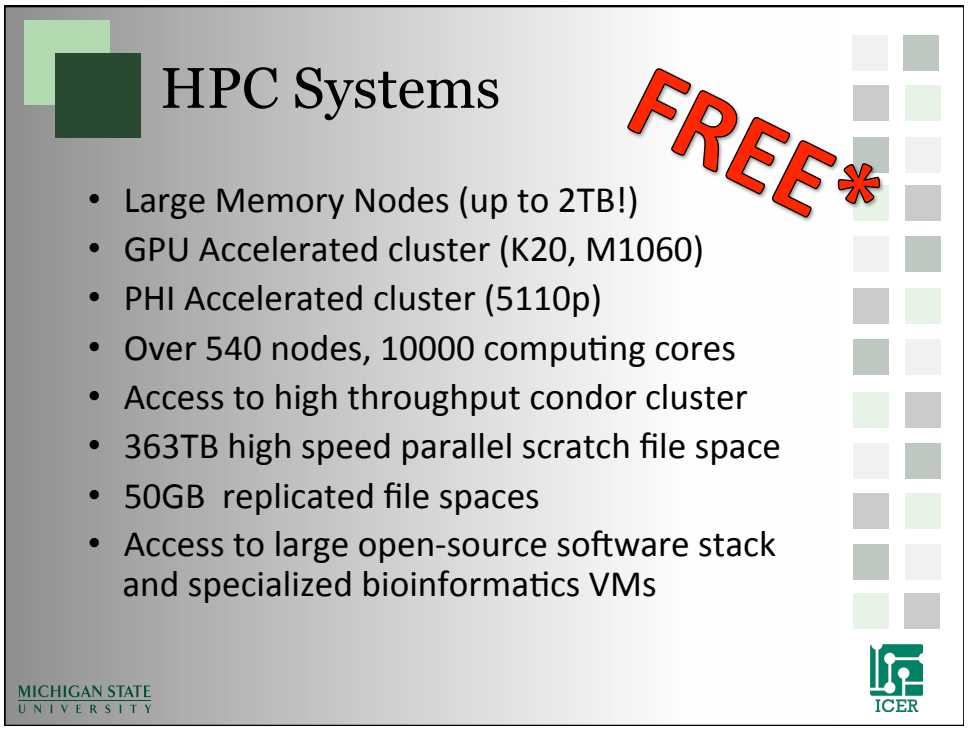
HPC Systems
FREE*
• Large Memory Nodes (up to 2TB!)
• GPU Accelerated cluster (K20, M1060)
• PHI Accelerated cluster (5110p)
• Over 540 nodes, 10000 computing cores
• Access to high throughput condor cluster
• 363TB high speed parallel scratch file space
• 50GB replicated file spaces
• Access to large open-source software stack and specialized bioinformatics VMs
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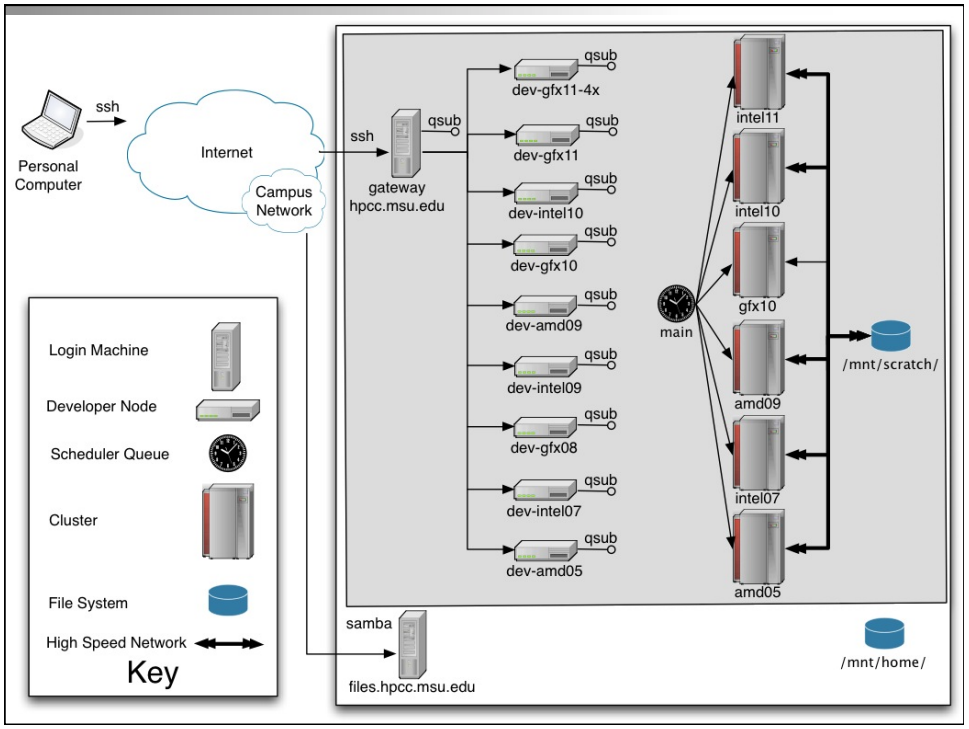

Commodity Cluster

- Most computers at HPCC fall into this category:
  - Racks of commodity Nodes
  - Connected with network
  - Uses a scheduler to run jobs.

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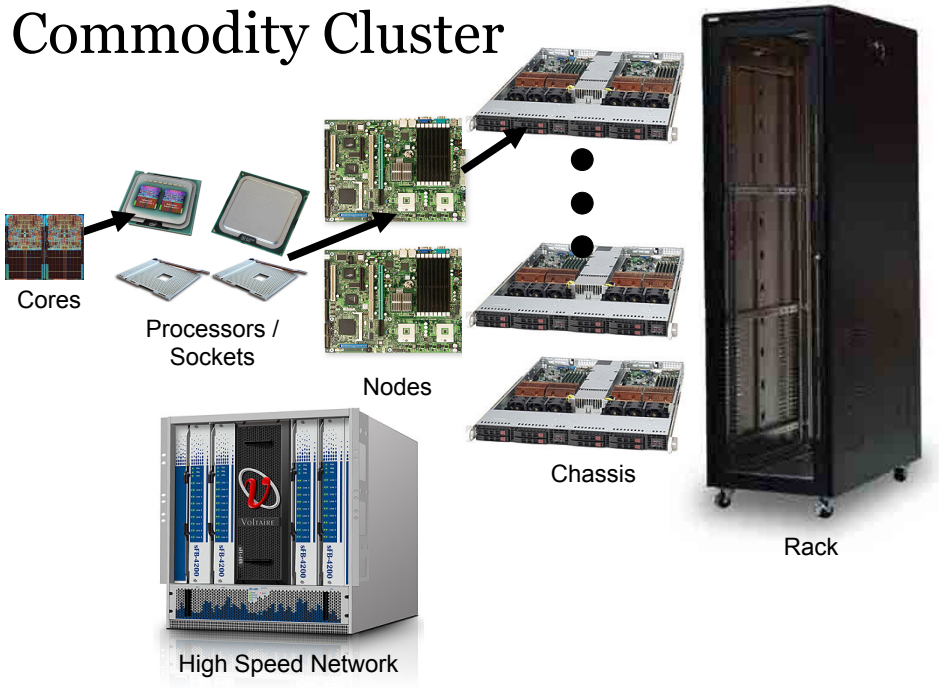
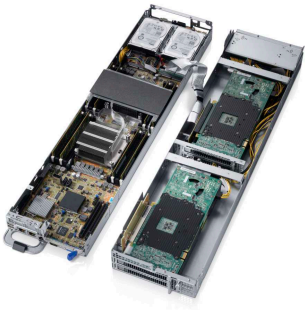
Commodity Cluster



Blade System (Cluster 14)



- General purpose base nodes
  - 20 cores, 64 gb
- 256gb nodes
- 256gb and 2xK20 GPU nodes
- 256gb and 2xPhi Card nodes

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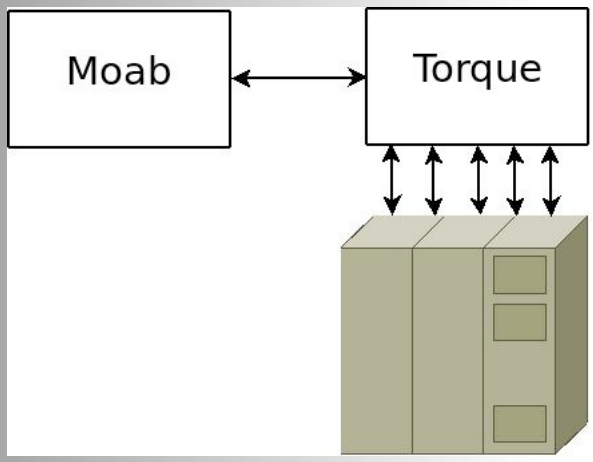
Resource Manager and scheduler



Not First In First Out!!

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Schedulers vs Resource Managers

- Scheduler
  (Moab)
  - Tracks and assigns
    - Memory
    - CPUs
    - Disk space
    - Software Licenses
    - Power / environment
    - Network
- Resource Manager
  (PBS/Torque)
  - Hold jobs for execution
  - Put the jobs on the nodes
  - Monitor the jobs and nodes

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Submission Script

1. List of required resources
2. All command line instructions needed to run the computation

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Typical Submission Script

Shell Comment

Define Shell

```
#!/bin/bash -login
#PBS -l walltime=10:00:00,mem=3Gb,nodes=10:ppn=1
#PBS -j oe

cd ${PBS_O_WORKDIR}

./myprogram -my input arguments

qstat -f ${PBS_JOBID}
```

Resource Requests

Shell Commands

Special Environment Variables

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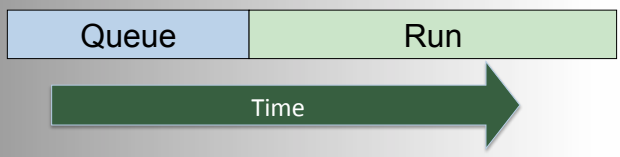
Submitting a job

- qsub –arguments <Submission Script>
  - Returns the job ID. Typically looks like the following:
    - 5945571.cmgr01
- Time to job completion



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Scheduling Priorities

- Jobs that use more resources get higher priority (because these are hard to schedule)
- Smaller jobs are backfilled to fit in the holes created by the bigger jobs
- Eligible jobs acquire more priority as they sit in the queue
- Jobs can be in three basic states:
  - Blocked, eligible or running

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What problems are we solving?

- Boundary Simulations
- Data Analysis
- Search

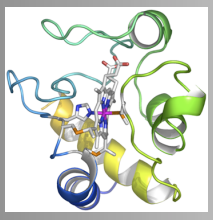
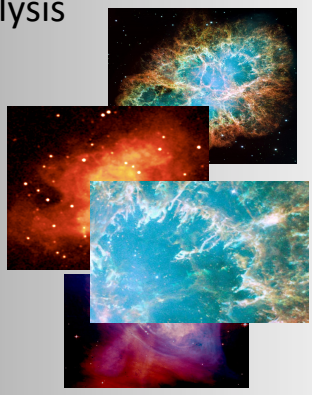


Image Provided by Dr. Warren F. Beck, MSU



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

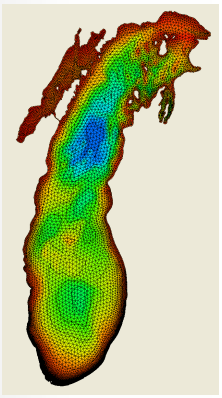


Image Provided by Dr. Mantha Phanikumar, MSU

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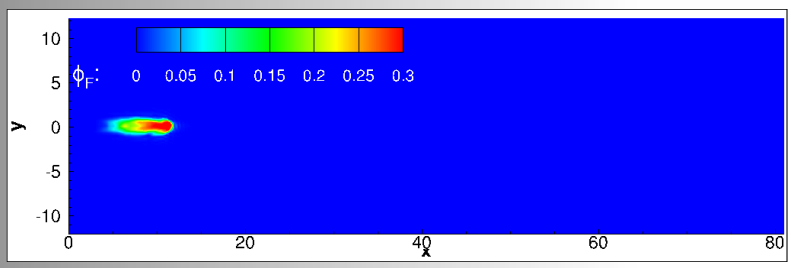
Boundary Simulations

- 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

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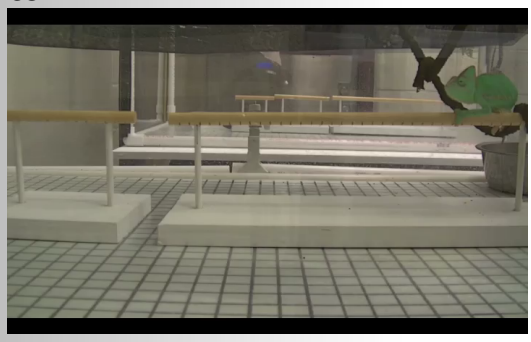
Data Analysis

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



Video Provided by Dr. Fred Dyer

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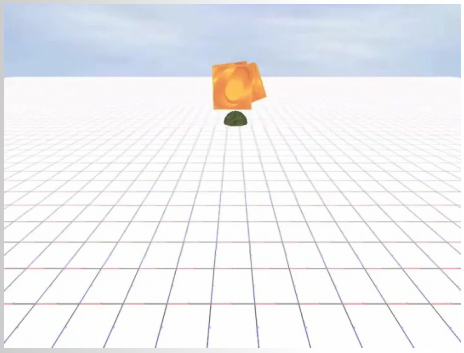
Search

- Genome sequencing
- Analytics
- Optimization
- Etc.



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

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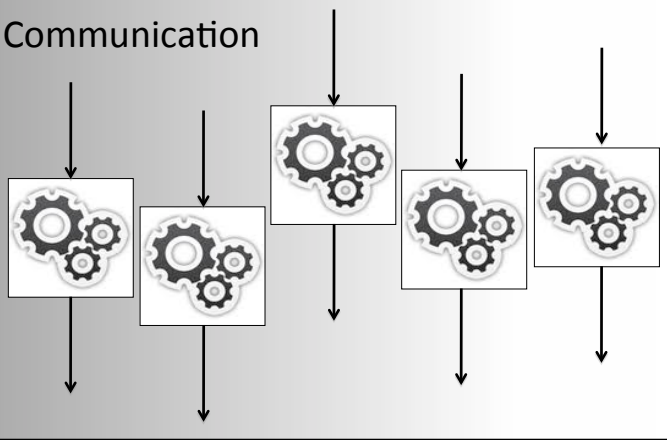
Pleasantly Parallel

- Lots-o-Computers
- Same thing different data
- No Communication



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Example

- Folder full of input files:

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

- Want folder full of output files:

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

- Command Syntax:
  - ./myprogram inputfile > outputfile

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Simple Job Array

```
#!/bin/bash -login
#PBS -l walltime=00:05:00,mem=2gb
#PBS -l nodes=1:ppn=1,feature=gbe
#PBS -t 1-200

cd ${PBS_O_WORKDIR}

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

qstat -f ${PBS_JOBID}
```

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Condor High Throughput Computing

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

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Communication

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

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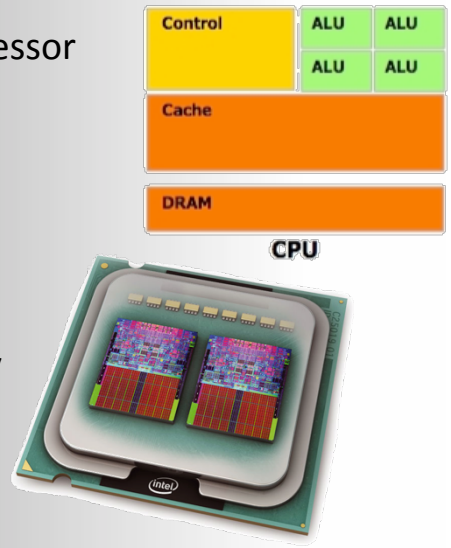
Shared Memory Communication

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



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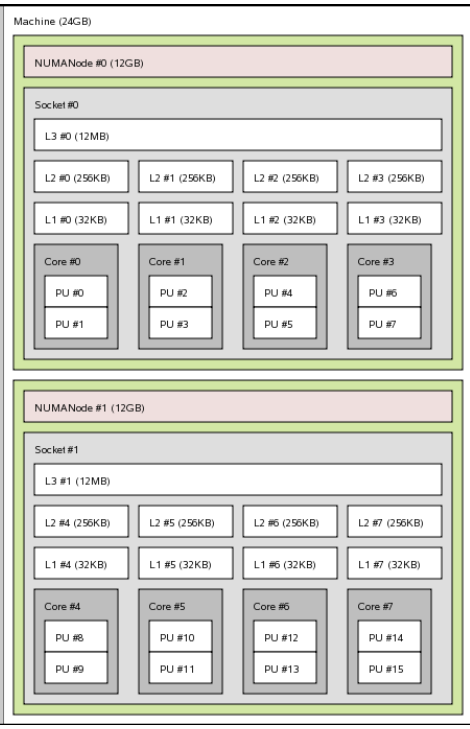
Intel10

- 8 cores
- 24 GB memory

Figure Generated using hwloc



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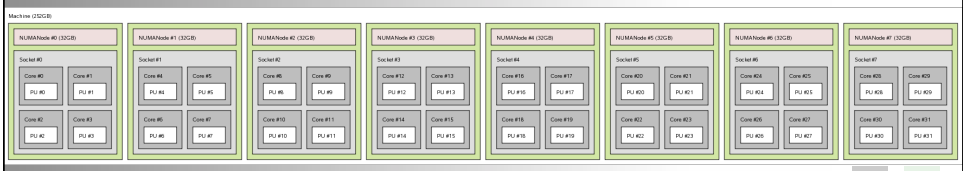
amd09

- 32 cores
- 256 GB memory



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

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Figure Generated using hwloc

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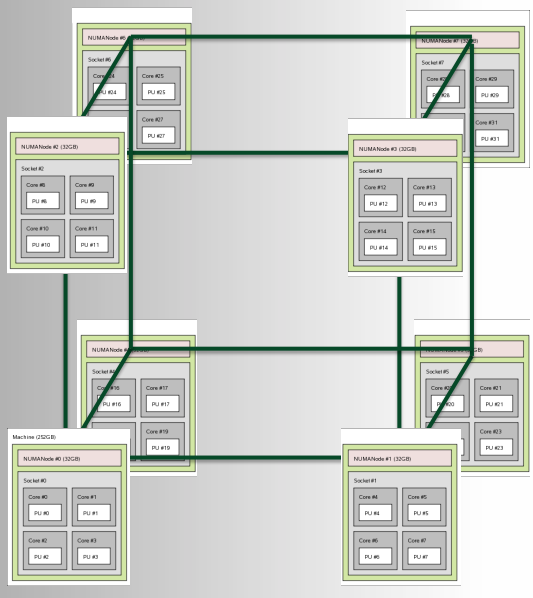
NUMA



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OpenMP

- Common Shared Memory parallelization
- C/C++/FORTRAN
- Single program runs in many cores
- 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 cpu version of code.

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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

Running OpenMP code

```
export OMP_NUM_THREADS=2

./myCode
```

OpenMP Job Script

```
#!/bin/bash -login
#PBS -l walltime=00:05:00,mem=7gb
#PBS -l nodes=1:ppn=8,feature=gbe

cd ${PBS_O_WORKDIR}
export OMP_NUM_TREADS=8

./myOMPprogram

qstat -f ${PBS_JOBID}
```

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Limits of Shared Memory

- Maximum 64-100 cores
- Even with a lot of cores doesn't always scale well

- How do we scale even bigger?

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Network parallelization

- High Speed Network
- What does the programming look like?

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MPI

- Message Passing Interface (MPI)
- C/FORTRAN library that allows programs to pass “messages” between computers over the internet.
- Works best with a high speed network such as 10gigE or Infiniband

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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);
```

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);
   }
```


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);
}
```

Compile MPI Jobs

- To compile an mpi program you need to use the mpi compiler wrappers:
  - mpicc
  - mpif90

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Using MPI

- MPI programs are run using the "mpirun" command:

  mpirun –np 10 –hostfile ./hosts ./myprogram

  - Number of processor cores
  - Hostefile:
    - Ipaddress
    - Computer names
- User needs to be able to remotely connect to each computer and run the program.

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MPI Job Script

```
#!/bin/bash -login
#PBS -l walltime=00:05:00,mem=7gb
#PBS -l nodes=100 ppn=1

cd ${PBS_O_WORKDIR}

mpirun ./myOMPprogram

qstat -f ${PBS_JOBID}
```

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Distributed Network Parallelization

- Map-Reduce (HADOOP)
- Fault tolerant
- Does not require high speed network
- Scales very well.
- Not all problems map well to map-reduce

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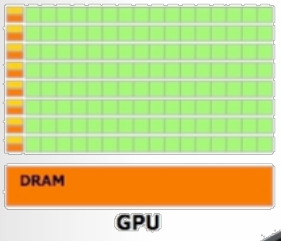
Dedicated Accelerators

- Small shared memory/network systems.
- HPC on a card
  - GPGPU (CUDA)
  - Phi Cards
  - FPGA

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!



GPU vs CPU

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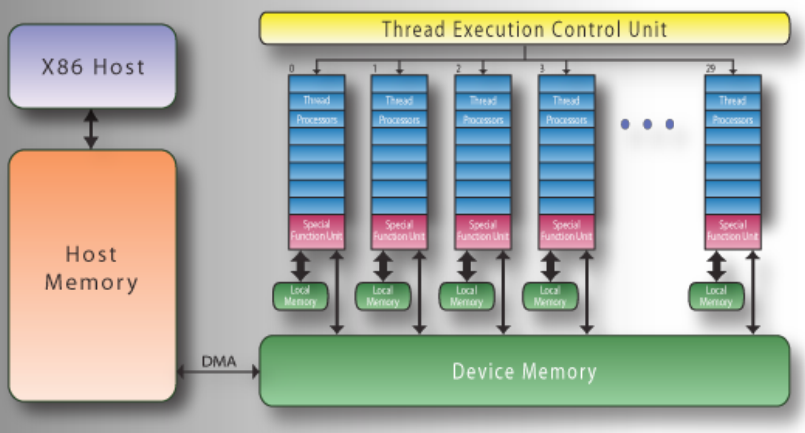
CPU and GPU working together



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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.

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)

```
__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;
}
```

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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GPGPU Job Script

```
#!/bin/bash -login
#PBS -l walltime=00:05:00,mem=7gb
#PBS nodes=1:ppn=1:gfx10,gres=gpu:1,feature=gpgpu

cd ${PBS_O_WORKDIR}

./myOMPprogram

qstat -f ${PBS_JOBID}
```

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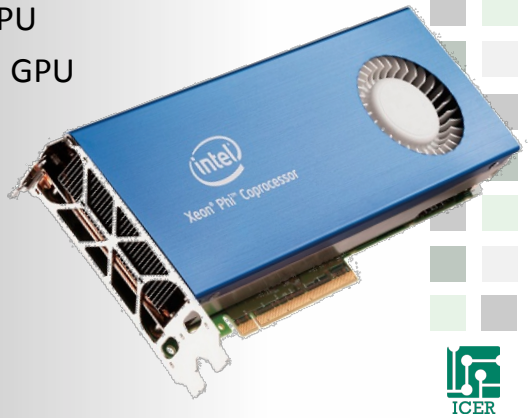
Intel Xeon Phi

- 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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QUESTIONS?

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