Parallel Compute Systems for Scientific Computing

Dirk Colbry, Director
High Performance Computing Center
Institute for Cyber-Enabled Research

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Agenda

- Computation's role in science
- Typical Computational Science problems
- Parallel paradigms and systems for solving Computational Science problems.

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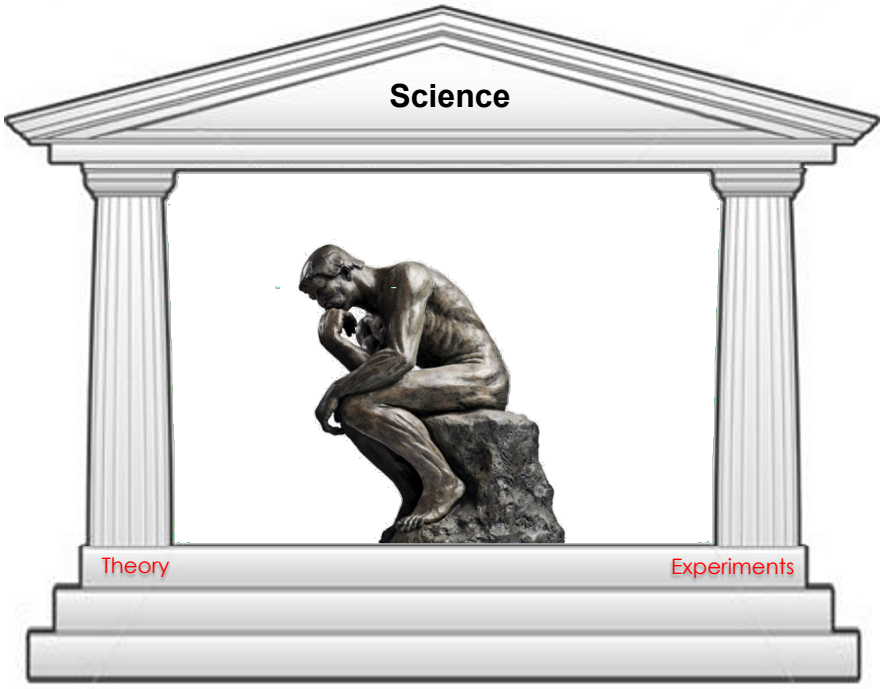

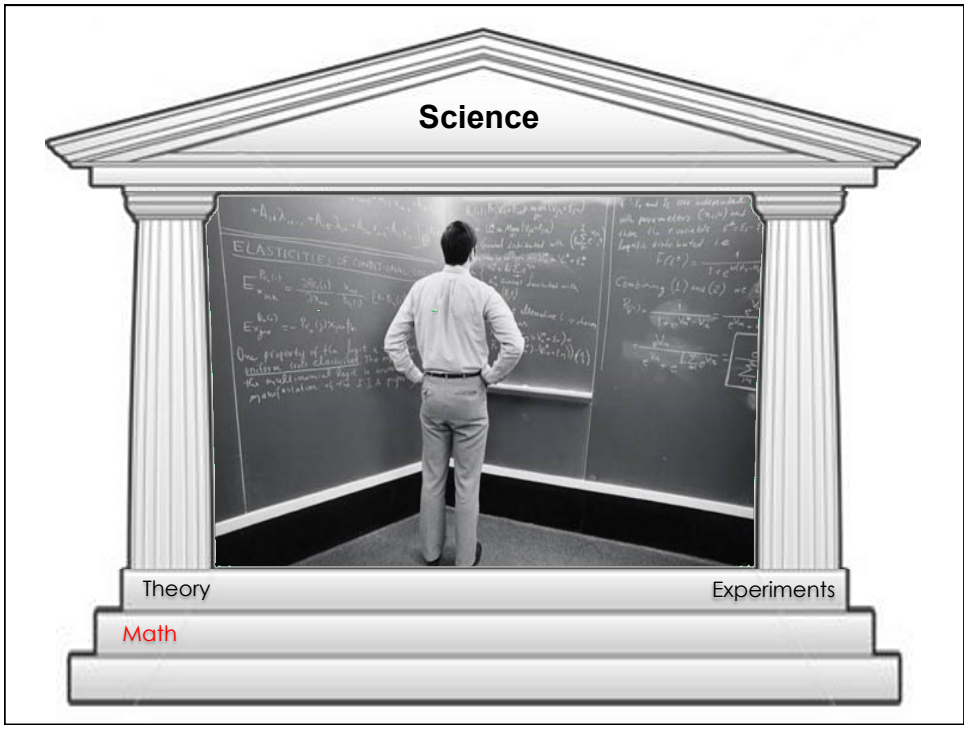
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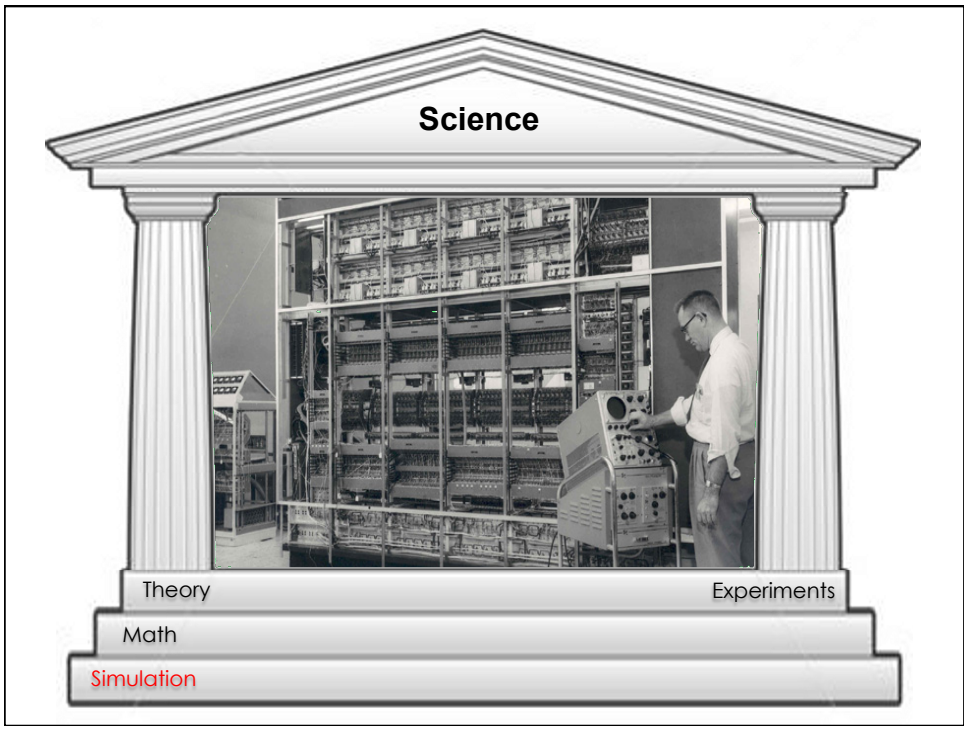
Theory
Experiments
Math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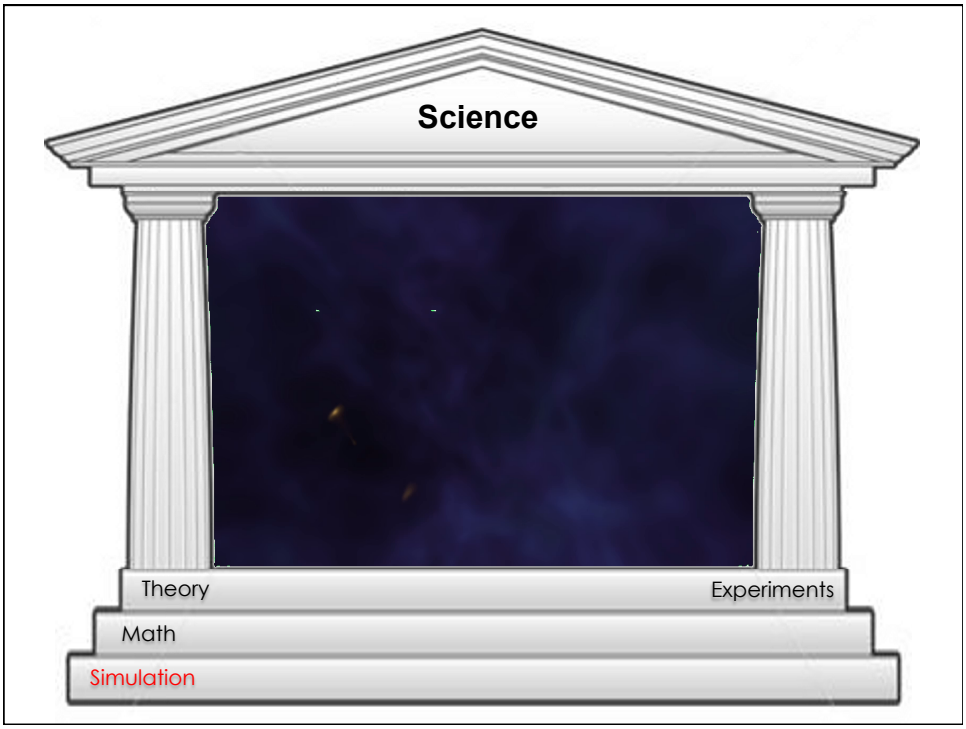
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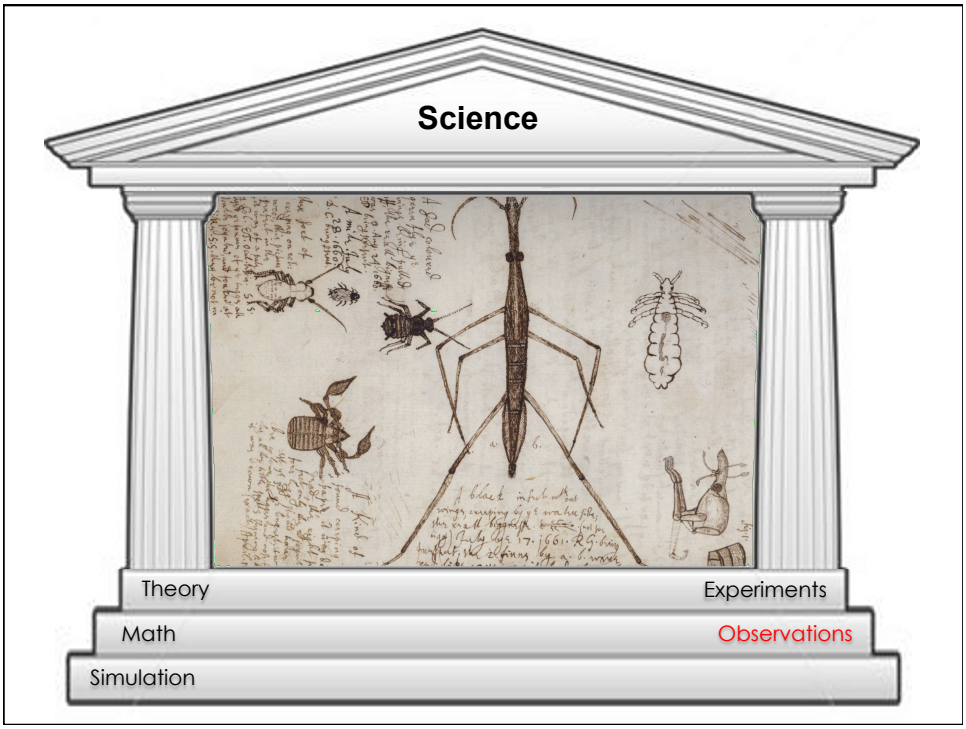
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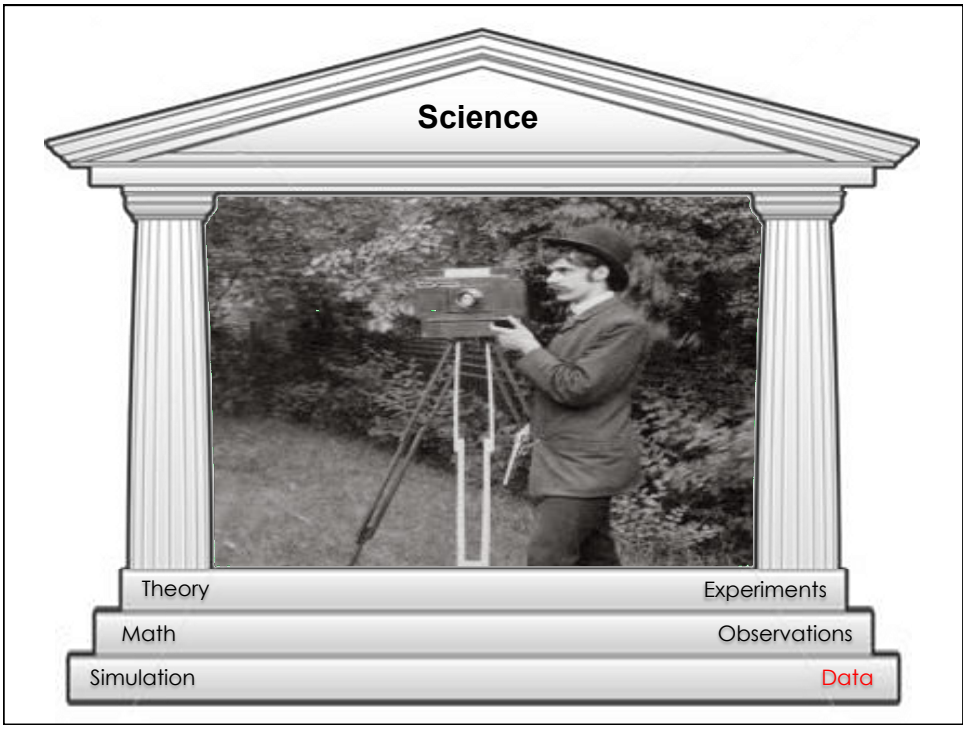
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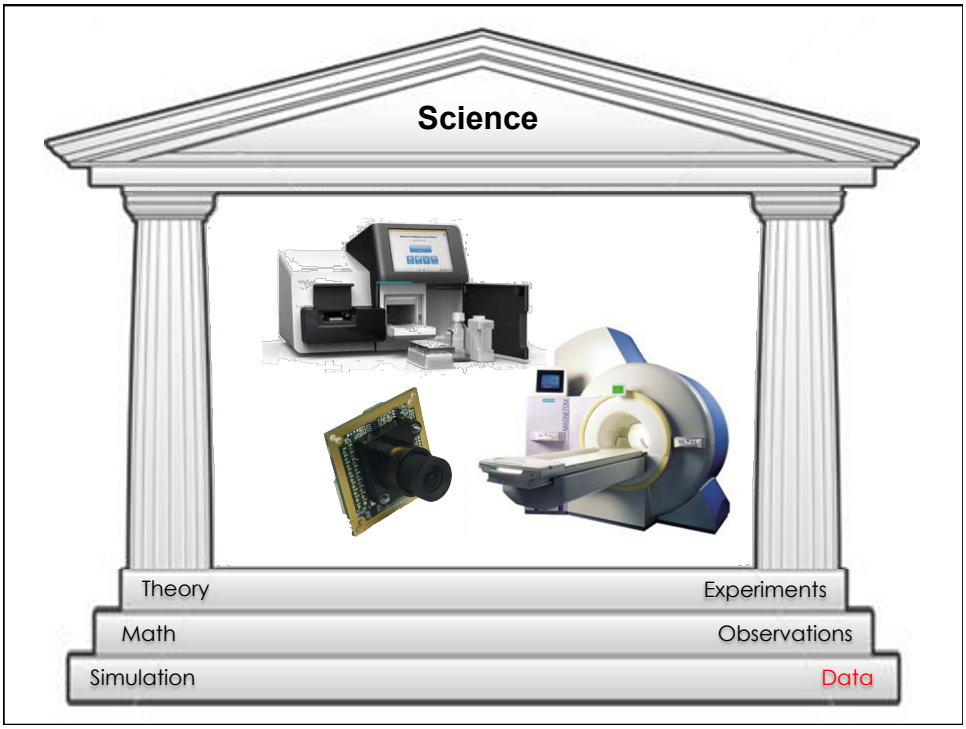
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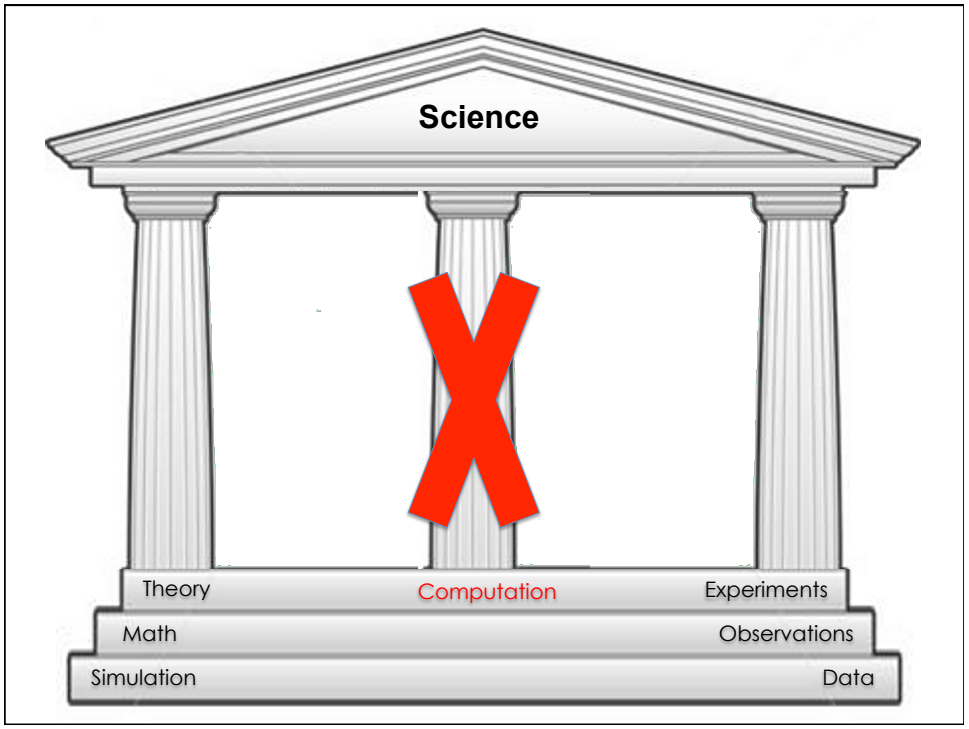
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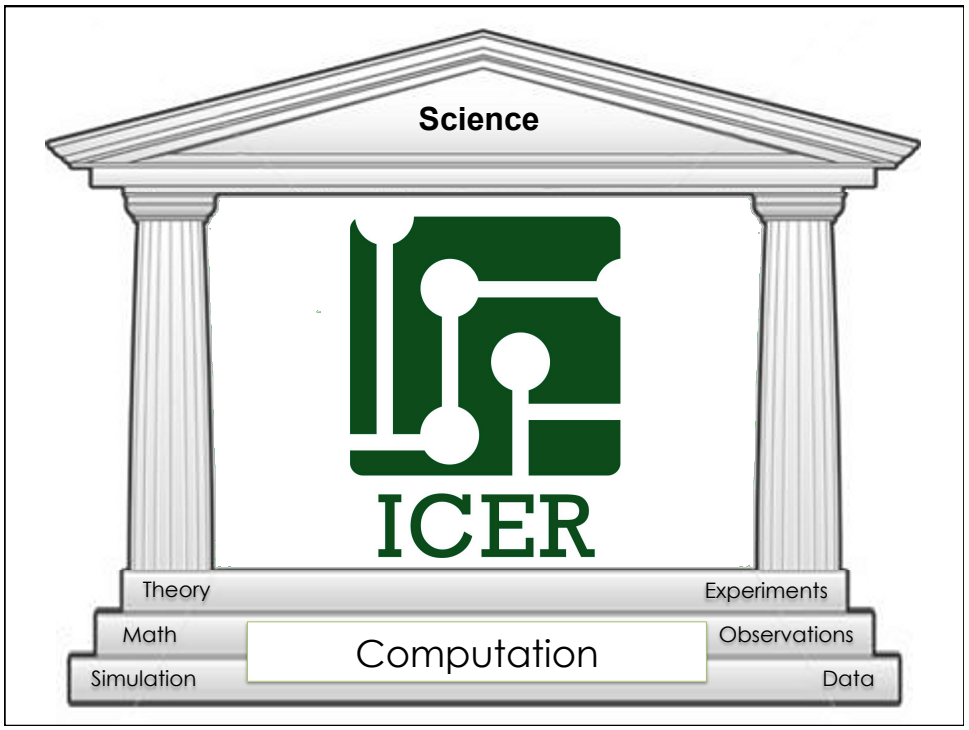
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Computational Research Resource

iCER is a research unit at MSU. We provide:

- Advanced computing hardware
- Software-as-a-service
- Training
- Consulting
- Proposal writing support

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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*

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Types of Problems

- Simulations
- Data Analysis
- Search

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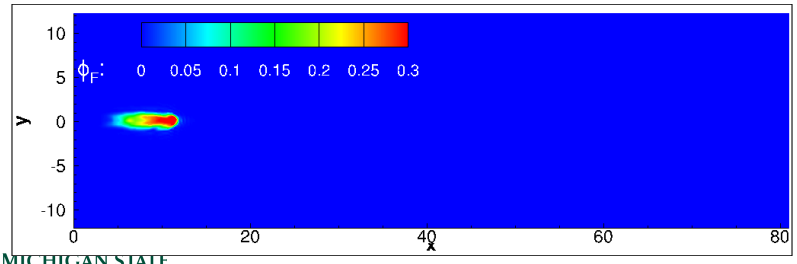
Simulations

- Typically System of PDE (Partial Differential equations)
  - Fluid dynamics
  - Finite element analysis
  - Molecular dynamics
  - Weather
  - Etc.
- Mathematically equivalent to inverse of a matrix



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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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Example: Boundary simulations

1. Divide a 2D or 3D simulation space into a grid of cells
2. Define information that is transferred at the boundary of the cells
3. Simulate the dynamics of the cell during a time interval
4. Repeat steps 2 and 3

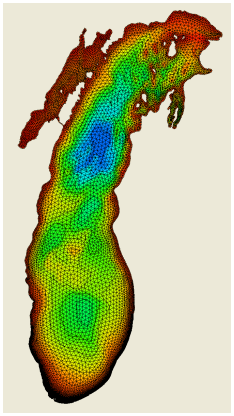

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Image Provided by Dr. Mantha Phanikumar, MSU

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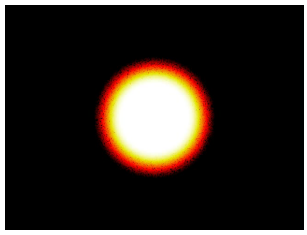
Kinetic Supernova

- Hydrodynamic Codes and Kinetic Codes
- "Meta" Particles
- Calculate position, velocity and collisions
- Can do more than Hydro Codes
- Scales better than Kinetic Codes



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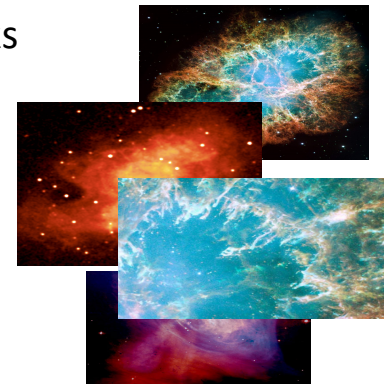
Data Analysis

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



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

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Who are you? -- Biometrics

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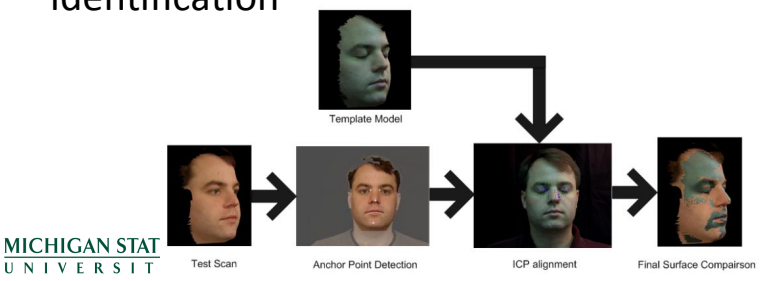
Pairwise-All Problem

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



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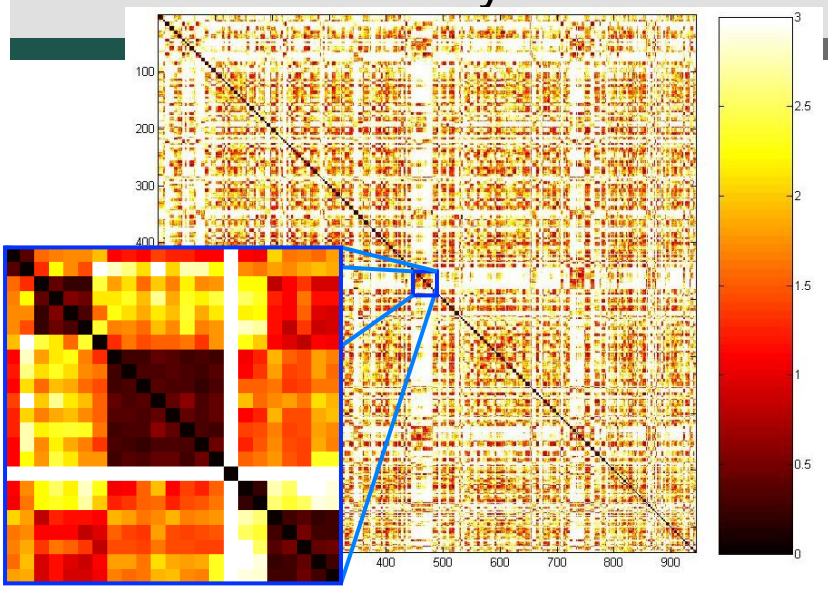
943 x 943 Similarity Matrix



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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

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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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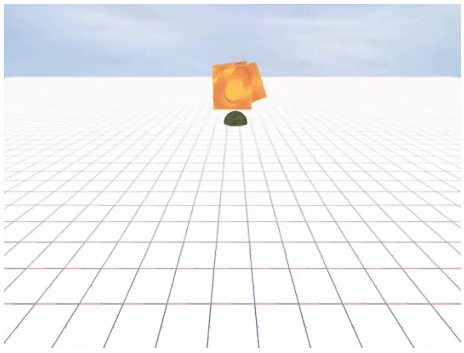
Search

- Genome sequencing
- Analytics
- Optimization
- Etc.



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

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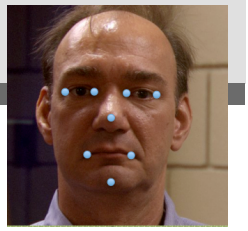
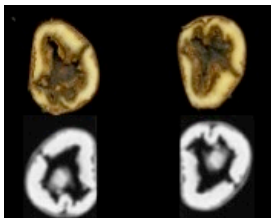
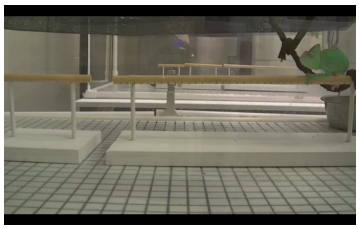
Scientific Imaging



- Point Selection
- Lots of algorithms to choose from
- Every Problem is Different





Video Provided by Dr. Fred Dyer

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How are digital images analyzed?

Graduate students are cheap…
Undergraduates are even cheaper!

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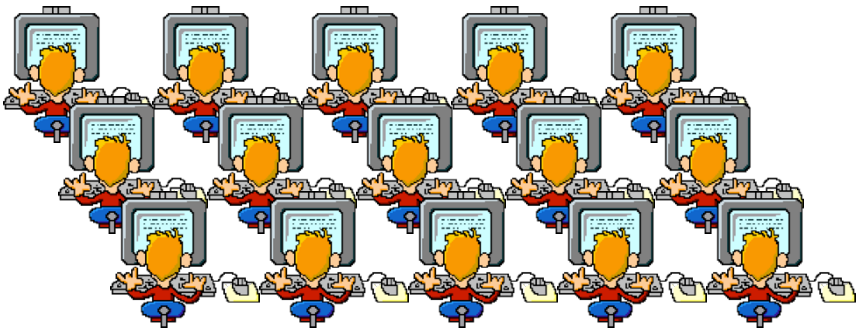
Also, easy to run in parallel



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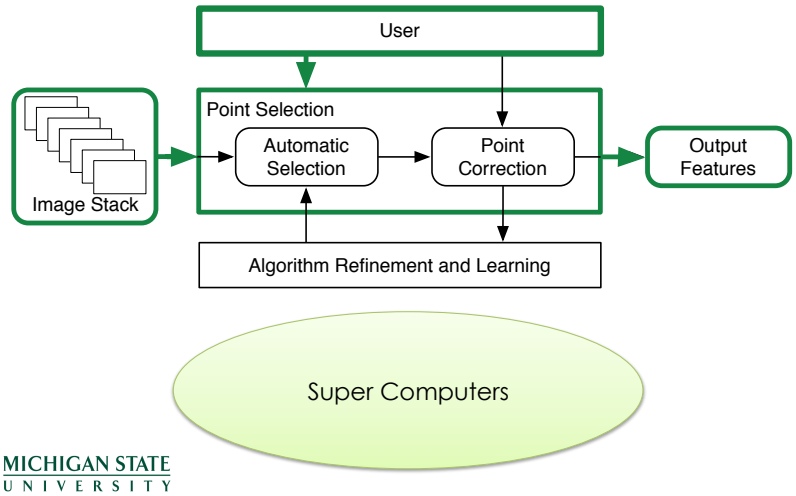
System Diagram



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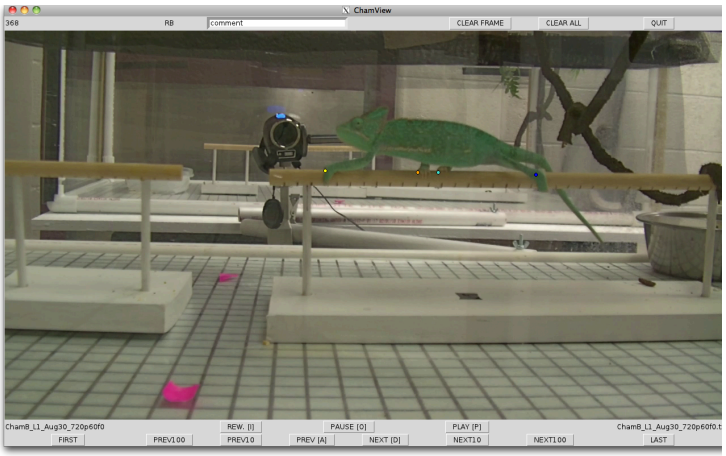
ChamView



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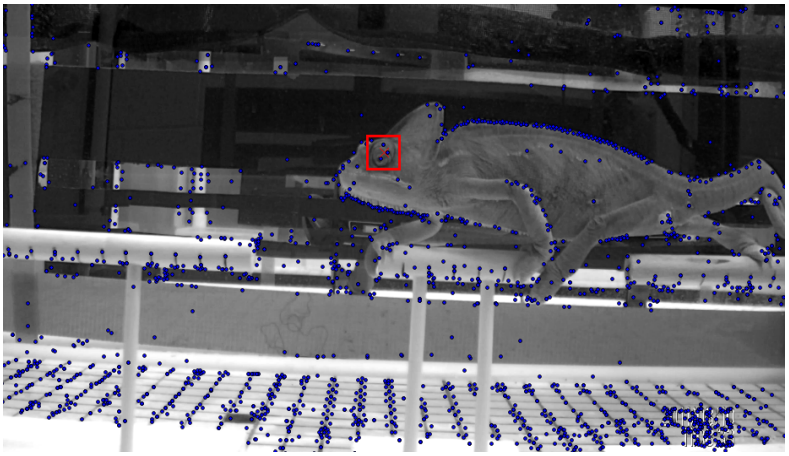
Point tracking on Chameleons



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Patrick Korth, CSE University of Michigan

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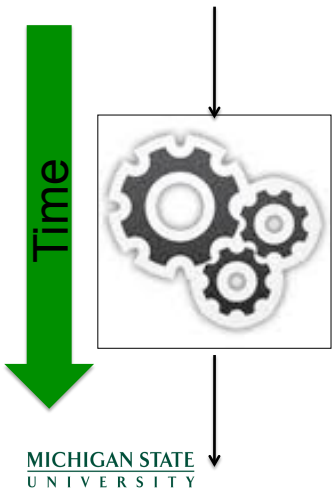
Single Thread Jobs



- One CPU can only run one thing at a time. (sort of)
- CPUs are not getting that much faster.

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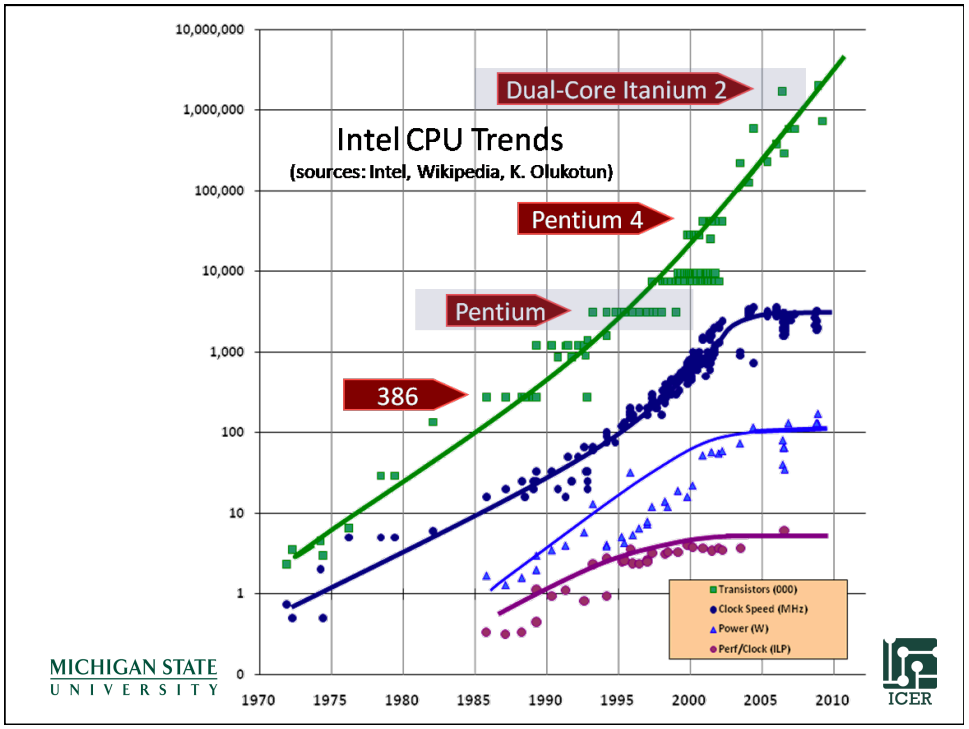

Communication

- Shared Memory
  - Ex. OpenMP
- Shared Network
  - Ex. MPI
- Distributed Network
  - Ex. Map-Reduce
- Dedicated Accelerators
  - Ex. GPGPU and Phi
- Hybrid Systems

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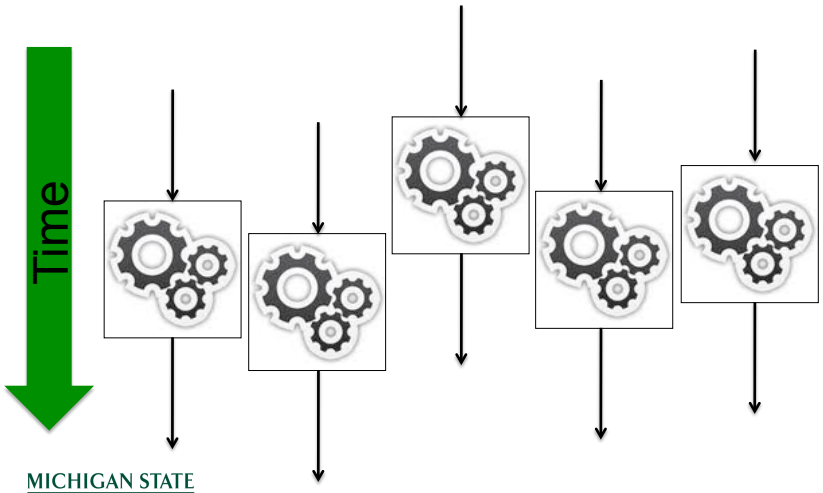
Pleasantly Parallel



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MSU HTCondor Cluster

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

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HTCondor
High Throughput Computing

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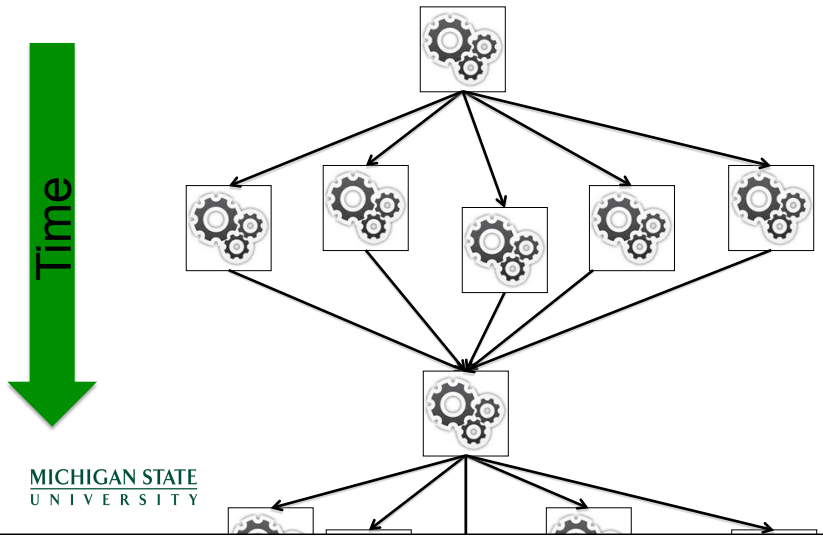
Loosely Coupled



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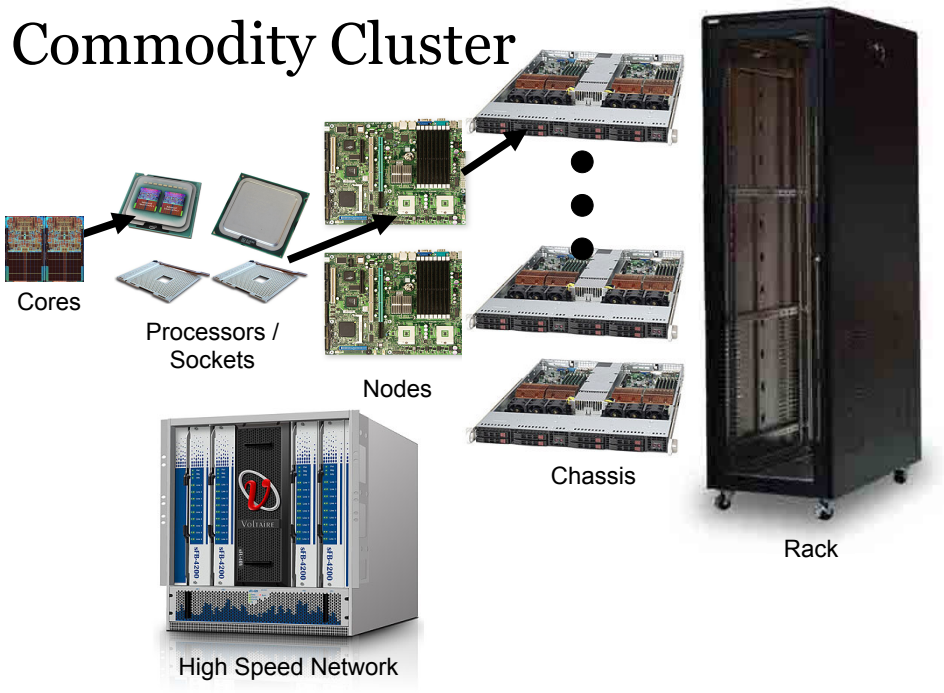
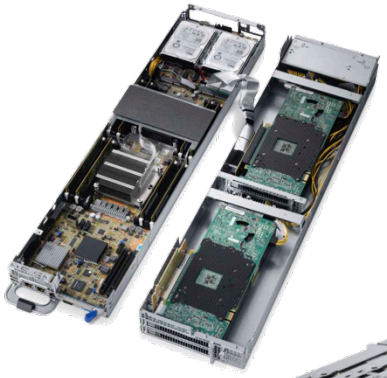
Commodity Cluster



MSU 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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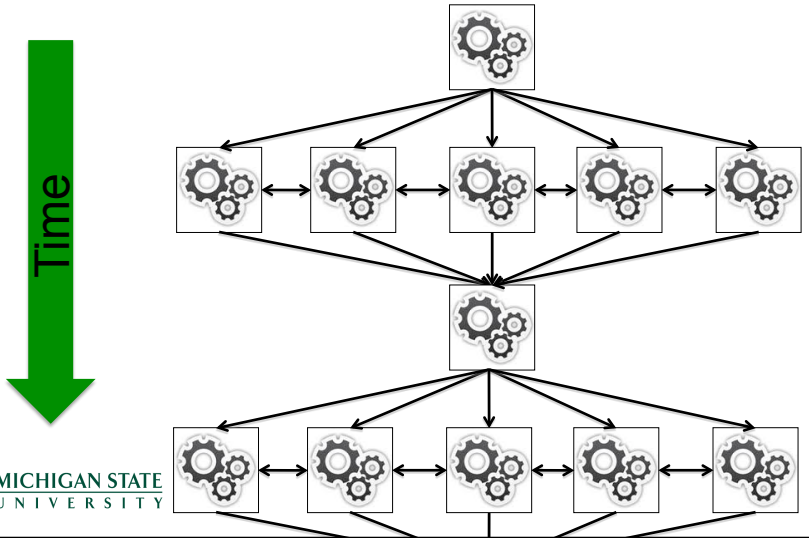
Tightly Coupled



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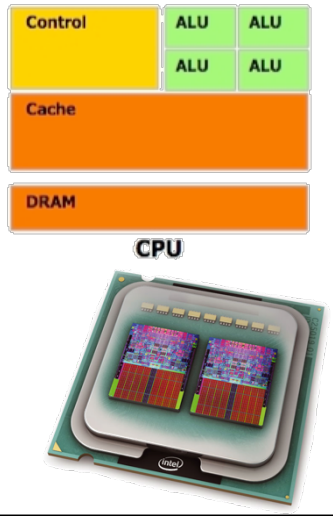
Shared Memory Communication

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



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Intel10

- 8 cores
- 24 GB memory

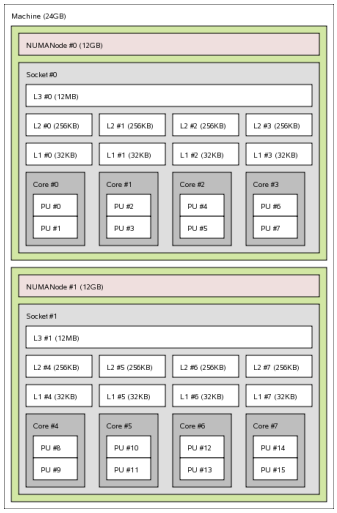

Figure Generated using hwloc

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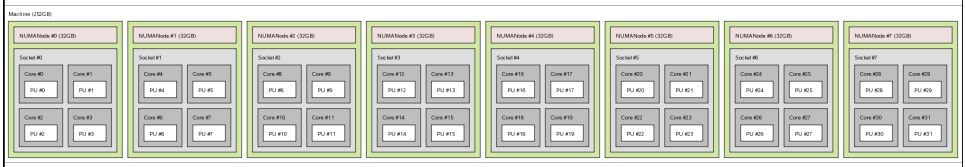
amd09

- 32 cores
- 256 GB memory



- We also have a node with 96 cores and 6TB of memory

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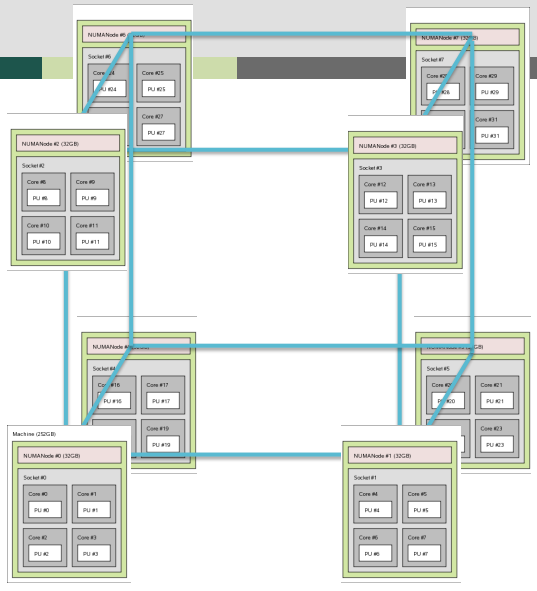
NUMA



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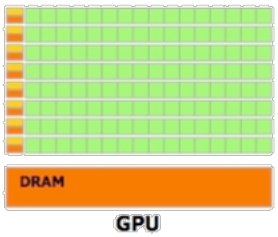
GPU

- 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!



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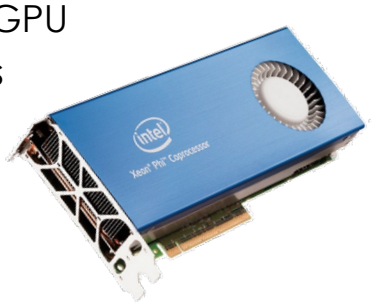
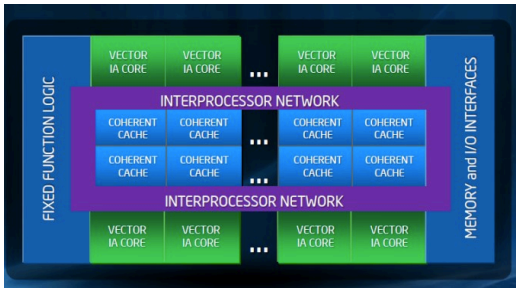
Intel Xeon Phi

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





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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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