Do More, Faster: Leveraging Computational Resources in Your Research

Dr. Dirk Colbry
Institute for Cyber Enabled Research
Adjunct Faculty, Electrical and Computer Engineering
Michigan State University

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Agenda

- **Who am I**
- Pillars of Science
- What is Advanced Computing Hardware?
- Common classes of problems
- Steps to High Performance

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I am an engineer

- Undergraduate Mechanical Engineering degree from Georgia Tech
- 3 years as a Mechanical Engineer for Delta Airlines in Atlanta
- 2 years as a Robotics Engineer for FANUC Robotics in Auburn Hills

Delta Air Lines

FANUC Robotics

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I am a Student

- M.S.E. in Computer Science and Engineering, University of Michigan
  - Artificial Intelligence
  - Thesis on Temporal Bayesian Networks
- Ph.D. in Computer Science and Engineering, Michigan State University
  - Pattern Recognition and Image Processing
  - 3D Face Recognition

THE UNIVERSITY OF MICHIGAN 1817

MICHIGAN STATE UNIVERSITY Founded 1855

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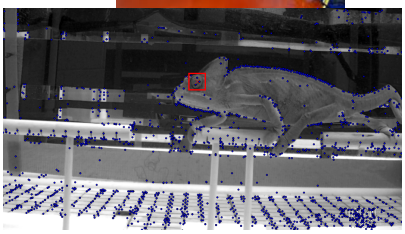
I am a Researcher

- Image Analysis in Research
- High Performance Computing
- Assistive Technologies



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I am a computational consultant

- One-on-one consulting
- HPC Programming
- Proposal Writing
- Training and Education
- Outreach

- Reduce the "Mean time to Science"

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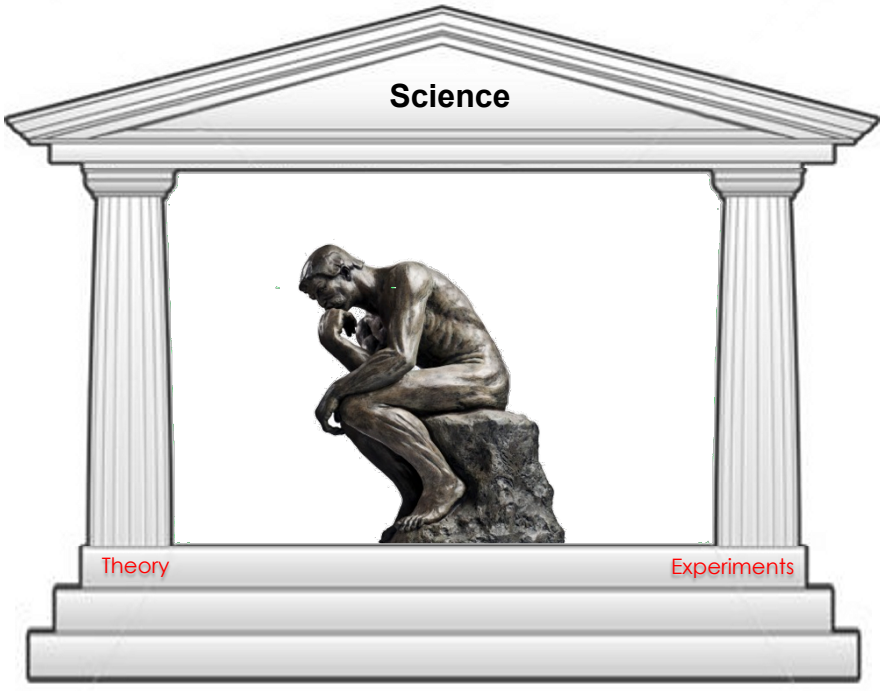
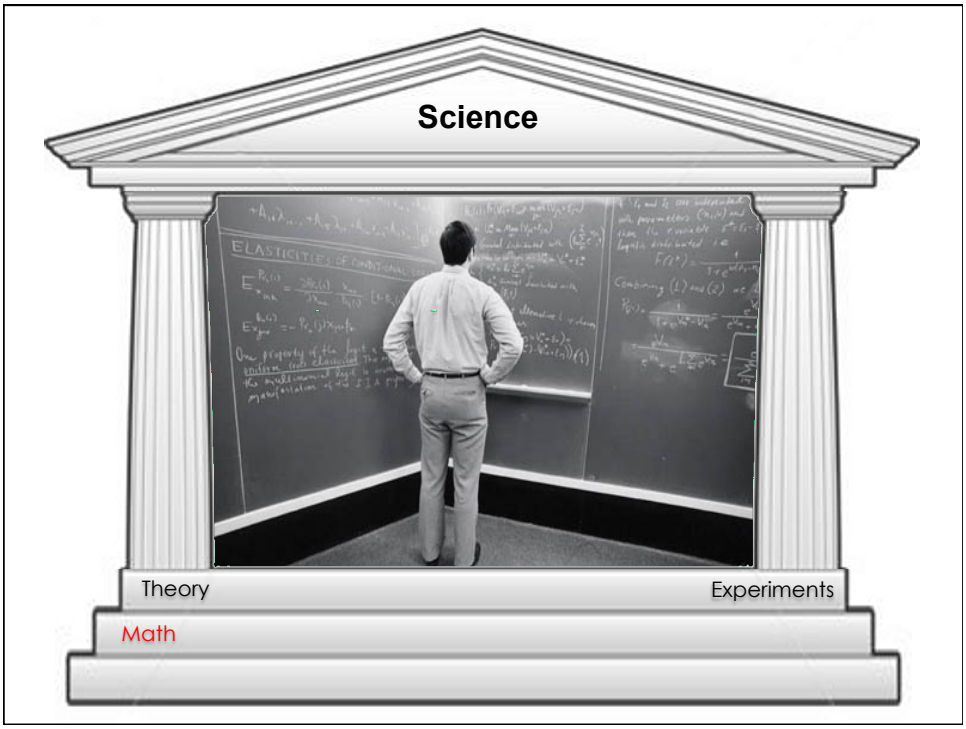
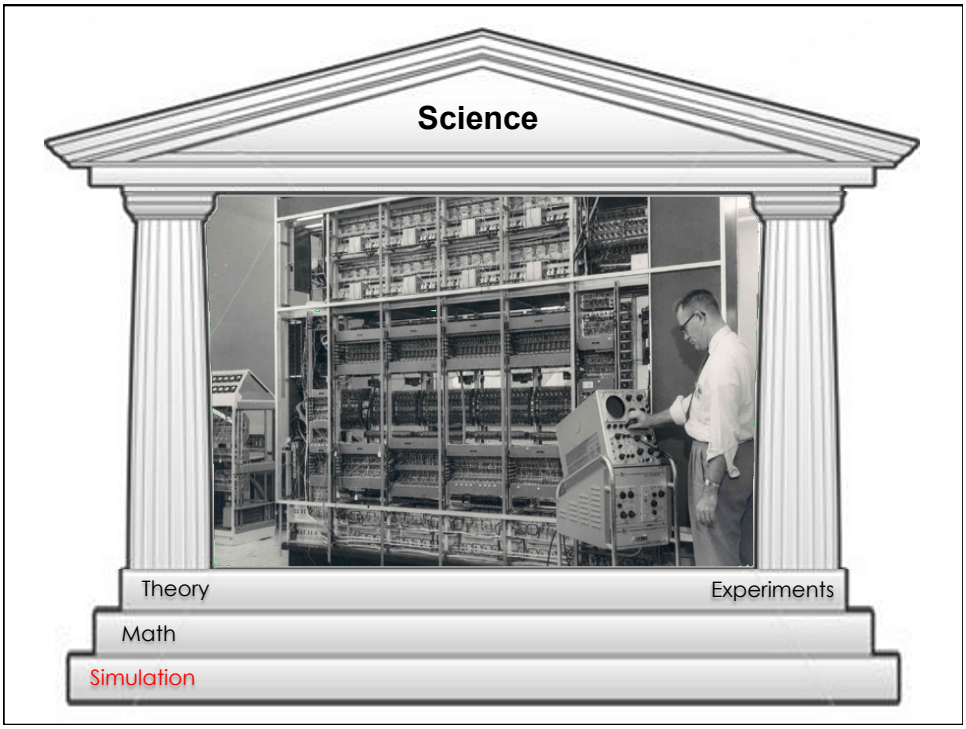



Science
Theory
Experiments
Math


Science
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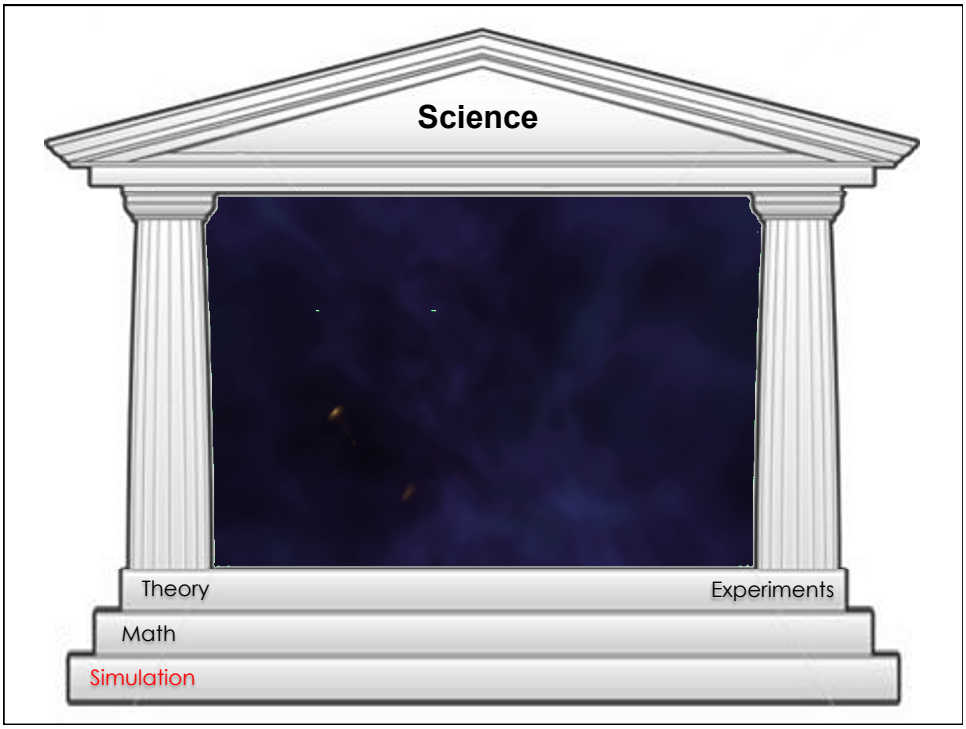
Simulation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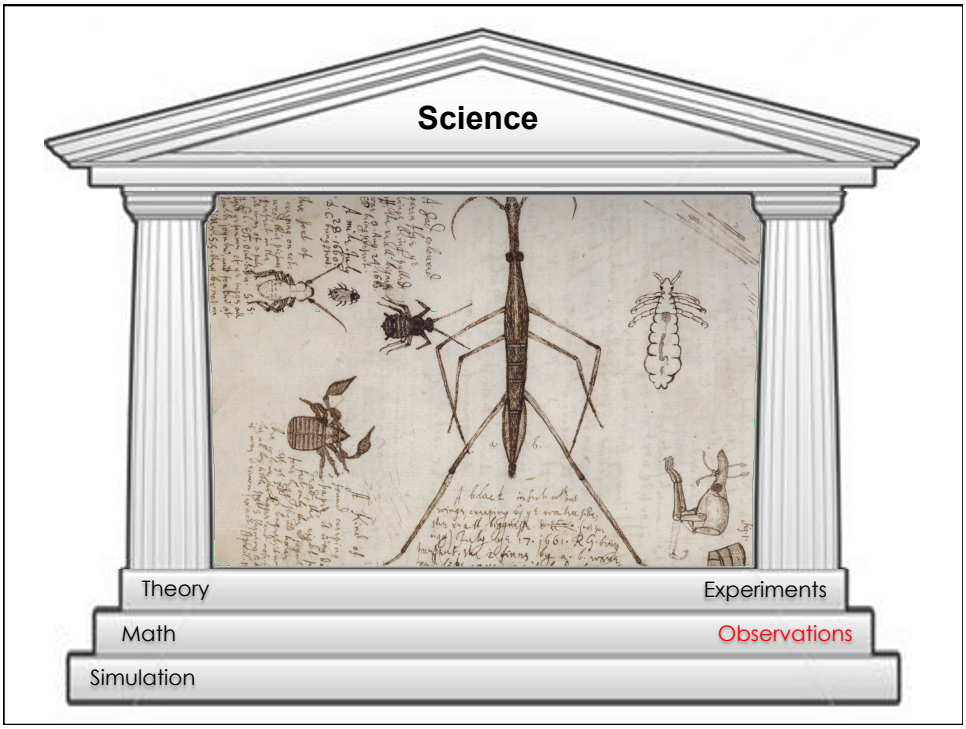
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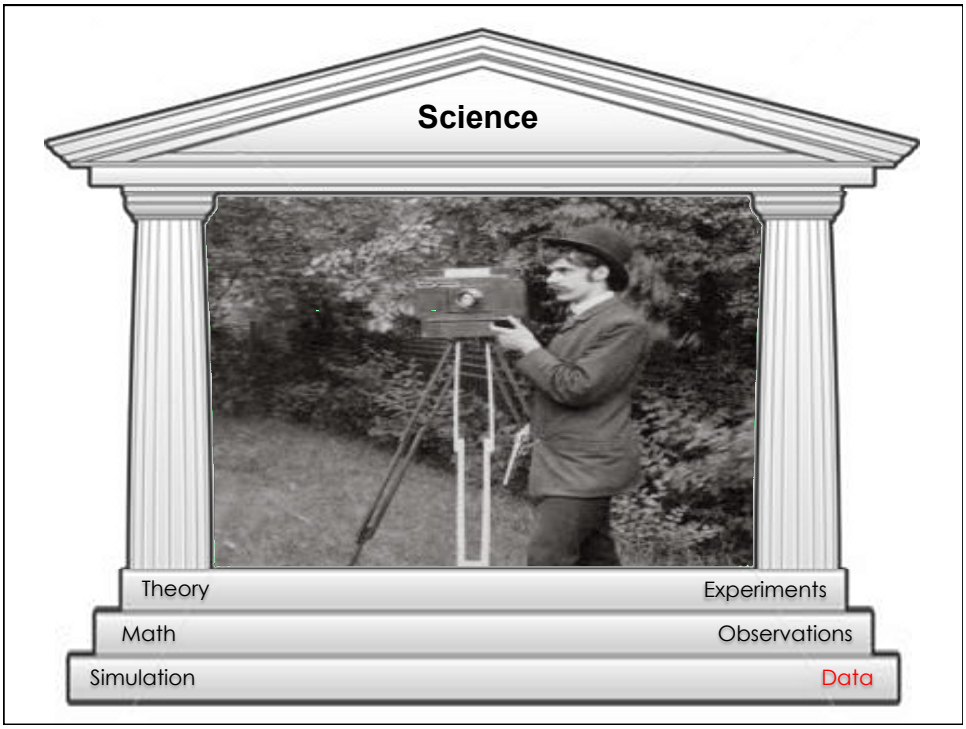
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Observations
Simulation
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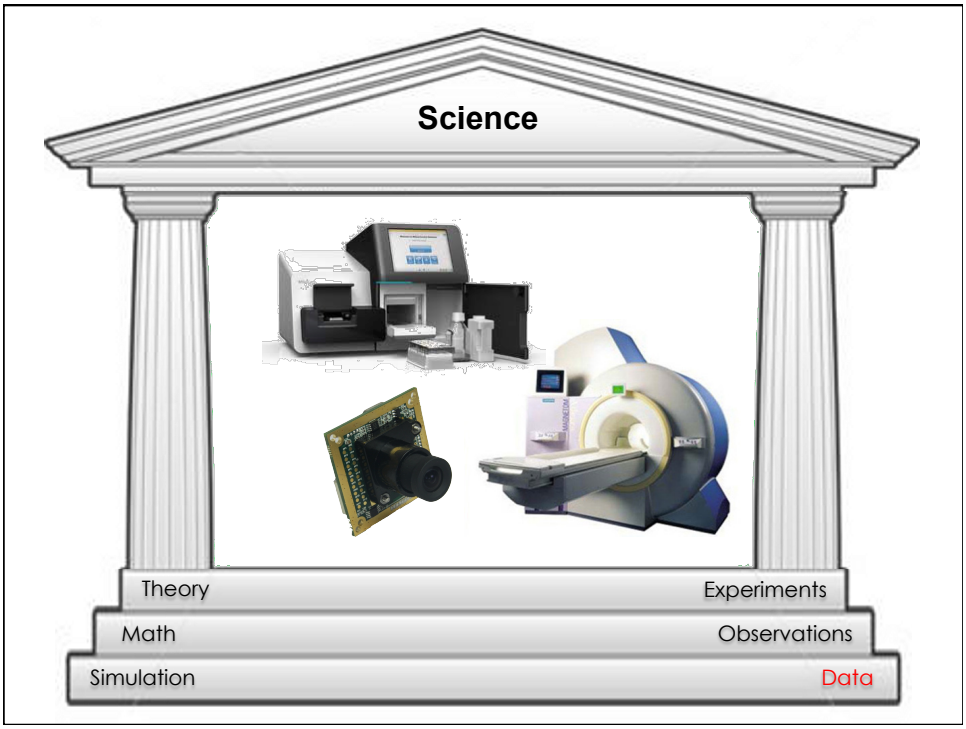
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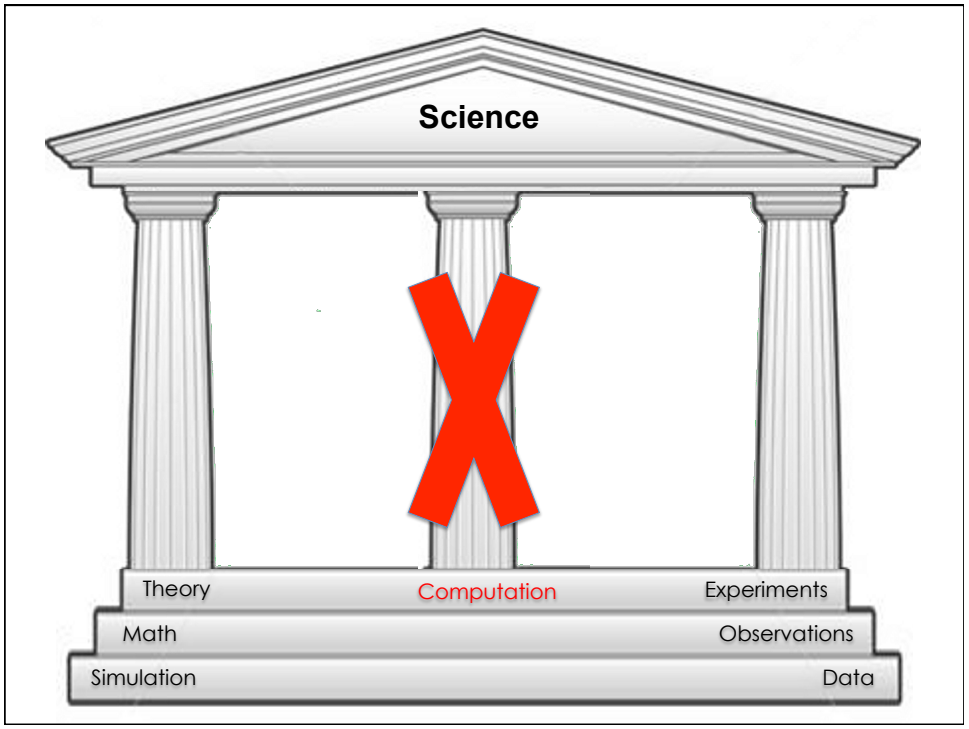
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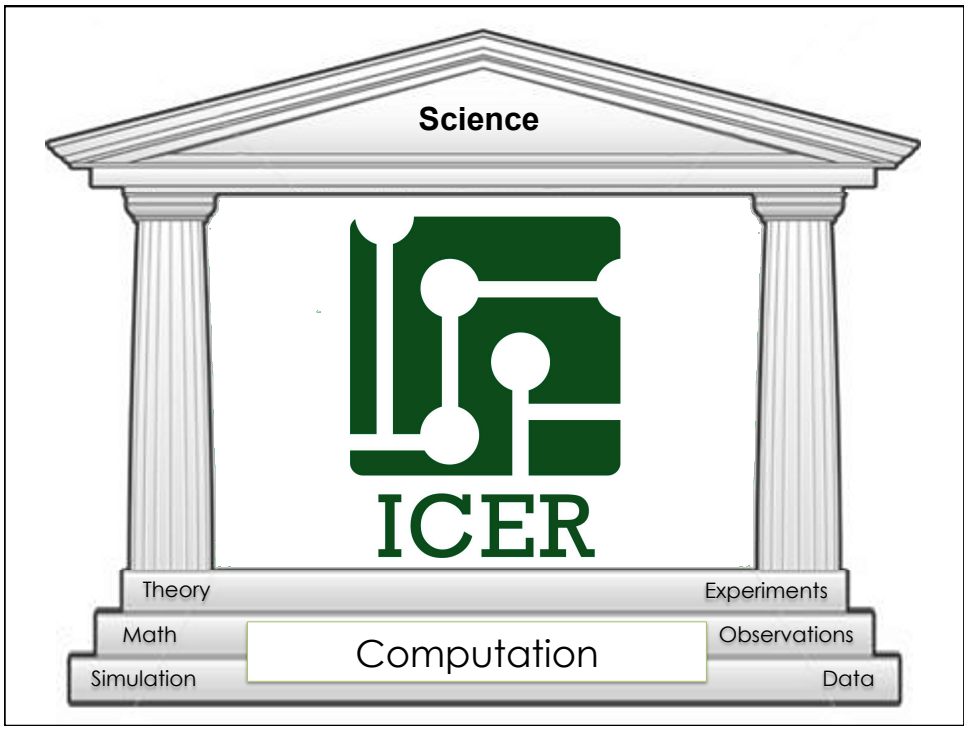
Science
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What is Advanced Computing Hardware?

- Anything more advanced than your desktop
- Local resources
  - Lab, Department, Institution (iCER)
- National resources
  - NSF (XSEDE), DOE (Jaguar) , Others
- Commercial Resources (cloud computing)
  - Amazon, Azure, Liquid Web, Others

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Why use Advanced Computing Hardware?

- Science takes too long
- Computation runs out of memory
- Run out of disk space
- Need licensed software
- Need advanced interface (visualization)

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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

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Available Software

- Center Supported Development Software
  - Intel compilers, openmp, openmpi, mvapich, totalview, mkl, pathscale, gnu...
- Center Supported Research Software
  - MATLAB, R, fluent, abaqus, HEEDS, amber, blast, ls-dyna, starp...
- Customer Software
  - gromacs, cmake, cuda, imagemagick, java, openmm, siesta…
  - For a more up to date list, see the documentation wiki:
    - http://wiki.hpcc.msu.edu/

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What if I need help?

- Ask us!

- Local Workshops
  - Software carpentry
  - Introduction to Linux and HPCC
  - Advanced HPCC

- Remote Training
  - VSCSE – Virtual School for Computer Science Education
  - XSEDE training Workshops

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XSEDE OpenMP Workshop

October 7, 2014

- Who? C and Fortran programmers
- What? Leave with a working knowledge of how to write scalable codes using OpenMP

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www.icer.msu.edu/events

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- Special guest speaker presentations
- Interactive workshops on a variety of topics
- Poster session showcasing CI-enabled research at MSU
- Resource fair featuring various CI resources available to MSU researchers
- Networking opportunities

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http://www.vprgs.msu.edu/ci-days

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CI Days Posters

Due, October 10, 2014

- Demonstrate a Direct connection to using Cyber-Infrastructure in your research
- In progress or Completed Research
- Cash Prizes!
- Networking opportunities

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CI Days Training

Thursday, October 23, 2014

- **10:00am-1:00pm**
  - Introduction to Python
  - Introduction to HPCC at MSU
  - Programming with MATLAB
- **2:00pm – 5:00pm**
  - Advanced Python
  - Advanced Topics in HPCC
  - Optimizing your MATLAB Code

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Computational Chemoinformatics & Docking Studies

November 3-6, 2014

- Who? Interested in molecular design and macromolecule-small molecule interactions
- Hands on computational exercises

  Topics include:
  - Protein-ligand interactions
  - Protein structure prediction
  - Virtual screening using molecular docking
  - Common pitfalls in protein-ligand docking

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Check our Website

++More Training Coming

- Open MPI
- Open ACC
- Big Data

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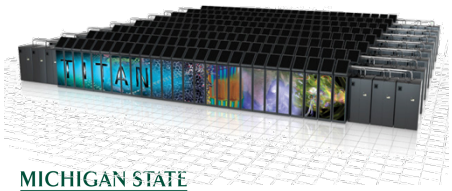
What if I want more?

XSEDE
Extreme Science and Engineering Discovery Environment

NASA

Open Science Grid

BLUE WATERS
SUSTAINED PETASCALE COMPUTING



amazon web services™

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What problems are we solving?

- Boundary Simulations
- Data Analysis
- Search

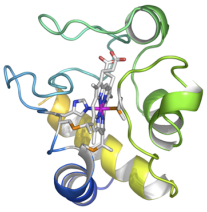

Image Provided by Dr. Warren F. Beck, MSU

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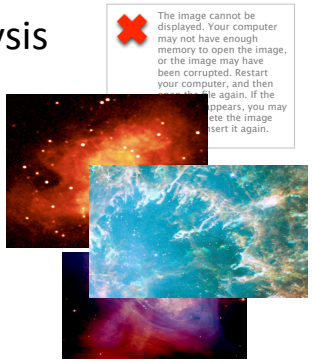

Images from, "Understanding the H_2 Emission from the Crab Nebula", C.T. Richardson, J.A. Baldwin, G.J. Ferland, E.D. Loh, Charles A. Huehn, A.C. Fabian, P.Salomé

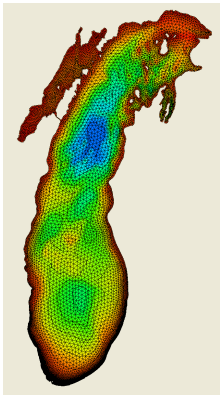

Image Provided by Dr. Mantha Phanikumar, MSU

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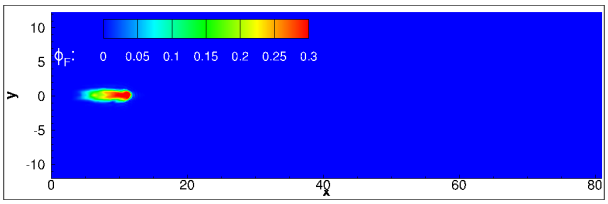
Boundary Simulations

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



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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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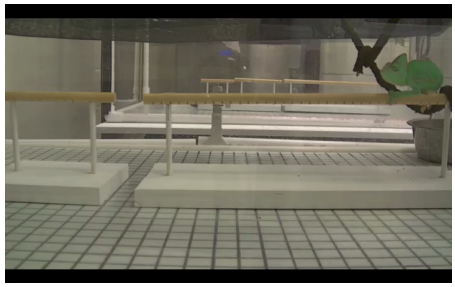
Data Analysis

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



Video Provided by Dr. Fred Dyer

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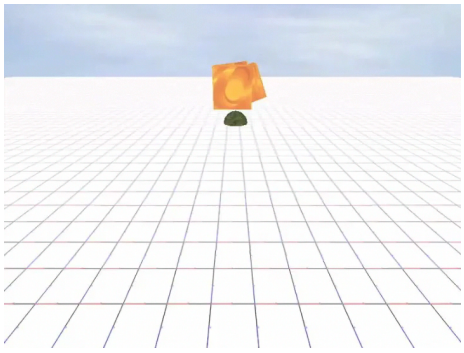
Search

- Genome sequencing
- Analytics
- Optimization
- Etc.



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

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Steps in Using the HPCC

1. Get an account (ask your advisor)
   https://contact.icer.msu.edu/account
2. Install needed software (SSH, SCP, X11)
3. Transfer input files and source code
4. Compile/Test programs on a developer node
5. Write a submission script
6. Submit the job
7. Get your results and write a paper!!

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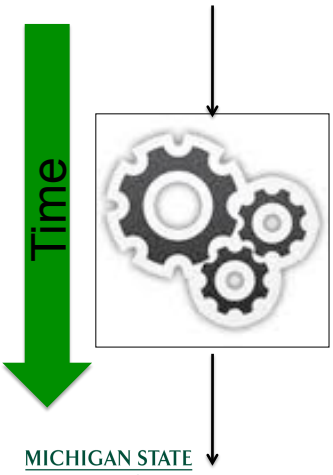
Single Thread Jobs



- 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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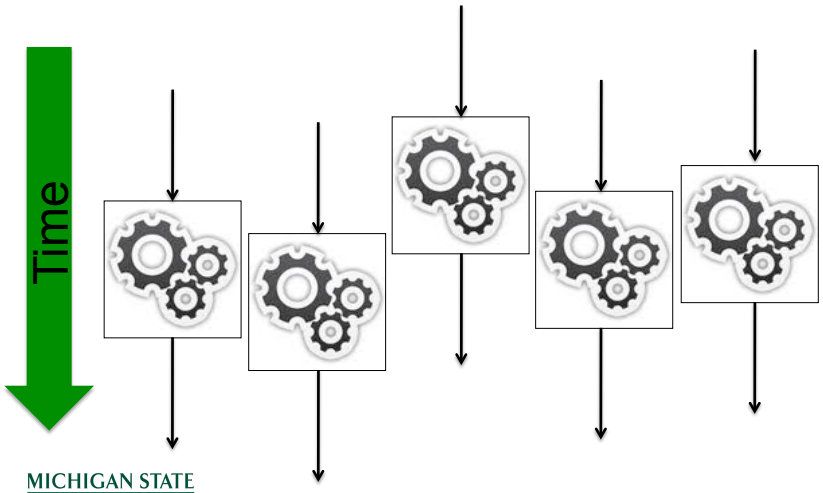
Pleasantly Parallel



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MSU HTCondor Cluster

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

HTCondor
High Throughput Computing

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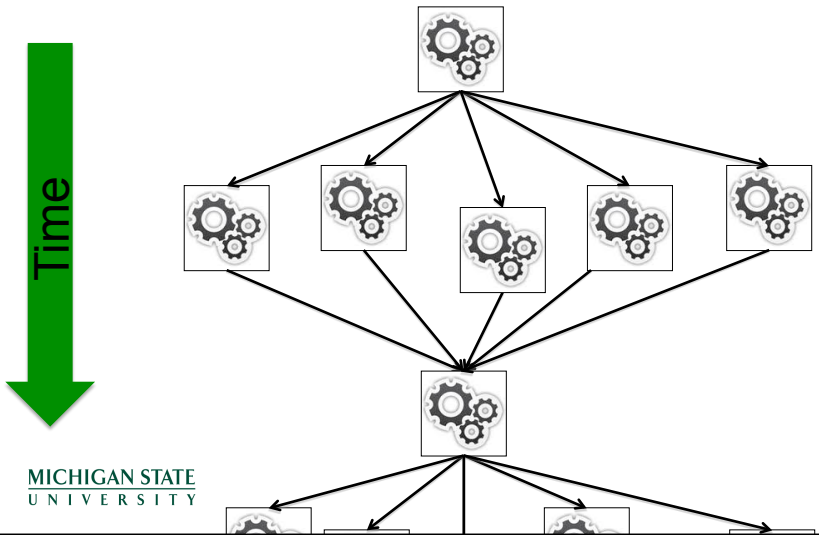
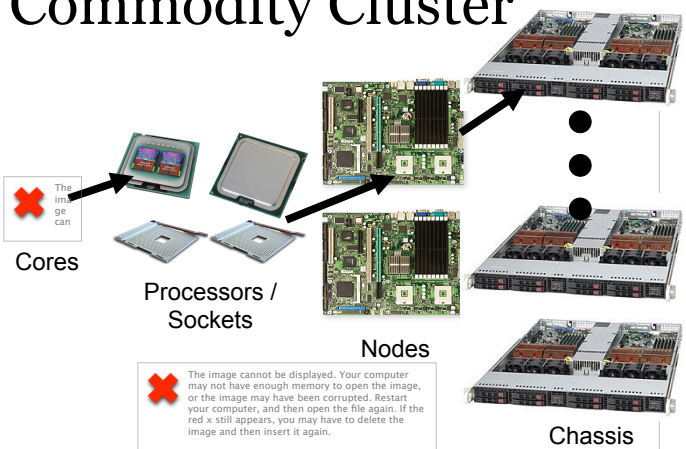
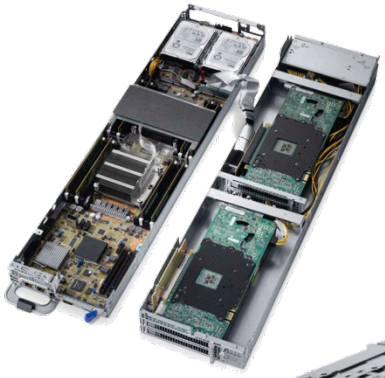
Loosely Coupled



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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Shared Network Communication

- Commodity Cluster
- High speed network
- MPI
  - Message Passing Interface
  - Programming standard
  - Ex Libraries: OpenMPI, MPICH/MVAPICH
- Parallel File systems
  - Lustre

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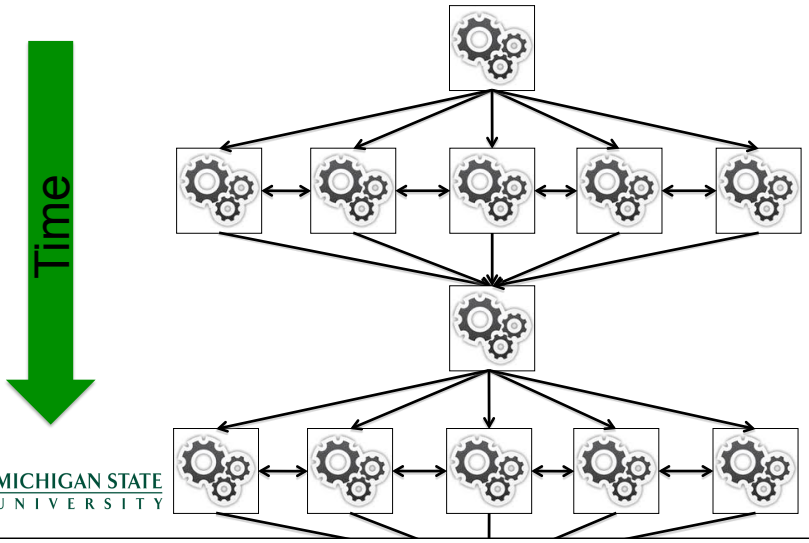
Tightly Coupled



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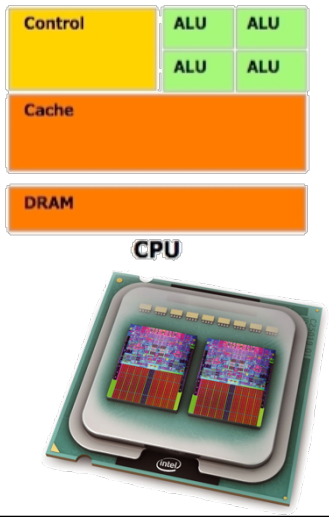
Shared Memory Communication

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



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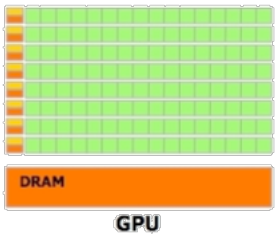
GPU

- 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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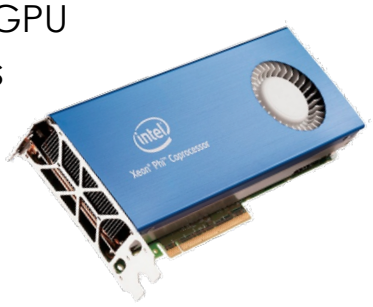
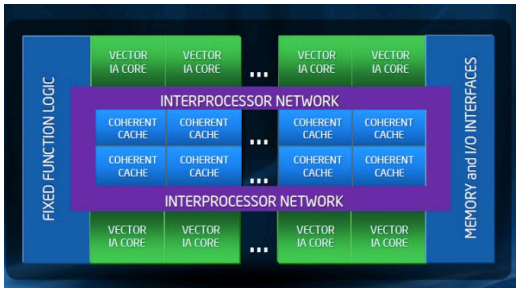
Intel Xeon Phi

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





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Summary of Hardware

- Pleasantly parallel
  - HTCondor
- Loosely Coupled
  - Commodity cluster
- Tightly Coupled
  - Fat Nodes
  - GPUs
  - Phi

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.

We are here to help

- www.hpcc.msu.edu/contact
  - Questions
  - Schedule Consultations
  - Code Reviews
  - Programming help
  - Hardware Purchasing
  - Help with Grants
  - Support for Grants

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