

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



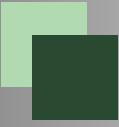
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Agenda

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



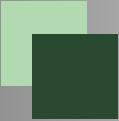
 I am an engineer

- 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








 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






I am a Researcher

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

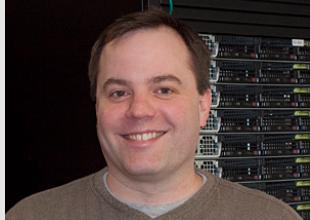


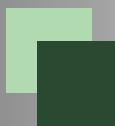




I am a computational consultant

- One-on-one consulting
- HPC Programming
- Proposal Writing
- Training and Education
- Outreach
- Reduce the “Mean time to Science”

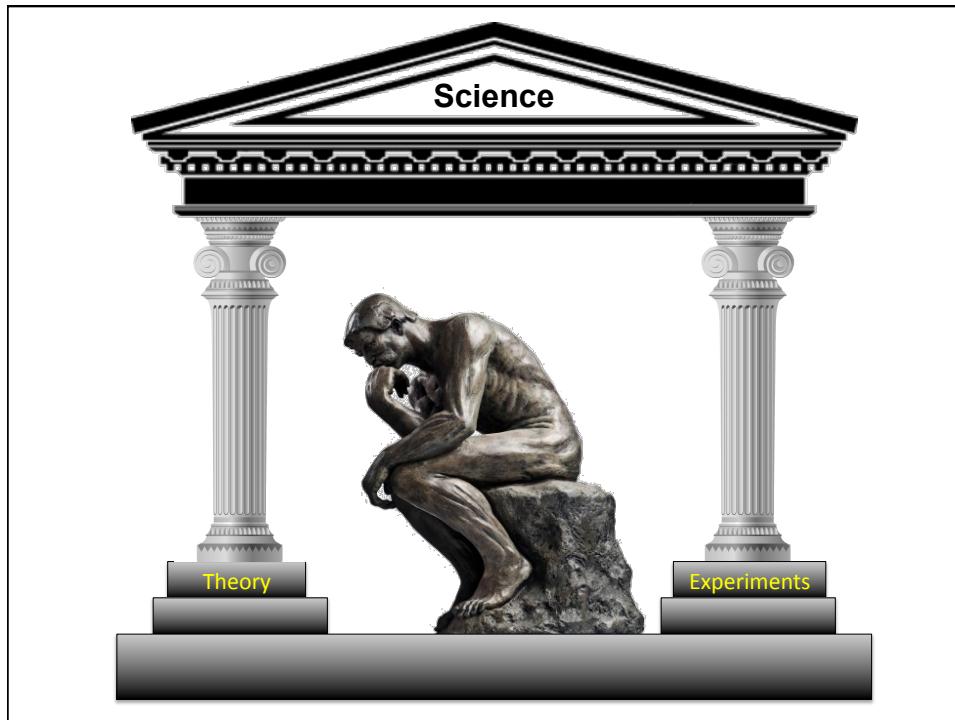



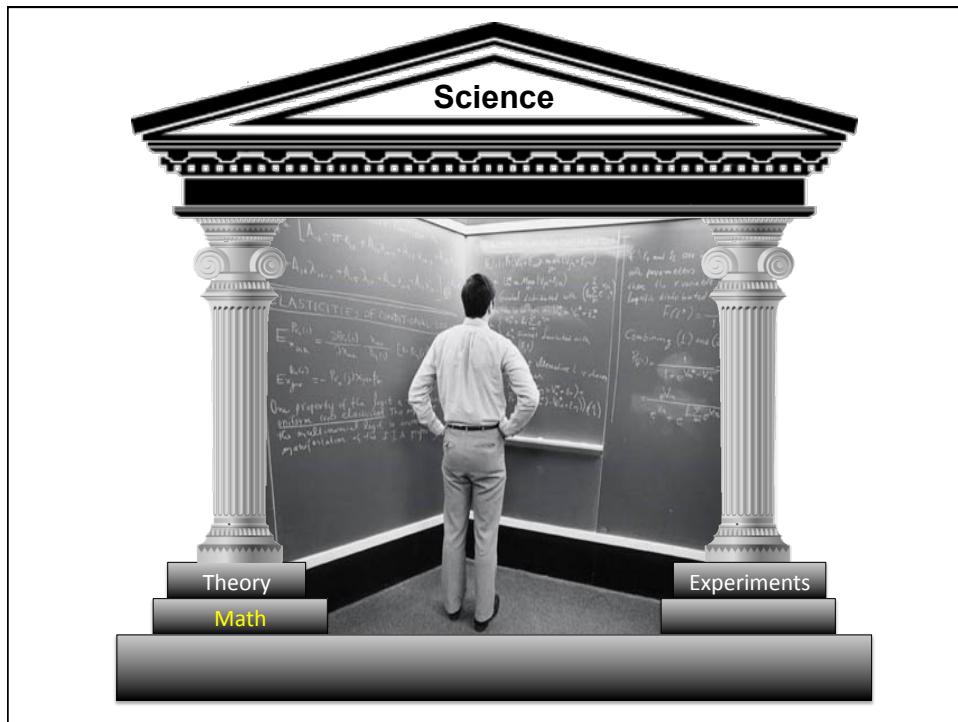
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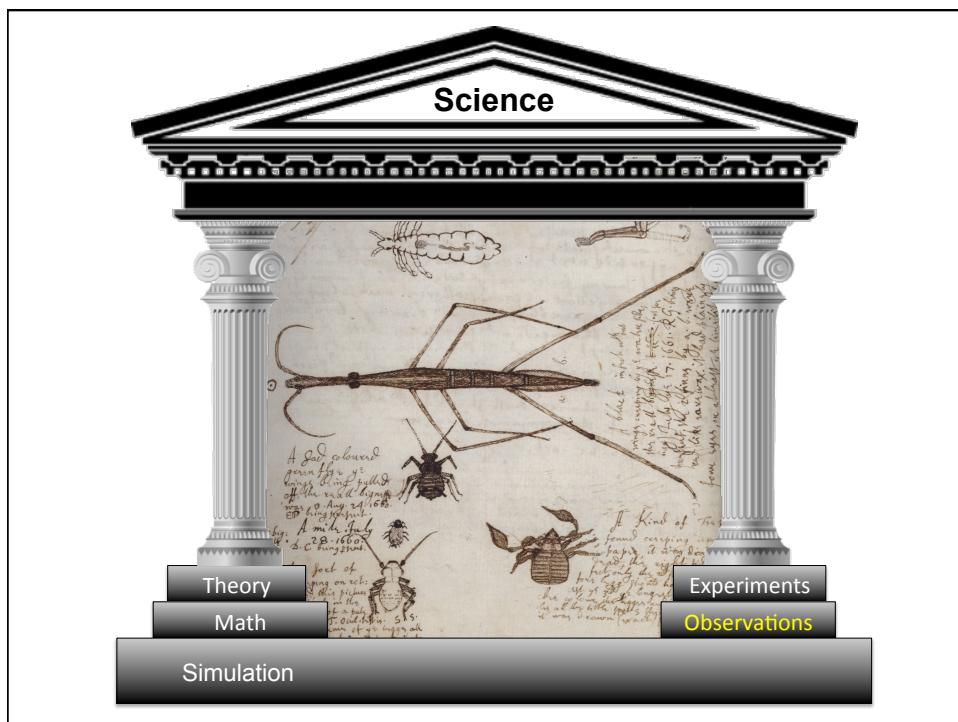
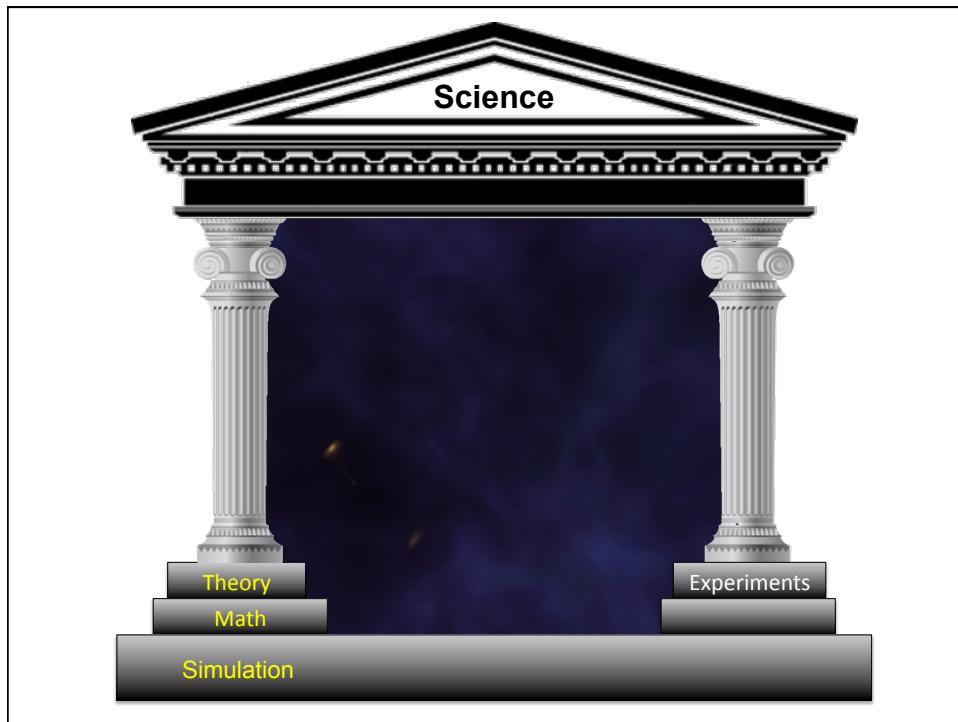
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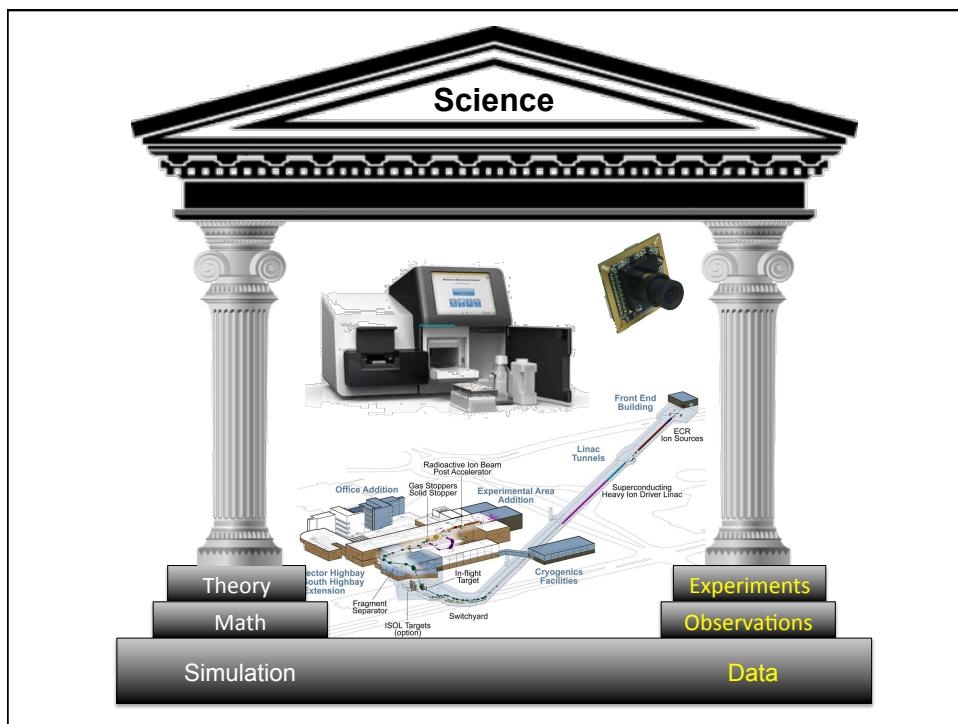


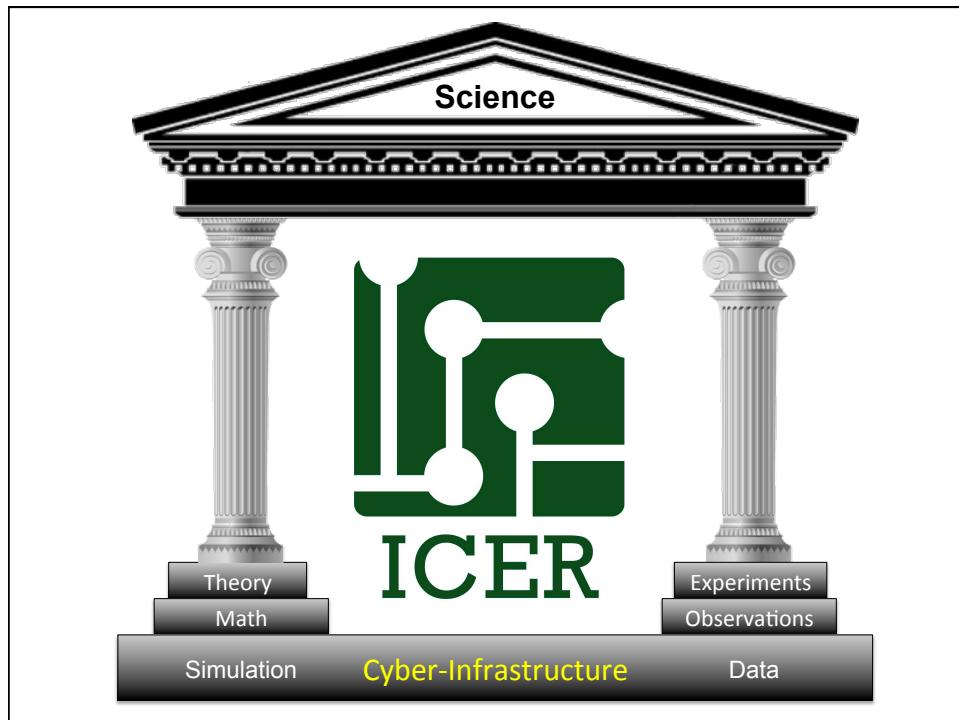
A vertical color palette on the right side of the slide, consisting of a 4x4 grid of squares in various shades of gray, light green, and dark green.











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What is Advanced Computing Hardware?

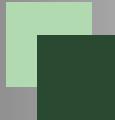
- Anything more advanced than your desktop
- Local resources
 - Lab, Department, Institution (iCER)
- National resources
 - NSF (XSEDE), DOE (Jaguar) , Others
- Commercial Resources (cloud computing)
 - Amazon, Azure, Liquid Web, Others

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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

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





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/>




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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Poster abstracts Due tomorrow

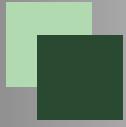


2013
CYBER INFRASTRUCTURE DAYS
 OCTOBER 24-25
 Save The Date!

<http://tech.msu.edu/CI-Days/>



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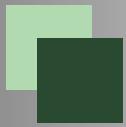


MSU Seminars in Research and Instructional Technology

Dec 17, 18, 2013

- Two days of no-cost seminars to faculty and graduate students on technology topics.
 - Morning sessions run from 8:30 to 11:30 am.
 - Afternoon sessions run from 1:30 to 4:30 pm.
 - Lunch is provided that will feature guest speakers on instructional technology.
 - Introduction to HPC
 - Advanced HPC

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What if I want more?



XSEDE
Extreme Science and Engineering
Discovery Environment



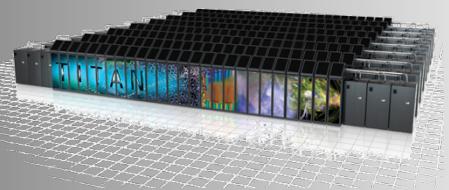
NASA



Open Science Grid



BLUE WATERS
SUSTAINED PETASCALE COMPUTING



TITAN



amazon
web services™

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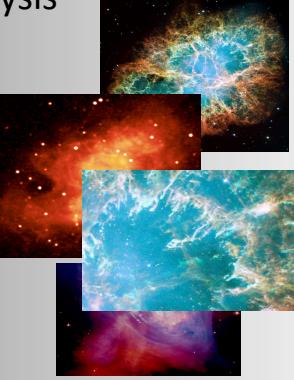
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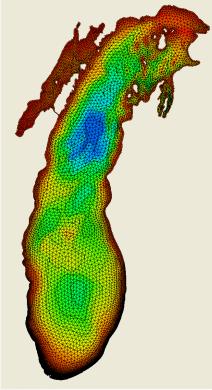


What problems are we solving?

- Boundary Simulations
- Data Analysis
- Search

 Image Provided by Dr. Warren F. Beck, MSU



 Image Provided by Dr. Mantha Phanikumar, MSU

Images from, "Understanding the H₂ 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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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.

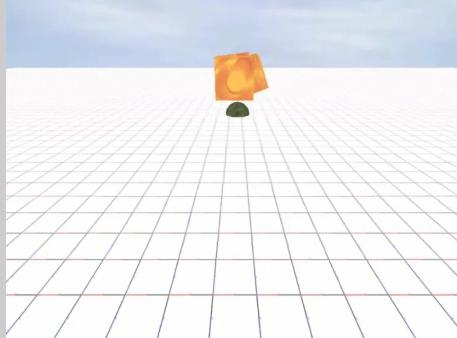
Video Provided by Dr. Fred Dyer

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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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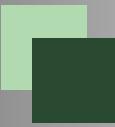
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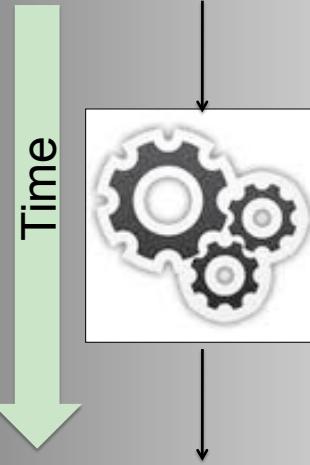


Steps in Using the HPCC

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!!



Single Thread Jobs



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



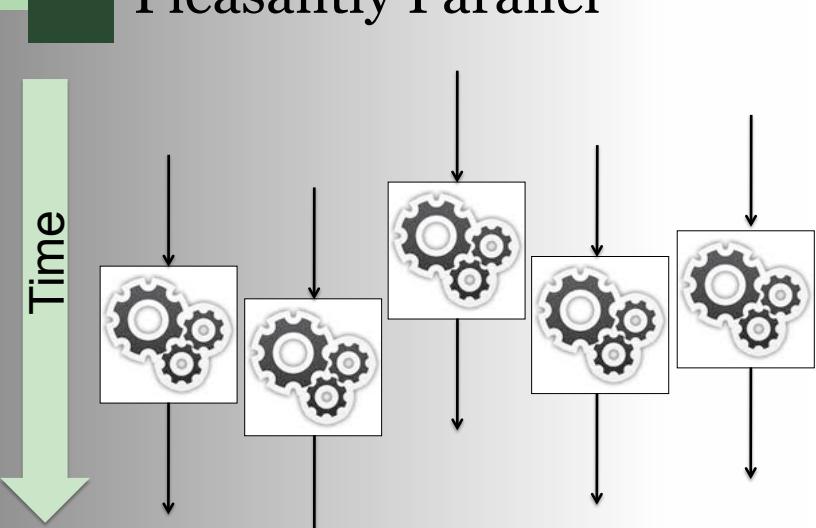


Communication

- 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

Time

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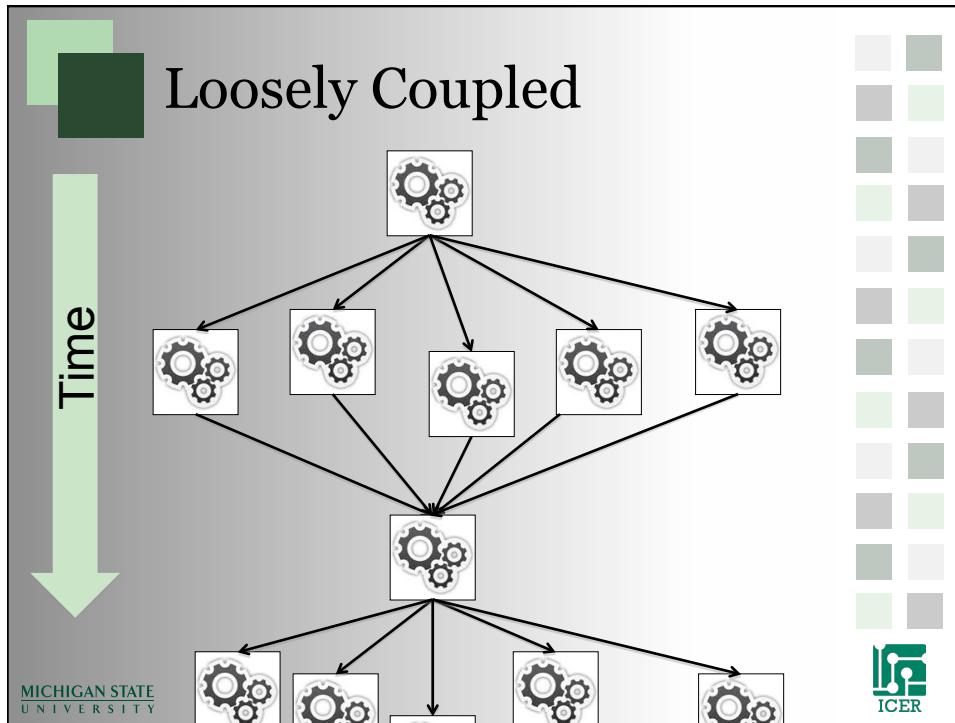
MSU HTCondor Cluster

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



 **HTCondor**
High Throughput Computing

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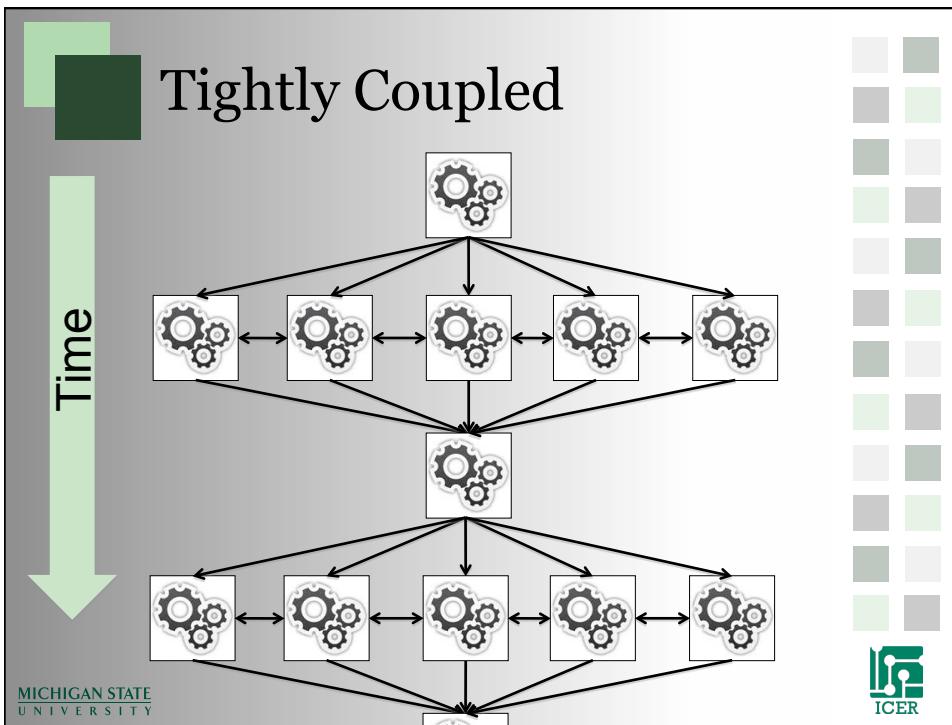


Shared Network Communication

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

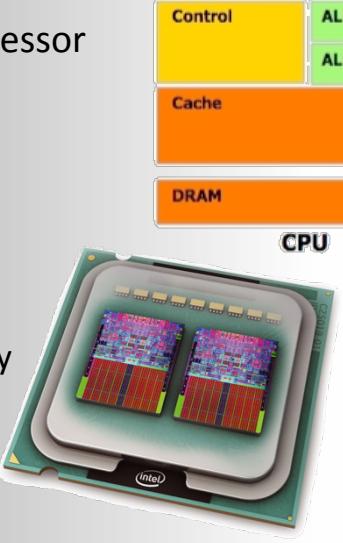
InfiniBand inside





Shared Memory Communication

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



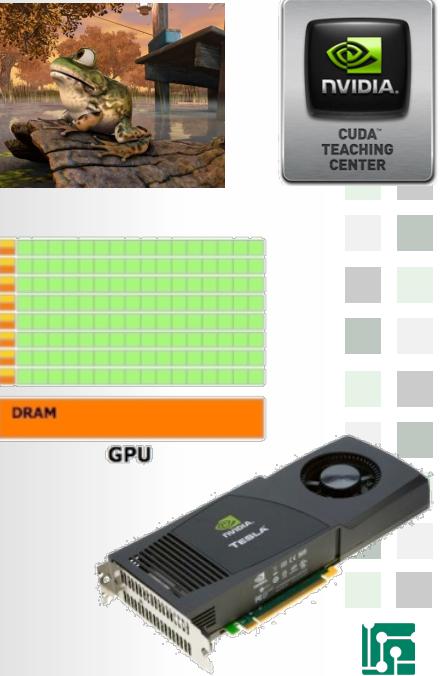
CPU

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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!



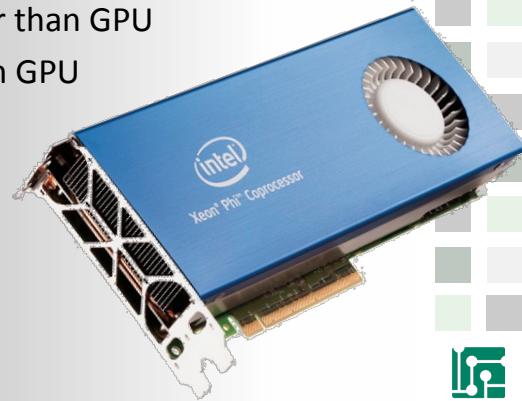
NVIDIA CUDA TEACHING CENTER

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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 GPU
- Very new



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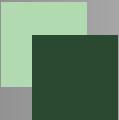
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Summary of Hardware

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

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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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