Do More, Faster: Leveraging Computational Resources in Your Research

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Agenda

- Who am I
- What is iCER / HPCC
- Steps to High Performance
- Common classes of computational science problems

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I am an engineer

- 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

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I am a researcher

- Ph.D. in CSE from MSU, focusing on image processing and pattern recognition
- Adjunct Faculty in ECE
- Research interests include optimizing image analysis workflows for researchers
- Currently collaborating with researchers in Engineering, Biology, Math and Statistics

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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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What is Advanced Computing Hardware?

- Anything more advanced than your desktop
- Local resources
  - Lab, Department, Institution (HPCC)
- 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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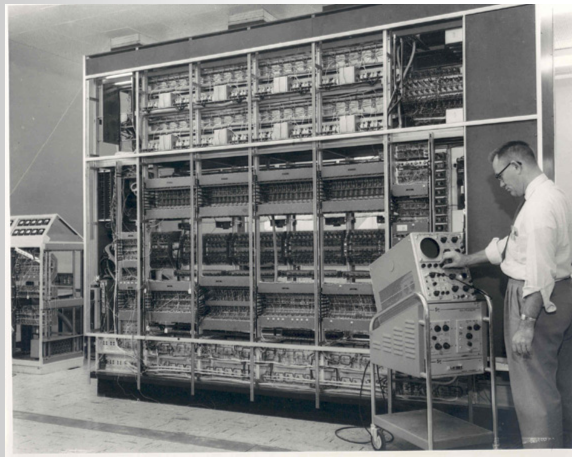
1957 MISTIC Mainframe

- 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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What is iCER?

- Institute for Cyber-Enabled Research
  - Established in 2009 to encourage and support the application of advanced computing resources and techniques by MSU researchers
  - Goal is to maintain and enhance the university's national and international standing in computational disciplines and research thrusts

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Bigger Science

- The goal of iCER is NOT:
  - Kflops
- Instead, the goal of iCER IS:
  - KSciences / second
- Doing More Science, Faster
  - Reducing the “Mean time to Science”
- iCER is designed to help researchers do their science and when appropriate scale them up to one of the national labs

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Hardwa

High speed network interconne
- MPI jobs
- High Speed Parallel Scratch Space

InfiniBand inside

General Purpose Graphics Cluster

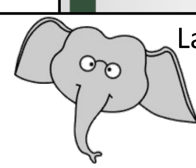
NVIDIA CUDA

GB of local

2010

2010

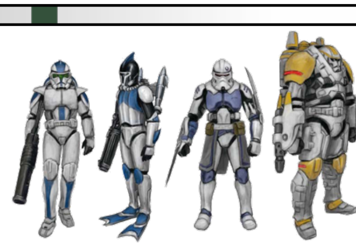
Large Capacity “FAT” Nodes
- Up to 2TB of RAM
- Up to 64 cores



512 core, 128 node cluster installed 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
- RHEL6.0
- Compile once
- Run anywhere



2011

1
512GB - 2TB RAM nodes
64 core 2.66 GHZ Xeon processors.

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Hardware Summary

FREE*

- Over 3110 Nodes
- Over 23072 CPU cores
- Over 363 TB of scratch memory 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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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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Accounts

- Each user has 50Gigs of backed-up personal hard drive space
  - /mnt/home/username/
- Users have access to 363TB of high speed parallel scratch space
  - /mnt/scratch/username/
- Shared group space is also available upon request

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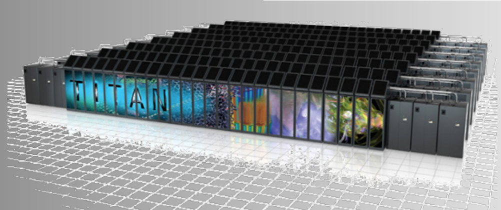
What if I want more?

XSEDE
Extreme Science and Engineering Discovery Environment

NASA

Open Science Grid

BLUE WATERS
SUSTAINED PETASCALE COMPUTING



amazon web services™

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MSU Seminars in Research and Instructional Technology

Dec 18 and 19, 2012

- 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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http://train.msu.edu/faculty/seminars/

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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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Steps in Using Resource

- Connect to Resource
- Determine required software
- Transfer required input files and source code
- Compile programs (if needed)
- Test software/programs on a developer node
- Write a submission script
- Submit the job
- Get your results and write a paper!!

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Types of problems

- CPU bound
  - Lots of computing (think simulation)
- Memory bound
  - Requires lots of memory (think genomics)
- I/O bound
  - Requires lots of data (think astronomy)

(many problems fall in more than one category)

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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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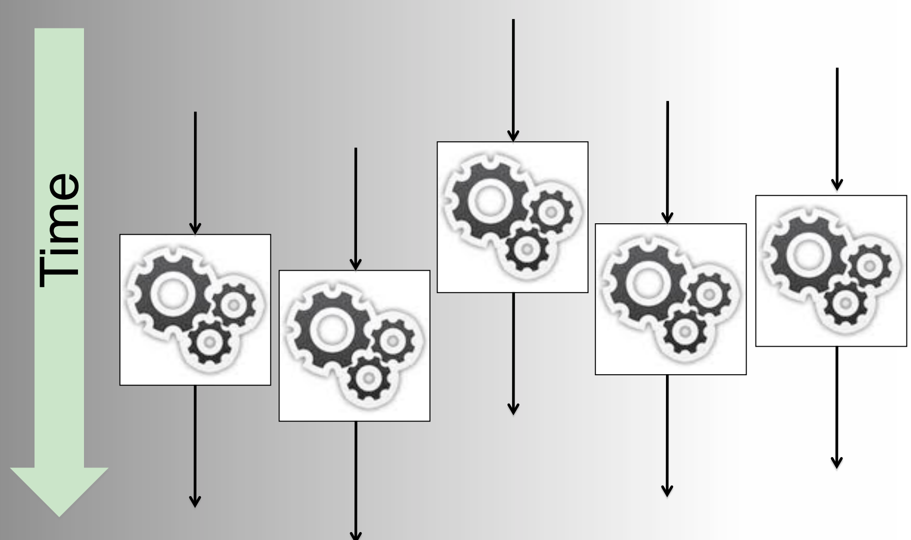
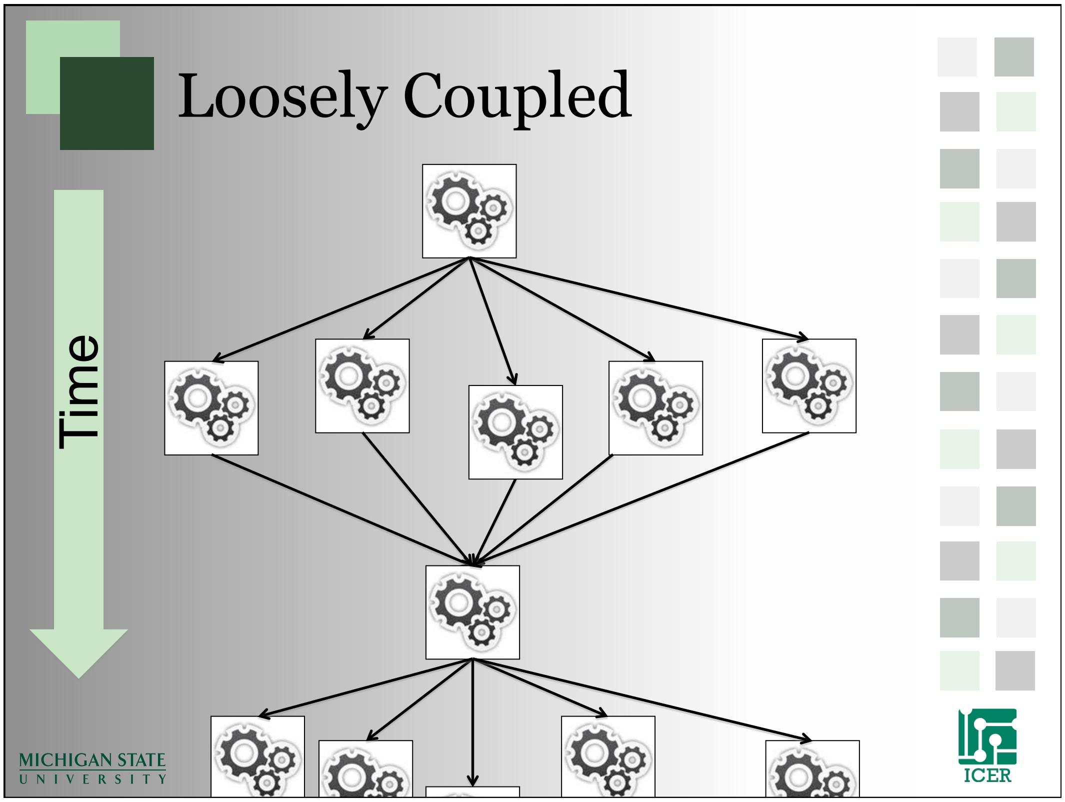
How much Communication?

- Pleasantly parallel
  - No communication required
- Loosely coupled
  - Typically sync at regular intervals
- Tightly coupled
  - Constant communication

Pleasantly Parallel




Loosely Coupled
Time
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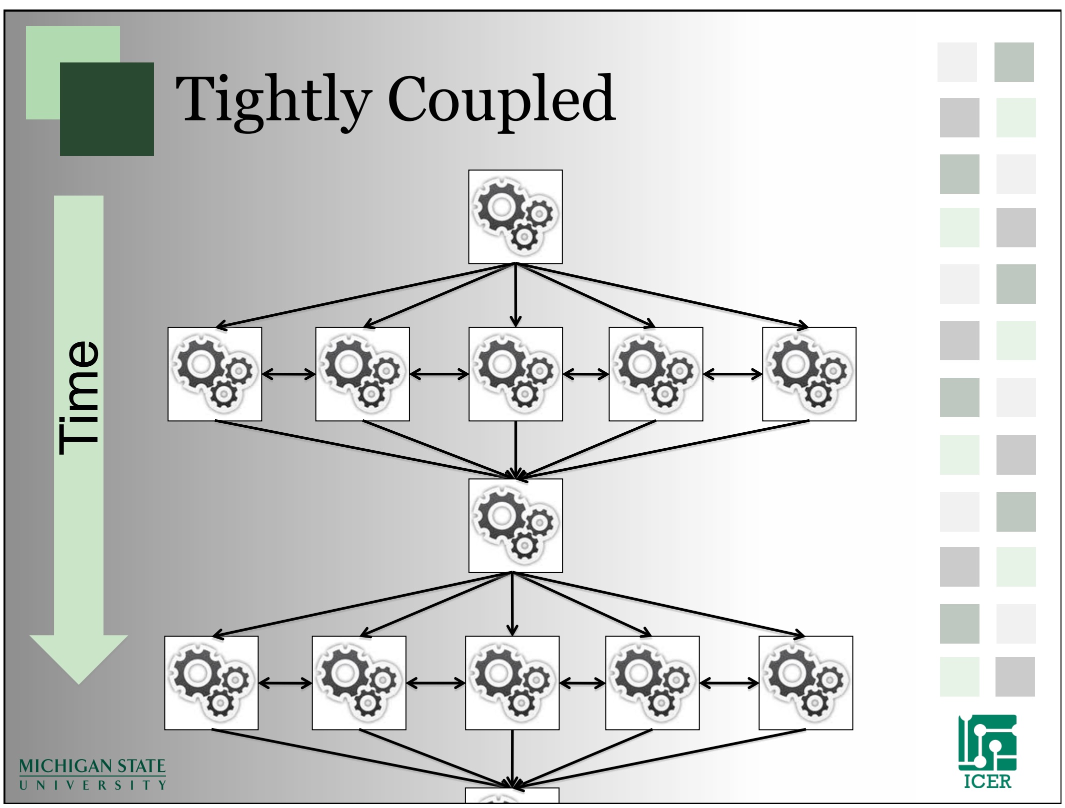
Tightly Coupled
Time
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Types of communication

- Shared Memory
  - Typically very fast
  - OpenMP and GPGPU interfaces (sort of)
  - Doesn't scale well
- Shared File System
  - Slower communication / locking issues
  - Very easy to use
  - Speed of the network is a bottleneck
- Shared Network
  - Speed of the network is a bottleneck
  - Scales well
  - MPI and Map-Reduce interfaces

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Example Problems

- Boundary Simulations
- Data Analysis
- Search

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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

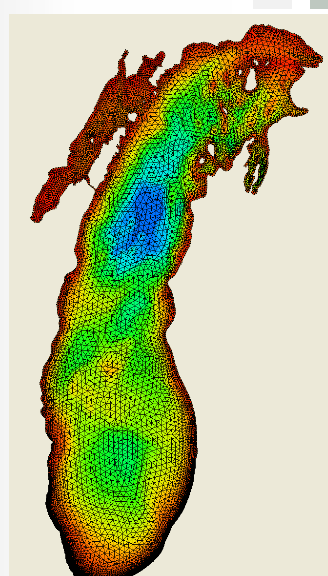

Image Provided by Dr. Mantha Phanikumar, MSU

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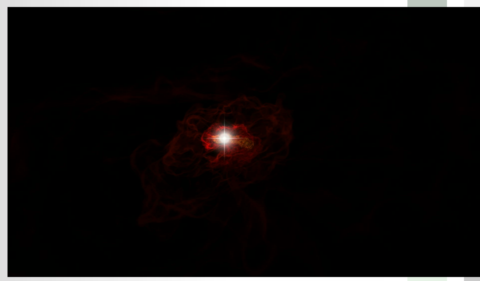
Boundary Simulations

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



O'Shea

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

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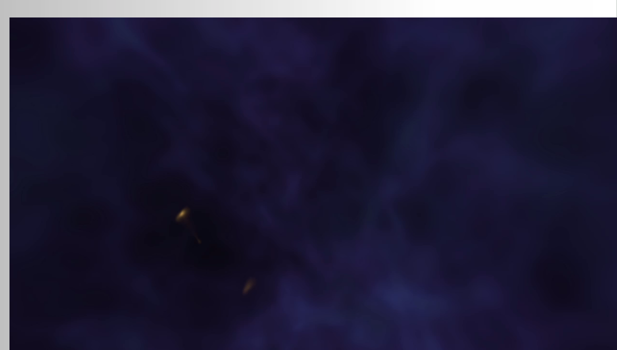
Boundary Simulation

- Tightly to loosely coupled
- Typically solved with MPI
- PDE solutions available for GPU and OpenMP



Turk, Smith, O'Shea

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Example: Data Analysis

1. Input data file
2. Find features, search or filter data in some way
3. Output Results

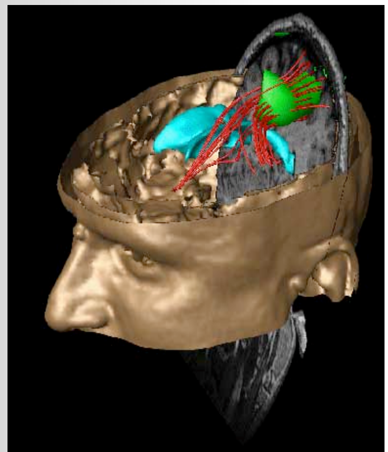
Image from OpenDX

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Data Analysis

- Computer vision tasks
- Bioinformatics
- Astrophysics
- Etc.

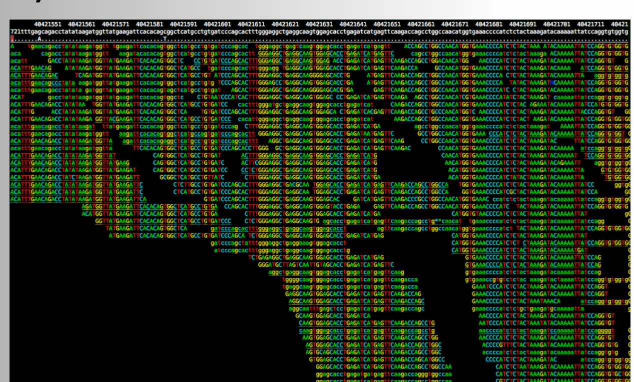
Image generated using SAMtools

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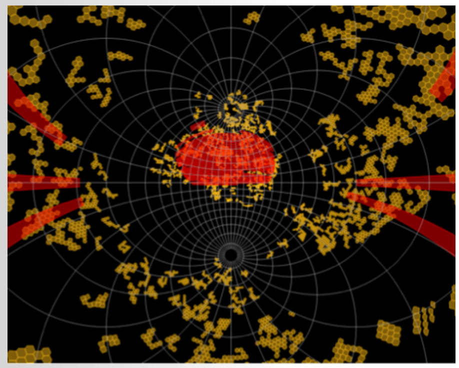
Data Analysis

- Loosely coupled
- Bulk of computation is typically pleasantly parallel
- Can be I/O bound



The footprints of the Sloan Digital Sky Survey's 5th Data Release and the Galaxy Evolution Explorer's 2nd Public Release

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Example: Search

- Randomly generate test candidates
- Evaluate the quality of solution
- Repeat until found

Image Provided by Dr. Warren F. Beck, MSU

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Search

- Evolution (Avida)
- Genetic Algorithms
- RANSAC
- Monte Carlo
- Etc.

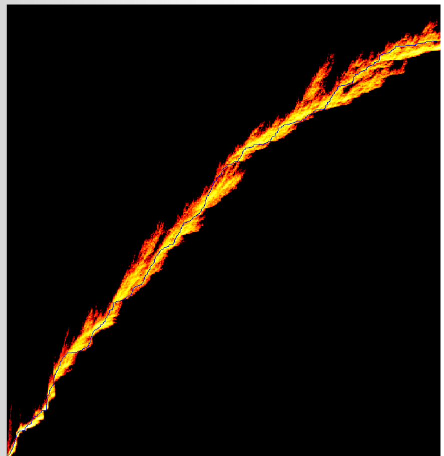
Image Provided by Dr. Charles Ofrea, MSU

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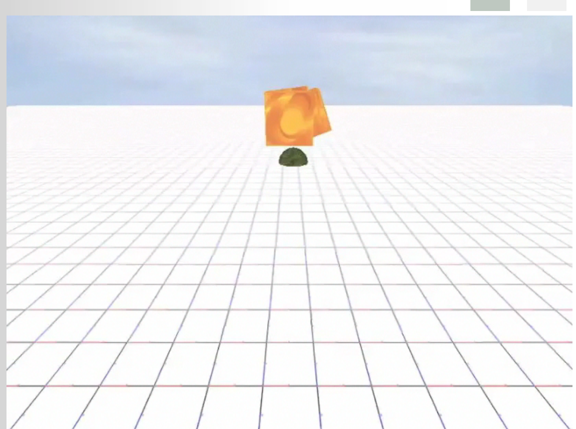
Search

- Pleasantly parallel
- The more the better
- Typically not I/O bound
- Typically not memory bound


BEACON, evolved foraging behavior, digital evolution study

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Summary

- Advanced computational hardware can help you do more science faster
- Advanced computing typically requires knowledge of a primitive interface (command line)
- When parallelizing your computation,
  think about where the loops are,
  what needs to be communicated,
  and where there are bottlenecks
- There are many existing computational resources that can help you get started

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Questions?

iCER Website:

http://icer.msu.edu

User Information on HPCC:

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

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