Do More, Faster:
Utilizing Advanced Computing Hardware

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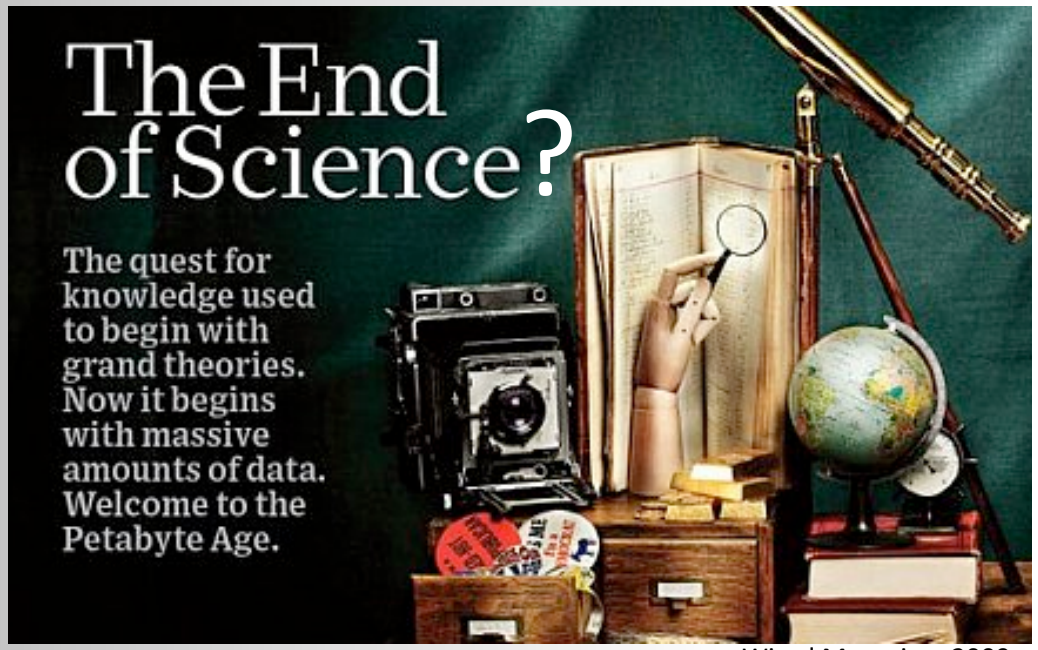
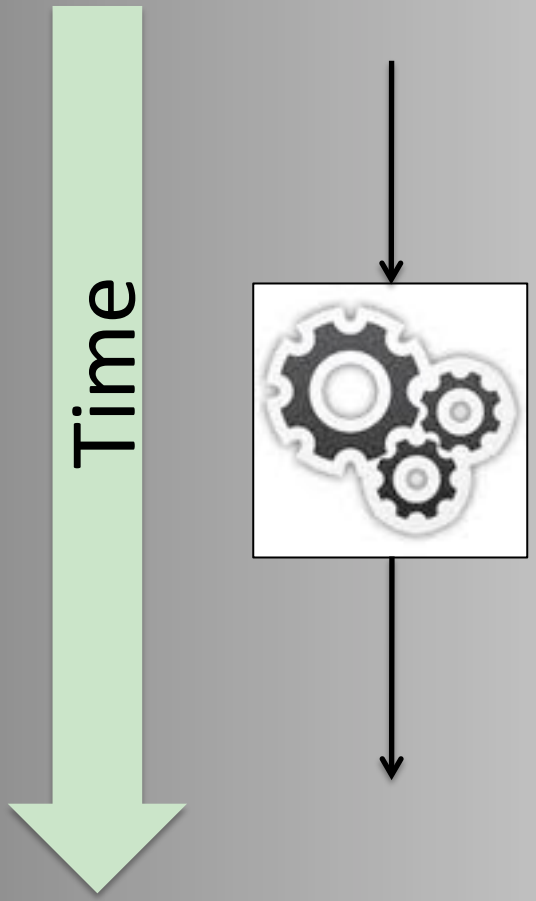
Science and Computation

- Pillars of Science:
  - Theory
  - Experimentation
  - Simulation
  - (Big) Data



Wired Magazine, 2009

Scientific Programming



Inputs (Data)

Computation

Outputs (Results)

Agenda

- Three Examples
  - Pleasantly Parallel
  - Shared Memory
  - Scaling up
- Advanced Computing at MSU

Problem Type: Data Analysis

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

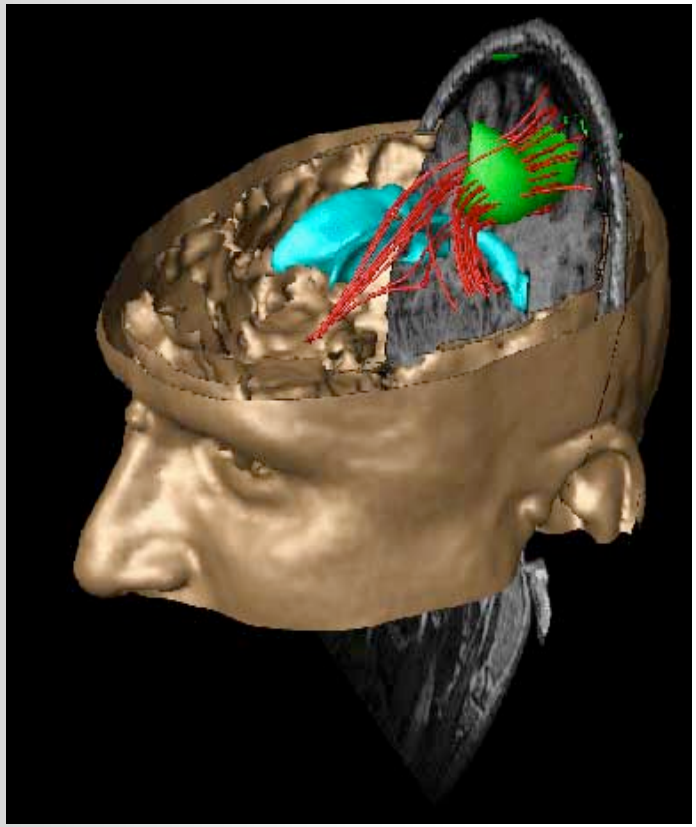


Image from OpenDX

Data Analysis

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

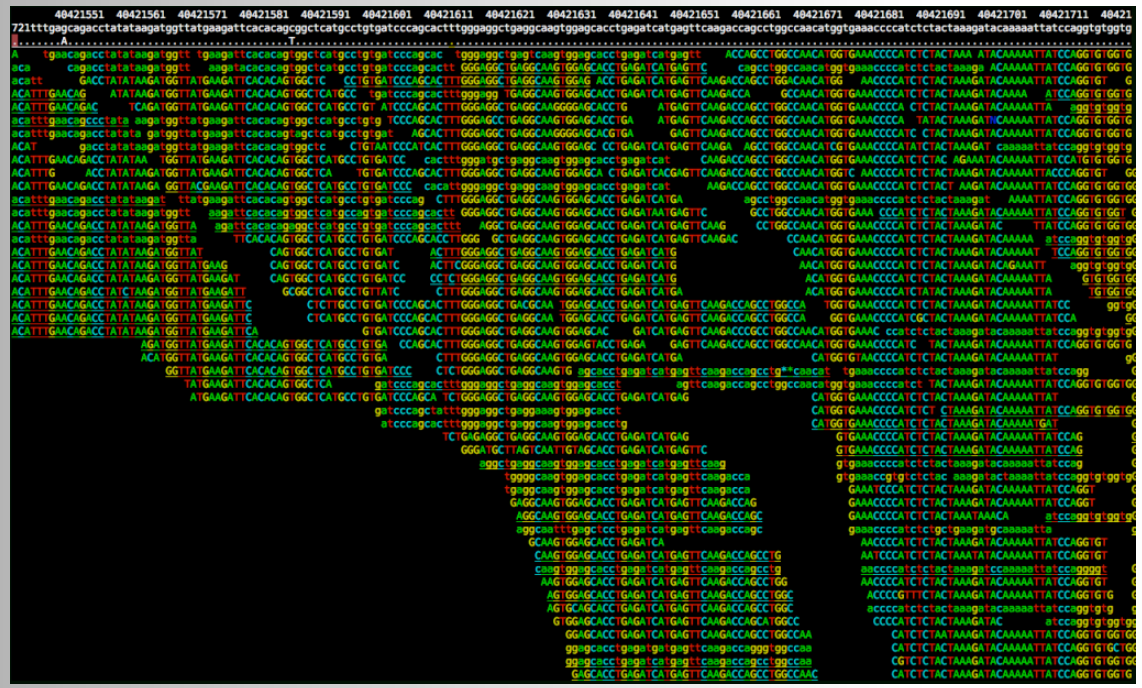
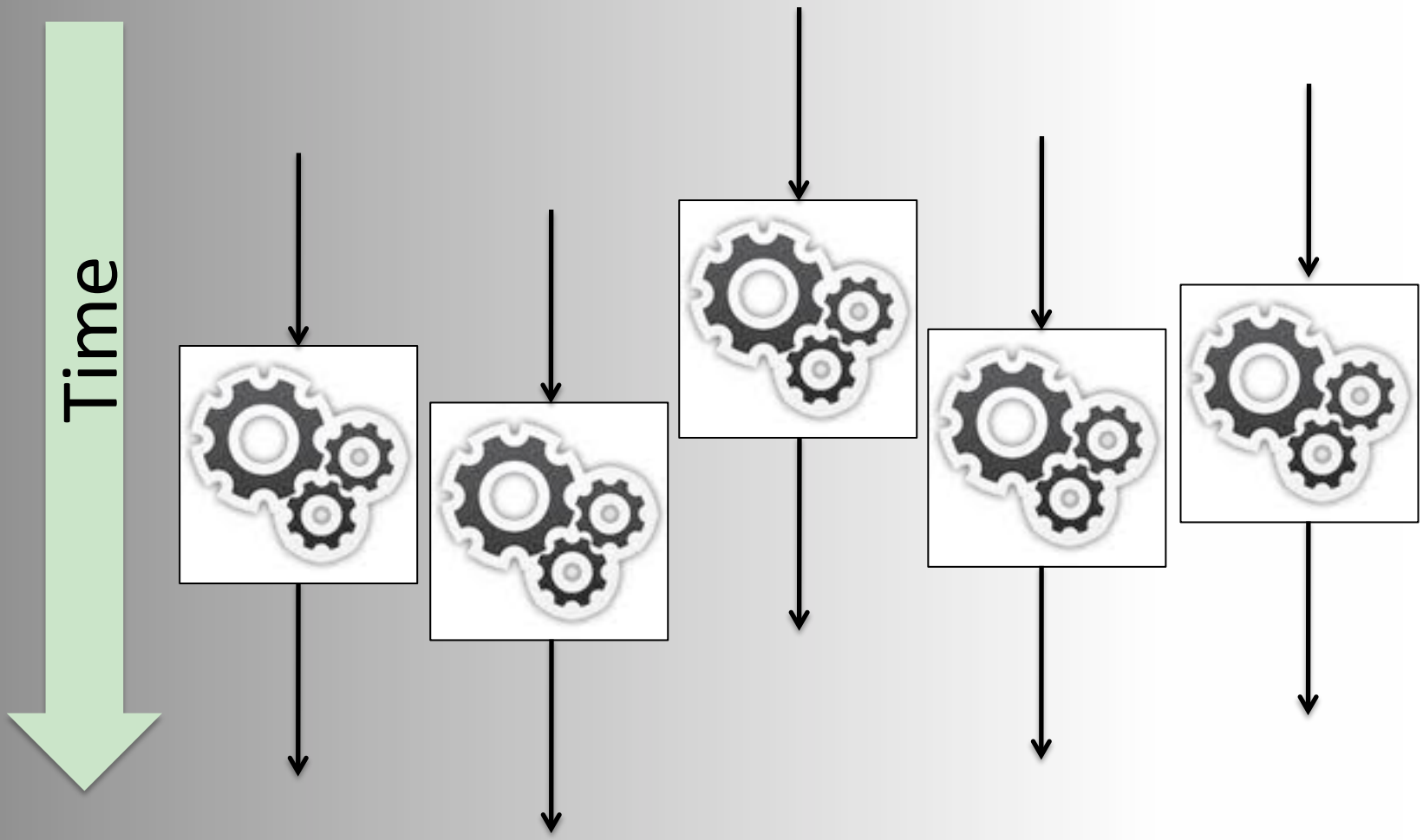
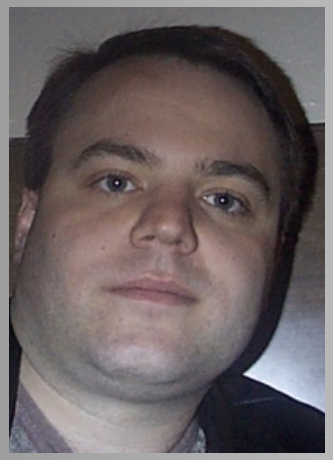


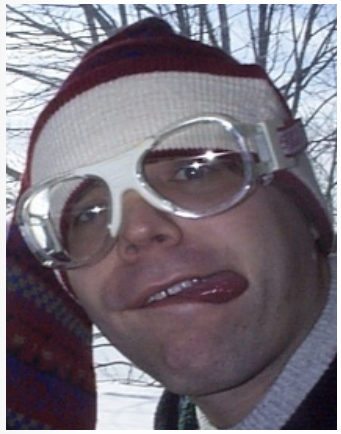
Image generated using SAMtools

Pleasantly Parallel



Who are you? -- Biometrics





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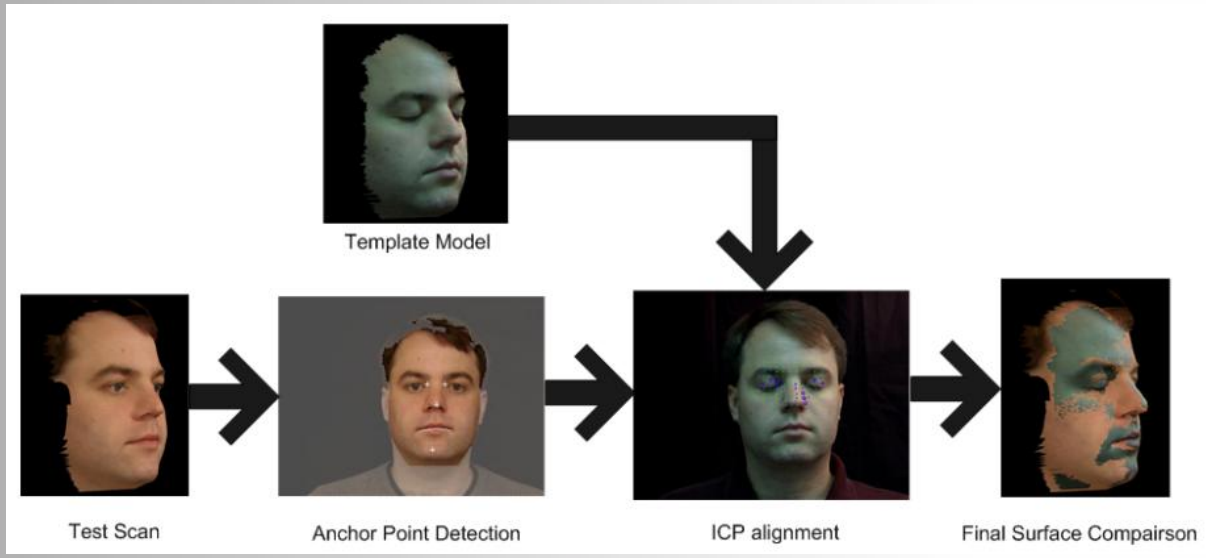
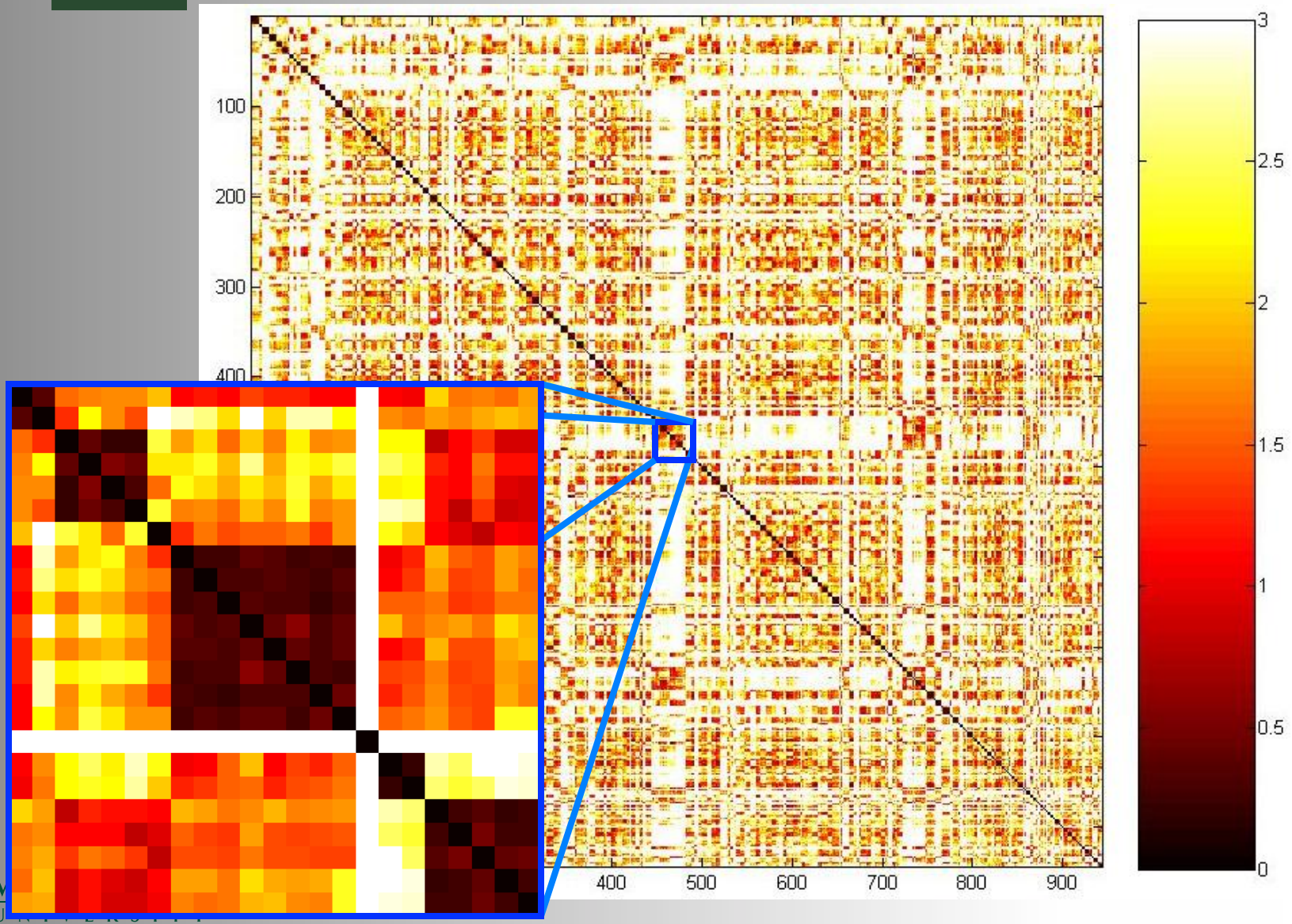
Pairwise-All Problem

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



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

- Running on 32 computers
  - < 1 day

How do we go even bigger?

- 5000 scans.
  - 1.5 years on a single processor computer
  - 13 days on 32 computers.
  - 3 days on 144 computers

High Throughput Computing (HTC)

- Problem easily split into small independent chunks
- Does not require large amounts of memory
- Does not require large network bandwidth

- Examples
  - SETI@home
  - Folding@home
  - Boinc
  - Condor

Condor High Throughput Computing

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

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Agenda

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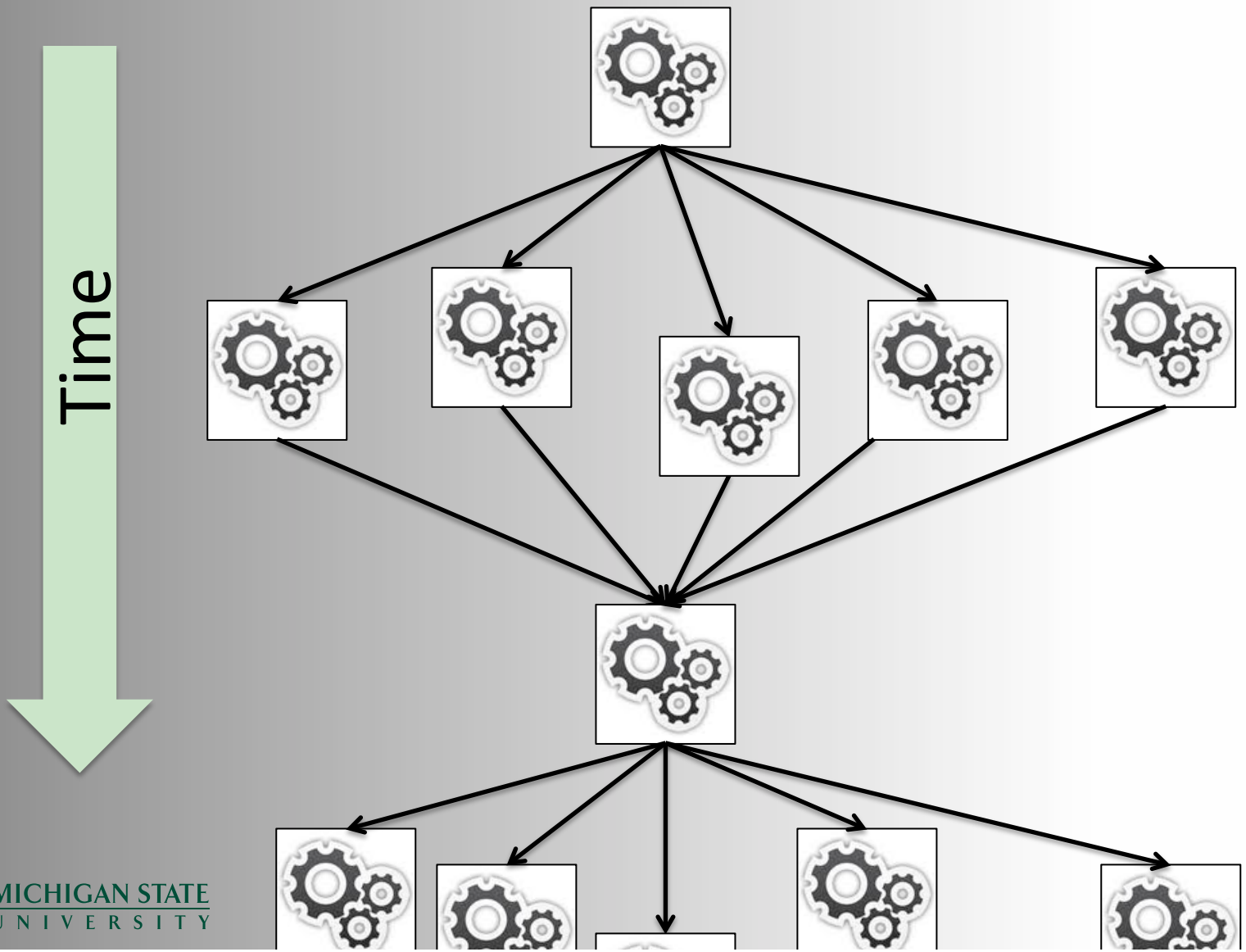
Loosely Coupled



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Problem Type: Search

- Search a parameter space
- Evaluate the quality of solution
- Repeat until found

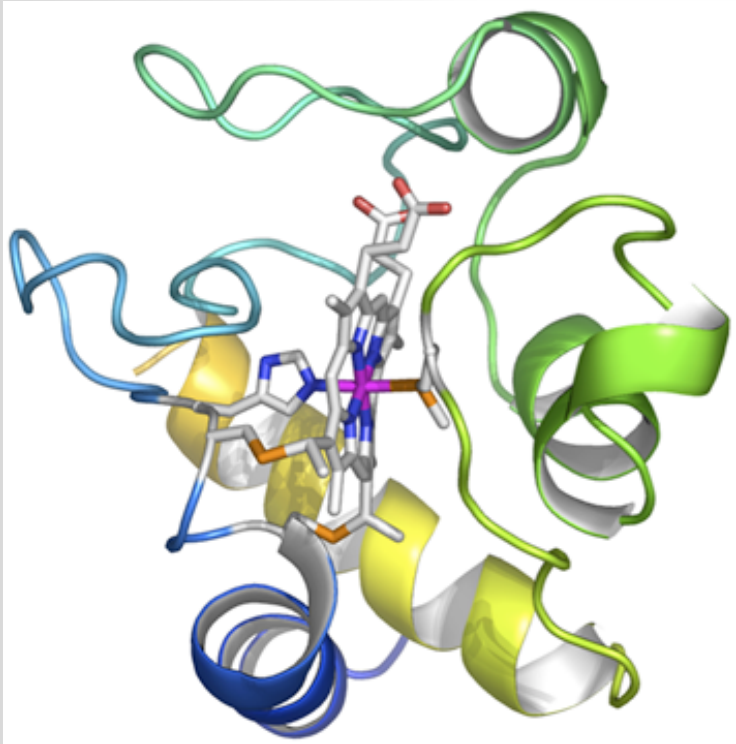

Image Provided by Dr. Warren F. Beck, MSU

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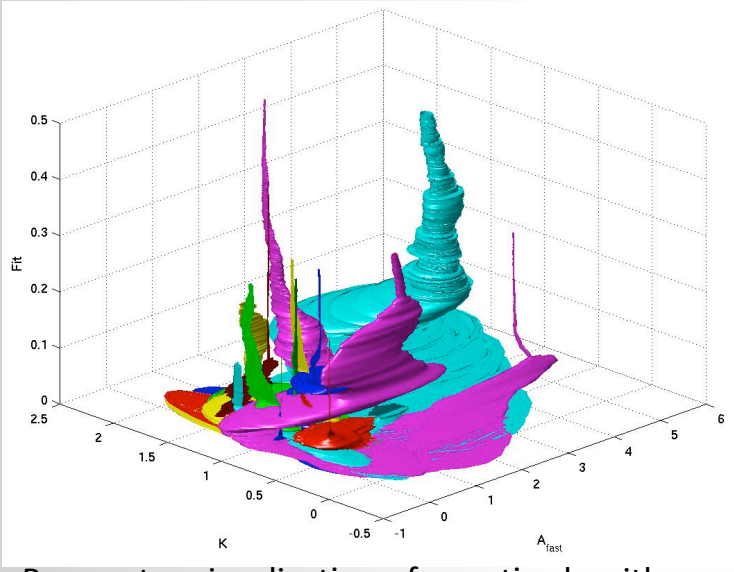
Search

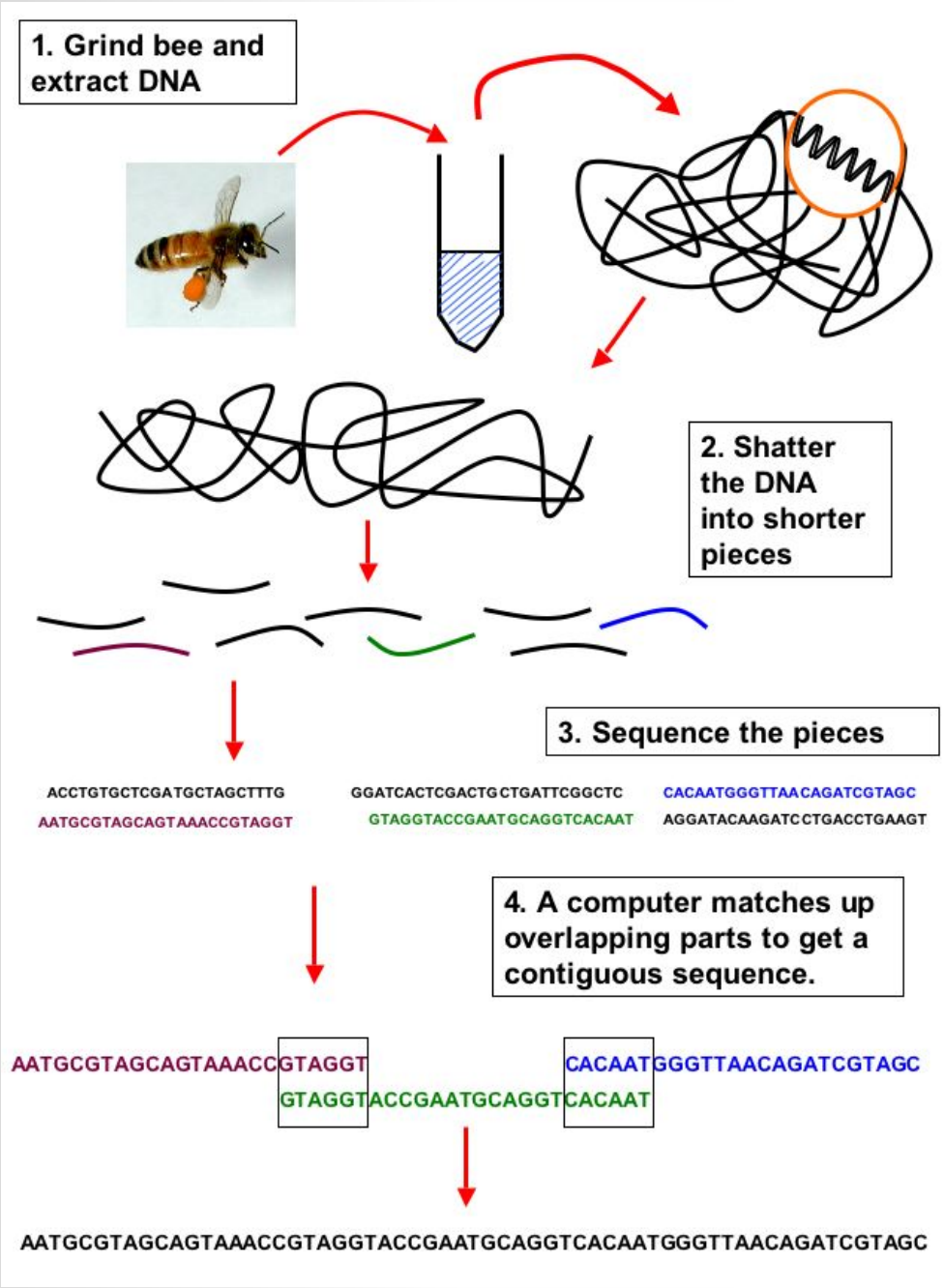
- Sometimes Pleasantly parallel
- What happens when it is memory bound?



Parameter visualization of genetic algorithm search for research conducted at Ohio University

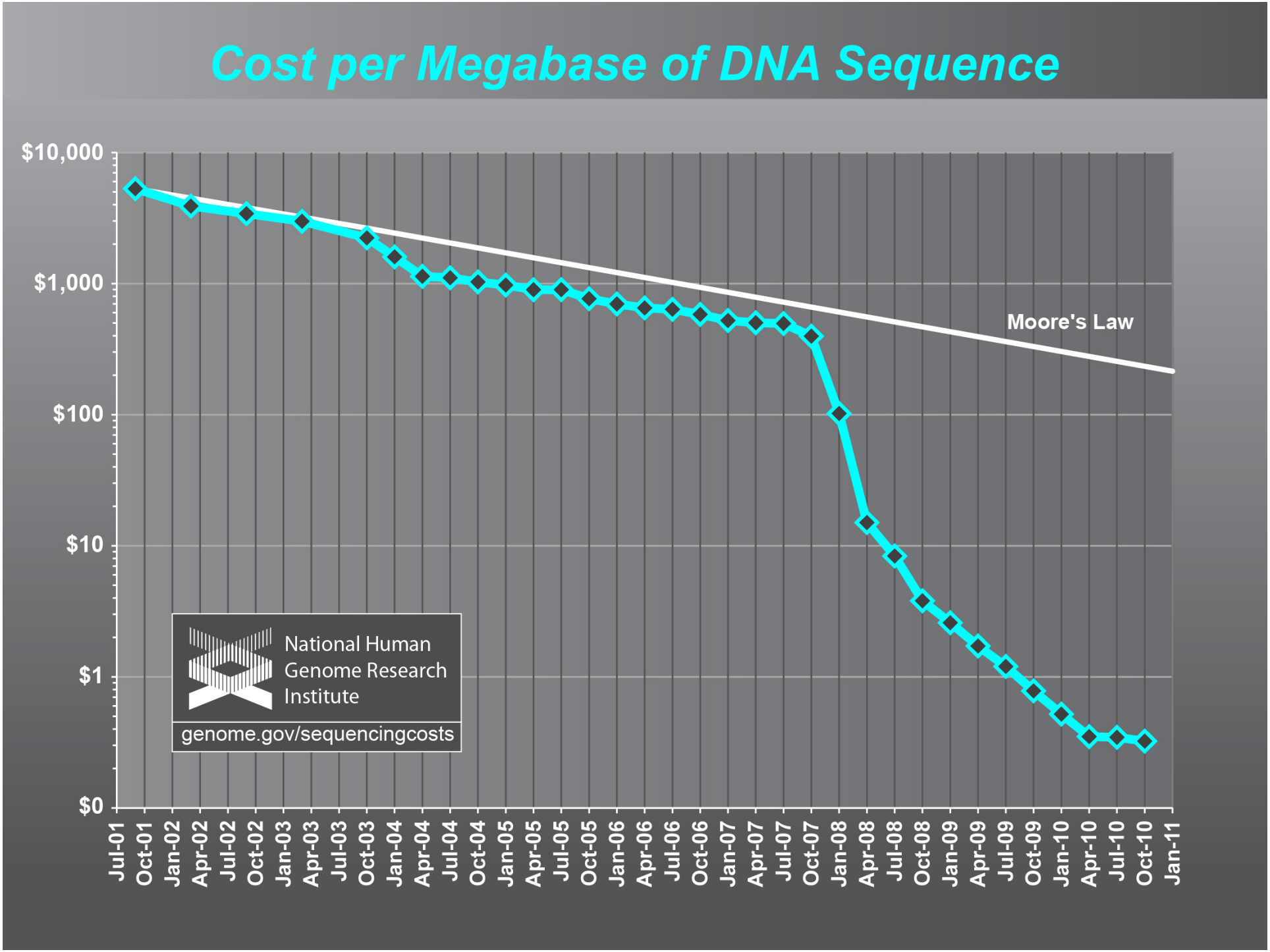
Genome Sequencing

- Assembly typically uses large tables to record all of the different possible overlaps.
- It takes a lot of memory and CPUS to assemble typical Genomes

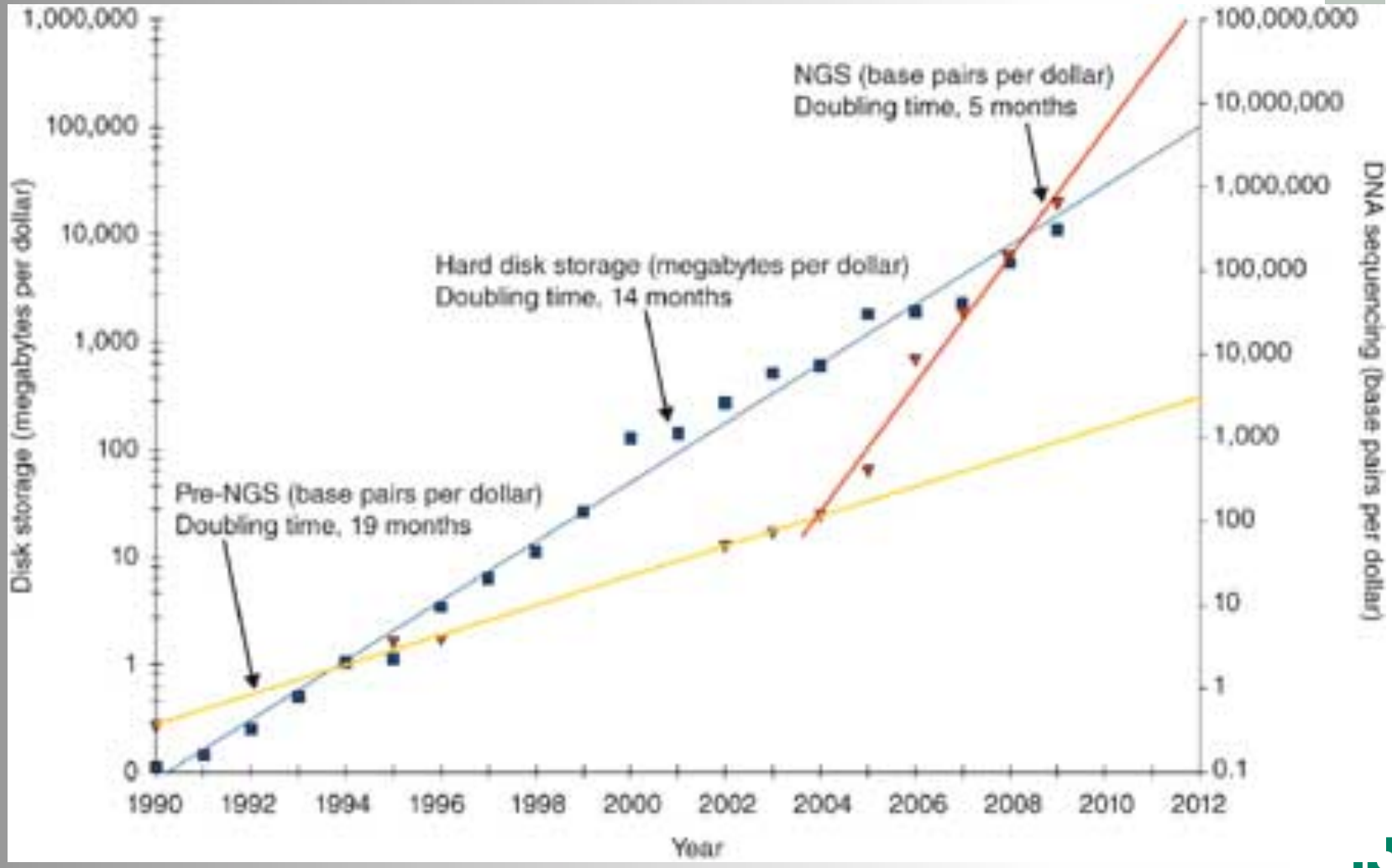


http://beespotter.mste.illinois.edu/

Cost per Megabase of DNA Sequence



Hard to keep up!



Stein, L.D. Genome Biol. 11, 207 (2010).

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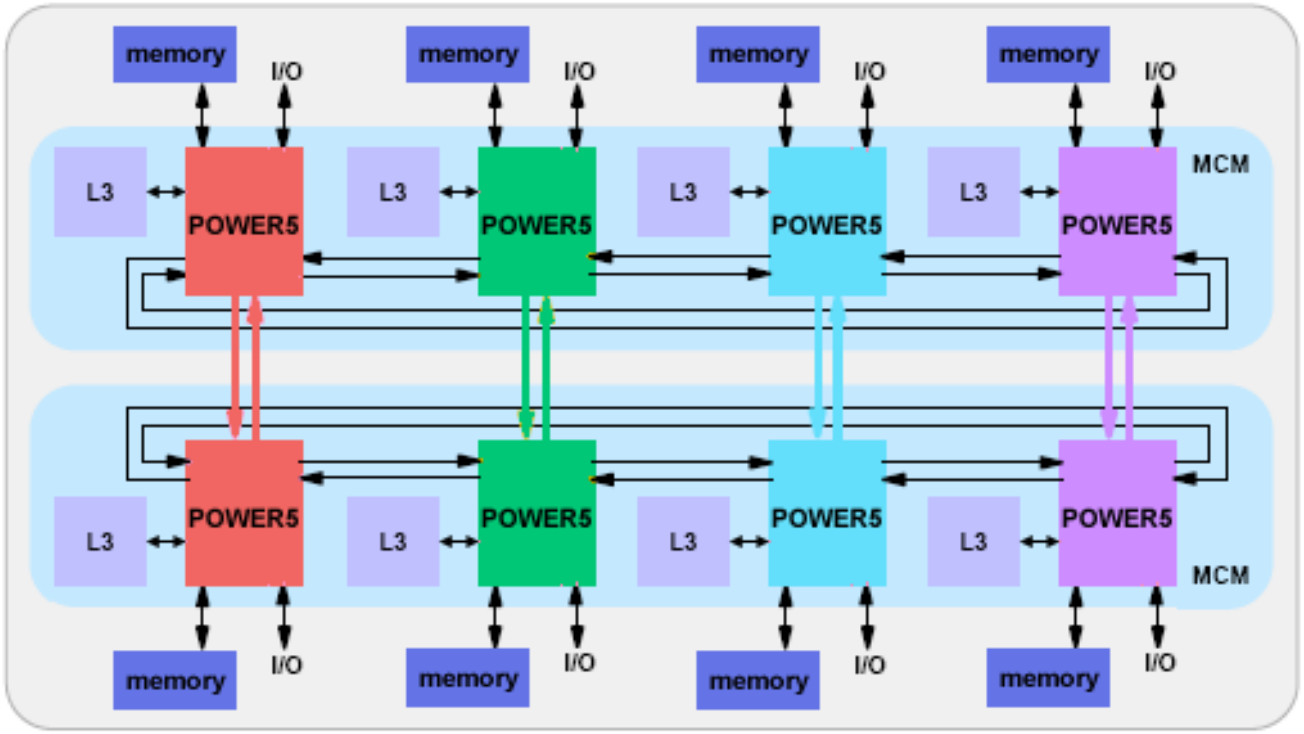
Shared Memory

- Symmetric Multiprocessor (SMP) machine
  - Many cores shared memory
- Current Machines:
  - 32-64 processing cores (CPUS)
  - 250GB – 2TB of memory
- All Communication can be done in memory so communication is very fast.

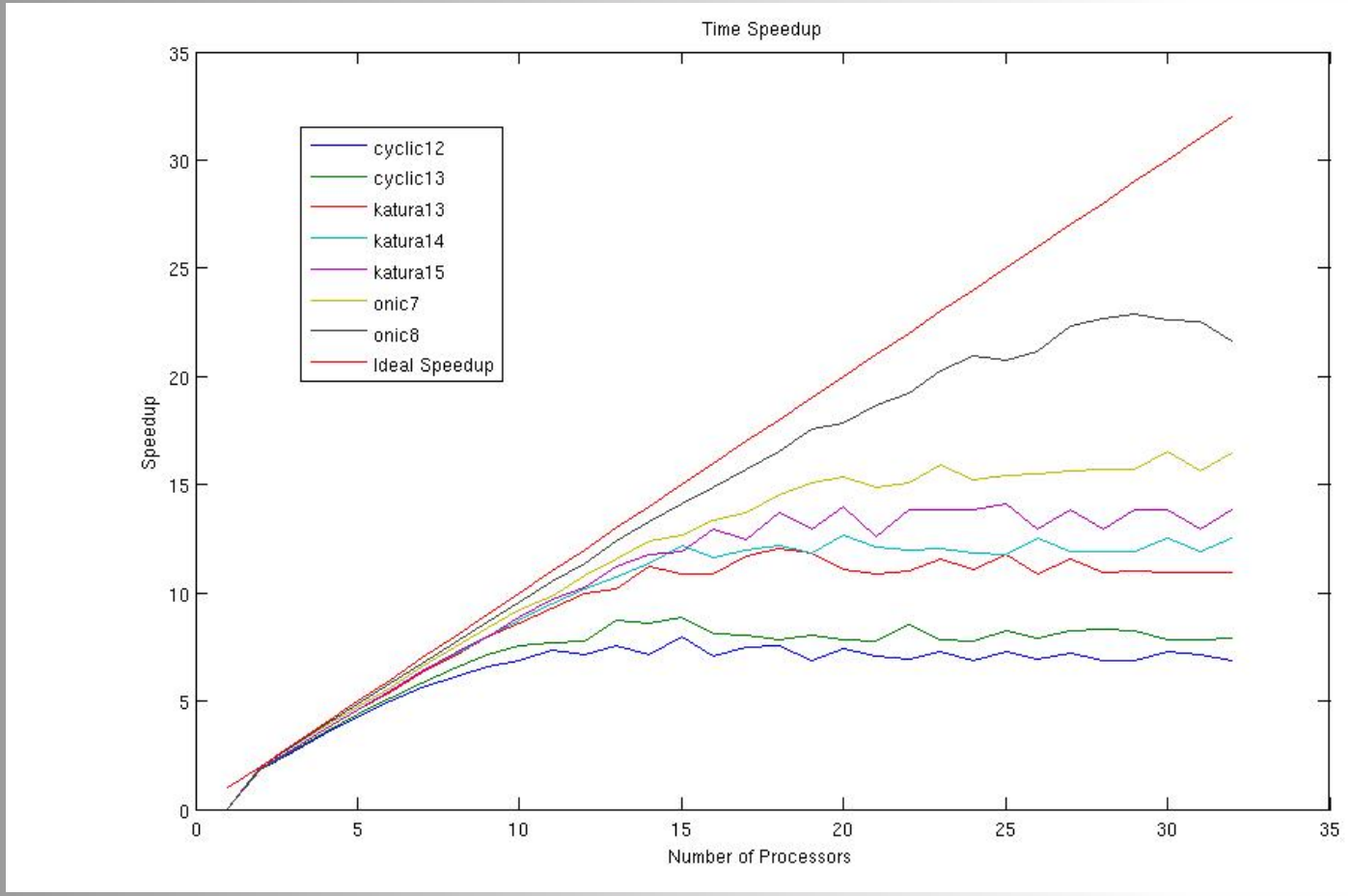
Shared Memory Libraries

- OpenMP
- Pthreads
- Cuda
- others



16-way SMP Building Block (book)

Limits to Shared memory computing



GPGPU

Agenda

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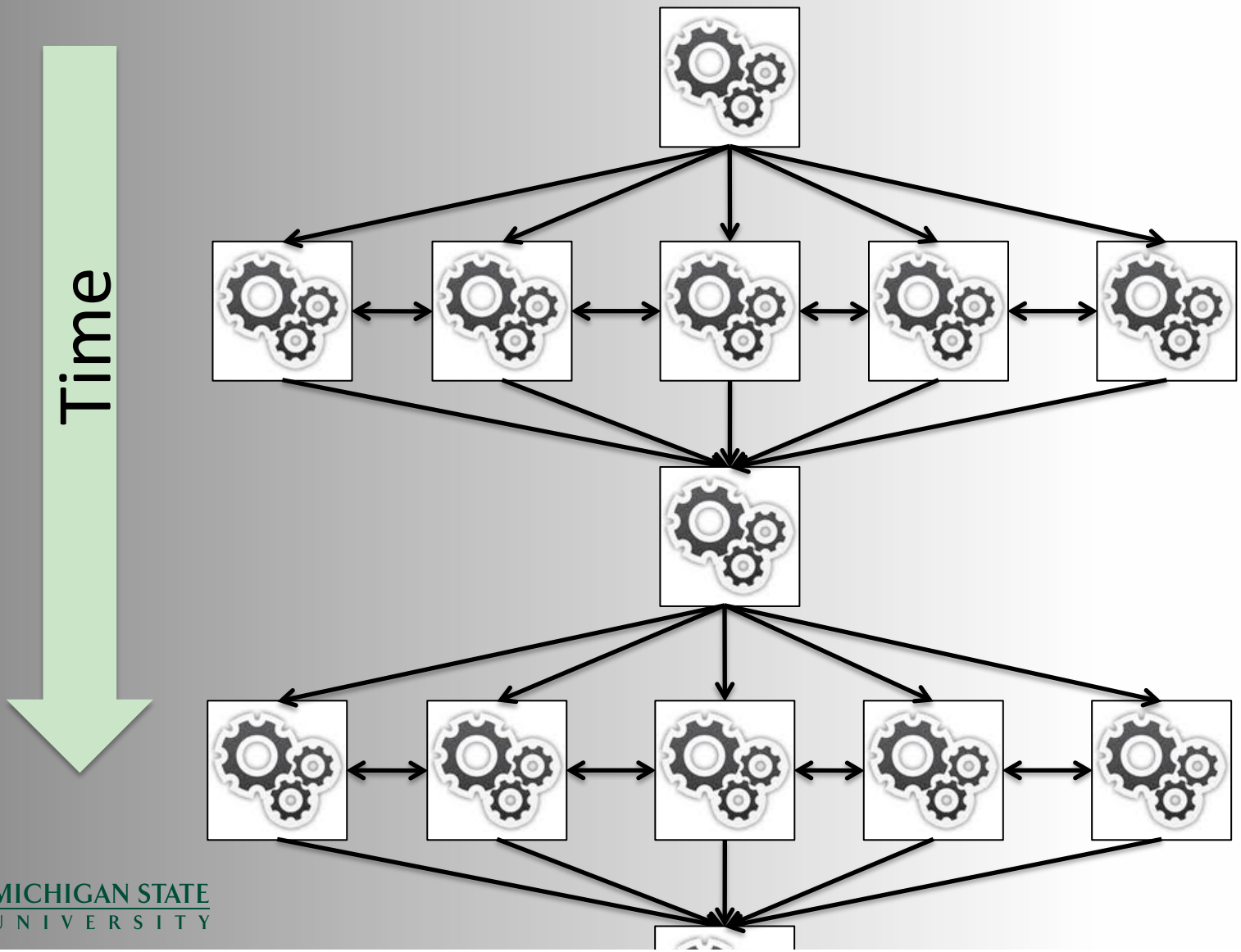
Tightly Coupled



Problem Type: 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

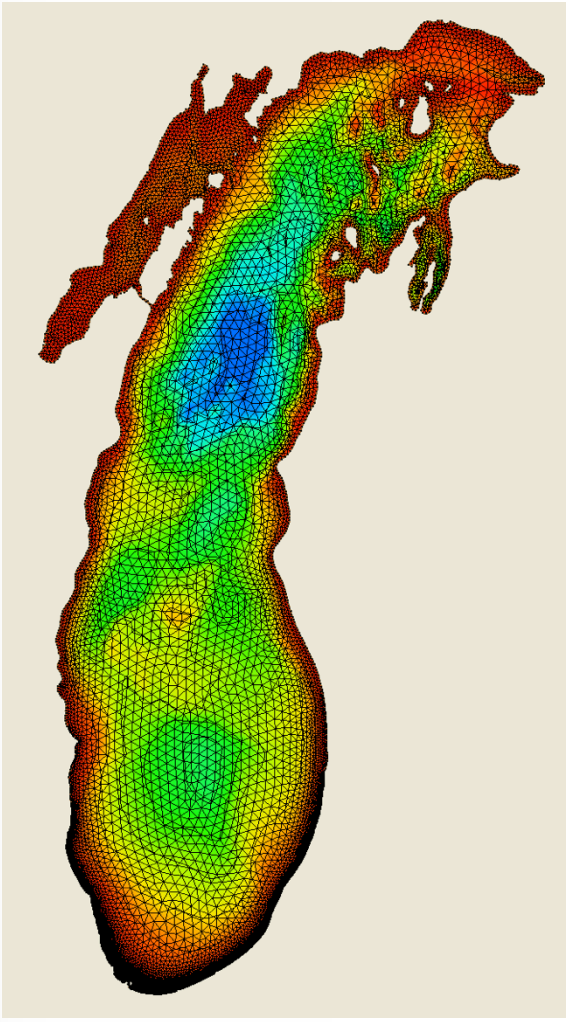
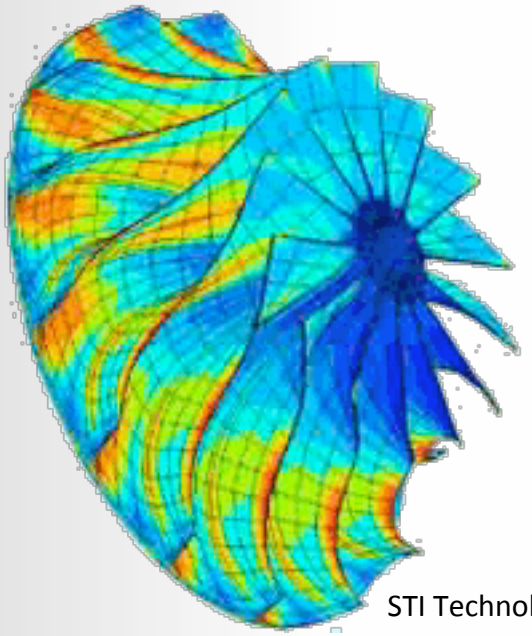


Image Provided by Dr. Mantha Phanikumar, MSU

Boundary simulations

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

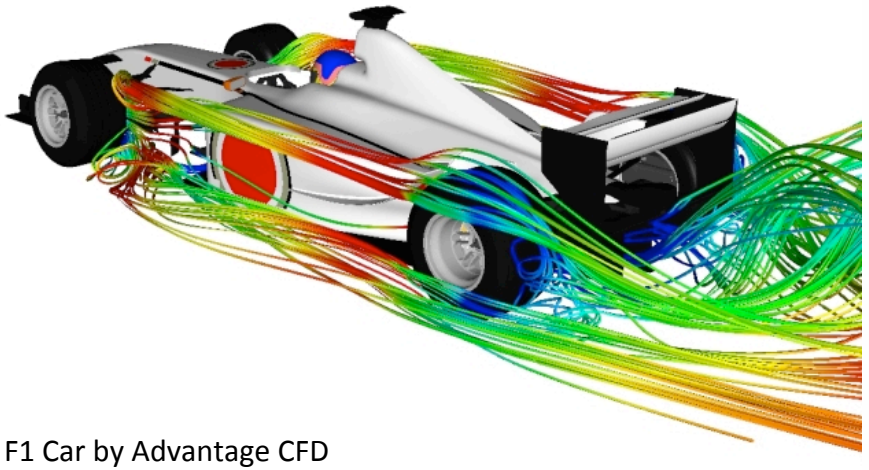


STI Technologies Inc.

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

Boundary Simulation

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

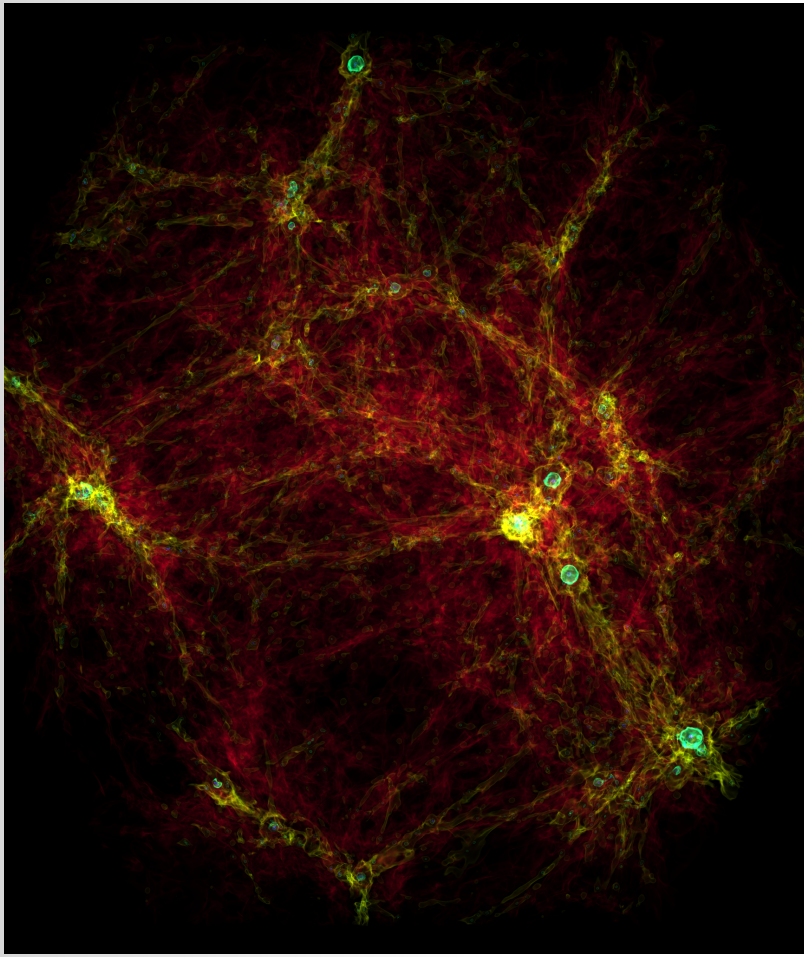


F1 Car by Advantage CFD

Simulating The Birth of Stars

- Subdivide the universe into a grid
- What Scale do you use?

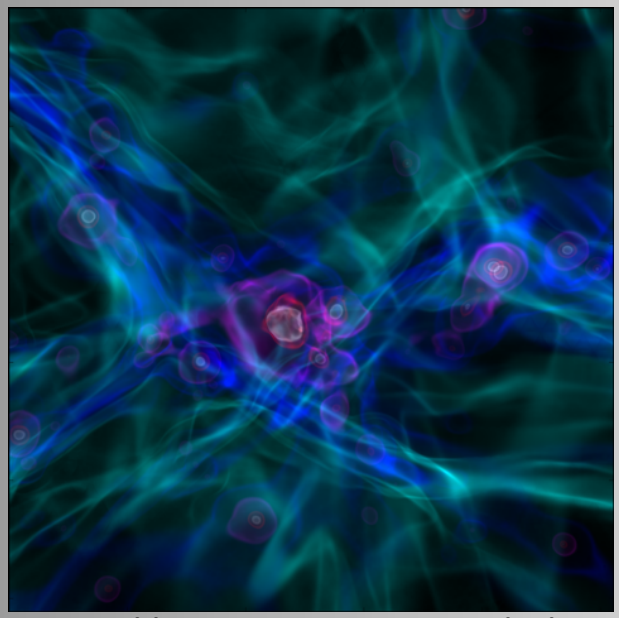
- No way to solve the problem at any one resolution!



http://code.google.com/p/enzo/

No scale is feasible

- Solution:
  - Change the scale dynamically



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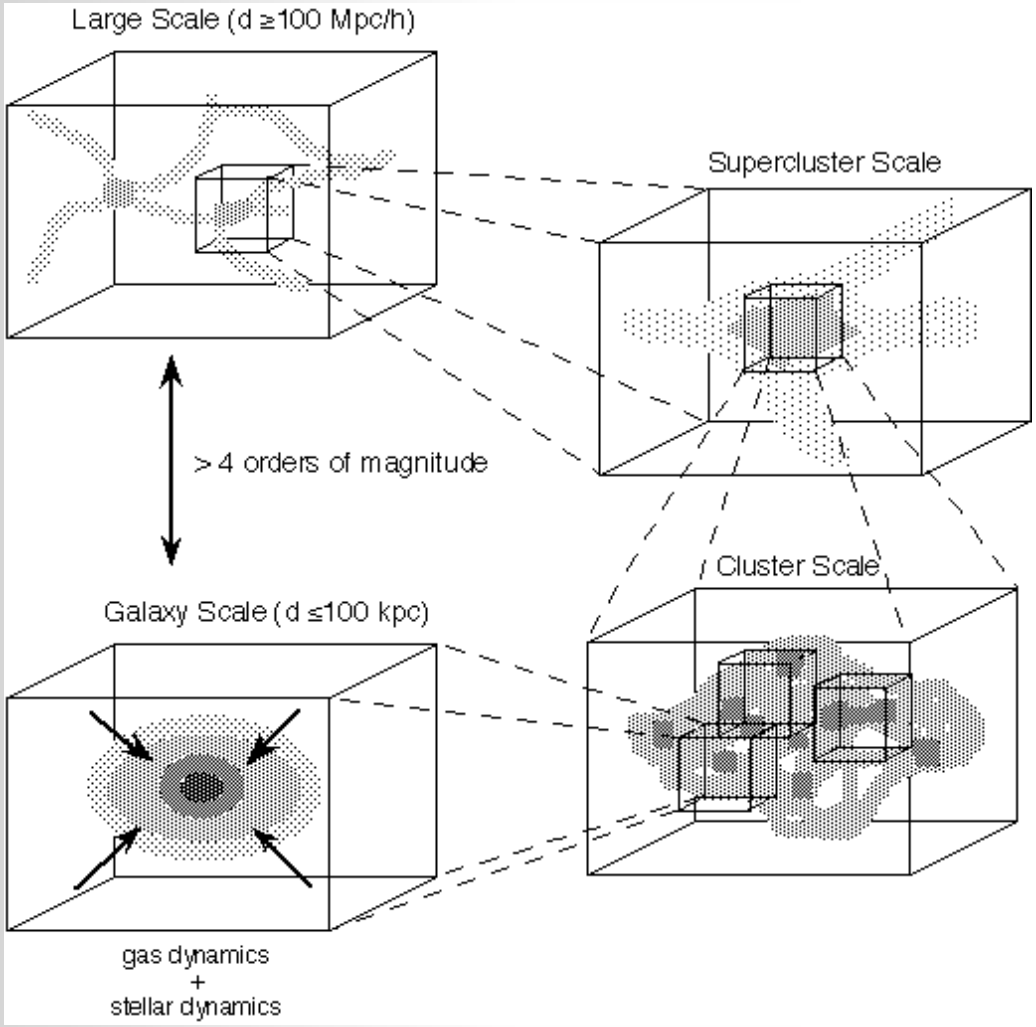

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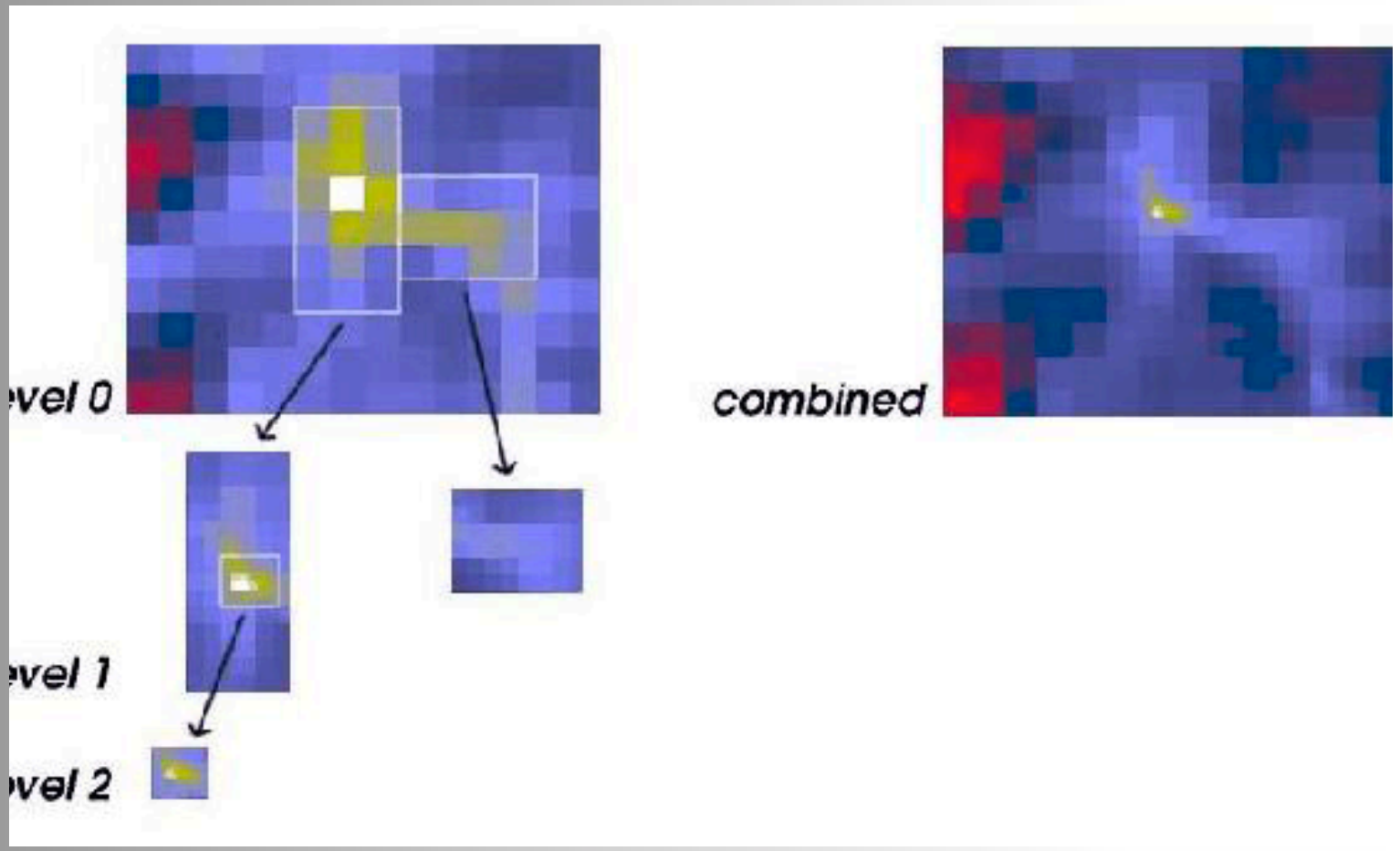
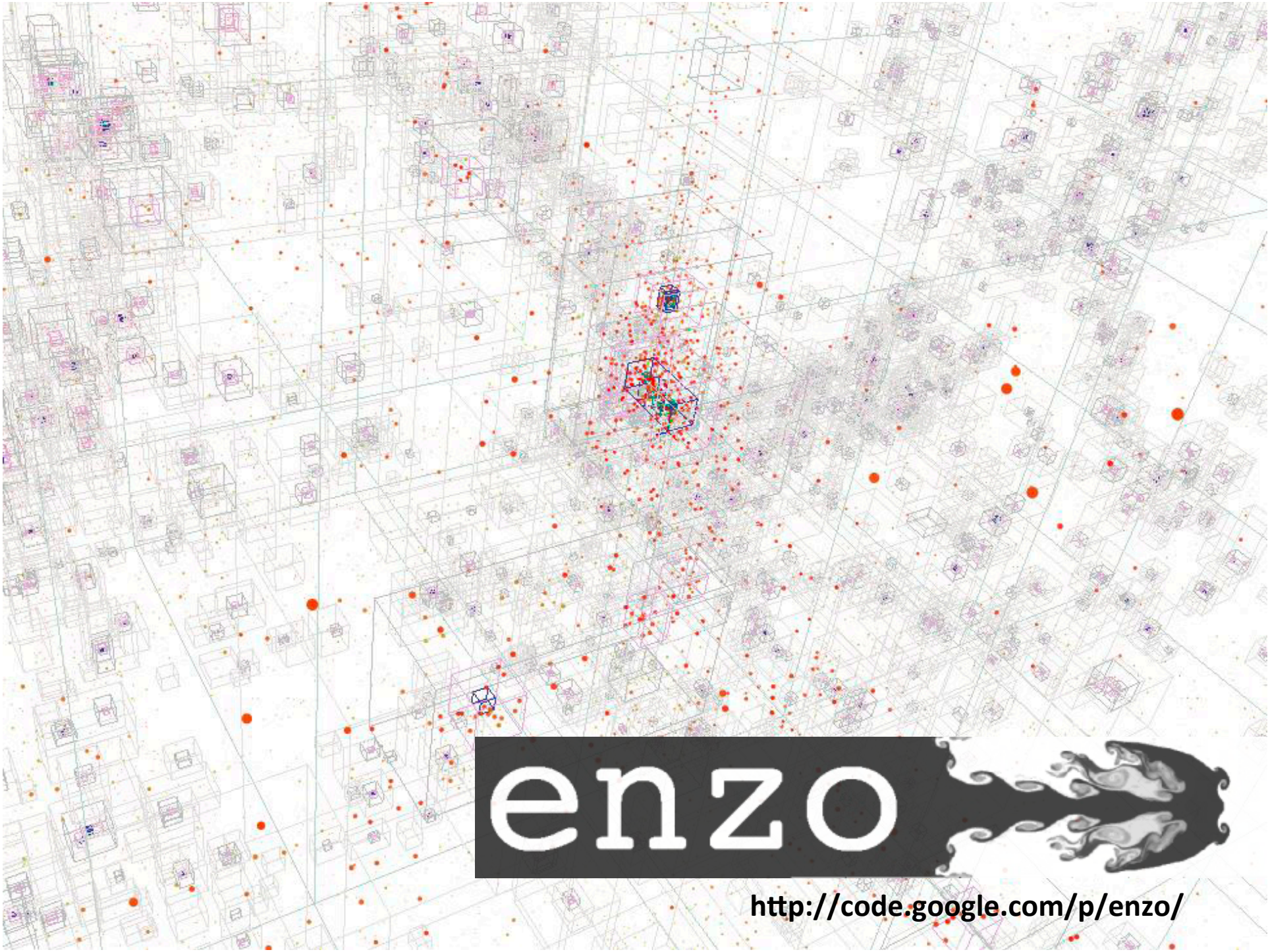
Structured Adaptive Mesh Refinement (Berger and Colella 1989)




enzo
http://code.google.com/p/enzo/

MPI

- MPI – Message Passing Interface
  - OpenMPI
  - MPICH2
  - Many others
- Send/Receive Messages between threads
- Typically one program is written and multiple copies get run

Agenda

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  - Pleasantly Parallel
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1957 MISTIC Mainframe

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

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.

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.

Bigger Science

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

2005

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2005

512 core, 128 nod
in 2005. Each n
2.2GHz AMD Opte
RAM, and 14

10

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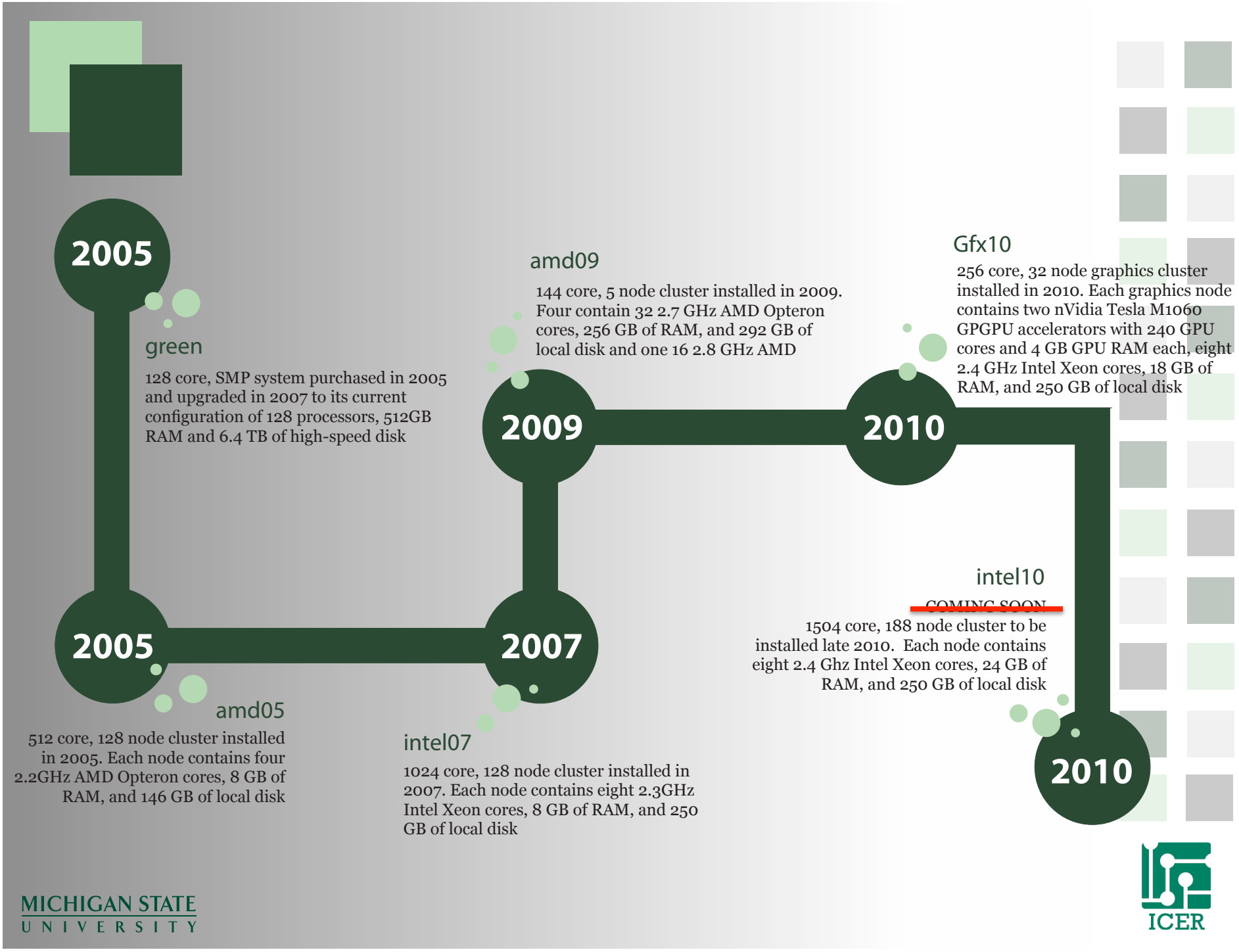
2005
green
128 core, SMP system purchased in 2005 and upgraded in 2007 to its current configuration of 128 processors, 512GB RAM and 6.4 TB of high-speed disk
amd09
144 core, 5 node cluster installed in 2009. Four contain 32 2.7 GHz AMD Opteron cores, 256 GB of RAM, and 292 GB of local disk and one 16 2.8 GHz AMD
Gfx10
256 core, 32 node graphics cluster installed in 2010. Each graphics node contains two nVidia Tesla M1060 GPGPU accelerators with 240 GPU cores and 4 GB GPU RAM each, eight 2.4 GHz Intel Xeon cores, 18 GB of RAM, and 250 GB of local disk
2009
2010
intel10
COMING SOON
1504 core, 188 node cluster to be installed late 2010. Each node contains eight 2.4 Ghz Intel Xeon cores, 24 GB of RAM, and 250 GB of local disk
2005
2007
2010
amd05
512 core, 128 node cluster installed in 2005. Each node contains four 2.2GHz AMD Opteron cores, 8 GB of RAM, and 146 GB of local disk
intel07
1024 core, 128 node cluster installed in 2007. Each node contains eight 2.3GHz Intel Xeon cores, 8 GB of RAM, and 250 GB of local disk
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Questions?