
N-body Simulations
On
GPU Clusters

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Outline

- Types of N-Body simulations
  - Small N (SS, GC)
  - Large N
- Need for Exascale
- GPU details
- Single node performance
- Scaling
- Multistepping issues

Cosmology at 130,000 years

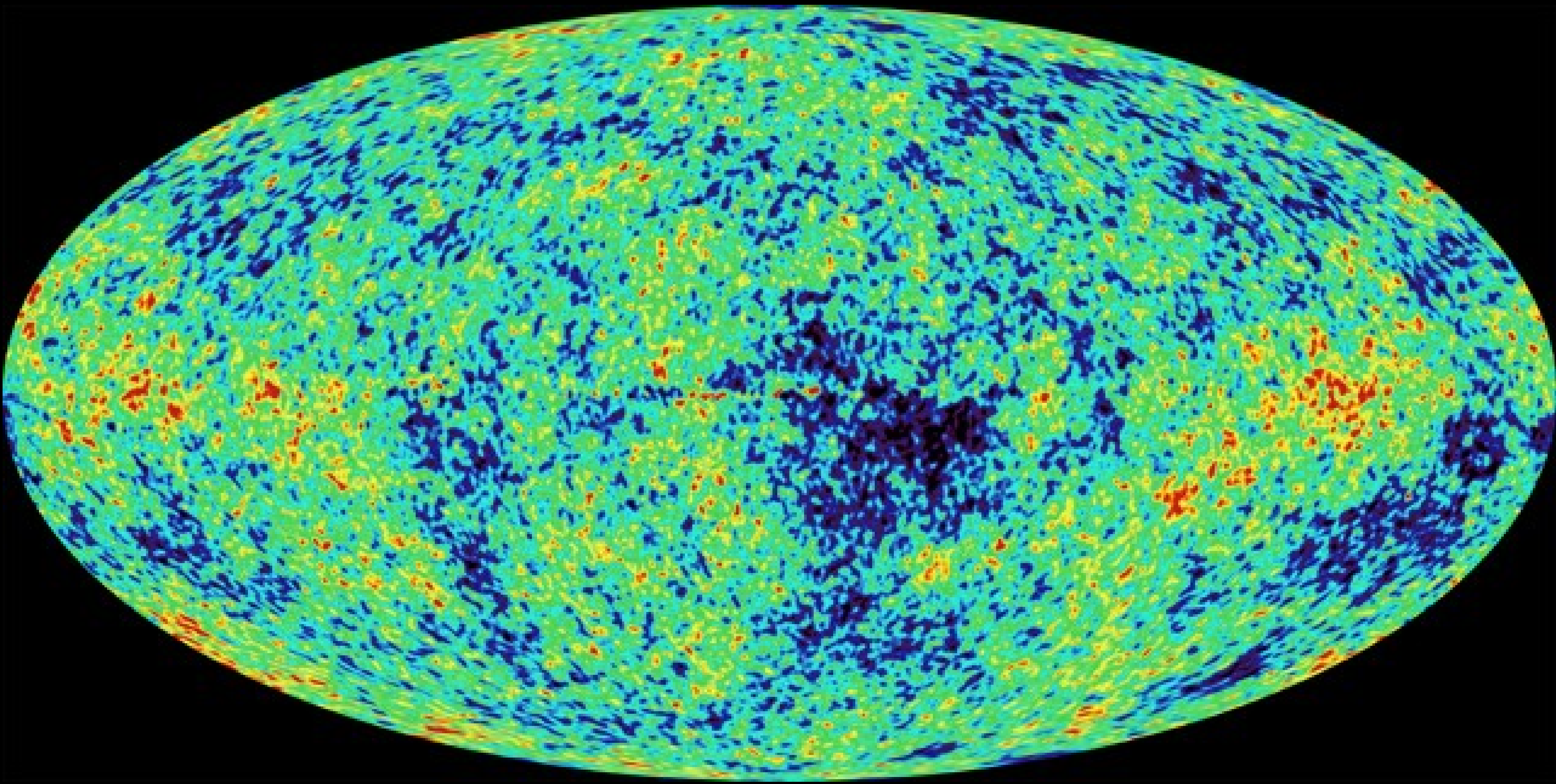
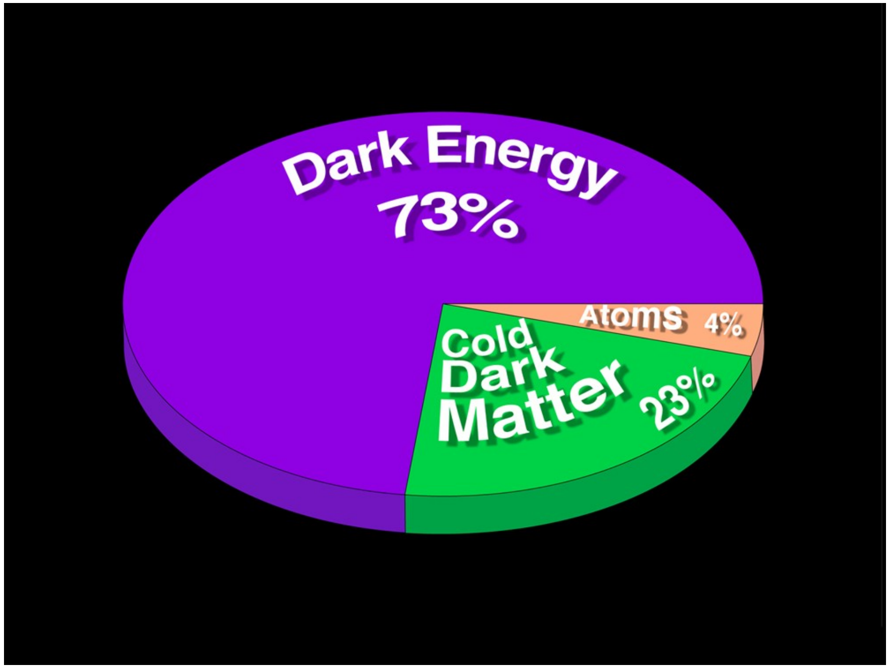


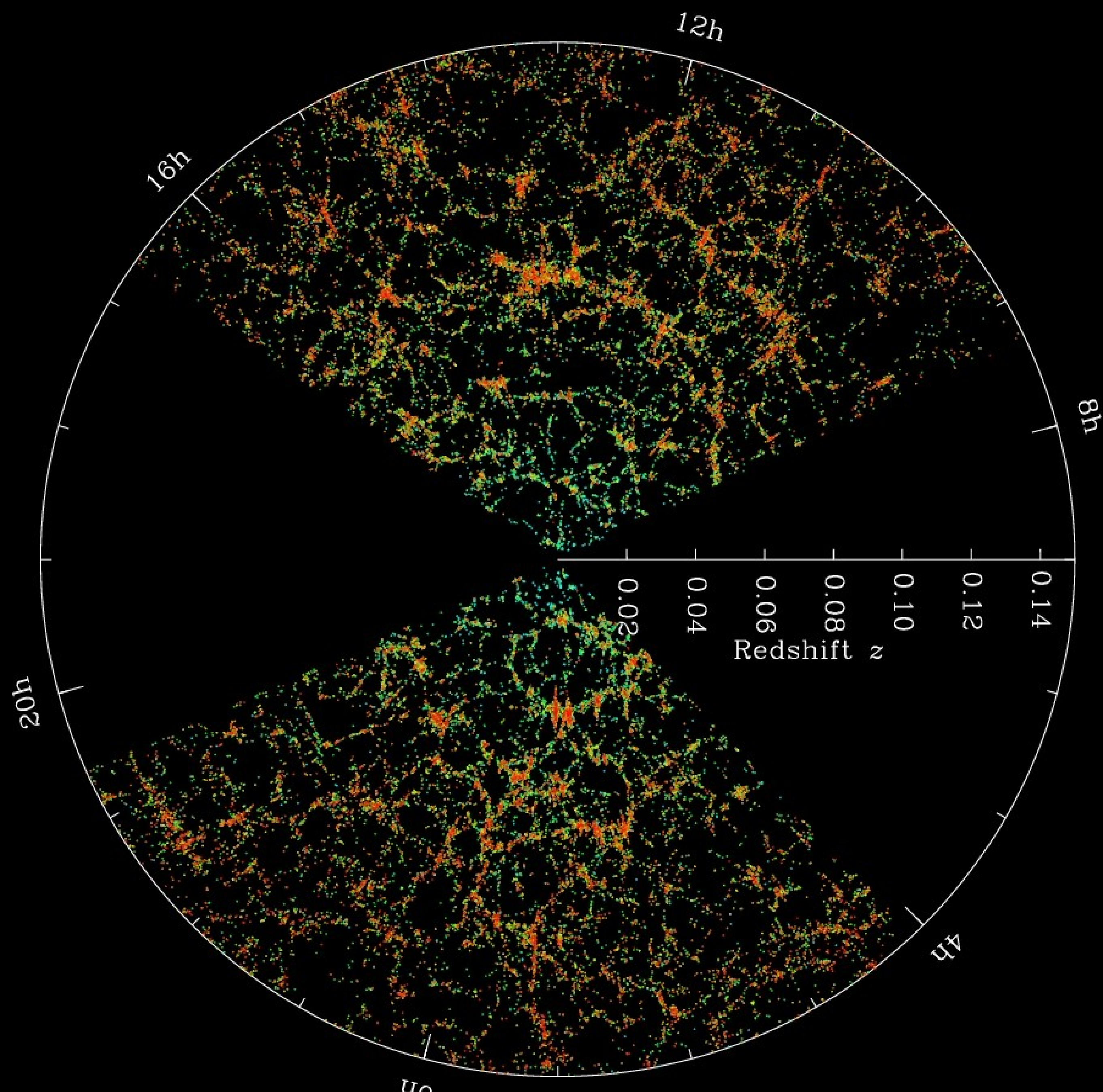
Image courtesy NASA/WMAP

Fundamental Problem: Dark Matter and Energy: What is it?

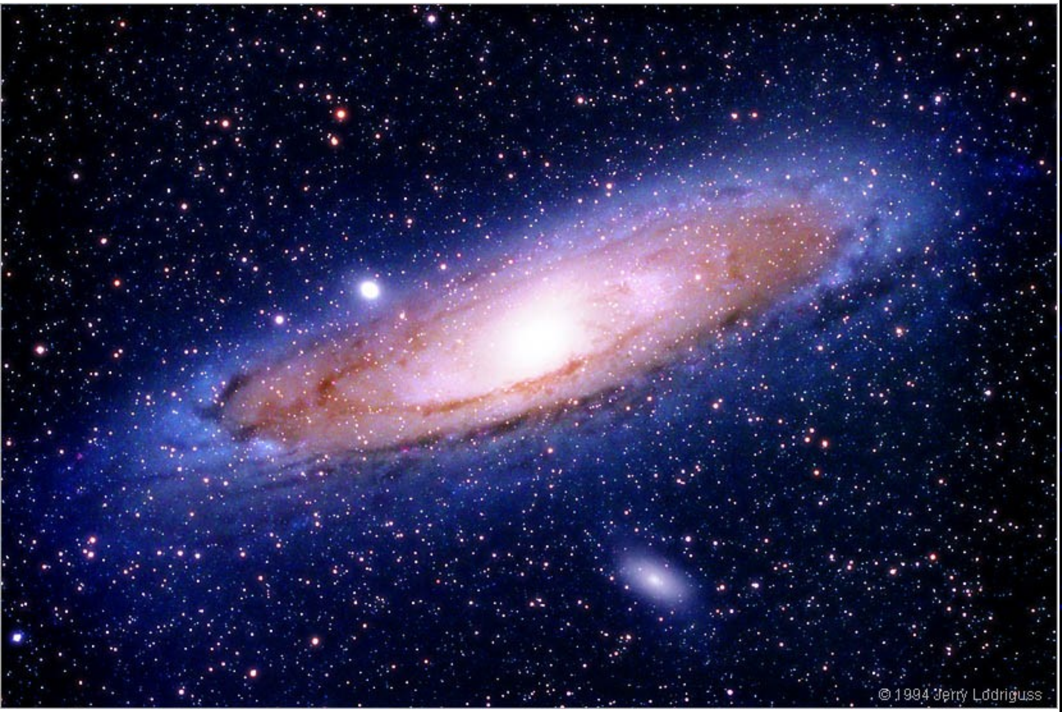
- Not baryons
- Simulations show: not known neutrinos
- Candidates:
  - Sterile Neutrinos
  - Axions
  - Lightest SUSY Particle (LSP)

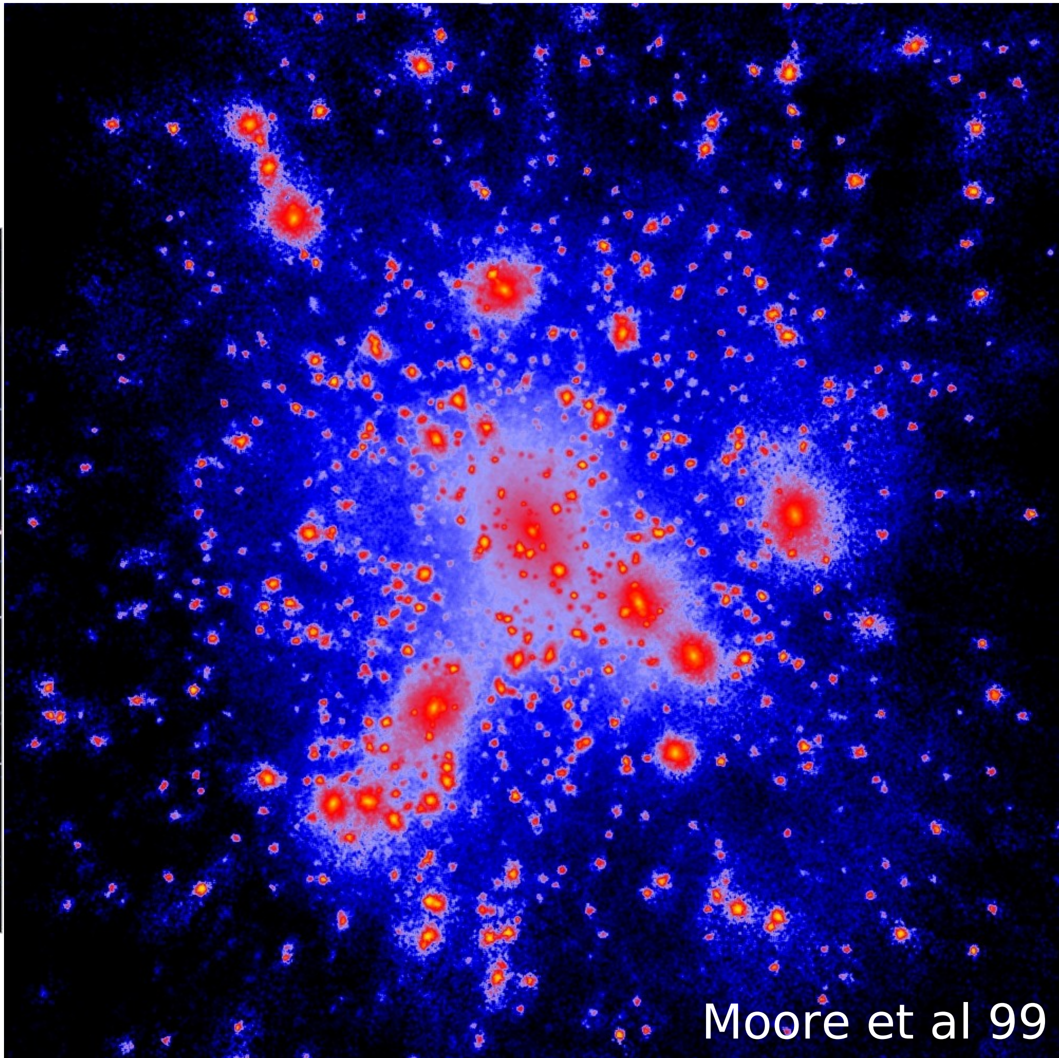


Cosmology at 13.6 Gigayears



Light vs. Matter





Computational Cosmology

- CMB has fluctuations of 1e-5
- Galaxies are overdense by 1e7
- It happens (mostly) through **Gravitational Collapse**
- Making testable predictions from a cosmological hypothesis requires
  - Non-linear, dynamic calculation
  - e.g. **Computer simulation**

What is N?

Are we solving for orbits of particles:

$$\ddot{\mathbf{x}}_i = -\sum_{j \neq i}^{N} \frac{G m_j \mathbf{r}_{ij}}{|r_{ij}|^3}?$$

We should be solving the Collisionless Boltzmann equation:

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \boldsymbol{\nabla} f - \boldsymbol{\nabla} \Phi \cdot \frac{\partial f}{\partial \mathbf{v}} = 0.$$

On the surface this is difficult, but we can use the method of characteristics where we follow the motion of packets of f:

$$\delta f(\mathbf{x}(t), \mathbf{v}(t)).$$

Now the equations of motion for these packets are:

$$\dot{\mathbf{x}} = \mathbf{v},$$

$$\dot{\mathbf{v}} = -\boldsymbol{\nabla} \Phi.$$

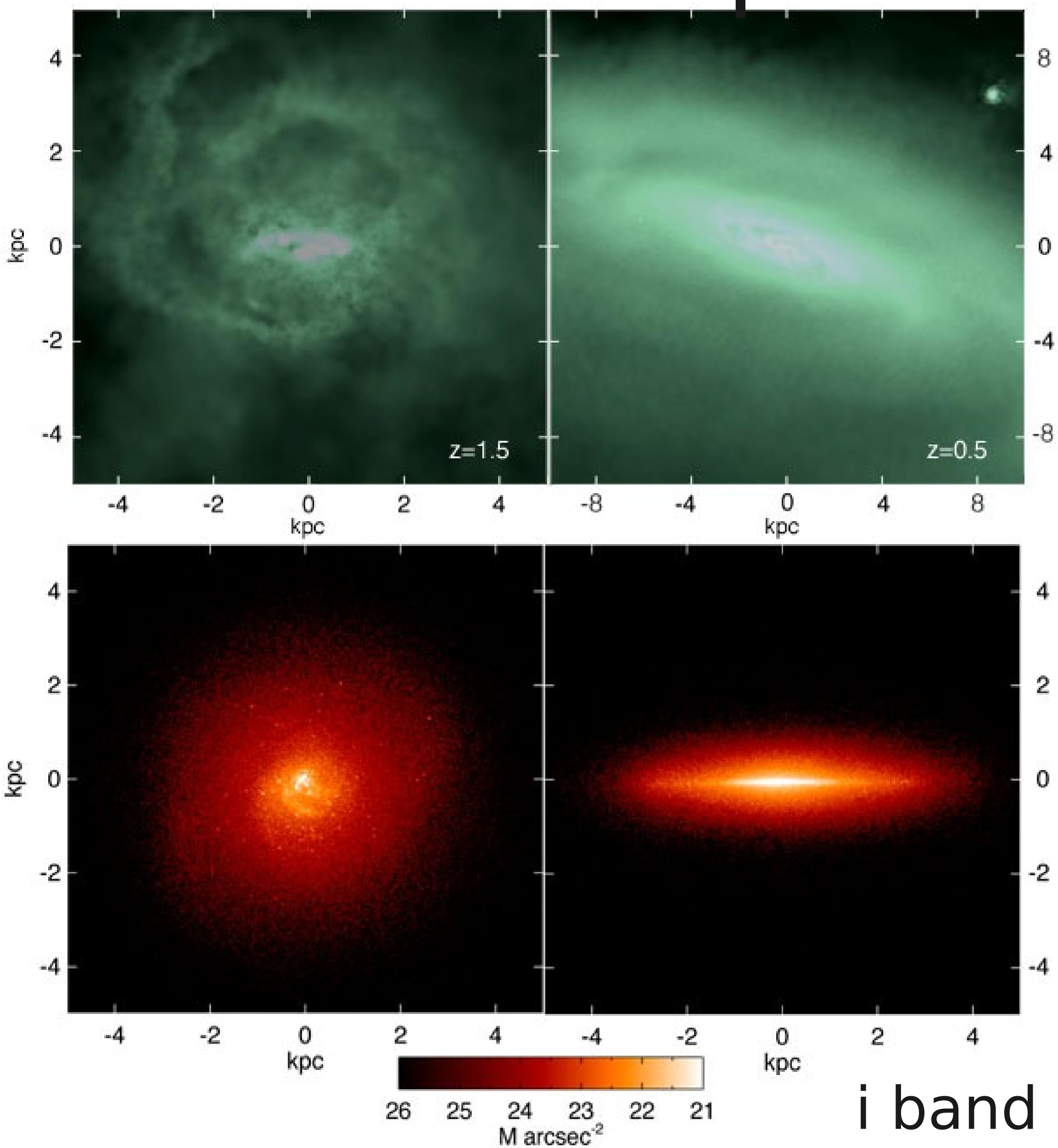
Smooth Particle Hydrodynamics

- Making testable predictions needs Gastrophysics
  - High Mach number
  - Large density contrasts
- Gridless, Lagrangian method
- Galilean invariant
- Monte-Carlo Method for solving Navier-Stokes equation.
- Natural extension of particle method for gravity.

Simulating Galaxy Formation: Current Methodology

- Full cosmological context with high resolution
  - Dynamic range of 1e5 in time and space
  - Treecode/SPH or similar adaptive method is required.
- Physically motivated subgrid effects of star formation and feedback
- Complete simulations to present epoch.
- Analyze with multiple simulated observations

Dwarf galaxy simulated to the present



Reproduces:
* Light profile
* Mass profile
* Star formation
* Angular momentum

i band image

Galactic structure in the local Universe: What's needed

- 1 Million particles/galaxy for proper morphology/heavy element production
- 25 Mpc volume
- 800 M core-hours
- Necessary for:
  - Comparing with Hubble Space Telescope surveys of the local Universe
  - Interpreting HST images of high redshift galaxies

Large Scale Structure: What's needed

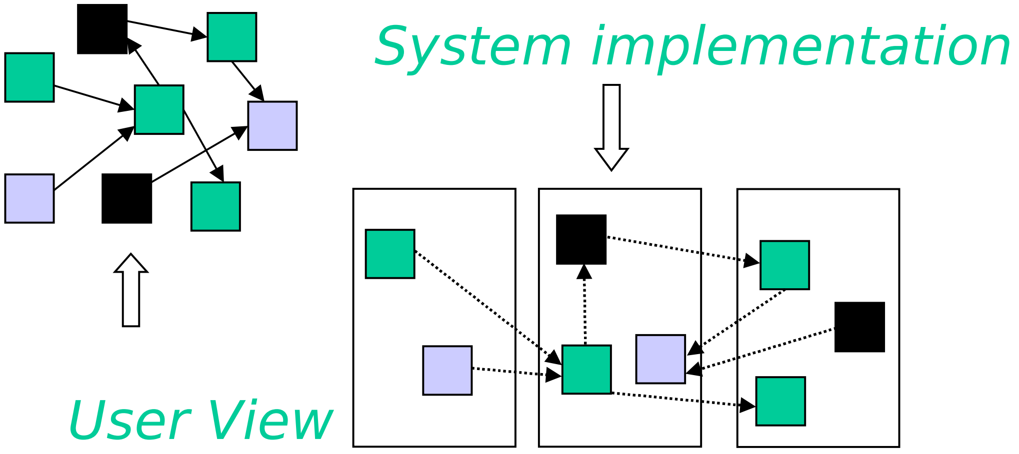
- 700 Megaparsec volume for "fair sample" of the Universe
- 18 trillion core-hours (~ exaflop year)
- Necessary for:
  - Interpreting future surveys (LSST)
  - Relating Cosmic Microwave Background to galaxy surveys

Charm++: Migratable Objects

Programmer: **[Over] decomposition into virtual processors**

Runtime: **Assigns VPs to processors**

Enables *adaptive runtime strategies*



Benefits

- Software engineering
  - Number of virtual processors can be independently controlled
  - Separate VPs for different modules
- Message driven execution
  - Adaptive overlap of communication
- Dynamic mapping
  - Heterogeneous clusters
    - Vacate, adjust to speed, share
  - Automatic checkpointing
  - Change set of processors used
  - Automatic dynamic load balancing
  - Communication optimization

Charm++ at scale

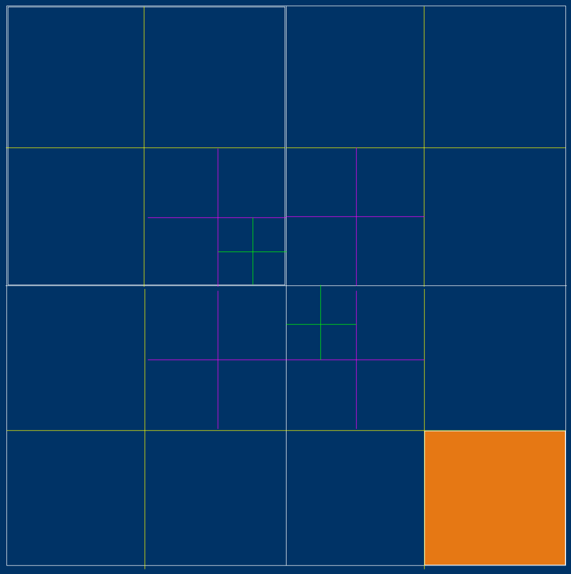
- Composability, object oriented
- Load balancing framework
  - Topology aware
- Available development tools:
  - Profiling at scale
  - Debugging at scale
  - Visualization at scale (http://hpcc.astro.washington.edu/tools/salsa)
  - Machine simulation

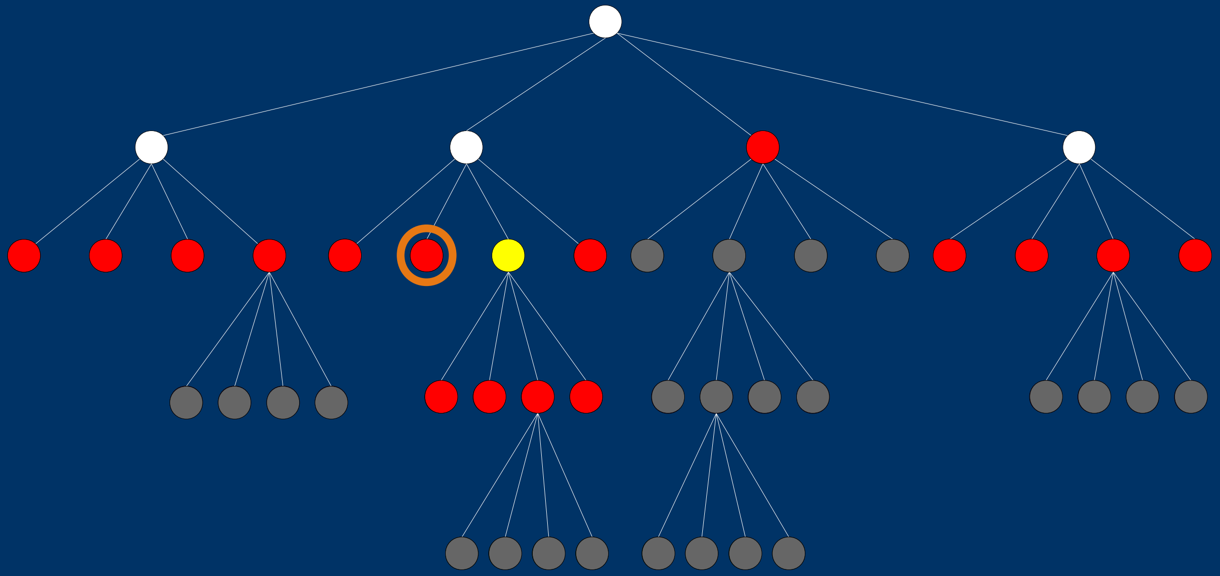
ChaNGa (CHArm N-body GrAvity) Features

- Tree-based gravity solver
- High order multipole expansion
- Periodic boundaries (if needed)
- Individual multiple timesteps
- Dynamic load balancing with choice of strategies
- Checkpointing (via migration to disk)
- Visualization

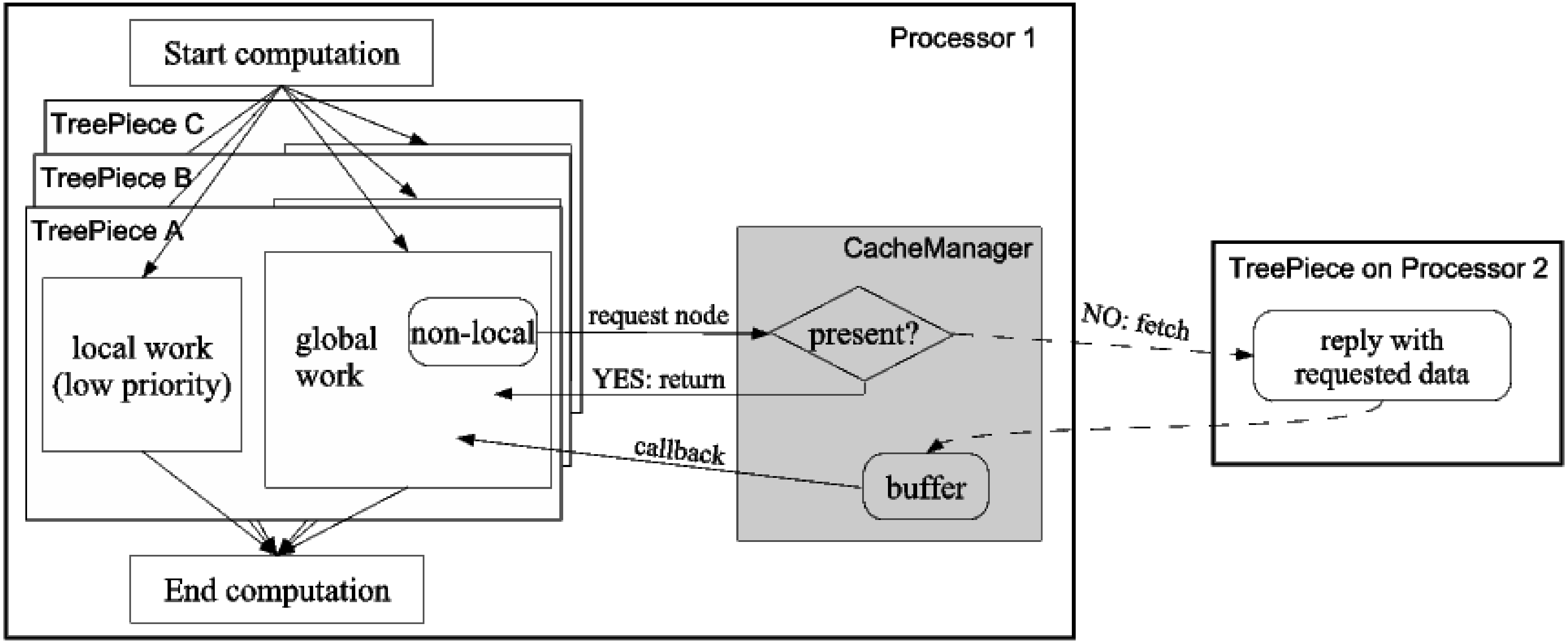
Basic Gravity algorithm ...

- Newtonian gravity interaction
  - Each particle is influenced by all others: O(n^2) algorithm
- Barnes-Hut approximation: O($n\log n$)
  - Influence from distant particles combined into center of mass

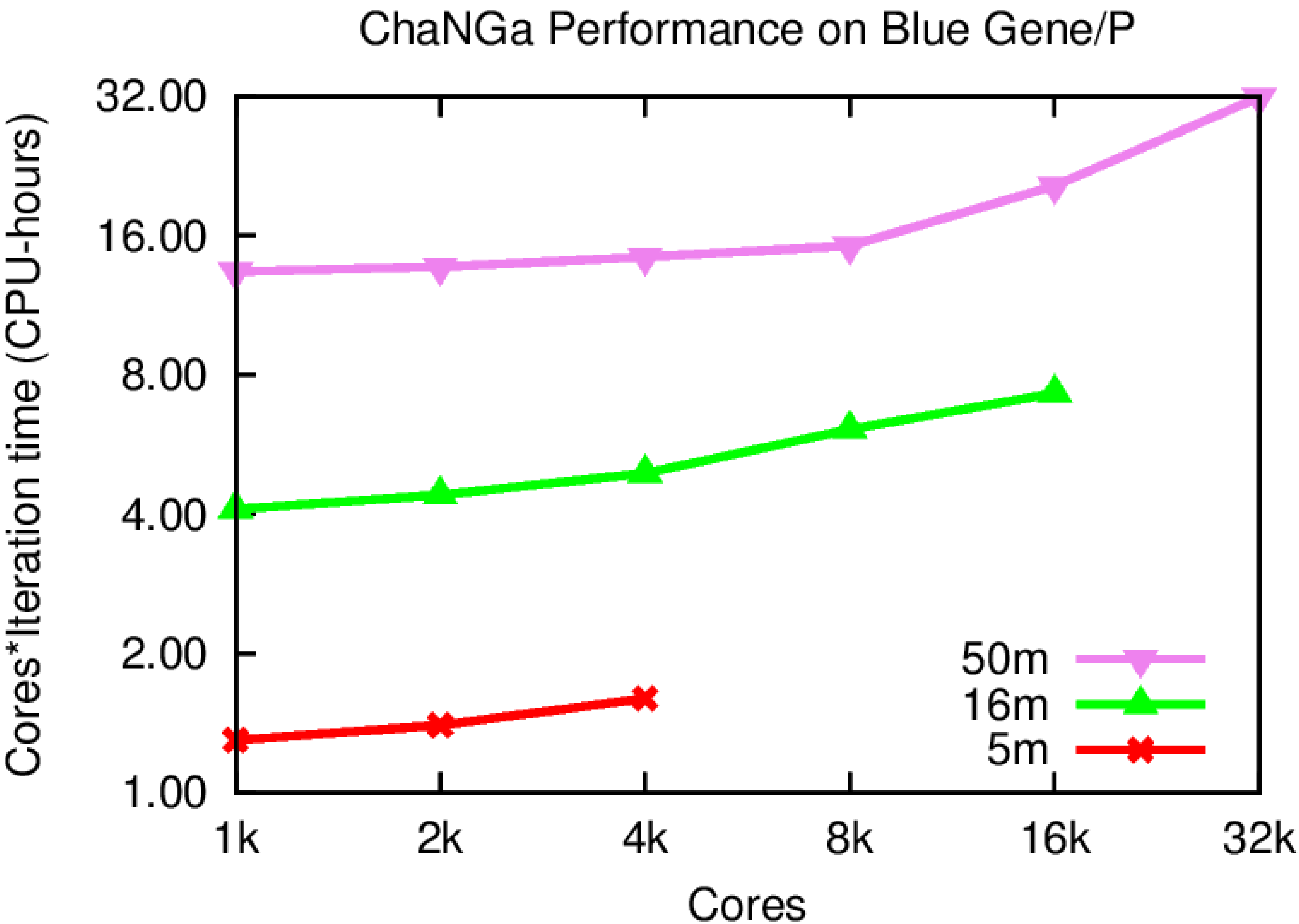




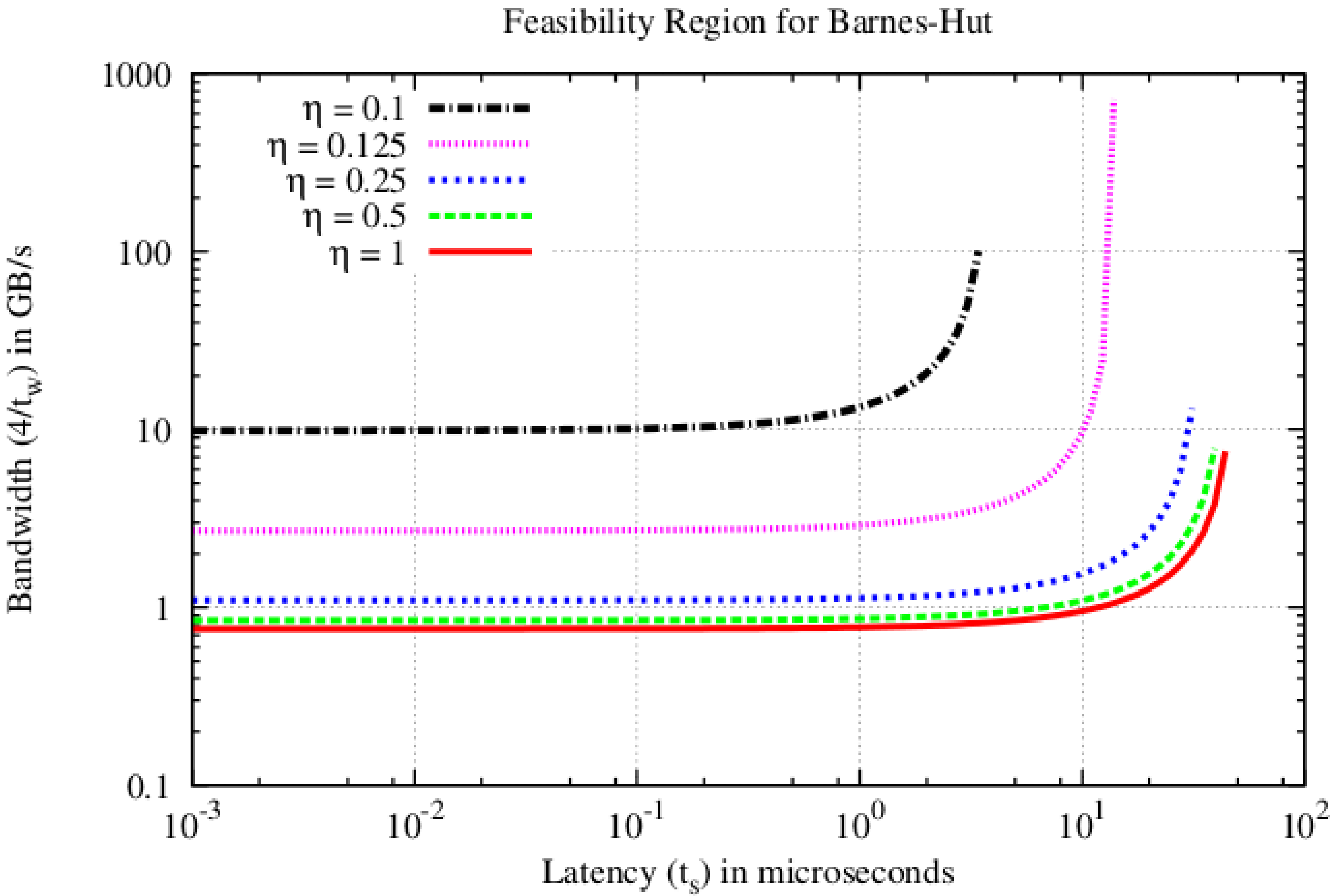
Overall Algorithm



Strong Scaling on BG/P



6.8e12 particles @ 1 Exaflop



200Mpc^3 volume at 1e4 Msun

Cosmology at Exascale

- The Universe is big
  - Build a computer and a cosmologist will fill it.
  - With compelling problems to solve
- Scaling to Exaflops is conceivable
  - Despite use of irregular algorithms/data structures
  - But with significant investment in newer languages/libraries

General Purpose GPUs

- Graphics chips adapted for general purpose programming
- Impressive floating point performance
  - 4.6 Tflops single precision (AMD Radeon HD 5970)
  - Cmp. 100 Gflop for 3 GHz quad-core quad-issue CPU
- Good for large scale data parallelism
- Consumer driven technology

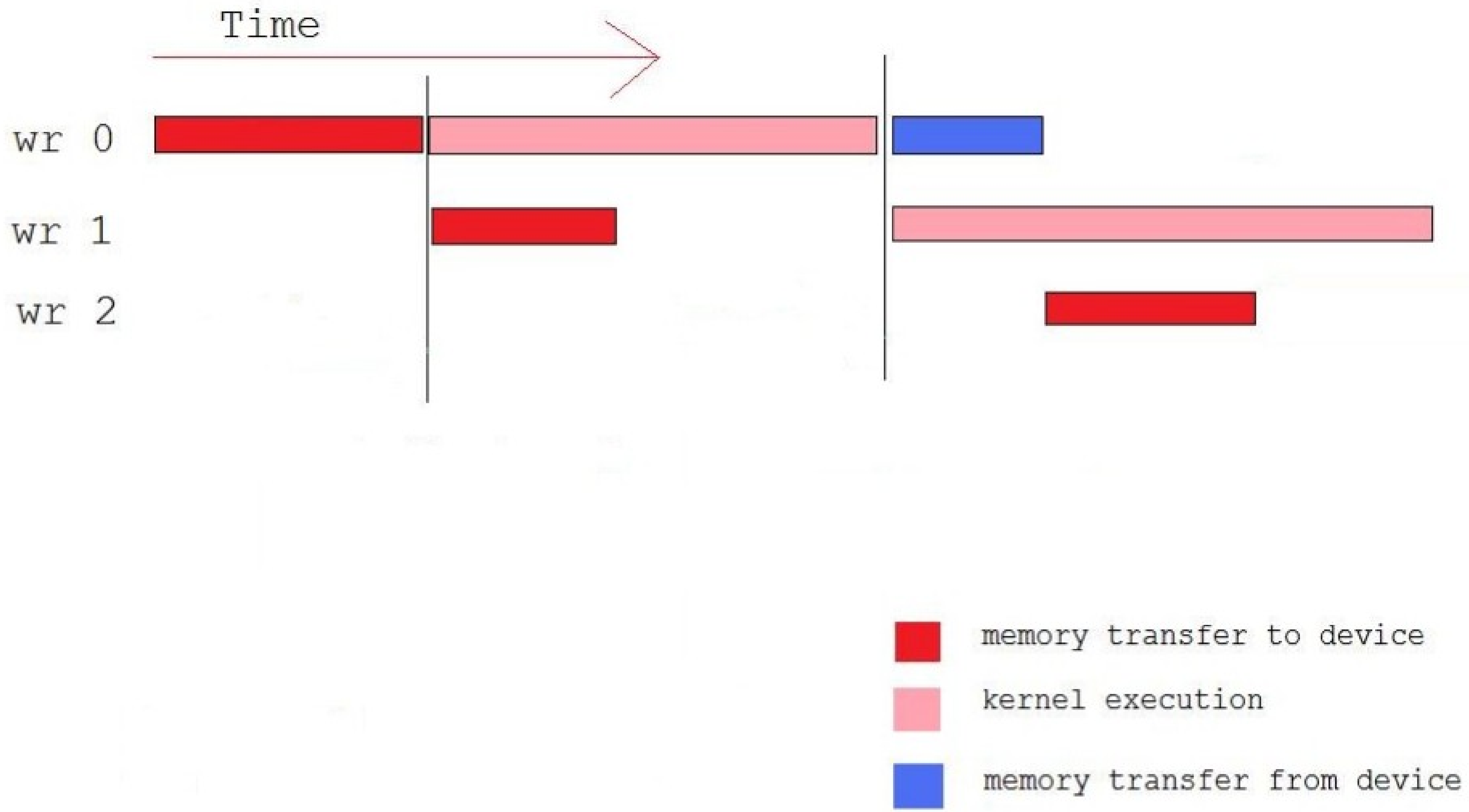
GPU Stream Management

- Common stream usage
  - CPU -> GPU data transfer
  - kernel_call
  - GPU -> CPU data transfer
  - Poll for completion
- Third operation blocks DMA engine until kernel is finished
- Avoid by delaying GPU -> CPU transfer until kernel is finished
  - Requires additional polling call

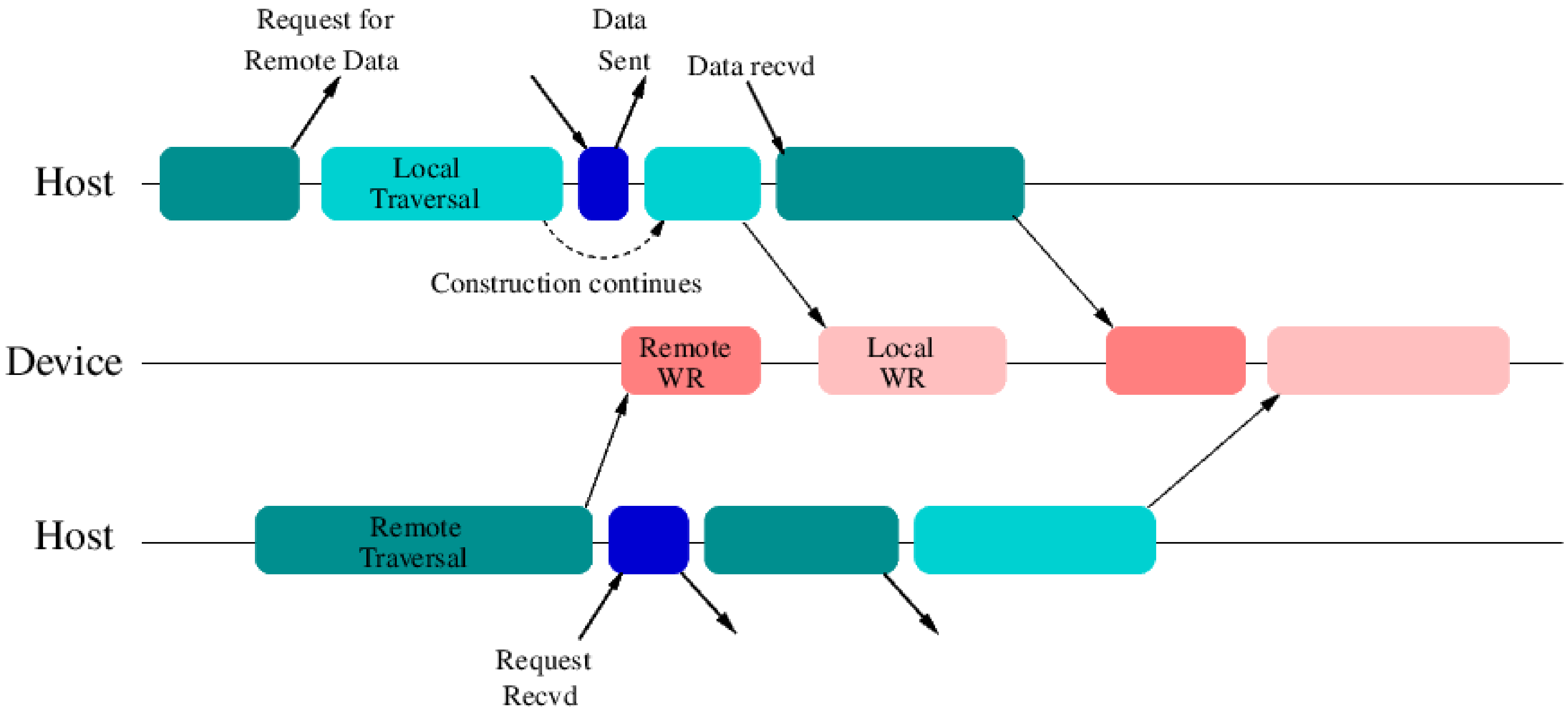
GPU Manager

- User submits “work requests” with GPU kernel, associated buffers and callback
- System transfers memory between CPU and GPU, executes kernel, and returns via a callback
- GPU operations performed asynchronously
- Pipelined execution
- Consistent with Charm++ model
- Charm++ tools (profiler) available

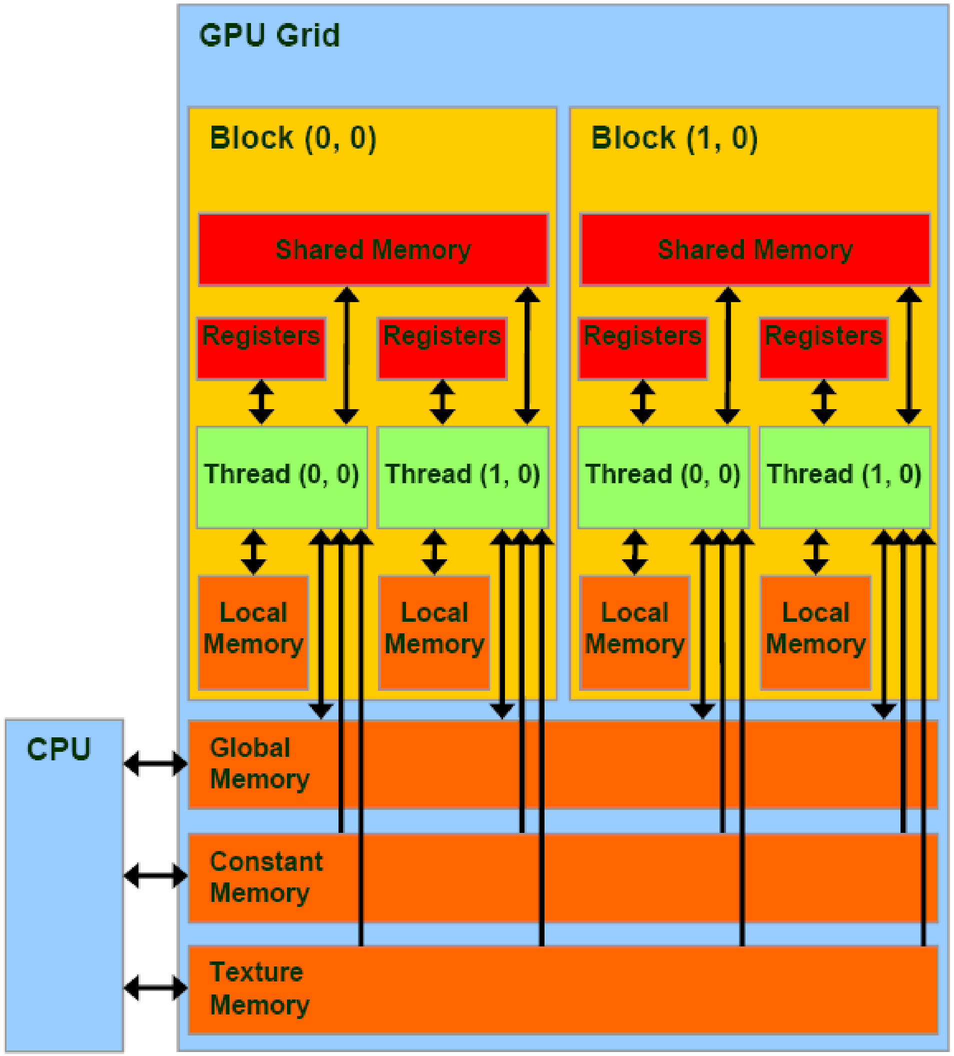
Execution of Work Requests



Overlapping CPU and GPU Work

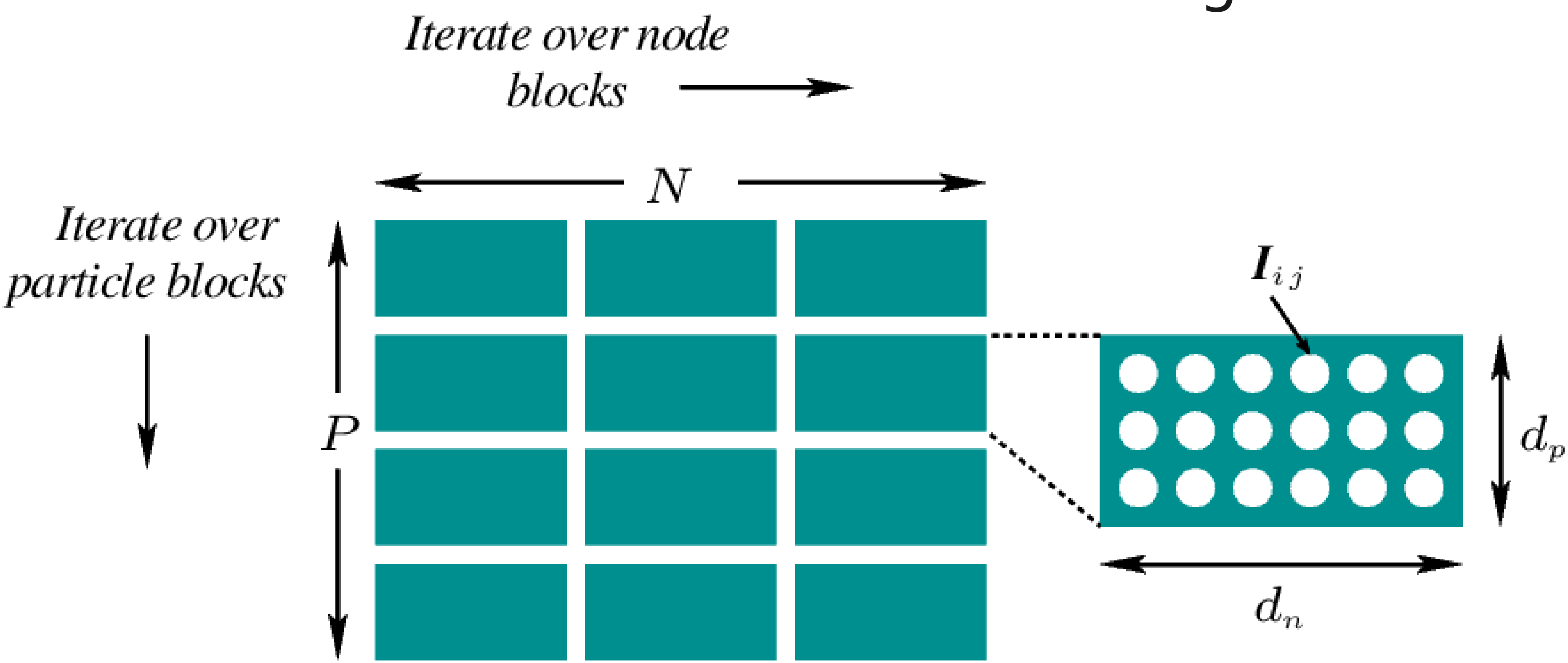


CUDA memory model

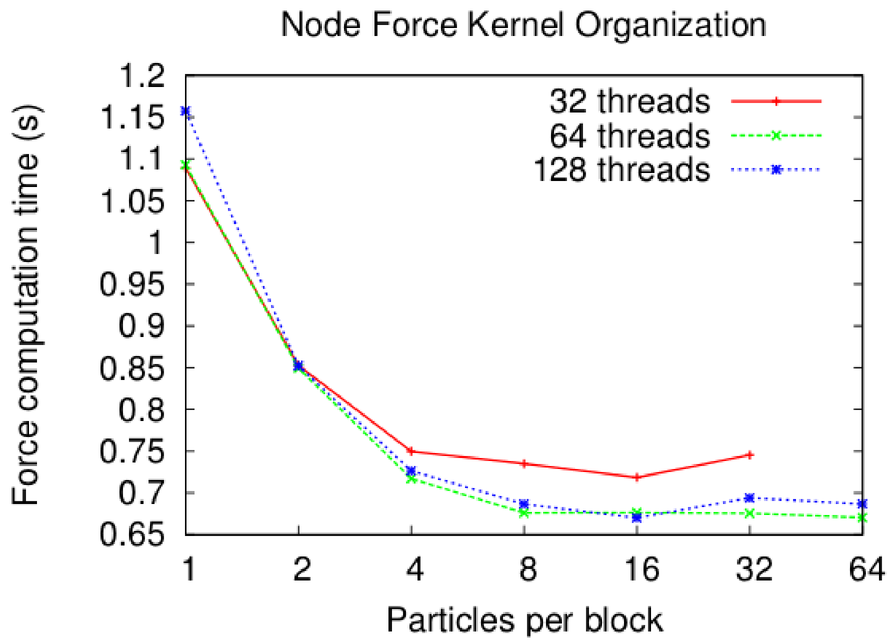


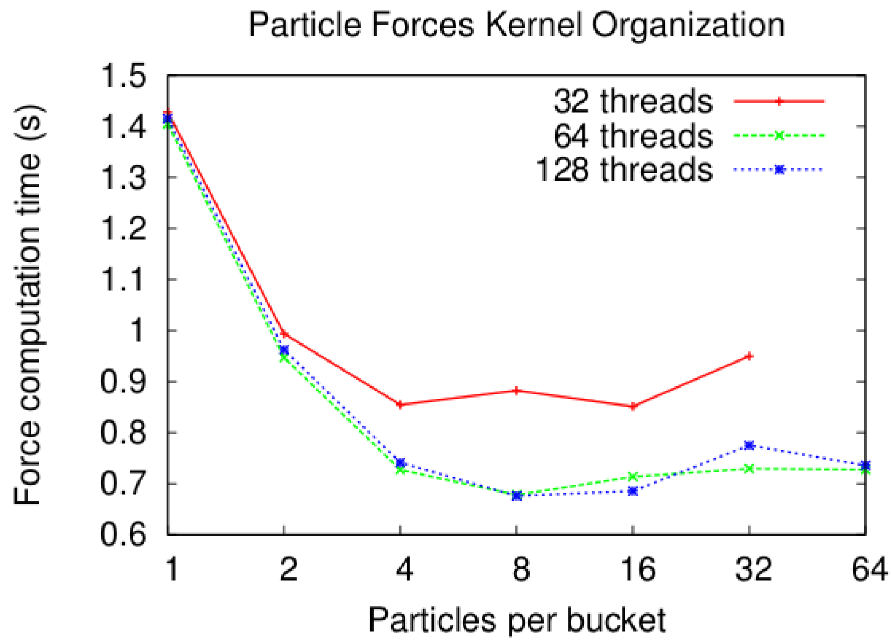
Force Kernel Optimization

More particles->fewer loads
More particles->larger shared memory use
Fewer executing blocks



Kernel Optimization Results





Optimum at 128 threads, 16 particles, 8 nodes/block

Ewald on the GPU

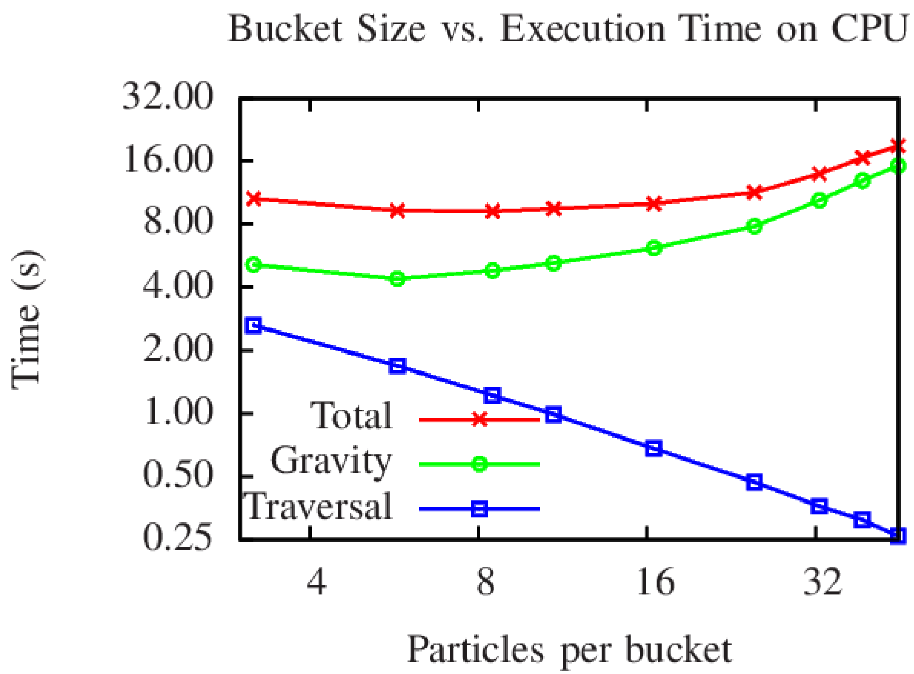
- Real space loop and Fourier space loop
- Separate kernels for each loop

  More concurrent blocks/SM
- Constant memory for cos/sin tables
- Factor of 20 speedup over CPU

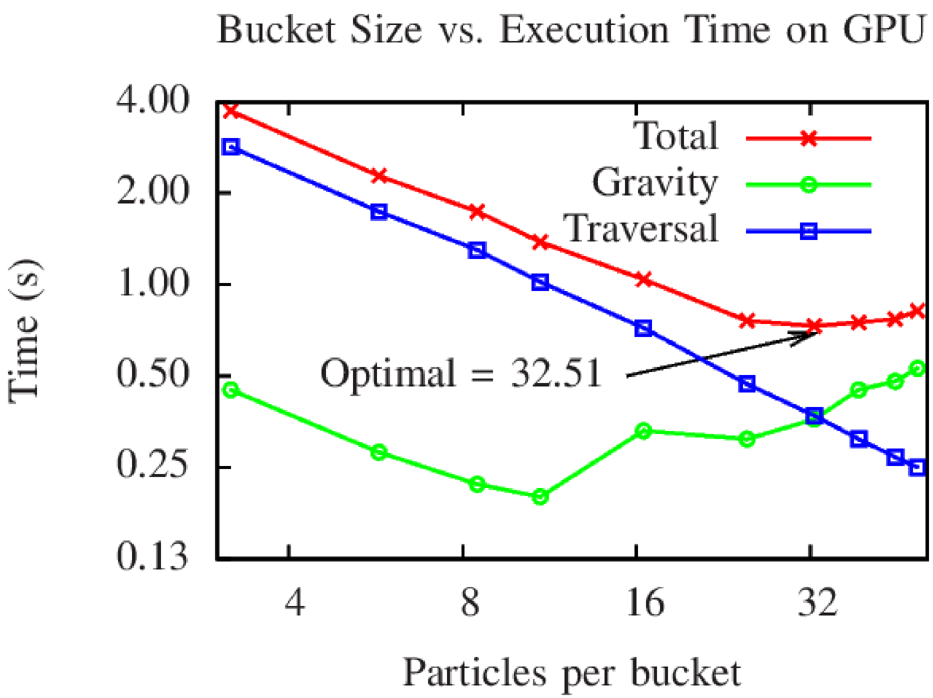
Tree Traversal and Computation

- GPU is hungry for work
  - CPU should hold back GPU
  - Decrease tree walk time to generate more computing
- Increase average bucket size
  - Tree is shallower: CPU less busy
  - More computation: GPU more busy
  - Balance for optimum

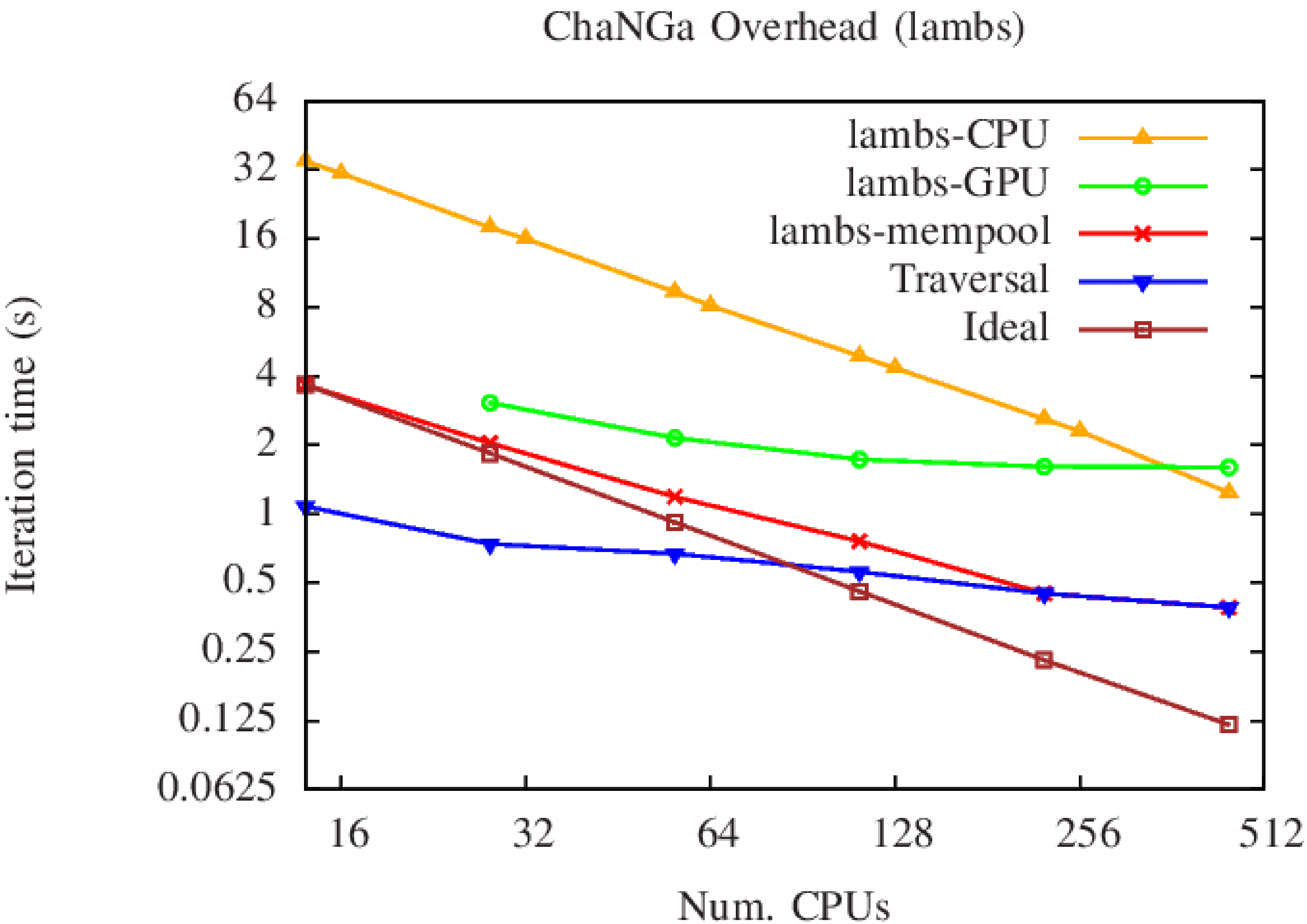
Work-throughput tradeoff

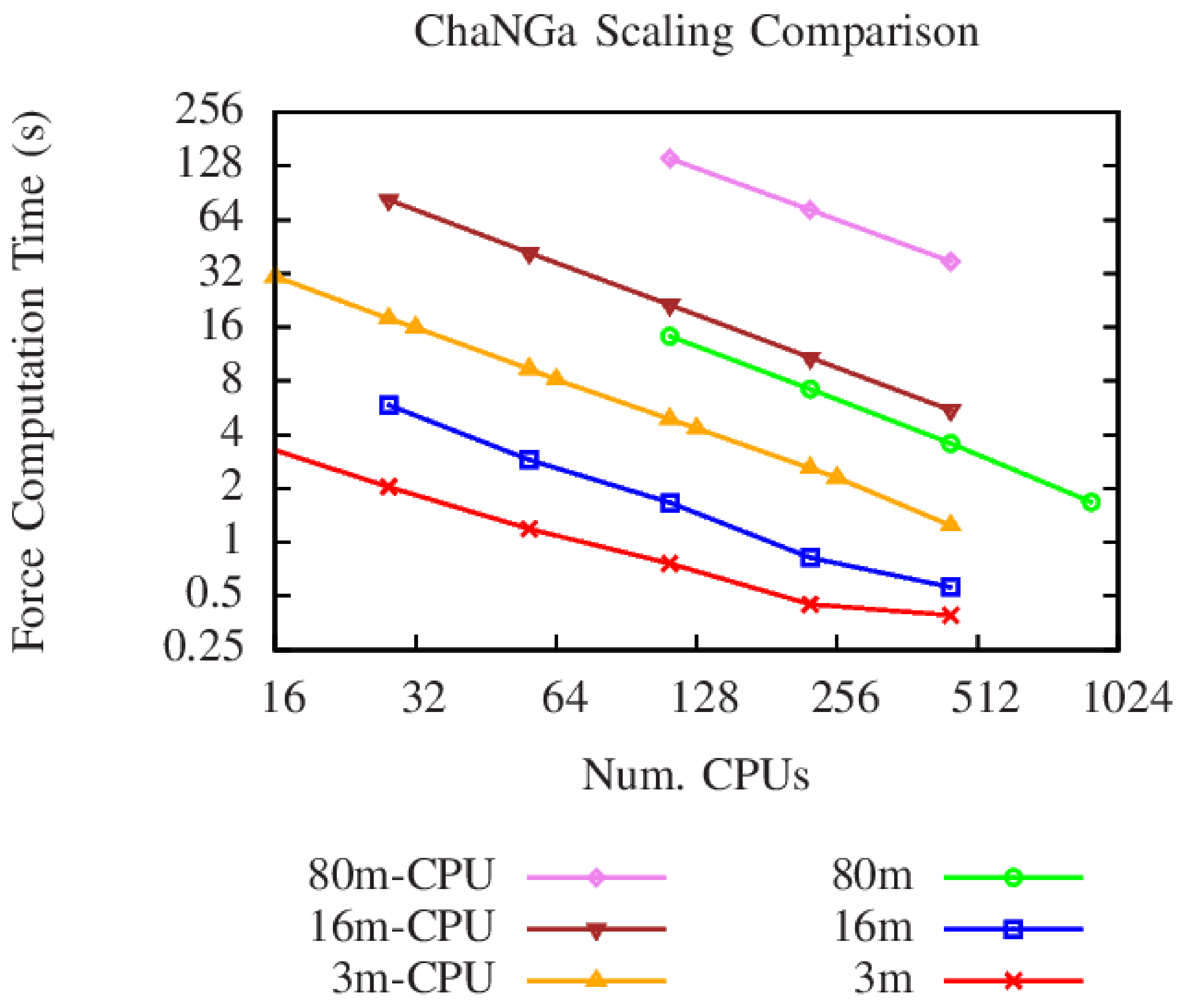


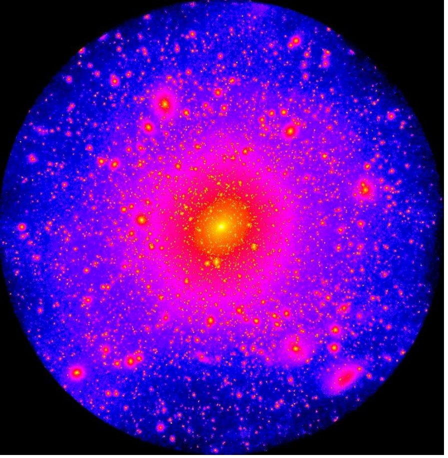
CPU



GPU

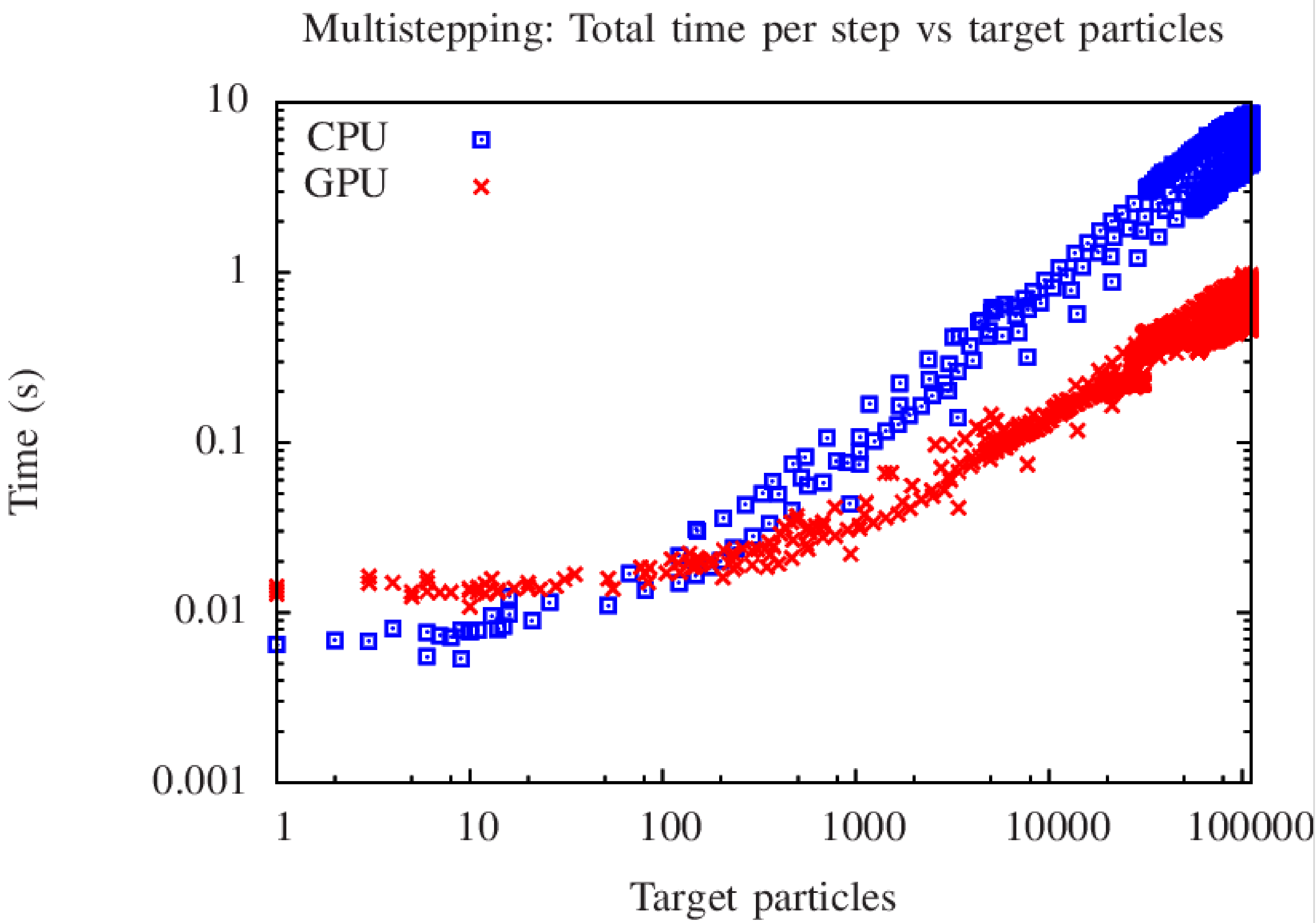

ChaNGa Overhead (lambs)
lambs-CPU
lambs-GPU
lambs-mempool
Traversal
Ideal
Iteration time (s)
64
32
16
8
4
2
1
0.5
0.25
0.125
0.0625
16
32
64
128
256
512
Num. CPUs


ChaNGa Scaling Comparison
Force Computation Time (s)
256
128
64
32
16
8
4
2
1
0.5
0.25
16
32
64
128
256
512
1024
Num. CPUs
80m-CPU
16m-CPU
3m-CPU
80m
16m
3m



Timestepping Challenges

- 1/*m* particles need *m* times more force evaluations
- Naively, simulation cost scales as N^(4/3)ln(N)
  - This is a problem when N ~ 1e9 or greater
- If each particle an individual timestep scaling reduces to N (ln(N))^2
- A difficult dynamic load balancing problem



Multistepping: Total time per step vs target particles
10
1
0.1
0.01
0.001
Time (s)
CPU
GPU
1
10
100
1000
10000
100000
Target particles

GPU Summary/prognosis

- Successfully kept the monster fed
- More floats yet better throughput
- More work to do:
  - Load balancing needs more sophistication
  - Higher order multipoles/single precision
  - Multistepping optimization
  - Tree traversal on the GPU?
  - Ease of Programming

hpcc.astro.washington.edu/tools/changa.html