Multi-GPU Simulations of the Infinite Universe

with STEreographically Projected cosmological Simulations

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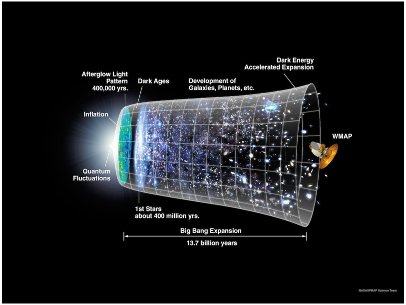
Outline

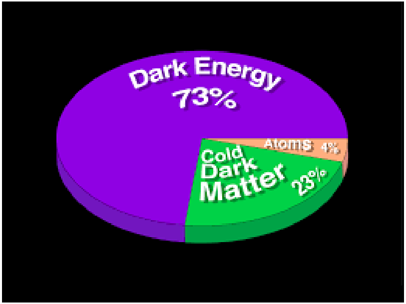
Concordance Model

The standard cosmological model: ΛCDM

- Cosmological constant (or Dark Energy) (Λ)
- Cold Dark Matter (CDM)
- 6 independent parameter
- Fits well with the measurements

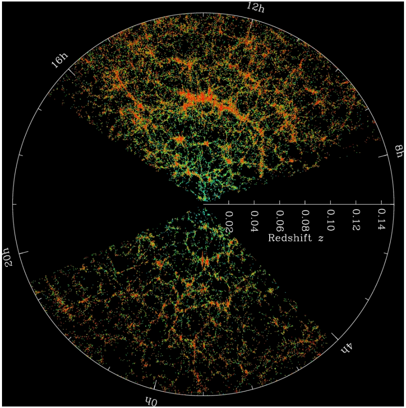


The ingredients of the Universe



- Ordinary matter (baryons, we know them)
- Dark Matter (no detection, some good ideas)
- Dark Energy (cosmological constant)

Large Scale Structure

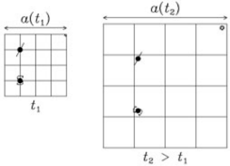


Large fluctuations in the galaxy distribution. Density field: $\rho/\rho_0 \simeq 10^6$

Comoving coordinates[1]

$$\mathbf{x}(t) = \mathbf{X}(t)/a(t),$$

where $\mathbf{X}(t)$ is the real coordinate of the particle, $\mathbf{x}(t)$ is the comoving coordinate, and $a(t)$ is the cosmic scale factor.



For a perfectly uniform expansion, the comoving position vectors $\mathbf{x}$ remain fixed for all particles

[1] https://ned.ipac.caltech.edu/level5/March02/Bertschinger/Bert1.html

How to calculate the matter distribution as a function of time?

These structures formed by gravitational instability
Initial conditions: CMB power spectra.
At early times:

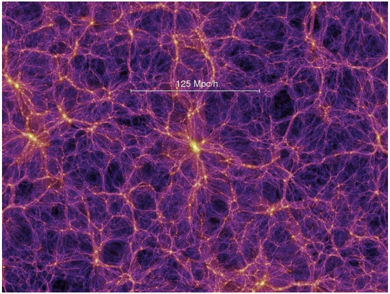
- The fluctuations are small
- Linear structure formation
- Perturbation theory can be used

Late times:

- Non-linear structure formation
- Linear theory cannot be used at small redshifts
- Cosmological simulations

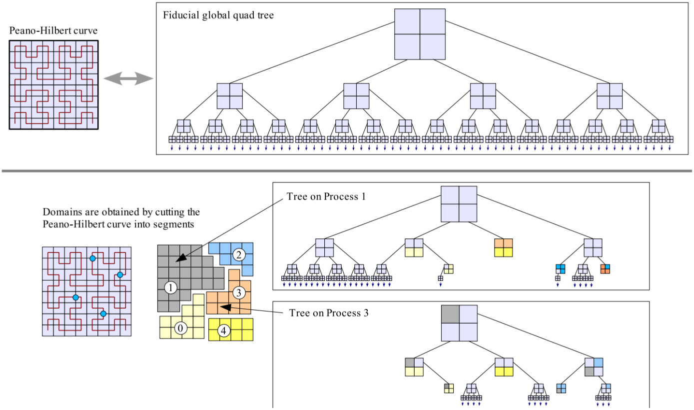
Periodic Cosmological Simulations

- N-body simulations
- Newtonian gravity in an expanding periodic box
- Tree, Tree-PM algorithm for force calculation
- Number of particles are very large: $N \sim 10^6 - 10^{12}$



The tree-algorithm

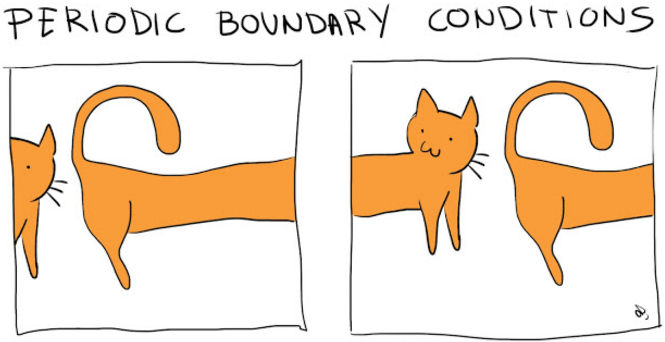
In GADGET-2[2]:



[2] Springel, V. 2005, Mon. Not. Roy. Astron. Soc., 364, 1105

Periodic boundary conditions: torus topology

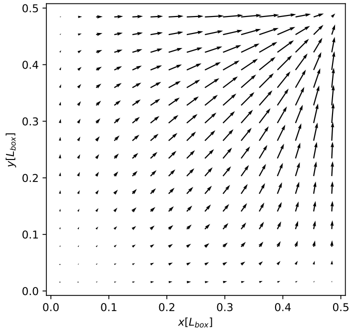
"Quantum cats have a lot of problems in their everyday life, but it's easier to solve them using periodic boundary conditions."[3]



3 http://dingercatadventures.blogspot.com/2012/09/17-boundary-conditions.html

Problems with the torus topology

- Unsupported by observations
- The gravitational force law is not isotropic in this case:

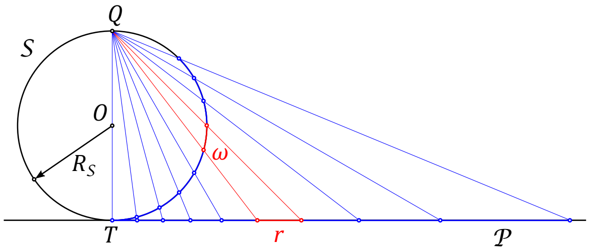


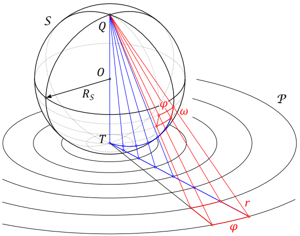
STEreographically Projected cosmological Simulations (StePS)

Our approach to calculate the cosmic matter distribution

- N-body simulations
- DM only (at the present state)
- Its fundamental geometry and topology match observations (no periodicity)
- Number of particles are small: $N \sim 10^6 - 10^7$
- The Mass resolution is decreasing in radial direction
- The last radial "bin" have infinite volume

Stereographic projection in 1 and 2 dimension



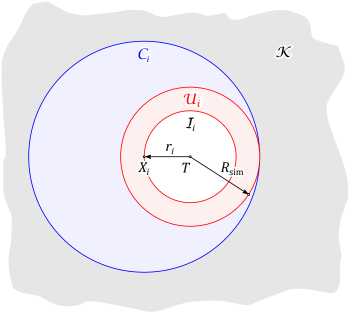


The basic idea of the StePS algorithm: Compactifying the infinite space

Instead of using periodic boundaries, we transform the infinite Universe into a compact, finite space with inverse stereographic projection:

- Our code bins the 4 dimensional spherical surface with using HEALPix or spherical glass in ϑ and φ coordinates, and with a simple equivalent size binning in the compact radial coordinate ω
- The particles are united in each bin
- After this, the code uses the stereographic projection to transform the coordinates of these particles back to cartesian coordinate system.

Force calculation



The equations of motion in spherical simulations with isotropic boundary conditions are

$$\ddot{\mathbf{x}}_i = \sum_{j=1;j\neq i}^{N} \frac{m_j \mathbf{F}(\mathbf{x}_i - \mathbf{x}_j, h_i + h_j)}{a(t)^3} - 2 \cdot \frac{\dot{a}(t)}{a(t)} \cdot \dot{\mathbf{x}}_i + \frac{4\pi G}{3} \overline{\rho} \mathbf{x}_i .$$

Force calculation on GPUs

Because the StePS method uses small number of particles (typically $N < 10^7$):

- Direct N^2 force calculation can be used
- Low memory requirements
  $\Longrightarrow$ All particle data can easily fit in one GPU
- Every GPU can store all of the simulation data in multiple GPU case
  $\Longrightarrow$ parallelisation without communication between the GPUs is possible

Our parallelisation strategy

Force calculation: $\sim N^2 \implies$ if N is large enough, the simulation time is dominated by the force calculation

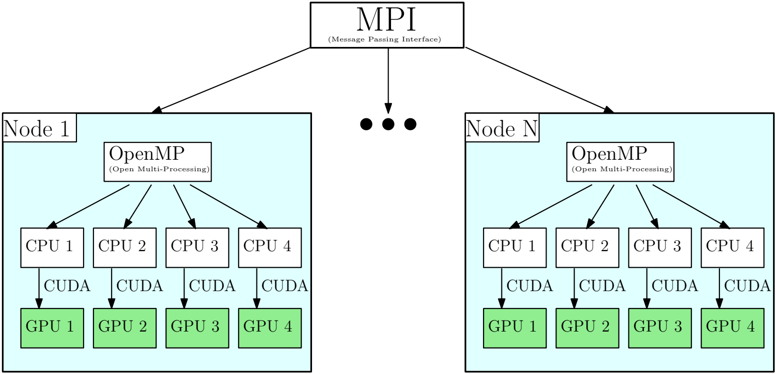
MPI-OpenMP-CUDA hybrid parallelisation

In every timestep

1. The master MPI thread Bcasts the particle coordinates
2. The nodes are calculating the forces with OpenMP-CUDA parallelisation
3. the calculated forces are collected by the master MPI thread, and this node integrates the equations of motion on the CPU

Even with this, the nodes most of the time are calculating forces ($\simeq$ 99.5% of the full simulation time)

Our parallelisation strategy



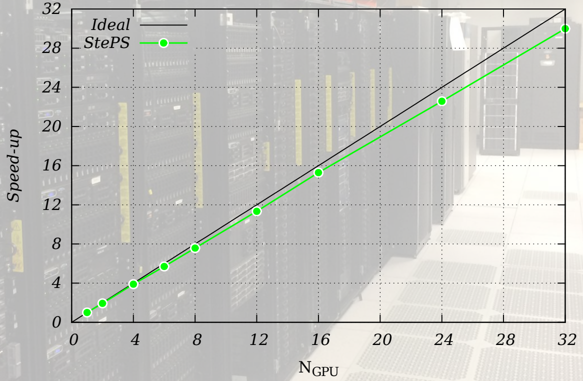
MARCC (Maryland Advanced Research Computing Center)[4]

Nodes	Type	Description	TFLOPs
676	Regular compute nodes	Intel Haswell dual socket, 12-core processors, 2.5GHz, 128GB RAM	648.9
50	Large memory nodes	Intel Ivy Bridge quad socket, 12-core processors, 3 GHz, 1024GB RAM	57.6
48	GPU nodes	Intel Haswell dual socket, 12-core processors, 2.5GHz, 128GB RAM, plus ***2 Nvidia K80 GPUs per node***	46 (cpu) + 279.36 (gpu)

4 https://www.marcc.jhu.edu/cyberinfrastructure/hardware/

The relative speed-up

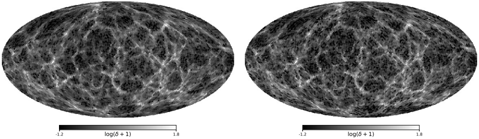
Speed-up test on MARCC with Nvidia Tesla K80 GPUs



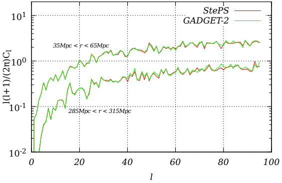
93.75% speed-up efficiency for $N_{GPU} = 32$

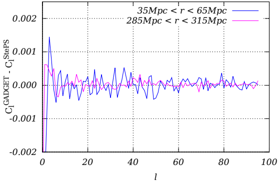
Results

- The StePS can easily reproduce the density field of larger simulations, even in a personal computer or a laptop

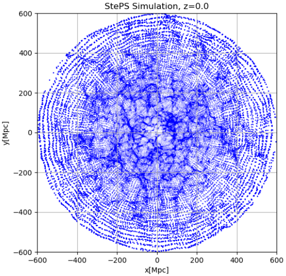


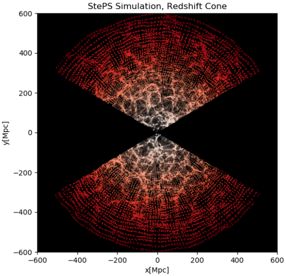
- The StePS $C_l(r)$ is matches with the corresponding Gadget-2 $C_l(r)$

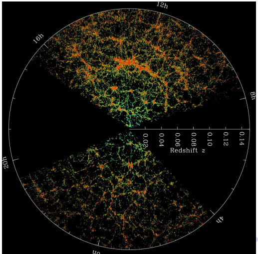




Generating mock-catalogues







Future plans

StePS

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- Resimulate the Millenium Simulation with our code with $\simeq 10^7$ particles (The original simulation had 10^{10} particles)
- Hubble-volume simulation
- Use these simulations to fit the cosmological parameters

Acknowledgements

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