

# Cosmological N-body simulations

## Techniques & Scope

Jayanti Prasad

National Center for Radio Astronomy  
Pune, India (411007)

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# Plan of the Talk

- Introduction
- Basic equations & approximations in N-body simulations
- Cosmological N-body simulations
- Some popular Cosmological N-body codes
- Applications of Cosmological N-body codes
- Summary and Conclusions

# Introduction

- The Newtonian equation of motion (EOM) cannot be solved analytically for a system of  $N > 2$  gravitating bodies.
- N-body simulations try to *integrate* the EOMs for a  $N > 2$  system of gravitating bodies *numerically*, using fast computers [Sellwood(1987), Hockney & Eastwood(1981), Aarseth(2003)].
- Any N-body problem can be broken into two parts:
  - ▶ Force Computation -  $N(N - 1)/2$  pairs of forces - Computational cost  $O(N^2)$
  - ▶ Moving Particles - updating  $N$  positions and velocities - Computational cost  $O(N)$

Cosmological N-body simulations use periodic boundary conditions & an expanding background [Bertschinger(1998), Efstathiou et al.(1985), Efstathiou, Davis, White, & Frenk].

## Force softening in N-body simulations

- For a system of  $N$  gravitating particles the relaxation time ( $\tau_r$ ) and the crossing time ( $\tau_c = R_h/v$ ) are related as

$$\frac{\tau_r}{\tau_c} = \frac{N}{\log_{10} \Lambda} \quad (1)$$

where  $\Lambda \approx 0.4N$  and  $R_h$  is the half mass radius. **There are more number of collisions if the same mass is distributed among lesser number of massive particles than more number of lighter particles.**

- In any N-body simulation the number of particles considered are always far less than the actual number of particles in the physical system therefore artificial collisions have to be avoided. Force softening is one of the ways to achieve this

$$\vec{F}_{ij} = -\frac{GM_i M_j \hat{r}_{ij}}{r_{ij}^2 + \epsilon^2} \quad (2)$$

- Softening at small scales prevent gravitational force from blowing up and helps to chose a time step for numerical integration: smaller softening demands for smaller time step and the computational cost goes up.
- Softened forces imply that a system of particles in equilibrium no longer satisfies the Virial theorem,  $2T + W = 0$ , where  $T$  and  $W$  are the total kinetic and potential energies of the system respectively.
- Softening can be regarded as replacing each point mass by a finite size "mass cloud" therefor sometime the codes are called "finite-size particle" codes.

## Types of N-body codes

On the basis of how the force is computed, N-body codes can be put into various classes:

- Direct N-body or Particle-Particle (PP):- These codes are the most accurate and computationally most expensive. All  $N(N - 1)/2$  pairs of force are computed and the force is accurate at all scales.
- Particle-Mesh (PM)  
[Efstathiou et al.(1985)Efstathiou, Davis, White, & Frenk, Bagla & Padmanabhan(1997)]:- Force is computed at the grid points of an artificial grid in Fourier space using the Fast Fourier Techniques (FFT). The force is inaccurate at sub-grid scales. Computational cost increases as  $O(N \log N)$ .
- Tree [Barnes & Hut(1986)]:- are based on the approximation that a group of particles at large distance can be considered a single large particle with representative mass, which reduces the number of pairs considerably. These codes are also inaccurate at small scales and computationally inexpensive  $O(N \log N)$

## N-body (hybrid) codes:

- Particle-Particle/Particle-Mesh (P3M) [Couchman(1991), Efstathiou et al.(1985)Efstathiou, Davis, White, & Frenk] :- By computing the force directly (particle-particle) at small scales ( $< 3 \times L_{grid}$ ) this method overcomes the shortcoming of PM method. However, it has the disadvantage that too easily the force computation gets dominated by the direct summation part.
- Tree-Particle (TreePM) [Bode & Ostriker(2003), Bagla(2002)]:- The force acting on a particle is splitted into two parts: the long range force and the short range force. The long range force is computed using the particle mesh (PM) method in Fourier space and the short range force is computed using tree method in real space.

$$\phi_k = -\frac{4\pi G\rho_k}{k^2}e^{-k^2r_s^2} - \frac{4\pi G\rho_k}{k^2} \left[1 - e^{-k^2r_s^2}\right] = \phi_k^l + \phi_k^s \quad (3)$$

## Nbody (adaptive) codes:

- Mesh-refined P3M [Couchman(1991)]:- “ adaptive mesh refinement in regions of high particle density.”
- Adaptive Refinement Tree [Kravtsov et al.(1997)Kravtsov, Klypin, & Khokhlov]:- “ mesh is generated to effectively match an arbitrary geometry of the underlying density field ... in a simulations the mesh structure is not created at every time step but is properly adjusted to the evolving particle distribution”.
- Multi-level adaptive particle mesh (MLAPM) [Knebe et al.(2001)Knebe, Green, & Binney]:- “ grid-based and uses a recursively refined Cartesian grid to solve Poisson’s equation for the potential, rather than obtaining the potential from a Green’s function. Refinements can have arbitrary shapes and in practice closely follow the complex morphology of the density field that evolves”.
- The Adaptive TreePM [Bagla & Khandai(2009)]:- “force softening length is reduced in high-density regions while ensuring that it remains well above the local inter-particle separation.”



## Nbody (hydro) codes:

- **Hydra**: an Adaptive-Mesh Implementation of P 3M-SPH  
[Couchman et al.(1995)Couchman, Thomas, & Pearce,  
Pearce & Couchman(1997)]:-

*an implementation of smoothed particle hydrodynamics (SPH) in an adaptive particle-particle-particle-mesh (AP3M) algorithm...evolves a mixture of purely gravitational particles and gas particles. SPH gas forces are calculated in the standard way from near neighbors.*

- **GADGET**: a code for collision-less and gas-dynamical cosmological simulations  
[Springel et al.(2001)Springel, Yoshida, & White, Springel(2005)]:-

*the simulation of interacting galaxies. GADGET evolves self-gravitating collision-less fluids with the traditional N-body approach, and a collisional gas by smoothed particle hydrodynamics*

# Cosmological N-body simulations

- Poisson Equation in co-moving coordinates ( $r(t) = a(t)x(t)$ ):

$$\nabla_r^2 \Phi(r, t) = 4\pi G \rho(r, t) \quad (4)$$

or

$$\nabla_r^2 (\phi_b(t) + \phi(x, t)) = 4\pi G \rho_b(t) (1 + \delta(x, t)) \quad (5)$$

or

$$\nabla_x^2 \phi(x, t) = 4\pi G \rho_b(t) \delta(x, t) = \frac{3\Omega_M H_0^2}{2} \frac{\delta(x, t)}{a(t)} \quad (6)$$

or

$$\nabla_x^2 \psi(x, t) = \frac{\delta(x, t)}{a(t)} \quad (7)$$

where

$$\psi(x, t) = \frac{2}{3H_0^2 \Omega_M} \phi(x, t); \quad \Omega_M = \frac{8\pi G \rho_b(t_0)}{3H_0^2}; \quad H_0 = \frac{\dot{a}(t_0)}{a(t_0)} \quad (8)$$

# Cosmological N-body simulations

- Equation of motion in an expanding background:

$$\ddot{\mathbf{r}}(t) = \ddot{a}(t)\mathbf{x}(t) + 2\dot{a}(t)\dot{\mathbf{x}}(t) + a(t)\ddot{\mathbf{x}}(t) = -\vec{\nabla}(\phi_b + \phi) \quad (9)$$

or

$$\ddot{a}(t)\mathbf{x}(t) = -\frac{\vec{\nabla}\phi_b}{a(t)} \quad (10)$$

and

$$a(t)\ddot{\mathbf{x}}(t) + 2\dot{a}(t)\dot{\mathbf{x}}(t) = -\vec{\nabla}\phi(\mathbf{x}) \quad (11)$$

or

$$\frac{d\mathbf{v}(t)}{dt} + H(t)\mathbf{v}(t) = -\frac{\vec{\nabla}\phi(\mathbf{x}, t)}{a(t)} \quad (12)$$

and

$$\frac{d\mathbf{x}(t)}{dt} = \frac{\mathbf{v}(t)}{a(t)} \quad (13)$$

# Cosmological N-body simulations

- Amplitude of growing mode as “time”: [Padmanabhan(1993)]

$$\ddot{\delta}_{\mathbf{k}} + 2\frac{\dot{a}}{a}\dot{\delta}_{\mathbf{k}} = 4\pi G\rho_b\delta_{\mathbf{k}} \quad (14)$$

where

$$b(t) \propto \frac{X^{1/2}}{a} \int^a \frac{da}{X^{3/2}} \quad (15)$$

$$X = 1 + \Omega_m \left( \frac{1}{a} - 1 \right) + \Omega_\Lambda (a^2 - 1) \quad (16)$$

$$\frac{d\mathbf{u}}{db} = -\frac{3}{2} \frac{Q}{b} (\mathbf{u} - \mathbf{g}) \quad (17)$$

where

$$\mathbf{u} = \frac{d\mathbf{x}}{db}; \quad \mathbf{g} = -\nabla\psi \quad \text{where} \quad \text{and} \quad Q = \left( \frac{\rho_b}{\rho_c} \right) \left( \frac{\dot{a}b}{ab} \right)^2 \quad (18)$$

## Special requirements of cosmological N-body simulations:

- Matter distribution in the universe is uniform at very large scales ( $> 100Mpc$ ), therefore there should be no structures in the universe at that scale in the final output.
- Physical scales in N-body simulations are incorporated from the normalization condition i.e.,  $\sigma^2(r = 8Mpc) = 1$ .
- For a simulation with box size  $L$  at  $z = 0$ ,  $N_{grid}$  number of grid points in one direction,  $N_{row}$  number of particles in one row and the density parameter  $\Omega_0$  the physical of the grid and mass of a particle are given by:

$$x_0 = 7.8 \text{ kpc} \left( \frac{L_{Mpc}}{L_{grid}/128} \right) \quad (19)$$

and

$$m_0 = 1.32 \times 10^5 (\Omega_0 h^2) \left( \frac{L_{Mpc}}{L_{row}/128} \right)^3 \quad (20)$$

- Periodic boundary conditions have to be incorporated.

# Particle Mesh Code

- Poisson equation is solved in Fourier space using FFT/FFTW. The potential is given by

$$\phi_k = -\frac{\delta_k}{k^2} \quad (21)$$

and the force

$$f_k = -i\phi_k \quad (22)$$

- Force is automatically softened at small scale due to finite size of the grid.
- Periodic boundary boundary conditions are automatically incorporated.
- Modes smaller than grid size and large than box size are ignored.
- There is no effect of mode smaller than the grid on the evolution of perturbations at large scales  
[Bagla et al.(2005)Bagla, Prasad, & Ray, Bagla & Prasad(2009)].

## Finite volume effects

- Modes greater than the box size leads to errors in physical quantities like two point correlation function and mass function  
[Bagla & Prasad(2006), Prasad(2007), Bagla et al.(2009)Bagla, Prasad, & Khandai].

$$\sigma^2(r) = \int_0^\infty \frac{dk}{k} \frac{k^3 P(k)}{2\pi^2} W^2(k, r) \quad (23)$$

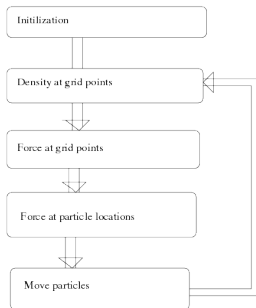
In N-body simulation:

$$\sigma^2(r, L_{\text{box}}) = \int_{2\pi/L_{\text{box}}}^{2\pi/L_{\text{grid}}} \frac{dk}{k} \frac{k^3 P(k)}{2\pi^2} W^2(k, r) = \sigma_0^2(r) - \sigma_1^2(r, L_{\text{box}}) \quad (24)$$

where

$$\sigma_1^2(r, L_{\text{box}}) = \int_0^{k_f = \frac{2\pi}{L_{\text{box}}}} \frac{dk}{k} \Delta^2(k) W^2(k, r) \quad (25)$$

# Particle Mesh Code





## Main steps in a PM force computation method:

- Assign mass/density to grid points

$$\rho(\mathbf{n}/M) = \frac{M^3}{N} \sum_{i=1}^{i=N} W(x_i - \mathbf{n}/M) \quad (26)$$

- Compute potential at grid points:

$$\phi(\mathbf{n}/M) = \frac{1}{M^3} \sum_{n'} \mathcal{G}\left(\frac{\mathbf{n} - \mathbf{n}'}{M}\right) \rho(\mathbf{n}'/M) \quad (27)$$

- Compute force at grid points:

$$F(\mathbf{n}/M) = -\frac{1}{N} \mathcal{D}_n \phi \quad (28)$$

- Calculate force on each particle:

$$F(x_i) = \sum_{i=1}^{i=N} W(x_i - \mathbf{n}/M) F(\mathbf{n}/M) \quad (29)$$

where:

$N$  : total number of particles in simulation

$M$  : total number of grid points along one direction

$n$  : an integer triple defining the center of a grid cell

$x_i$  : position vector of  $i$ th particle

$W$  : weighting scheme uses to assign mass to grid points

$\mathcal{G}$  : an approximation to green function for Poisson equation

$\mathcal{D}$  : differentiation scheme

The optimal choice of  $W$ ,  $\mathcal{G}$ ,  $\mathcal{D}$  and  $M$  depends on a trade of between force accuracy and computational cost.

## Integrating equation of motion:

- Euler's method:

$$x(t + \Delta t) = x(t) + v(t)\Delta t + O((\Delta t)^2) \quad (30)$$

and

$$v(t + \Delta t) = v(t) + a(t)\Delta t + O((\Delta t)^2) \quad (31)$$









- Leap-Frog method:







$$x(t + \Delta t) = x(t) + v(t + \Delta t/2)\Delta t + O((\Delta t)^3) \quad (32)$$

and

$$v(t + 3\Delta t/2) = v(t + \Delta t/2) + a(t)\Delta t + O((\Delta t)^3) \quad (33)$$

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