N-body Simulations

Techniques & Scope

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Plan of the Talk

- Introduction
- Gravitational N-body simulations
- Cosmological N-body simulations
- Cosmological N-body codes
- Discussion

Computer simulations

COMPUTER EXPERIMENTS USING PARTICLE MODELS 5

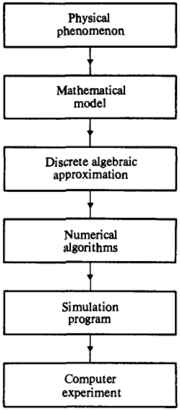


Figure 1-1 The principal steps in setting up a computer experiment.

Computer Experiments/Simulations

- In computer experiments or simulations, physical system of interest is represented by a mathematical model which is discretized using some approximation.
- On the basis of the method of approximation, simulations are divided into three broad categories: finite difference, finite elements and particles [Hockney & Eastwood(1981)].
- Particle method is a generic term used for the class of simulations where the discrete representation of the physical phenomenon involves interactions of particles. Particle methods are quite useful for evolutionary systems i.e., initial value - boundary value problems.
- Most often particles in simulations can be directly identified with the physical particles and can posses properties like mass, charge, momentum etc.
- There are two main approaches to study the dynamics of particles: (1) Lagrangian and (2) Eulerian.

Lagrangian and Eulerian methods

- In the Lagrangian approach, in order to compute the physical properties of particles, their trajectories are evolved in time. For example, we can calculate a physical quantity $S(x,t)$ at position x and time t, for a particle labeled by the initial coordinate q by computing x:

$$x(q,t) = q + v(q) * t; \tag{1}$$

- In the Eulerian methods, physical quantities are computed at space-time grid or mesh points. Time evolution of a physical quantity $S(x,t)$ is given by the convective derivative:

$$\frac{DS}{DT} = \left.\frac{dS}{dt}\right|_x + \mathbf{v}.\ \nabla \mathbf{S} \tag{2}$$

- Problem: If the velocity field is given by $u(x,t) = ax + bt$ find the total rate of change of the scalar field $S(x,t) = S_0 \sin(\omega t) + mt$ at some point A.

Particle systems

Table 1-1 Examples of physical systems represented by particle models
Scale lengths L are in meters and times T in seconds. N_p is the number of particles in L^3.

Example	Computer particles	Particle attributes	Physical N_p	Physical L	Physical T	Computer model N_p	Computer model L	Computer model T
1. *Correlated systems*								
Covalent liquids	Atoms or molecules	Strength constants related to quantum-mechanical dipole and quadruple interactions, mass, force, position, velocity	10^5	10^{-8}	10^{-12}	10^3-10^4	$10^{-8}-10^{-9}$	10^{-12}
Ionic liquids	Positive ions, Negative ions	Charge, mass, force, position, velocity, radius	10^5	10^{-8}	10^{-12}	10^3-10^4	$10^{-8}-10^{-9}$	10^{-12}
Stellar clusters	Stars	Mass, position, velocity, force, radius	10^2-10^3	10^{17}	10^{15}	10^2-10^3	10^{17}	10^{15}
Galaxy clusters	Galaxies	Mass, position, velocity, force, radius	10^4-10^5	10^{23}	10^{17}	10^4-10^5	10^{23}	10^{17}
2. *Collisionless systems*								
Collisionless plasma	"Superparticle" $\simeq 10^8$ electrons or 10^8 ions	Charge, mass, position, velocity, radius	10^9-10^{12}	$10^{-5}-10^{-2}$	$10^{-9}-10^{-12}$	$<10^5$	$10^{-5}-10^{-2}$	$10^{-9}-10^{-12}$
Galaxies—spiral structures	"Superparticle" $\simeq 10^6$ stars	Mass, position, velocity, radius	$10^{10}-10^{11}$	10^{21}	10^{13}	$<10^5$	10^{21}	10^{13}
3. *Collisional systems*								
Submicron Semiconductor devices (microscopic Monte-Carlo model)	"Superparticle" $= 10^4$ electron wavepackets	Charge, mass, position, wavenumber, radius	10^8	10^{-7}	10^{-10}	$<10^5$	10^{-7}	10^{-10}
4. *Collision-dominated systems*								
Semiconductor devices (diffusion model)	"Superparticle" $= 10^4$ electrons or holes	Charge, position	10^9	10^{-6}	10^{-9}	$<10^5$	10^{-6}	10^{-9}
Inviscid, incompressible fluids (vortex)	Vortex element	Vorticity, position	continuum	$10^{-3}-10^6$	$10^{-3}-10^5$	$<10^5$	$10^{-3}-10^6$	$10^{-3}-10^5$

Gravitational N-Body simulations

- Solving the equation of motion (Newtonian) for N gravitating bodies numerically is called the Gravitational N-body simulation.
- The applications of gravitational N-body simulations range from a few bodies in the solar systems to millions of galaxies in cosmological simulations.
- The relevant dynamics in the astrophysical context for a system of N gravitating bodies is Newton's law, plus an external potential field(if there is any).
- The force $\mathbf{F}_i$ acting on a particle of mass m_i is given by:

$$\mathbf{F}_i = -\sum_{j=1,j\neq i}^{j=N} G \frac{m_i m_j(\mathbf{r}_i - \mathbf{r}_j)}{|(\mathbf{r}_i - \mathbf{r}_j)|^3} - \nabla.\phi_{ext}(\mathbf{r}_i) \qquad (3)$$

Force softening

- The force given by the equation (4) presents a singularity (which can lead to arbitrary large relative velocities) when the distance between two particles approaches to zero.
- The singularity can be avoided by modifying the gravitational force at small scales:

$$\mathbf{F}_i = -\sum_{j=1, j\neq i}^{j=N} G\frac{m_i m_j(\mathbf{r}_i - \mathbf{r}_j)}{(|(\mathbf{r}_i - \mathbf{r}_j)|^2 + \epsilon^2)^{3/2}} - \nabla.\phi_{ext}(\mathbf{r}_i) \qquad (4)$$

where $\epsilon > 0$ is the length scale below which the force is modified.

Collisions

- For a system of N gravitating bodies with total mass M, dimension R, the crossing time T_{cr} (time taken by a particle to cross the systems which is also equal to the time that the system needs to settle in the Virial equilibrium) is defined as:

$$T_{cr} \approx \frac{1}{\sqrt{GM/R^3}} \tag{5}$$

- Evolution of a gravitating system in dynamic equilibrium is possible due to two-body collisions which leads to thermodynamics equilibrium and equipartition of energy. The time-scale for this processes is called the relaxation time T_{rel} defined as:

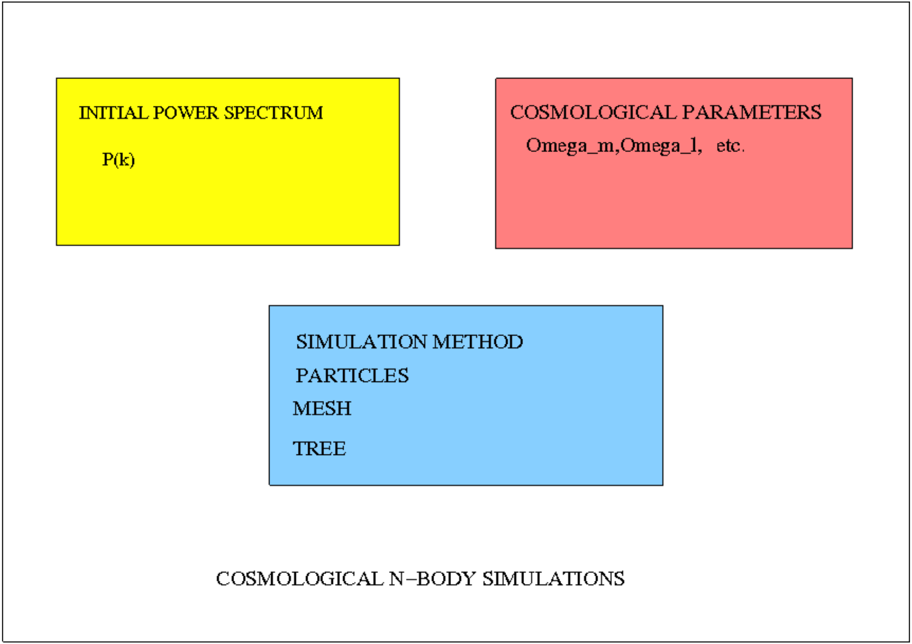
$$T_{rel} \propto \frac{N}{\log(0.11N)} T_{cr} \tag{6}$$

- N-body systems such and galaxies and dark matter haloes have a relaxation time much longer than the age of the Universe and are thus considered collision-less systems. Softening at small scales avoids collisions.

A typical N-body simulation

A typical N-body simulation have the following three steps:

1. Setting initial conditions: The position and velocities of all the particles need to be specified at some initial time $t = t_{in}$. In general, the particles are perturbed from the uniform distribution using the initial power spectrum.
2. Force Computation:- Force between particles is computed at every time step. It involves computation of $N(N-1)/2$ pairs of forces and the computational cost increases as $O(N^2)$.
3. Moving Particles: Once force acting on every particle is computed its position and velocity cab be updated.


INITIAL POWER SPECTRUM
P(k)
COSMOLOGICAL PARAMETERS
Omega_m,Omega_l, etc.
SIMULATION METHOD
PARTICLES
MESH
TREE
COSMOLOGICAL N–BODY SIMULATIONS

Cosmological N-body simulations

- In cosmological N-body simulations a representative volume of the Universe is considered and periodic boundary conditions are often i.e., $x + L_{box} \longrightarrow x, -x \longrightarrow x + L_{box}$
- One needs to make sure that the distribution of mass remains uniform at the final epoch also: there should be no power at the scale of the simulation box i.e., $P(k) = 0$ for $k < 2\pi/L_{box}$.
- In cosmological N-body simulations the mass resolution is decided by the number of particles used:

$$N_p \times m_p = l_{box}^3 \times \Omega_m \times \rho_c \tag{7}$$

or

$$m_p \approx \left(\frac{l_{box}}{128Mpc}\right)^3 \times \left(\frac{128^3}{N_p}\right) \times \Omega_m h^2 \times 2.77 \times 10^{11} M_\odot \tag{8}$$

- The spatial resolution is decided by the grid spacing and/or the softening length. Note that physical length scale is introduced by the normalization condition i.e., $\sigma^2(r = 8Mpc) = 1$.

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):- The force acting on particles is computed in pairs (Lagrangian approach). These codes are the most accurate and computationally most expansive $O(N^2)$.
- Particle-Mesh (PM):- An artificial grid is used and the physical quantities (force) are computed at the grid points and then interpolated at particle positions. Force is computed in the Fourier space using FFT which brings down computational cost from $O(N^2)$ to $O(N \log N)$. These methods are inaccurate at small scales.
- Tree [Barnes & Hut(1986)]:- These methods 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 and the force computation becomes $O(N \log N)$.

Particle Mesh Code

In a typical particle mesh code the following steps are followed:

1. Density is interpolated from the particle position to the grid points.

$$(x_i, y_i, zi, m_i) \longrightarrow \rho(x, y, z) \tag{9}$$

2. From the density at grid points, force at the grid points is computed:

$$\nabla^2\phi(x, y, z) = 4\pi G\rho(x, y, z) \text{ or } \tilde{\phi}(k_x, k_y, k_z) = -4\pi G\tilde{\rho}(k_x, k_y, k_z)/| \mathbf{k}| \tag{10}$$

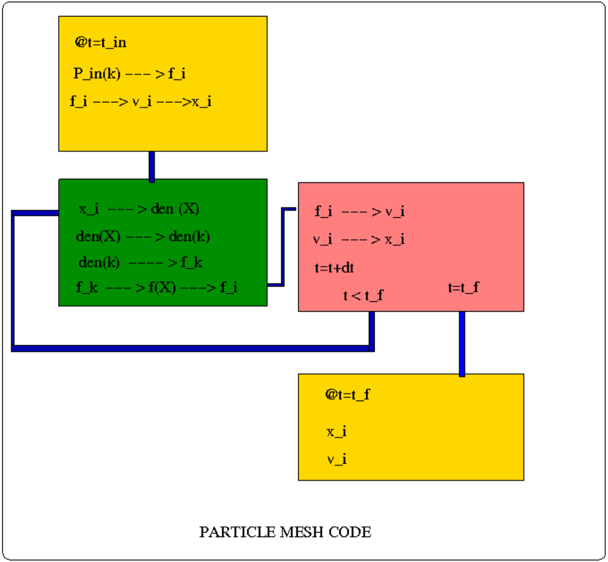
3. From the potential at grid points force at grid points is calculated:

$$f(x, y, z) = -\nabla\phi(x, y, z) \text{ or } \tilde{f}(k_x, k_y, k_z) = -i\,\mathbf{k}\tilde{\phi}(k_x, k_y, k_z) \tag{11}$$

4. Force is extrapolated from the grid points to the particle locations.
5. The positions and velocities of particles are updated.

Automatically softening + Periodic boundary boundary conditions

Particle-Mesh Codes



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 split ted 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.

$$\phi_k = -\frac{4\pi G\rho_k}{k^2} e^{-k^2 r_s^2} - \frac{4\pi G\rho_k}{k^2}\left[1 - e^{-k^2 r_s^2}\right] = \phi_k^l + \phi_k^s \qquad (12)$$

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*

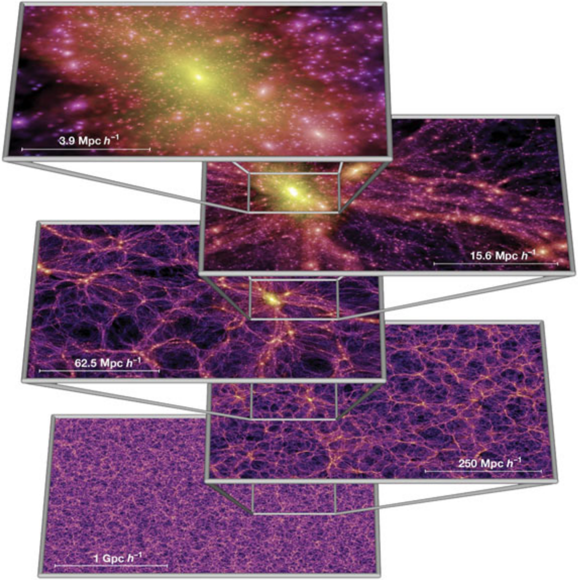
In this lecture I talked about :

- Computer simulations using particles
- Gravitational N-body simulations and cosmological simulations
- PP, PM and Tree, and some hybrid methods

I could not talk about:

- Interplay between theory, experiments/observations and simulations
- Computational aspects of N-body simulations and their limitations
- Hydrodynamical simulations
- Results from N-body simulations

Millennium simulation



Thank You !

- Aarseth, S. J. 2003, Gravitational N-Body Simulations (Cambridge, UK: Cambridge University Press, November 2003.)
- Bagla, J. S. 2002, Journal of Astrophysics and Astronomy, 23, 185
- Bagla, J. S., & Khandai, N. 2009, Monthly Notices of Royal Aastron. Society, 396, 2211
- Bagla, J. S., & Padmanabhan, T. 1997, Pramana, 49, 161
- Bagla, J. S., & Prasad, J. 2006, Monthly Notices of Royal Aastron. Society, 370, 993
- —. 2009, Monthly Notices of Royal Aastron. Society, 393, 607
- Bagla, J. S., Prasad, J., & Khandai, N. 2009, Monthly Notices of Royal Aastron. Society, 395, 918
- Bagla, J. S., Prasad, J., & Ray, S. 2005, Monthly Notices of Royal Aastron. Society, 360, 194
- Barnes, J., & Hut, P. 1986, Nature, 324, 446

- Bertschinger, E. 1998, Ann. Rev. Astron. Astrophys., 36, 599
- Bode, P., & Ostriker, J. P. 2003, Astrophical Journal Suppliment, 145, 1
- Couchman, H. M. P. 1991, Astrophical Journal Letters, 368, L23
- Couchman, H. M. P., Thomas, P. A., & Pearce, F. R. 1995, Astrophical Journal, 452, 797
- Efstathiou, G., Davis, M., White, S. D. M., & Frenk, C. S. 1985, Astrophical Journal Suppliment, 57, 241
- Hockney, R. W., & Eastwood, J. W. 1981, Computer Simulation Using Particles (New York: McGraw-Hill, 1981)
- Knebe, A., Green, A., & Binney, J. 2001, Monthly Notices of Royal Aastron. Society, 325, 845
- Kravtsov, A. V., Klypin, A. A., & Khokhlov, A. M. 1997, Astrophical Journal Suppliment, 111, 73

- Padmanabhan, T. 1993, Structure Formation in the Universe (Cambridge, UK: Cambridge University Press, June 1993.)
- Pearce, F. R., & Couchman, H. M. P. 1997, New Astronomy, 2, 411
- Prasad, J. 2007, Journal of Astrophysics and Astronomy, 28, 117
- Sellwood, J. A. 1987, Ann. Rev. Astron. Astrophys., 25, 151
- Springel, V. 2005, Monthly Notices of Royal Aastron. Society, 364, 1105
- Springel, V., Yoshida, N., & White, S. D. M. 2001, New Astronomy, 6, 79