N-BODY SIMULATION TECHNIQUES:

IT'S FOR EVERYBODY (CONT.)...

Neal Katz

Particle Mesh Codes (PM) $O(M \ln M)$

- Use fast Fourier transforms (**FFT**'s) to calculate the gravitational accelerations. Done on a regular rectangular grid.

- Schematically the algorithm proceeds as follows:

  - Assign masses of particles to the grid to determine the density at the grid points through interpolation.

  - Compute the gravitational potential at the grid points by solving the Poisson equation on the grid.

  - Compute gravitational accelerations by at the grid points by finite-differencing the potential. Forces are automatically softened on the grid scale.

  - Calculate the acceleration at each particle position using the same interpolation scheme used in the mass assignment to ensure momentum conservation.

References:

Efstathiou, G., Davis, M., Frenk, C.S., & White, S.D.M. 1985, *Ap. J. Suppl.* **57**, 241.

Mass Assignment

- Assign mass points to the grid using

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

  where N is total number of particles, M is the number of grid cells along one dimension, and $\mathbf{n}$ is an integer triple defining the center of each grid cell. W defines the interpolation scheme. Throughout the discussion of PM codes assume that the length of the entire grid is one and that the total mass is one.

- In three dimensions W can be expressed as the product of three one dimensional functions of the one dimensional displacement of a particle from the cell center $\delta\mathbf{x} = \mathbf{x} - \mathbf{n}/M$, i.e. $W_{ijk} = w_i w_j w_k$.

- There is a hierarchy of W's of increasing order p where a mass point is assigned to p^3 cells.

1) $p = 1$ (NGP): the density is discontinuous across cell boundaries.

$$w_i = 1, \qquad M|\delta x_i| \leq \frac{1}{2}$$

1) $p = 2$ (CIC): the density is continuous across cell boundaries but the first derivative is discontinuous.

$$w_i = 1 - M|\delta x_i|, \qquad M|\delta x_i| < 1$$

1) $p = 3$ (TSC): both the density and its first derivative is continuous across cell boundaries but higher order derivatives are discontinuous.

$$w_i = \begin{cases} \frac{3}{4} - M^2 \delta x_i^2, & M|\delta x_i| \leq \frac{1}{2} \\ \frac{1}{2}\left(\frac{3}{2} - M|\delta x_i|\right)^2, & \frac{1}{2} \leq M|\delta x_i| \leq \frac{3}{2} \end{cases}$$

$w_i = 0$ outside the above ranges.

Determining the Potential

- The potential ϕ is determined from the density field by solving Poisson's equation

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

where G is an approximation to the Green's function of Poisson's equation.

- The convolution can be solved rapidly in Fourier space using FFT's

$$\phi(l, m, n) = \sum_{p,q,r} \hat{\mathcal{G}}_{p,q,r} \hat{\rho}_{p,q,r} e^{2\pi i(pl+qm+rn)/M}$$

where circumflexes denote Fourier transforms and the subscripts are integer triples denoting a grid point.

- The usual Green's function for the Laplacian is

$$\hat{\mathcal{G}}_{p,q,r} = \begin{cases} 0, & l = m = n = 0 \\ \frac{-G}{\pi(p^2+q^2+r^2)} & \text{otherwise} \end{cases}$$

- Another choice is the seven point finite difference approximation to the Laplacian

$$\hat{\mathcal{G}}_{p,q,r} = \begin{cases} 0, & l = m = n = 0 \\ \frac{-G\pi}{M^2}\left[\sin^2(\pi p/M) + \sin^2(\pi q/M) + \sin^2(\pi r/M)\right] & \text{otherwise} \end{cases}$$

Computing the Accelerations

- The accelerations are calculated by finite differencing the grid of gravitational potential energies.

$$\mathbf{a}(\mathbf{n}/M) = \frac{-1}{N}\mathbf{D}_n \phi$$

where the operator $\mathbf{D}_n$ represents the differencing scheme used.

- One choice is the two point finite difference approximation

$$a_x(\mathbf{n}/M) = \frac{M}{2N}\left(\phi_{l-1,m,n} - \phi_{l+1,m,n}\right)$$

with similar terms for the other two directions.

- Another choice is the four point finite difference approximation

$$a_x(\mathbf{n}/M) = \frac{2M}{3N}\left(\phi_{l-1,m,n} - \phi_{l+1,m,n}\right) + \frac{7M}{12N}\left(\phi_{l-2,m,n} - \phi_{l+2,m,n}\right)$$

- The acceleration are interpolated to each particle location using

$$\mathbf{a}(\mathbf{x}_i) = \sum_n W(\mathbf{x}_i - \mathbf{n}/M)\mathbf{a}(\mathbf{n}/M)$$

- The W used in the force interpolation has to be the same as that in the mass assignment to conserve momentum.

- To reduce small scale errors that can lead to poor energy conservation the Green's function can be *shaped*.

PPPM ($\mathbf{P^3M}$)

- To gain better force resolution at small scales can add the direct summation (PP) of particles within a grid cell to the PM forces.
- Choose the PM Green's function and the PP softening to make the forces as continuous as possible.
- Particles within a grid cell are found using a linked list approach.
- The method becomes inefficient if there are too many particles in a few grid cells, i.e. it becomes $O(n^2)$.
- Can fix this problem using a hierarchical series of grids, i.e. put a subgrid in the cells with a lot of particles.

Reference:

Couchman, H.M.P. 1991, *Ap. J.* **368**, 23.

Boundary Conditions

- Two main choices for boundary conditions:
  - Periodic–good for simulating pieces of larger structures like in cosmological simulations.
  - Vacuum–good for simulating isolated objects like galaxies.
- The *natural* boundary conditions for a PM code are periodic and the *natural* boundary conditions for a tree code are vacuum.
- Can make a tree code fully periodic using **Ewald summation**.
- Can make a PM code not periodic by:
  - padding-adding zeros around the volume in effect making the calculation 8 times larger.
  - Introduce a series of negative charges on the edges of the box. Used in codes that subgrid.

Reference:

Hernquist, L., Bouchet, F.R., & Suto, Y. 1991 *Ap. J. Suppl.* **75**, 231 (Ewald).

Comoving Coordinates

- For cosmological simulations it is expedient to work with coordinates comoving with the expansion, $\mathbf{x}$, which are related to proper coordinates, $\mathbf{r}$, and the expansion factor through

$$\mathbf{x} = \frac{\mathbf{r}}{a}$$

  where $a = 1./(1+z)$

- The momentum of a particle with mass m in these coordinates is

$$\mathbf{p} = ma^2\dot{\mathbf{x}}$$

  where $\dot{\mathbf{x}} \equiv d\mathbf{x}/dt$.

- a evolves according to

$$\left(\frac{\dot{a}}{a}\right)^2 - \frac{8\pi}{3}G\rho = \frac{\Lambda}{3} - \frac{kc^2}{a}$$

  where ρ is the mean mass density, Λ is the cosmological constant, and $k = -1, 0$, or 1 for closed, flat, and open universes.

- It is customary to express the mean mass density of the universe in terms of the critical density for $k = 0$ and $\Lambda = 0$ by $\Omega \equiv \rho/\rho_c$, where

$$\rho_c = \frac{3H^2}{8\pi G}$$

and $H(t) \equiv \dot{a}/a$ is the Hubble parameter.

- Employ the convention that at the present time, t_0, the expansion factor is $a(t_0) = 1$. Then, for example the solution for a flat universe with no cosmological constant is

$$a(t) = \left(\frac{3H_0 t}{2}\right)^{2/3}$$

- The equations of motion for the i-th particle are

$$\dot{\mathbf{x}}_i = \frac{d\mathbf{x}_i}{dt}$$

and

$$\ddot{\mathbf{x}}_i + 2H\dot{\mathbf{x}}_i - \frac{1}{a}\mathbf{g}_i = 0.$$

Therefore, if the spatial coordinates are known at time step $n - 1/2$ and the velocities are known at time step n, the values of $\mathbf{x}_i$ at time step $n + 1/2$, $\mathbf{x}_i^{n+1/2}$ are

$$\mathbf{x}_i^{n+1/2} = \mathbf{x}_i^{n-1/2} + \delta t \dot{\mathbf{x}}_i^n.$$

These new spatial coordinates are then used to estimate the peculiar acceleration at time step $n+1/2$, making it possible to update velocities according to

$$\dot{\mathbf{x}}_i^{n+1} = \dot{\mathbf{x}}_i^n \frac{1 - H^{n+1/2}\delta t}{1 + H^{n+1/2}\delta t} + \frac{\delta t}{a^{n+1/2}} \frac{\mathbf{g}_i^{n+1/2}}{1 + H^{n+1/2}\delta t}$$

where $a^{n+1/2}$ and $H^{n+1/2}$ are the values of the expansion factor and the Hubble parameter at the intermediate time.