N-Body Simulation

Solving the CBE with a 6-D grid takes too many cells. Instead, we use a Monte-Carlo method.

Example: Monte-Carlo calculation of $\pi$. Scatter $n$ points in square; count number $n_{\text{circle}}$ falling within circle.

$$\pi = 4A_{\text{circle}}/A_{\text{square}} \approx 4n_{\text{circle}}/n$$

Typical uncertainty:

$$|\pi_{\text{est}} - \pi| = O(n^{-1/2})$$
Representing the Distribution Function

Replace smooth distribution with bodies:

\[ f(\vec{r}, \vec{v}) \rightarrow \{(m_i, \vec{r}_i, \vec{v}_i) \mid i = 1, \ldots, N\} \]

\[
f(\vec{r}, \vec{v}) \simeq \sum_{i=1}^{N} m_i \delta^3(\vec{r} - \vec{r}_i) \delta^3(\vec{v} - \vec{v}_i)
\]

This requires that for any phase-space volume \( V \),

\[
\int_V d\vec{r} d\vec{v} f(\vec{r}, \vec{v}) = \left\langle \sum_{(\vec{r}_i, \vec{v}_i) \in V} m_i \right\rangle
\]

E.g., select \((\vec{r}_i, \vec{v}_i)\) with probability proportional to \(f(\vec{r}_i, \vec{v}_i)\), and assign all bodies equal mass:

\[
m_i = \frac{1}{N} \int d\vec{r} d\vec{v} f(\vec{r}, \vec{v})
\]
Advancing Time

Move bodies along phase flow (method of characteristics):

\[ (\dot{\vec{r}}_i, \dot{\vec{v}}_i) = (\vec{v}_i, - (\nabla \Phi)_i) \]

Estimate potential from N-body representation:

\[ \nabla^2 \Phi \bigg|_{\vec{r}} = 4\pi G \sum_{i=1}^{N} m_i \delta^3(\vec{r} - \vec{r}_i) \]

This will yield the usual N-body equation for point masses. But singular potentials are awkward, so we smooth the density field:

\[ \delta^3(\vec{r} - \vec{r}_i) \rightarrow \frac{3}{4\pi} \frac{\epsilon^2}{\left( |\vec{r} - \vec{r}_i|^2 + \epsilon^2 \right)^{3/2}} \]

Plummer (1911) smoothing

This substitution yields the following equations of motion:

\[ \frac{d\vec{r}_i}{dt} = \vec{v}_i \]

\[ \frac{d\vec{v}_i}{dt} = \sum_{j \neq i}^{N} \frac{G m_j (\vec{r}_j - \vec{r}_i)}{\left( |\vec{r}_j - \vec{r}_i|^2 + \epsilon^2 \right)^{3/2}} \]

Aarseth (1963)
Comments

1. N-body models relax at roughly the same rate as real stellar systems with the same $N$; the relaxation time is

$$t_r \simeq \frac{N}{8 \ln(R/\varepsilon)} t_c$$

2. Sampling proportional to $f(\vec{r}_i, \vec{v}_i)$ is the simplest option, but not the only one; other weighting schemes are also possible.

E.g., use different masses when sampling $f_s(\vec{r}, \vec{v})$ and $f_d(\vec{r}, \vec{v})$, or make $m_i$ depend on $f(\vec{r}_i, \vec{v}_i)$. But note effect on relaxation time!

3. Plummer smoothing is just one of many possibilities, and may not be optimal; one alternative with less of a “tail” is

$$\delta^3(\vec{r} - \vec{r}_i) \rightarrow \frac{15 \varepsilon^4}{8\pi (|\vec{r} - \vec{r}_i|^2 + \varepsilon^2)^{7/2}}$$

Dehnen (2001)
Force Calculation: Direct Summation

Simplest method: sum over all other bodies.

\[ \vec{a}_i = \sum_{j \neq i}^{N} \frac{G m_j (\vec{r}_j - \vec{r}_i)}{(|\vec{r}_j - \vec{r}_i|^2 + \varepsilon^2)^{3/2}} \]

Advantages: robust, accurate, completely general.

Disadvantage: computational cost per body is \( O(N) \); need \( O(N^2) \) operations to compute forces on all bodies.

However, direct summation is a good fit with
1. Individual timesteps (see Sverre’s lectures)
2. Specialized hardware (see Simon’s lectures)
Tree Codes

Long-range gravitational field dominated by monopole term:

$$\phi \approx -\frac{Gm}{r} + O(r^{-3})$$

Divide system into hierarchy (i.e. “tree”) of compact cells:

Replace sum over $N$ bodies with sum over $N_c \approx O(\log N)$ cells; cost to find forces on all bodies is $O(N \log N)$.
1. To compute potential at $\vec{r}$ due to a cell $c$:  
   a) if $c$ is “too close” to $\vec{r}$, sum the potentials of its sub-cells;  
   b) otherwise, approximate the potential as $-\frac{Gm_c}{|\vec{r} - \vec{r}_c|}$. 

2. “too close” can be defined in various ways; e.g.:  
   a) geometrically: $|\vec{r} - \vec{r}_c| < \ell_c/\theta$ (BH86) or $< \ell_c/\theta + \delta_c$ (B95),  
   b) dynamically: $|\vec{r} - \vec{r}_c|^4 < GM_c\ell^2_c/\alpha|\vec{a}|$ (GADGET-2: Springel 2005). 

3. Different tree structures give roughly equivalent results:  
   a) oct-trees: 1 cube $\rightarrow$ 8 cubes (Barnes & Hut 1986),  
   b) kd trees: divide at median along $x, y, z$ (Dikaiakos & Stadel 1996),  

4. Higher moments improve accuracy:  
   a) quadrupole potential term: $\frac{1}{2}G \delta \vec{r} \cdot \vec{Q}_c \cdot \delta \vec{r} / \delta r^5$ (Hernquist 1987),  
   b) source/sink symmet. $\Rightarrow$ momentum cons., $O(N)$ (Dehnen 2000).
Self-Consistent Field Method

Represent potential and density as sums:

\[ \Phi(\vec{r}) = \sum_k A_k \Phi_k(\vec{r}) \quad \text{and} \quad \rho(\vec{r}) = \sum_k A_k \rho_k(\vec{r}) \]

where \(A_k\) are coefficients and the basis functions \(\Phi_k\) and \(\rho_k\) are bi-orthogonal and satisfy the PE:

\[ I_k \delta_{kk'} = \int d\vec{r} \rho_k(\vec{r}) [\Phi_{k'}(\vec{r})]^* \quad \text{and} \quad \nabla^2 \Phi_k = 4\pi G \rho_k \]

The coefficients are computed using overlap integrals:

\[ A_k = \frac{1}{I_k} \int d\vec{r} \rho(\vec{r}) [\Phi_k(\vec{r})]^* = \frac{1}{I_k} \sum m_i [\Phi_k(\vec{r}_i)]^* \]

The cost of calculating forces on all bodies is just \(O(N)\).

With the right basis set, SCFM yields good forces for spheroidal systems with only a few terms (Hernquist & Ostriker 1992).
Time Step Algorithms

The underlying symmetry of the N-body equation of motion becomes evident in Hamiltonian formulation:

\[
\frac{d\vec{r}}{dt} = \frac{\partial H}{\partial \vec{p}}, \quad \frac{d\vec{p}}{dt} = -\frac{\partial H}{\partial \vec{r}}
\]

This symmetry has important consequences:
1. dynamical evolution conserves phase space volume
2. Hamiltonian systems have no attractors
3. dynamical evolution is reversible.

Hamiltonian systems are not structurally stable; most integrators will not preserve these properties.

An integration algorithm with Hamiltonian symmetry is desirable; such an integrator is known as \textit{symplectic}.
Leapfrog Integrator

This very simple integrator explicitly preserves the symmetry of the Hamiltonian equations of motion:

\[
\begin{align*}
\vec{r}_{i}^{[k+1]} &= \vec{r}_{i}^{[k]} + \Delta t \vec{v}_{i}^{[k+1/2]} \\
\vec{v}_{i}^{[k+3/2]} &= \vec{v}_{i}^{[k+1/2]} + \Delta t \vec{a}_{i}(\vec{r}^{[k+1]})
\end{align*}
\]

In addition, it is accurate to second order, meaning that the error is \(O(\Delta t^3)\) per step, and requires very little storage.

A drawback of the leapfrog is that velocities are a half-step out of sync with positions; this can be avoided as follows:

\[
\begin{align*}
\vec{v}_{i}^{[k+1/2]} &= \vec{v}_{i}^{[k]} + \frac{\Delta t}{2} \vec{a}_{i}(\vec{r}^{[k]}) \\
\vec{r}_{i}^{[k+1]} &= \vec{r}_{i}^{[k]} + \Delta t \vec{v}_{i}^{[k+1/2]} \\
\vec{v}_{i}^{[k+1]} &= \vec{v}_{i}^{[k+1/2]} + \frac{\Delta t}{2} \vec{a}_{i}(\vec{r}^{[k+1]})
\end{align*}
\]

This formulation introduces a one-time error of \(O(\Delta t^2)\) but is otherwise equivalent to the standard leapfrog.
Individual Time Steps?

 Leapfrog becomes inaccurate if $\Delta t$ is not constant and identical for all bodies. This seems inefficient.

 However, the symplectic properties of the leapfrog give it much more stability than most integrators.

 Algorithms in which $\Delta t$ is determined by current conditions are not reversible. Symmetrizing the time step between endpoints $t$ and $t + \Delta t$ works but imposes a significant overhead (Hut et al. 1995).

 A 4th order symplectic scheme allowing individual and adaptive time-steps is now available (Farr & Bertschinger 2007).
Errors and Relaxation

N-body simulations diverge from exact solutions of CBE and PE for several reasons:
1. Roundoff errors.
2. Truncation in time stepping.
3. Force calculation approximations.
4. Density field smoothing.
5. Relaxation due to finite $N$.

In theory, these effects can all be controlled — at a price. Error #1 is seldom an issue, while errors #2 and #3 are easily limited. Smoothing and relaxation are harder to balance; high resolution demands shorter timesteps and more bodies.

Finally, all N-body systems with $N > 2$ are potentially chaotic, while the role of chaos in real galaxies is unclear.
Parameter Choices

The number of bodies $N$ is the key parameter:

— 2-body relaxation time: $t_r \simeq N t_c / 8 \ln(R/\varepsilon)$
— Monte-Carlo errors: $O(N^{-1/2})$

Maximum duration of simulation must be $t \ll t_r$.

Typical errors in acceleration should be $|\delta a/a| \lesssim N^{-1/2}$.

Global energy should be conserved to $|\delta E/E| \lesssim N^{-1/2}$.

Smoothing length is typically $R N^{-1/2} < \varepsilon < R N^{-1/3}$.

Leapfrog time-step should be $\Delta t \lesssim 0.03 t_{\text{min}} \simeq 0.09 (G \rho_{\text{max}})^{-1/2}$.

**WARNING**: these rules are not definitive. Tests with different parameter values are useful; a skeptical attitude is advised!
Introduction to Smoothed Particle Hydrodynamics

Fluid equations in conservation form:

mass:
\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \]

momentum:
\[ \frac{\partial \vec{v}}{\partial t} + (\vec{v} \cdot \nabla)\vec{v} = -\nabla \Phi + \frac{1}{\rho} \nabla P \]

energy or entropy:
\[
\begin{align*}
\frac{\partial u}{\partial t} + (\vec{v} \cdot \nabla) u &= -\frac{P}{\rho} \\
\frac{\partial a}{\partial t} + (\vec{v} \cdot \nabla) a &= (\gamma - 1) \rho^{1-\gamma} \ddot{u}
\end{align*}
\]

Equation of state (ideal gas):
\[ P = (\gamma - 1) \rho u \quad P = a(S) \rho^\gamma \]
SPH Formalism

Particle representation (c.f. N-body):

\[ \rho(\vec{r}), \vec{v}(\vec{r}), u(\vec{r}), a(\vec{r}) \rightarrow \{(m_i, \vec{r}_i, \vec{v}_i, u_i, a_i) \mid i = 1, \ldots, N\} \]

Density estimate uses smoothing kernel \( W(\vec{x}, h) \) with scale \( h \):

\[ \rho(\vec{r}) \approx \sum_{i} m_i W(\vec{r} - \vec{r}_i, h) \]

where \( \int d\vec{x} W(\vec{x}, h) = 1 \); estimates of gradients become sums involving gradients of \( W(\vec{x}, h) \).

Dynamical equations:

\[
\begin{align*}
\frac{d\vec{r}_i}{dt} &= \vec{v}_i \\
\frac{d\vec{v}_i}{dt} &= (-\nabla \Phi)_i + \left(-\frac{1}{\rho}\nabla P\right)_i + \vec{a}^{\text{visc}}_i \\
\frac{du_i}{dt} &= \left(-\frac{P}{\rho}\nabla \cdot \vec{v}\right)_i + \dot{u}_i + \dot{u}^{\text{visc}}_i \\
\frac{da_i}{dt} &= (\gamma - 1) \rho_i^{1-\gamma} (\dot{u}_i + \dot{u}^{\text{visc}}_i)
\end{align*}
\]
Comments

1. The smoothing kernel \( W(\vec{x}, h) \) has compact support, so only nearby bodies are included in the sums. Most SPH codes adapt the smoothing length \( h \) to the local particle density.

2. Adaptive timesteps are generally necessary to satisfy the Courant condition; most SPH integrators are not symplectic.

3. Artificial viscosity is required to keep particles from streaming through shocks. The best formulation is not entirely clear.

4. SPH is often criticized as a poor approximation to proper gas dynamics. However, the ISM is much more complex than an ideal gas. In the context of galaxy-scale simulations, momentum and energy conservation may be all we can expect of a code.