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Lecture Notes for

Modern Computational Astrophysics: Concepts and Applications

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January 14, 2021

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8 Collisionless particle systems

According to the ΛCDM paradigm, the matter density of our Universe is dominated by *dark matter*, which is thought to be composed of a yet unidentified, non-baryonic elementary particle (e.g. Bertone et al., 2005). A full description of the dark mass in a galaxy would hence be based on following the trajectories of each dark matter particle – resulting in a gigantic N-body model. This is clearly impossible due to the large number of particles involved. Similarly, describing all the trajectories of electrons in a plasma is infeasible. In this chapter we discuss why we can nevertheless describe these systems as discrete N-body systems, but composed of far fewer particles than there are in reality.

8.1 N-particle ensembles

The state of an N-particle ensemble at time t can be specified by the *exact* particle distribution function (Hockney & Eastwood, 1988), in the form

$$F(\boldsymbol{x},\boldsymbol{v},t) = \sum_{i=1}^{N} \delta(\boldsymbol{x}-\boldsymbol{x}_i(t)) \cdot \delta(\boldsymbol{v}-\boldsymbol{v}_i(t)). \tag{8.1}$$

This gives effectively the number of particles at phase-space point $(\boldsymbol{x},\boldsymbol{v})$ at time t. Let now

$$p(\boldsymbol{x}_1,\boldsymbol{x}_2,\ldots,\boldsymbol{x}_N,\boldsymbol{v}_1,\boldsymbol{v}_2,\ldots,\boldsymbol{v}_N)\,\mathrm{d}\boldsymbol{x}_1\,\mathrm{d}\boldsymbol{x}_2\cdots\mathrm{d}\boldsymbol{x}_N\,\mathrm{d}\boldsymbol{v}_1\,\mathrm{d}\boldsymbol{v}_2\cdots\mathrm{d}\boldsymbol{v}_N \tag{8.2}$$

be the probability that the system is in the given state at time t. Then a reduced statistical description is obtained by *ensemble averaging*:

$$f_1(\boldsymbol{x},\boldsymbol{v},t) = \langle F(\boldsymbol{x},\boldsymbol{v},t)\rangle = \int F\cdot p\cdot \mathrm{d}\boldsymbol{x}_1\,\mathrm{d}\boldsymbol{x}_2\cdots\mathrm{d}\boldsymbol{x}_N\,\mathrm{d}\boldsymbol{v}_1\,\mathrm{d}\boldsymbol{v}_2\cdots\mathrm{d}\boldsymbol{v}_N. \tag{8.3}$$

For each of the N terms in $F(\boldsymbol{x},\boldsymbol{v},t)$ we can integrate out the two Dirac delta-functions in F to obtain

$$\begin{aligned} f_1(\boldsymbol{x},\boldsymbol{v},t) &= \int p\,[\delta(\boldsymbol{x}-\boldsymbol{x}_1(t))\delta(\boldsymbol{v}-\boldsymbol{v}_1(t)) + \delta(\boldsymbol{x}-\boldsymbol{x}_2(t))\delta(\boldsymbol{v}-\boldsymbol{v}_2(t)) \\ &\quad +\cdots+\delta(\boldsymbol{x}-\boldsymbol{x}_N(t))\delta(\boldsymbol{v}-\boldsymbol{v}_N(t))]\,\mathrm{d}\boldsymbol{x}_1\,\mathrm{d}\boldsymbol{x}_2\cdots\mathrm{d}\boldsymbol{x}_N\,\mathrm{d}\boldsymbol{v}_1\,\mathrm{d}\boldsymbol{v}_2\cdots\mathrm{d}\boldsymbol{v}_N \\ &= \int [\underbrace{p(\boldsymbol{x},\boldsymbol{x}_2,\ldots,\boldsymbol{x}_N,\boldsymbol{v},\boldsymbol{v}_2,\ldots,\boldsymbol{v}_N)\,\mathrm{d}\boldsymbol{x}_2\cdots\mathrm{d}\boldsymbol{x}_N\,\mathrm{d}\boldsymbol{v}_2\cdots\mathrm{d}\boldsymbol{v}_N+\ldots}_{N\text{ terms}}] \\ &= N\int p(\boldsymbol{x},\boldsymbol{x}_2,\ldots,\boldsymbol{x}_N,\boldsymbol{v},\boldsymbol{v}_2,\ldots,\boldsymbol{v}_N)\,\mathrm{d}\boldsymbol{x}_2\cdots\mathrm{d}\boldsymbol{x}_N\,\mathrm{d}\boldsymbol{v}_2\cdots\mathrm{d}\boldsymbol{v}_N. \end{aligned} \tag{8.4}$$

Note that we can permute the arguments in p where $\boldsymbol{x}$ and $\boldsymbol{v}$ appear. $f_1(\boldsymbol{x}, \boldsymbol{v}, t)\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{v}$ now gives the *mean number* of particles in a phase-space volume $\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{v}$ around $(\boldsymbol{x}, \boldsymbol{v})$.

Similarly, the ensemble-averaged two-particle distribution ("the mean product of the numbers of particles at $(\boldsymbol{x}, \boldsymbol{v})$ and $(\boldsymbol{x}', \boldsymbol{v}')$") is given by

$$\begin{aligned} f_2(\boldsymbol{x}, \boldsymbol{v}, \boldsymbol{x}', \boldsymbol{v}', t) &= \langle F(\boldsymbol{x}, \boldsymbol{v}, t) F(\boldsymbol{x}', \boldsymbol{v}', t) \rangle \\ &= N(N-1) \int p(\boldsymbol{x}, \boldsymbol{x}', \boldsymbol{x}_3, \ldots, \boldsymbol{x}_N, \boldsymbol{v}, \boldsymbol{v}', \boldsymbol{v}_3, \ldots \boldsymbol{v}_N)\,\mathrm{d}\boldsymbol{x}_3 \cdots \mathrm{d}\boldsymbol{x}_N\,\mathrm{d}\boldsymbol{v}_3 \cdots \mathrm{d}\boldsymbol{v}_N. \end{aligned} \tag{8.5}$$

Likewise one may define $f_3, f_4, \ldots$ and so on. This yields the so-called BBGKY (Bogoliubov-Born-Green-Kirkwood-Yvon) chain (e.g. Kirkwood, 1946), see also Hockney & Eastwood (1988) for a detailed discussion.

8.2 Uncorrelated (collisionless) systems

The simplest closure for the BBGKY hierarchy is to assume that particles are *uncorrelated*, i.e. that we have

$$f_2(\boldsymbol{x}, \boldsymbol{v}, \boldsymbol{x}', \boldsymbol{v}', t) = f_1(\boldsymbol{x}, \boldsymbol{v}, t)\, f_1(\boldsymbol{x}', \boldsymbol{v}', t). \tag{8.6}$$

Physically, this means that a particle at $(\boldsymbol{x}, \boldsymbol{v})$ is completely unaffected by one at $(\boldsymbol{x}', \boldsymbol{v}')$. Systems in which this is approximately the case include

- electrons in a plasma
- stars in a galaxy
- dark matter particles in the universe

We will later consider in more detail under which conditions a system is collisionless.

Let's now go back to the probability density $p(\boldsymbol{w})$ which depends on the N-particle phase-space state $\boldsymbol{w} = (\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N, \boldsymbol{v}_1, \boldsymbol{v}_2, \ldots \boldsymbol{v}_N)$. The conservation of probability in phase-space means that it fulfills a continuity equation

$$\frac{\partial p}{\partial t} + \boldsymbol{\nabla}_{\boldsymbol{w}} \cdot (p\, \dot{\boldsymbol{w}}) = 0. \tag{8.7}$$

We can cast this into

$$\frac{\partial p}{\partial t} + \sum_i \left(p \frac{\partial \dot{\boldsymbol{x}}_i}{\partial \boldsymbol{x}_i} + \frac{\partial p}{\partial \boldsymbol{x}_i} \cdot \dot{\boldsymbol{x}}_i + p \frac{\partial \dot{\boldsymbol{v}}_i}{\partial \boldsymbol{v}_i} + \frac{\partial p}{\partial \boldsymbol{v}_i} \cdot \dot{\boldsymbol{v}}_i \right) = 0. \tag{8.8}$$

Now we recall Hamiltonian dynamics with the equations of motion $\dot{\boldsymbol{x}} = \frac{\partial H}{\partial \boldsymbol{p}}$ and $\dot{\boldsymbol{p}} = -\frac{\partial H}{\partial \boldsymbol{x}}$ (Goldstein, 1950). We can differentiate them to get $\frac{\partial \dot{\boldsymbol{x}}}{\partial \boldsymbol{x}} = \frac{\partial^2 H}{\partial \boldsymbol{x} \partial \boldsymbol{p}}$, and $\frac{\partial \dot{\boldsymbol{p}}}{\partial \boldsymbol{p}} = -\frac{\partial^2 H}{\partial \boldsymbol{x} \partial \boldsymbol{p}}$. Hence it follows $\frac{\partial \dot{\boldsymbol{x}}}{\partial \boldsymbol{x}} = -\frac{\partial \dot{\boldsymbol{v}}}{\partial \boldsymbol{v}}$. Using this we get

$$\frac{\partial p}{\partial t} + \sum_i \left(\boldsymbol{v}_i \cdot \frac{\partial p}{\partial \boldsymbol{x}_i} + \boldsymbol{a}_i \cdot \frac{\partial p}{\partial \boldsymbol{v}_i} \right) = 0, \tag{8.9}$$

where $\boldsymbol{a}_i = \dot{\boldsymbol{v}}_i = \boldsymbol{F}_i/m_i$ is the particle acceleration. This is *Liouville's theorem*.

Now, in the collisionless/uncorrelated limit, this directly carries over to the one-point distribution function

$$f = f_1 = N \int p(\boldsymbol{x}, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N, \boldsymbol{v}, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_N)\, \mathrm{d}\boldsymbol{x}_2 \cdots \mathrm{d}\boldsymbol{x}_N\, \mathrm{d}\boldsymbol{v}_2 \cdots \mathrm{d}\boldsymbol{v}_N. \tag{8.10}$$

To proceed, we multiply Eqn. (8.9) by $F(\boldsymbol{x}, \boldsymbol{v}, t)$ and integrate it over $6N$-dimensional phase space. The first term yields $\partial f/\partial t$. The second term reads upon exchanging the integral and the sum as follows:

$$\begin{aligned}
&\sum_i \int F \cdot \left(\boldsymbol{v}_i \cdot \frac{\partial p}{\partial \boldsymbol{x}_i} \right) \mathrm{d}\boldsymbol{x}_1 \cdots \mathrm{d}\boldsymbol{x}_N\, \mathrm{d}\boldsymbol{v}_1 \cdots \mathrm{d}\boldsymbol{v}_N \\
&= \int \Bigg[\underbrace{\boldsymbol{v} \cdot \frac{\partial p}{\partial \boldsymbol{x}} \mathrm{d}\boldsymbol{x}_2 \cdots \mathrm{d}\boldsymbol{x}_N\, \mathrm{d}\boldsymbol{v}_2 \cdots \mathrm{d}\boldsymbol{v}_N + \ldots}_{N \text{ terms}} \Bigg] \\
&= \boldsymbol{v} \cdot \frac{\partial}{\partial \boldsymbol{x}} \int [\underbrace{p \cdot \mathrm{d}\boldsymbol{x}_2 \cdots \mathrm{d}\boldsymbol{x}_N\, \mathrm{d}\boldsymbol{v}_2 \cdots \mathrm{d}\boldsymbol{v}_N + \ldots}_{N \text{ terms}}] = \boldsymbol{v} \cdot \frac{\partial f}{\partial \boldsymbol{x}}.
\end{aligned} \tag{8.11}$$

The last term can be computed by analogy. To this end, we write $\boldsymbol{a}_i = \mathrm{d}\boldsymbol{v}_i/\mathrm{d}t$ and pull the time derivative out of the intergral so that the delta distribution $\delta(\boldsymbol{v} - \boldsymbol{v}_i(t))$ can act on the velocity variables to eventually yield $\boldsymbol{a}\, \partial f/\partial \boldsymbol{v}$. Summarizing, we arrive at the *Vlasov equation*, also known as collisionless Boltzmann equation:

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \frac{\partial f}{\partial \boldsymbol{x}} + \boldsymbol{a} \cdot \frac{\partial f}{\partial \boldsymbol{v}} = 0. \tag{8.12}$$

The close relation to Liouville's equation means that also here the phase space-density stays constant along characteristics (i.e. along orbits of individual particles) of the system.

What about the accelerations?

In the limit of a collisionless system, the accelerations cannot be due to a single other particle. However, collective effects, for example from the gravitational or electric field produced by the whole system are still allowed.

For example, the source field of self-gravity can be described as

$$\rho(\boldsymbol{x}, t) = m \int f(\boldsymbol{x}, \boldsymbol{v}, t)\, \mathrm{d}\boldsymbol{v}. \tag{8.13}$$

This then produces a gravitational field through Poisson's equation,

$$\boldsymbol{\nabla}^2 \Phi = 4\pi G \rho, \tag{8.14}$$

which yields the accelerations as

$$\boldsymbol{a} = -\frac{\partial \Phi}{\partial \boldsymbol{x}}. \tag{8.15}$$

One can also combine these equations to yield the Poisson-Vlasov system, given by

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \frac{\partial f}{\partial \boldsymbol{x}} - \frac{\partial \Phi}{\partial \boldsymbol{x}} \cdot \frac{\partial f}{\partial \boldsymbol{v}} = 0, \tag{8.16}$$

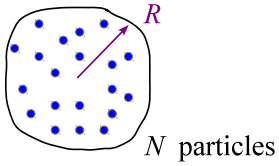
$$\boldsymbol{\nabla}^2 \Phi = 4\pi G m \int f(\boldsymbol{x}, \boldsymbol{v}, t)\, \mathrm{d}\boldsymbol{v}. \tag{8.17}$$

This holds in an analogous way also for a plasma where the mass density is replaced by a charge density.

It is interesting to note that in this description the particles have basically completely vanished and have been replaced with a continuum fluid description. Later, for the purpose of solving the equations, we will have to reintroduce particles as a means of discretizing the equations (but these are then not the real physical particles any more, rather they are fiducial macro particles that sample the phase-space in a Monte-Carlo fashion).

8.3 When is a system collisionless?

Consider a system of size R containing N particles.



The time for one crossing of a particle through the system is of order

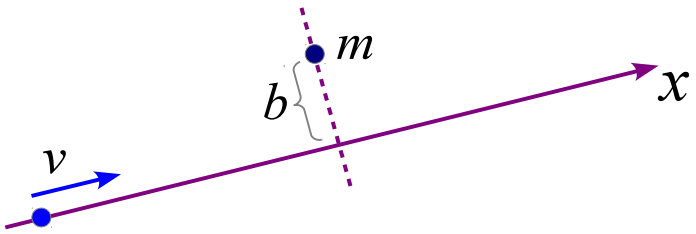
$$t_{\mathrm{cross}} = \frac{R}{v}, \tag{8.18}$$

where v is the typical particle velocity (Binney & Tremaine, 1987, 2008; Thorne & Blandford, 2017). For a self-gravitating system of that size we expect according to the virial theorem

$$v^2 \simeq \frac{GNm}{R} = \frac{GM}{R}, \tag{8.19}$$

where $M = N\,m$ is the total mass.

We now want to estimate the rate at which a particle experiences weak deflections by other particles, which is the process that violates perfect collisionless behavior and which induces relaxation.



If the deflection angle is small, $\theta_{\rm d} \ll 1$, we can approximate its value by computing the perpendicular impulse exerted by the gravitational field of another perturber particle (that is assumed to be stationary for simplicity), integrating along the original particle's unperturbed straight line trajectory (the "Born approximation")

$$\begin{aligned}
\Delta p_\perp &= m\Delta v_\perp \approx mv\theta_{\rm d} \approx -m\int_{-\infty}^{\infty} \boldsymbol{\nabla}_\perp \Phi {\rm d}t \approx -\int_{-\infty}^{\infty} \frac{\partial}{\partial b}\left(\frac{Gm^2}{\sqrt{b^2+v^2t^2}}\right){\rm d}t \\
&= \int_{-\infty}^{\infty} \frac{Gm^2 b\,{\rm d}t}{(b^2+v^2t^2)^{3/2}} = \frac{Gm^2}{v}\int_{-\infty}^{\infty}\frac{b\,{\rm d}x}{b^2(1+x^2)^{3/2}} \\
&= \frac{Gm^2}{vb}\left.\frac{x}{\sqrt{1+x^2}}\right|_{-\infty}^{\infty} = \frac{2Gm^2}{bv}, \qquad (8.20) \\
\Rightarrow \theta_{\rm d} &= \frac{b_0}{b} \quad \text{for} \quad b \gg b_0 = \frac{2Gm}{v^2}, \qquad (8.21)
\end{aligned}$$

where we adopted the small-angle approximation $\sin\theta_{\rm d} \approx \theta_{\rm d}$ and we defined a critical impact parameter b_0 in the last step at which the transverse velocity perturbation becomes as large as the velocity itself.

If the dominant source of this deflection were a single large-angle scattering event, then the relevant cross section would be $\sigma = \pi b_0^2$ (since all impact parameters $\lesssim b_0$ produce large-angle scatterings), and the resulting mean deflection fequency $\nu_{\rm d,\,single}$ and time $t_{\rm d,\,single}$ would be

$$\nu_{\rm d,\,single} \equiv \frac{1}{t_{\rm d,\,single}} = n\sigma v = n\pi b_0^2 v. \qquad (8.22)$$

The cumulative, random-walk effects of many small-angle scatterings of perturber particles produce a net deflection of order a radian in a shorter time as we will now see. Because the direction of the individual scatterings are random, the mean deflection angle after many scatterings vanishes, $\langle\theta\rangle = 0$. However, $\langle\theta^2\rangle$ will not vanish and we obtain

$$\langle\theta^2\rangle = \sum_{\text{all encounters}} \theta_{\rm d}^2 = \sum\left(\frac{b_0}{b}\right)^2. \qquad (8.23)$$

The number of encounters that occur with impact parameters between $[b, b+{\rm d}b]$ during time t is ${\rm d}N = nvt2\pi b\,{\rm d}b$. Hence, the mean square deflection angle accumulates up to

$$\langle\theta^2\rangle = \int_{b_{\rm min}}^{b_{\rm max}}\left(\frac{b_0}{b}\right)^2 {\rm d}N = n2\pi b_0^2 vt\ln\Lambda, \qquad (8.24)$$

where

$$\ln\Lambda = \ln\left(\frac{b_{\rm max}}{b_{\rm min}}\right) \qquad (8.25)$$

is the so-called Coulomb logarithm. The value of t that implies $\langle\theta^2\rangle \approx 1$ is the deflection time $t_{\rm d}$:

$$\nu_{\rm d} \equiv \frac{1}{t_{\rm d}} = n2\pi b_0^2 v\ln\Lambda = \nu_{\rm d,\,single}\,2\ln\Lambda. \qquad (8.26)$$

We find that the deflection frequency in the case of multiple weak deflections is larger by a factor of $2 \ln \Lambda$ than the frequency in Eqn. (8.22) for a single large-angle scattering event.

Relating the number of perturbers N to their number density n in a cylinder of radius R via $N = vt\pi R^2 n$, we obtain a mean square change of perpendicular velocity:

$$\langle (\Delta v_\perp)^2 \rangle \approx v^2 \langle \theta^2 \rangle = 2N \left(\frac{v b_0}{R} \right)^2 \ln \Lambda = 8N \left(\frac{Gm}{Rv} \right)^2 \ln \Lambda. \tag{8.27}$$

We can now define the relaxation time as

$$t_{\rm relax} \equiv \frac{v^2}{\langle (\Delta v_\perp)^2 \rangle / t_{\rm cross}}, \tag{8.28}$$

i.e., after this time the individual perturbations have reached $\sim 100\%$ of the typical squared velocity, and one certainly cannot neglect the interactions any more. With our result for $\langle (\Delta v_\perp)^2 \rangle$, and using equation (8.19) this now becomes

$$t_{\rm relax} = \frac{N}{8 \ln \Lambda} \, t_{\rm cross}. \tag{8.29}$$

But we still have to clarify what we can sensibly use for $b_{\rm min}$ and $b_{\rm max}$ in the Coulomb logarithm. For $b_{\rm max}$, we adopt the size of the system, i.e. $b_{\rm max} \simeq R$ and we impose as a lower limit for the impact parameter $b_{\rm min} \equiv b_0 = 2Gm/v^2$, where strong (large-angle) deflections occur (Eqn. 8.21) and below which impact parameter we do not get a substantial contribution to the mean square deflections. This then yields $b_{\rm min} = 2R/N$. We hence get for the Coulomb logarithm $\ln \Lambda \simeq \ln(N/2)$. But a factor of 2 in a logarithm might as well be neglected in this coarse estimate, so that we expect $\ln \Lambda \sim \ln N$. We hence arrive at the final result (Chandrasekhar, 1943):

$$t_{\rm relax} = \frac{N}{8 \ln N} \, t_{\rm cross}. \tag{8.30}$$

A system can be viewed as collisionless if $t_{\rm relax} \gg t_{\rm age}$, where $t_{\rm age}$ is the time of interest. We note that $t_{\rm cross}$ depends only on the size and mass of the system, but *not* on the particle number N or the individual masses of the N-body particles. We therefore clearly see that the primary requirement to obtain a collisionless system is to use a sufficiently large N.

Examples

- globular star clusters have $N \sim 10^5$, $t_{\rm cross} \sim \frac{3\,{\rm pc}}{6\,{\rm km/sec}} \simeq 0.5\,{\rm Myr}$, implying $t_{\rm relax} = 10^3 \, t_{\rm cross} \sim 0.5$ Gyr. This shows that such systems are strongly affected by collisions over the age of the Universe, $t_{\rm age} = \frac{1}{H_0} \sim 10\,{\rm Gyr}$.

- stars in a typical galaxy: Here we have $N \sim 10^{11}$, $t_{\rm cross} \sim \frac{1}{100\,H_0}$, implying $t_{\rm relax} = 5 \cdot 10^8 \, t_{\rm cross} \sim 5 \cdot 10^6 \, t_{\rm age}$. This means that these large stellar systems are collisionless over the age of the Universe to extremely good approximation.

- dark matter in a galaxy: Here we have $N \sim 10^{77}$ if the dark matter is composed of a $\sim 100\,\mathrm{GeV}$ weakly interacting massive particle (WIMP). In addition, the crossing time is longer than for the stars, $t_{\mathrm{cross}} \sim \frac{1}{10\,H_0}$, due to the larger size of the 'halo' relative to the embedded stellar system, implying $t_{\mathrm{relax}} = 10^{74}\,t_{\mathrm{cross}} \sim 10^{73}\,t_{\mathrm{age}}$. Clearly, the dark matter represents the mother of all collisionless systems.

8.4 N-body models of collisionless systems

We now reintroduce particles in order to discretize the collisionless fluid described by the Poisson-Vlasov system. We use however *far fewer* particles than in real physical systems, and we correspondingly give them a higher mass (and/or charge). These are hence fiducial macro-particles. Their equations of motions in the case of gravity are written as:

$$\ddot{\boldsymbol{x}}_i = -\boldsymbol{\nabla}\Phi(\boldsymbol{x}_i), \tag{8.31}$$

$$\Phi(\boldsymbol{x}) = -G\sum_{j=1}^{N}\frac{m_j}{[(\boldsymbol{x}-\boldsymbol{x}_j)^2+\epsilon^2]^{1/2}}. \tag{8.32}$$

A few comments are in order here:

- Provided we can ensure $t_{\mathrm{relax}} \gg t_{\mathrm{sim}}$ despite the smaller N than in the real physical system, the numerical model keeps behaving as a collisionless system over the simulated time-span t_{sim}, and the collective gravitational potential is sufficiently smooth.

- The mass of the macro-particles used to discretize the collision system does not enter in the equations of motion. Provided there are enough particles to describe the gravitational potential well, the orbits of the macro-particles will be just as valid as the orbits of the real physical particles.

- The N-body model gives only one (quite noisy) realization of the one-point function. It does not give the ensemble average directly (this would require multiple simulations).

- The equations of motion contain a **softening length** ϵ. The purpose of the force softening is to avoid large angle scatterings and the numerical expense that would be needed to integrate the orbits with sufficient accuracy in singular potentials. Also, we would like to prevent the possibility of the formation of bound particle pairs – they would obviously be highly correlated and hence strongly violate collisionless behaviour. We don't get bound pairs if

$$\left\langle v^2\right\rangle \gg \frac{Gm}{\epsilon}, \tag{8.33}$$

which can be used as a simple condition on reasonable softening settings. The adoption of a softening length also implies the introduction of a smallest resolved length-scale. The specific softening choice one makes ultimately represents a compromise between spatial resolution, discreteness noise in the orbits and the gravitational potential, computational cost, and the relaxation effects that may negatively influence results.

9 Tree algorithms

Once we have discretized a collisionless fluid in terms of an N-body system, two questions come up:

1. How do we integrate the equations of motion in time?

2. How do we compute the right hand side of the equations of motion, i.e. the gravitational forces?

For the first point, we can simply use one of our ODE integration schemes, preferably a symplectic one since we are dealing with a Hamiltonian system. The second point seems also straightforward at first, as the accelerations (forces) can be readily calculated through *direct summation*:

$$\ddot{\boldsymbol{x}}_i = -G \sum_{j=1}^{N} \frac{m_j}{[(\boldsymbol{x}_i - \boldsymbol{x}_j)^2 + \epsilon^2]^{3/2}} (\boldsymbol{x}_i - \boldsymbol{x}_j). \tag{9.1}$$

This calculation is *exact*, but for each of the N equations we have to calculate a sum with N partial forces, yielding a computational cost of order $\mathcal{O}(N^2)$. This quickly becomes prohibitive for large N, and causes a conflict with our urgent need to have a large N!

Perhaps a simple example is in order to show how bad the N^2 scaling really is in practice. Suppose you can do $N = 10^6$ in a month of computer time, which is close to the maximum that one may want to do in practice. A particle number of $N = 10^{10}$ would then already take of order 10 million years.

We hence need faster, approximative force calculation schemes. We shall discuss three different possibilities:

- Hierarchical multipole methods ("tree-algorithms")

- Fourier-transform based methods ("particle-mesh algorithms")

- Iterative solvers for Poisson's equation ("relaxation methods", multigrid-methods)

Various combinations of these approaches may also be used, and sometimes they are also applied together with direct summation on small scales. The latter may also be accelerated with special-purpose hardware (e.g. the GRAPE board), or with graphics processing units (GPUs) that are used as fast number-crunshers.

9.1 Multipole expansion

The central idea is here to use the multipole expansion of a distant group of particles to describe its gravity (Barnes & Hut, 1986), instead of summing up the forces from all individual particles.

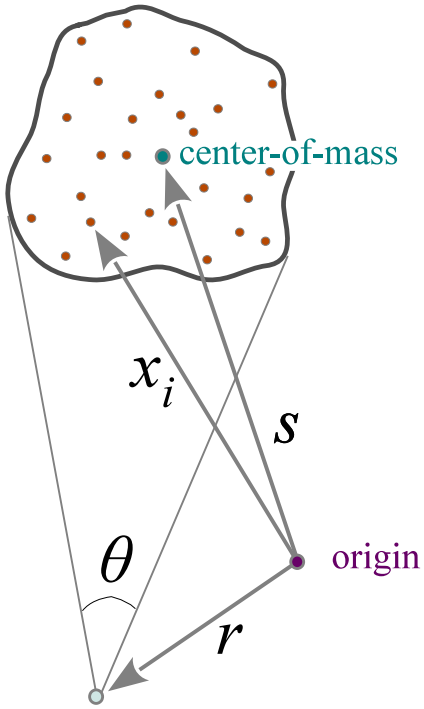


Figure 9.1: Multipole expansion for a group of distant particles. Provided the reference point $\boldsymbol{r}$ is sufficiently far away, the particles are seen under a small opening angle θ, and the field created by the particle group can be approximated by the monopole term at its center of mass, augmented with higher order multipole corrections if desired.

The potential of the group is given by

$$\Phi(\boldsymbol{r}) = -G \sum_i \frac{m_i}{|\boldsymbol{r} - \boldsymbol{x}_i|}, \tag{9.2}$$

which we can re-write as

$$\Phi(\boldsymbol{r}) = -G \sum_i \frac{m_i}{|\boldsymbol{r} - \boldsymbol{s} + \boldsymbol{s} - \boldsymbol{x}_i|}. \tag{9.3}$$

Now we expand the denominator assuming $|\boldsymbol{x}_i - \boldsymbol{s}| \ll |\boldsymbol{r} - \boldsymbol{s}|$, which will be the case provided the *opening angle* θ under which the group is seen is sufficiently small, see the sketch of Figure 9.1. We can then use the Taylor expansion

$$\frac{1}{|\boldsymbol{y} + \boldsymbol{s} - \boldsymbol{x}_i|} = \frac{1}{|\boldsymbol{y}|} - \frac{\boldsymbol{y} \cdot (\boldsymbol{s} - \boldsymbol{x}_i)}{|\boldsymbol{y}|^3} + \frac{1}{2} \frac{\boldsymbol{y}^T \left[3(\boldsymbol{s} - \boldsymbol{x}_i)(\boldsymbol{s} - \boldsymbol{x}_i)^T - (\boldsymbol{s} - \boldsymbol{x}_i)^2\right] \boldsymbol{y}}{|\boldsymbol{y}|^5} + \ldots, \tag{9.4}$$

where we introduced $\boldsymbol{y} \equiv \boldsymbol{r} - \boldsymbol{s}$ as a short-cut. The first term on the right hand side gives rise to the monopole moment, the second to the dipole moment, and the third to the quadrupole moment. If desired, one can continue the expansion to ever higher order terms.

These multipole moments then become properties of the group of particles:

$$\text{monopole:} \quad M = \sum_i m_i \tag{9.5}$$

$$\text{dipole:} \quad \boldsymbol{D} = \sum_i m_i(\boldsymbol{s} - \boldsymbol{x}_i) \tag{9.6}$$

$$\text{quadrupole:} \quad Q_{ij} = \sum_k m_k \left[3(\boldsymbol{s} - \boldsymbol{x}_k)_i(\boldsymbol{s} - \boldsymbol{x}_k)_j - \delta_{ij}(\boldsymbol{s} - \boldsymbol{x}_k)^2\right] \tag{9.7}$$

The dipole expresses how much mass is asymmetrically distributed with respect to the centre of mass, given by

$$\boldsymbol{s} = \frac{1}{M}\sum_i m_i \boldsymbol{x}_i. \tag{9.8}$$

As we have constructed the expansion around the centre of mass there is exactly as much mass on either side and the dipole vanishes. If we restrict ourselves to terms of up to quadrupole order, we hence arrive at the expansion

$$\Phi(\boldsymbol{r}) = -G\left(\frac{M}{|\boldsymbol{y}|} + \frac{1}{2}\frac{\boldsymbol{y}^T\mathbf{Q}\boldsymbol{y}}{|\boldsymbol{y}|^5}\right); \quad \boldsymbol{y} = \boldsymbol{r} - \boldsymbol{s}, \tag{9.9}$$

from which also the force can be readily obtained through differentiation. Recall that we expect the expansion to be accurate if

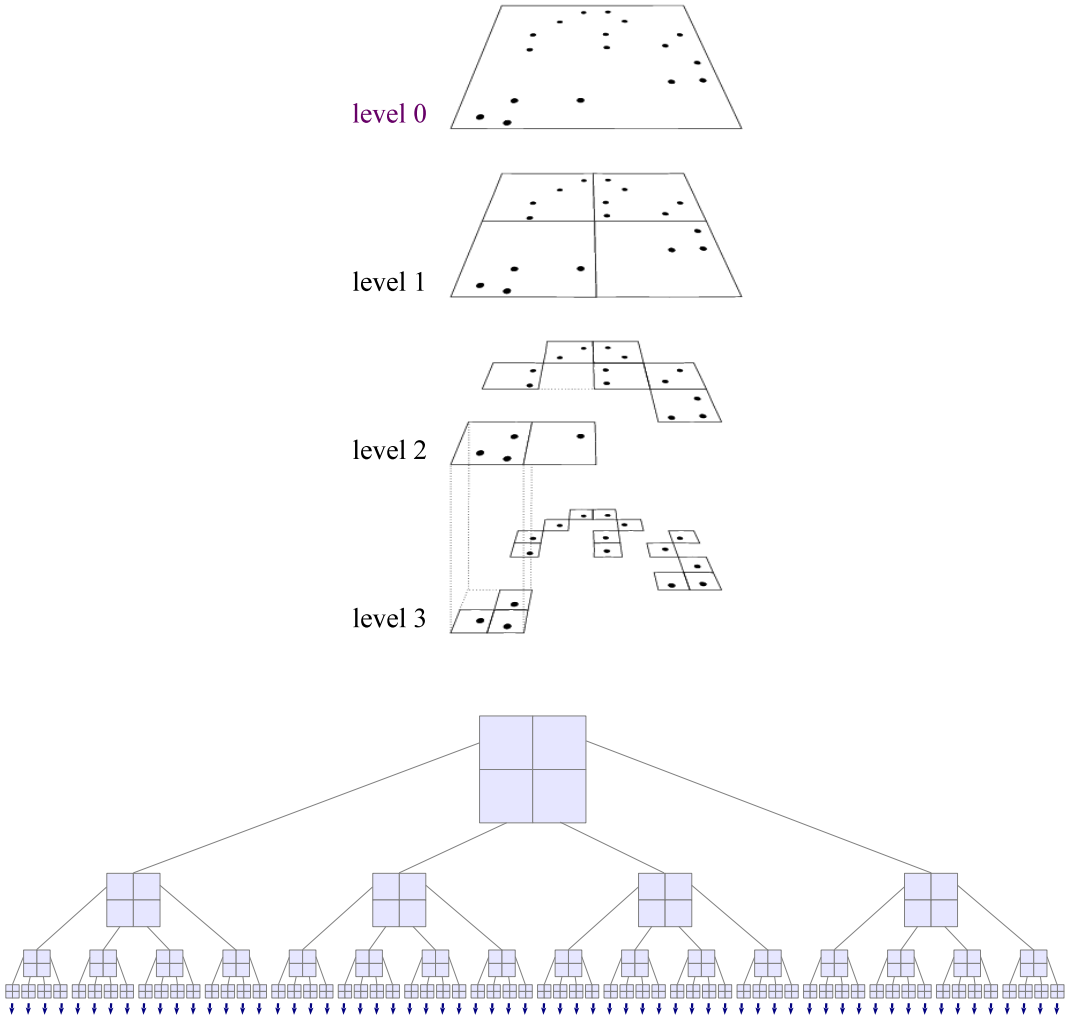
$$\theta \simeq \frac{\langle|\boldsymbol{x}_i - \boldsymbol{s}|\rangle}{|\boldsymbol{y}|} \simeq \frac{l}{y} \ll 1, \tag{9.10}$$

where l is the radius of the group.

9.2 Hierarchical grouping

Tree algorithms are based on a hierarchical grouping of the particles, and for each group, one then pre-computes the multipole moments for later use in approximations of the force due to distant groups. Usually, the hierarchy of groups is organized with the help of a tree-like data structure, hence the name "tree algorithms".

There are different strategies for defining the groups. In the popular Barnes & Hut (1986) oct-tree, one starts out with a cube that contains all the particles. This cube is then subdivided into 8 sub-cubes of half the size in each spatial dimension. One continues with this refinement recursively until each subnode contains only a single particle. Empty nodes (sub-cubes) need not be stored. Here is schematic sketch how this can look like in two dimensions (where one has a 'quad-tree'):



The sketch at the top shows the topological organization of the tree.

- We note that the oct-tree is not the only possible grouping strategy. Sometimes also so-called kd-trees (Stadel, 2001), or other binary trees are used where subdivisions are done along alternating spatial axes.

- An important property of such hierarchical, tree-based groupings is that they are geometrically fully flexible and adjust to any clustering state the particles may have. They are hence automatically adaptive.

- Also, there is no significant slow-down when severe clustering starts.

- The simplest way to construct the hierarchical grouping is to sequentially insert particles into the tree, and then to compute the multipole moments recursively.

9.3 Tree walk

The force calculation with the tree then proceeds by *walking the tree*. Starting at the root node, one checks for every node whether the opening angle under which it is seen is smaller than a prescribed tolerance angle θ_c (see also Salmon & Warren, 1994). If this is the case, the multipole expansion of the node can be accepted, and the corresponding partial force is evaluated and added to an accumulation of the total force. The tree walk along this branch of the tree can then be stopped. Otherwise, one must open the tree node and consider all its sub-nodes in turn.

The resulting force is then approximate in nature by construction, but the overall size of the error can be conveniently controlled by the tolerance opening angle θ_c. If one makes this smaller, more nodes will have to be opened. This will make the residual force errors smaller, but at the price of a higher computational cost. In the limit of $\theta_c \to 0$ one gets back to the expensive direct summation force.

An interesting variant of this approach to walk the tree is obtained by not only expanding the potential on the source side into a multipole expansion, but also around the target coordinate. This can yield a substantial additional acceleration and results in so-called fast multipole methods (FFM). The FALCON code of Dehnen (2000, 2002) employs this approach. A further advantage of the FFM formulation is that force anti-symmetry is manifest, so that momentum conservation to machine precision can be achieved. Unfortunately, the speed advantages of FFM compared to ordinary tree codes are significantly alleviated once individual time-step schemes are considered. Also, FFM is more difficult to parallelize efficiently on distributed memory machines.

Cost of the tree-based force computations

How do we expect the total cost of the tree algorithm to scale with particle number N? For simplicity, let's consider a sphere of size R containing N particles that are approximately homogeneously distributed. The mean particle spacing of these particles will then be

$$d = \left[\frac{(4\pi/3)R^3}{N}\right]^{1/3}. \tag{9.11}$$

We now want to estimate the number of nodes that we need for calculating the force on a central particle in the middle of the sphere. We can identify the computational cost with the number of interaction terms that are needed. Since the used nodes must tessellate the sphere, their number can be estimated as

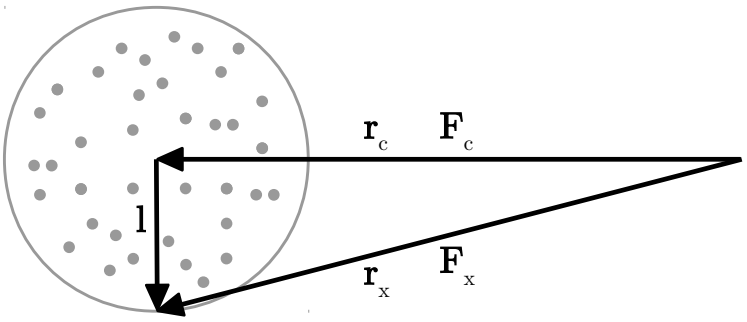
$$N_{\rm nodes} = \int_d^R \frac{4\pi r^2\,{\rm d}r}{l^3(r)}, \tag{9.12}$$

where $l(r)$ is the expected node size at distance r, and d is the characteristic distance of the nearest particle. Since we expect the nodes to be close to their maximum

allowed size, we can set $l \simeq \theta_c r$. We then obtain

$$N_{\rm nodes} = \frac{4\pi}{\theta_c^3} \ln \frac{R}{d} \propto \frac{\ln N}{\theta_c^3}. \tag{9.13}$$

The total computational cost for a calculation of the forces for all particles is therefore expected to scale as $\mathcal{O}(N \ln N)$. This is a very significant improvement compared with the N^2-scaling of direct summation.



We may also try to estimate the expected typical force errors. If we keep only monopoles, the error in the force per unit mass from one node should roughly be of the order of the truncation error, i.e. about

$$\begin{aligned}
\Delta F_{\rm node} &\sim |F_{\rm c} - F_{\rm x}| && (9.14)\\
&= \left| \frac{GM_{\rm node}}{r^2} - \frac{GM_{\rm node}}{r_x^2} \right| && (9.15)\\
&= \left| \frac{GM_{\rm node}}{r^2} - \frac{GM_{\rm node}}{r^2 + l^2} \right| && (9.16)\\
&= \frac{GM_{\rm node}}{r^2} \frac{l^2}{r^2} && (9.17)\\
&= \frac{GM_{\rm node}}{r^2} \theta_{\rm c}^2, && (9.18)
\end{aligned}$$

where we have used the expansion $1/(1+x) \approx 1 - x$ for $x \ll 1$. The errors from multipole nodes will add up in quadrature, hence

$$(\Delta F_{\rm tot})^2 \sim N_{\rm node} (\Delta F_{\rm node})^2 = N_{\rm node} \left(\frac{GM_{\rm node}}{r^2} \theta_{\rm c}^2 \right)^2 \propto \frac{\theta_{\rm c}^4}{N_{\rm node}} \propto \theta_{\rm c}^7, \tag{9.19}$$

where in the second-to-last approximation we compute the average mass of a node by $M_{\rm node} = M_{\rm tot}/N_{\rm node}$. The force error for a scheme with monopoles only therefore scales as $(\Delta F_{\rm tot}) \propto \theta_{\rm c}^{3.5}$, roughly inversely as the invested computational cost. A much more detailed analysis of the performance characteristics of tree codes can be found, for example, in Hernquist (1987).

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