

Exercises for the lecture
Fundamentals of Simulation Methods
WS 2016/17

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Exercise sheet 3 (*due date: Nov 10, 2016, 11:59pm*)

Collisionless dynamics and the tree code

1) Collisionless system in equilibrium (10 points)

The energy per unit mass of a particle in a *stationary* collisionless system can be written as

$$\epsilon = \frac{1}{2}v^2 + \Phi, \quad (1)$$

where v is the speed of the particle and Φ is the value of the gravitational potential. Prove that the total energy of the system is equal to

$$E = \frac{1}{3}M \langle \epsilon \rangle, \quad (2)$$

where $\langle \epsilon \rangle$ is the mass-weighted average of ϵ for all particles, and M is the total mass of N particles. (Hint: Use *Virial Theorem*, which does not necessarily have to be proven for a stable system consisting of N particles, bound by potential forces.)

2) Tree code (40 points)

Tree algorithms can approximately calculate the forces in an N-body system by means of a hierarchical multipole expansion. This reduces the computational cost to something of order $\mathcal{O}(N \ln N)$. On the Moodle page of the lecture, a simple skeleton tree code (in C) can be downloaded (note that this implementation uses only monopole order and is not optimized for speed or memory consumption). You can use this template for this exercise, either directly or translated to another language, or if you wish, you may also write your own tree code from scratch.

Consider N particles of total mass $M_{\text{tot}} = 1$ placed randomly into a cubical box of unit side-length. For definiteness, we assume all particles have the same mass, and we adopt $G = 1$. Assume that the gravitational potential of individual particles is Plummer-softened with a gravitational softening length $\epsilon = 0.001$, i.e. we adopt the potential

$$\phi(\mathbf{r}) = -\frac{m}{(\mathbf{r}^2 + \epsilon^2)^{1/2}} \quad (3)$$

for a single particle of mass m .

Calculate the gravitational forces for all N particles with an oct-tree and determine the typical force accuracy and calculational time in comparison with direct summation, both as a function of N and of the opening angle parameter θ^* . To this end, carry out the following steps:

- (a) The provided code template is incomplete, so start by filling in the missing pieces. Places where you have to complete the code are marked with the comment ‘to be filled in’. In particular, you need to add the computation of the multipole moments of tree nodes from their subnodes, as well as the partial force calculation from a tree node that is used in the tree walk. Also, please add a calculation of the *exact* forces by direct summation. When you’re done, verify that the force approximation delivered by the tree code is roughly correct by adding suitable output to the code.
- (b) To allow a more quantitative analysis, add an automatic measurement of the average force error after all forces have been calculated by the tree and direct summation. To this end, consider the relative force error

$$\eta = \frac{|\mathbf{a}_{\text{tree}} - \mathbf{a}_{\text{exact}}|}{|\mathbf{a}_{\text{exact}}|} \quad (4)$$

for each particle, and determine a simple arithmetic average $\langle \eta \rangle$ of the mean relative force error¹. Also, add diagnostic code that tells you the average number of particle-node interactions per particle, i.e. how many nodes the multipole expansion on average involves.

- (c) Make a little grid of calculations for $N = 5000, 10000, 20000$ and 40000 , and opening angles $\theta^* = 0.2, 0.4$ and 0.8 . In each case, measure the calculation time for the tree-based force calculation and for direct summation, as well as $\langle \eta \rangle$ and the mean number of terms the tree code used per particle. Report the results in a table.
- (d) Using the previous results, make a plot of the execution time of the force calculation with the tree as a function of N (for the $\theta^* = 0.4$ case). Use logarithmic axis and fit a regression line (in the log) to the 4 data points you obtained. Also include the results for direct summation. Estimate the time needed for 10^{10} particles for both methods by extrapolating your timing results.

¹Note that a more careful analysis of the errors should really consider the full distribution of the errors. It could well be that there are occasionally very large, catastrophic errors that go unnoticed in a simple average such as $\langle \eta \rangle$. To diagnose this, one needs to look at the error distribution function.