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Scientific Computing II

Molecular Dynamics

Exercise 13: Multi-Centered Molecules

For single-centered molecules, the force on molecule i equals the sum of all forces between molecule i and all other molecules: $\vec{F}_i = \sum_{j \neq i} \vec{F}_{ij}$.

Using the force, the acceleration of molecule i is given by the following formula:

$$\ddot{\vec{x}}_i = \frac{\vec{F}_i}{m_i} = \frac{\sum_{j \neq i} \vec{F}_{ij}}{m_i}$$

For multi-centered molecules, there are some more values to be considered to be able to represent rotations:

- values considered for single-centered molecules: force $\vec{F}$, mass m, acceleration $\ddot{\vec{x}}$.
- values only to be considered for multi-centered molecules: torque T, moment of inertia I, angular acceleration $\ddot{\omega}$.

Find the formula for the angular acceleration that is analogue to the formular for the acceleration $\ddot{\vec{x}}$.

Exercise 14: Linked Cells algorithm

Assume we simulate a molecular dynamics scenario with N molecules. If we explicitely compute the forces between all pairs of molecules, O(N^2) operations are necessary. For short-range potentials, we neglect interactions between particles that have a mutual distance bigger than a certain cut-off radius. This reduces the number of required operations to O(N).

(a) Someone tries to convince you that this is not true:

Assume that a simululation with N molecules requires C operations for the force calculations. Double the number of molecules in the domain. Then we of course have to compute forces for twice as many molecules. But, in addition, the number of molecules within the cut-off radius of a certain molecule doubles, too. Thus, we need 4C operations, which means that the number of operations behaves like O(N^2).

Why is that argumentation wrong?

(b) In 3D, apart from the cell itself, 26 additional cells have to be examined (8 cells in 2D). By reducing the size of the cells, more cells have to be used, but the volume covered by these cells is smaller. As the covered volume corresponds to the number of distance calculations, smaller cell sizes can increase the performance. Calculate the covered volume for $l = rc$, $l = \frac{rc}{2}$, $l = \frac{rc}{4}$ and $l \to 0$ in 2D and 3D.

	$l = rc$	$l = \frac{rc}{2}$	$l = \frac{rc}{4}$	$\ldots$	$L \to 0$
$2D$					
(% unnecessary)					
$3D$					
(% unnecessary)					

Exercise 15: Parallel Linked Cells algorithm

Now consider the simulation of a nucleation process. The simulation is started with a million molecules in gas phase, so the distribution of the molecules in the domain is homogenous. Over time, small droplets will evolve and the distribution of the molecules will become increasingly inhomogenous.

(a) For the simulation we will use the parallel linked cell algorithm. Describe a scalable implementation of the algorithm.

(b) Initially, every computer is assigned an equally sized part of the domain. Then, during the run of the simulation, a load imbalance will occur. What are suitable criteria for repartitioning?