Summary of SI2530 Computational Physics

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7 september 2021

Sammanfattning

Innehåll

1 Basic Concepts

Molecular Dynamics Molecular dynamics is a class of simulation based on simulating a collection of atoms as a set of material points which move according to Newton's laws and consider only forces that arise as interactions between two atoms.

Equilibration Equilibration is the process of using some scheme that fixes a certain set of quantities and running a molecular dynamics simulation until these quantities have stabilized to the desired value.

The Radial Distribution Function The radial distribution function is defined as

$$g(r) = \frac{1}{\rho} \left. \frac{\mathrm{d}N}{\mathrm{d}V} \right|_r .$$

Verlet's Method Euler's method does not respect the laws of physics. Instead we consider a different scheme, based on the Taylor expansions

$$x_{n\pm1} = x_n \pm v_n\tau + \frac{1}{2}a_n\tau^2.$$

This nets two equations

$$v_n = \frac{x_{n+1} - x_{n-1}}{2\tau}, \; x_{n+1} = 2x_n - x_{n-1} + a_n\tau^2.$$

This integration scheme is called Verlet's scheme, or the leapfrog method. Note that it is not self-starting. The way that is usually solved is through integrating a single step from the initial conditions using Euler's method and proceeding with the Verlet scheme from there.