1 Discrete time Molecular Dynamics

The Verlet algorithms provide an efficient tool for solving the Newtonian equations of motion of interacting particles. In this problem, we plan to review some qualities and drawbacks of these methods. Let us consider a system of N identical point particles of mass m interacting by a pairwise potential. The corresponding Hamiltonian is given by

$$H = \sum_{i=1}^{N} \frac{m\vec{v}^2}{2} + \frac{1}{2}\sum_{i\neq j} u(r_{ij}) \tag{1}$$

where $\vec{v}$ is the three-dimensional velocity of particle i, $u(r)$ the pair interaction potential and r_{ij} the distance between particles i and j.

The Verlet velocity algorithm is given by

$$\vec{r}_i(t+\Delta t) = \vec{r}_i(t) + \vec{v}_i(t)\Delta t + \frac{(\Delta t)^2}{2m}\vec{F}_i(t) \tag{2}$$

$$\vec{v}_i(t+\Delta t) = \vec{v}_i(t) + \frac{\Delta t}{2m}(\vec{F}_i(t) + \vec{F}_i(t+\Delta t)) \tag{3}$$

1. Express $\vec{F}_i(t)$ as a function of the interaction potential.
2. Show that the total momentum of the system is conserved along the simulation.
3. The initial configuration of a simulation is given by choosing velocities along each axis according a Gaussian distribution. Give a method to generate random gaussian numbers. For a finite system of N particles, give a simple method in order to start the simulation with a zero total momentum.

   In order to test the robustness of the algorithm, we now consider a one-dimensional harmonic oscillator with the Hamiltonian

   $$H = \frac{m}{2}\left(\frac{dx}{dt}\right)^2 + \frac{k}{2}x^2 \tag{4}$$

   The continous-time expectation that the momentum is the conjugate variable to the spatial coordinate is not satisfied by using a discrete time discretization. We illustrate this point with the Harmonic oscillator. One denotes $\Omega_0 = \sqrt{k/m}$.
4. Write the position Verlet algorithm for the oscillator between $x((n+1)\Delta t)$, $x(n\Delta t)$ and $x((n-1)\Delta t)n$ The timestep is called Δt.
5. Knowing that the exact solution of the equation of motion is given by $x(t) = ARe(e^{i\Omega_0 t})$, we plan to compare the exact solution to the solution of the discretized equation. By using the Verlet position algorithm and the ansatz $x(n\Delta t) = ARe(e^{ni\Delta t\Omega_v})$ where Ω_v is the pulsation of the discrete time Verlet algorithm, show that $\cos(\Omega_v\Delta t) = 1 - \frac{(\Omega_0\Delta t)^2}{2}$.
6. Express the discrete velocity $v(n\Delta t)$ as a function of $x(n\Delta t)$. What happens for $\Omega_0\Delta t = \sqrt{2}$

7. Calculate the total energy of the oscillator $E(n\Delta t)$ as a function of time $n\Delta t$. Show that the total energy oscillates around a mean value E_v to be determined. E_v is a function which depends on the exact total energy E_{ex}, Ω_0 and Δt.
8. Can the total energy $E(n\Delta t)$ reach E_{ex} ?. Show that the total energy can be expressed as
$$E = E_{ex}(1 - \frac{(\Omega_0 \Delta t)^2}{4} \sin^2(\Omega_v \Delta t)$$
9. Why does the discretized solution underestimate the kinetic energy ?.

2 Structure factor in different situations

In order to characterize the spatial correlations between particles, knowledge of the structure factor is essential. One proposes to show that the structure factor is suitable for exhibiting the specific features of particle correlations in different situations.

Consider N particles inside a box of volume V. The microscopic density is given as

$$\rho(\mathbf{r}) = \sum_{i=1}^{N} \delta(\mathbf{r} - \mathbf{r}_i) \tag{6}$$

where $\mathbf{r}_i$ denotes the position of particle i. One defined the structure factor as

$$S(\mathbf{k}) = \frac{< \tilde{\rho}(\mathbf{k})\tilde{\rho}(-\mathbf{k}) >}{N} \tag{7}$$

where $\tilde{\rho}(\mathbf{k})$ is the Fourier transform of the microscopic density and the brackets $< ... >$ denote the average over the available configurations of the system.

1. Express the structure factor $S(\mathbf{k})$ as a function in terms of $< e^{-i\mathbf{k}\mathbf{r}_{ij}} >$, where $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ with $i \neq j$.
2. Show that $S(\mathbf{k}) \to 1$ when $\mathbf{k} \to +\infty$.
3. One considers a simulation with a cubic box with a linear dimension L and we are using periodic boundary conditions. What is the smallest wave vectors $\mathbf{k}$ accessible in simulation ?
4. Consider a lattice gas with a lattice step a. Particles occupy lattice sites, show that it exists a ultraviolet cutoff of accessible wave vectors. By using periodic boundary conditions, compute the number of wave vectors available in simulation.

   One now considers a finite one-dimensional lattice with a step a (with periodic boundary conditions, i.e. a ring). Each site is occupied by a particle.
5. Calculate $\tilde{\rho}(k)$ and infer the structure factor associated with this configuration. Taking the thermodynamic limit ($N \to \infty$) show that the structure factor vanishes within the Brillouin zone ($-\frac{\pi}{a} < k < \frac{\pi}{a}$) (see Glossary).

Each particle is split into two particles which are identical and shifted symmetrically from the lattice node to a distance u. The distance is chosen randomly from the probability distribution $p(u)$. The microscopic density is given by

$$\rho_d(\mathbf{r}) = \sum_{i=1}^{N} (\delta(\mathbf{r} - \mathbf{r}_i - u_i) + \delta(\mathbf{r} - \mathbf{r}_i + u_i)) \tag{13}$$

and the structure factor becomes

$$S_d(\mathbf{k}) = \frac{< \tilde{\rho}_d(\mathbf{k}) \tilde{\rho}_d(-\mathbf{k}) >}{2N}. \tag{14}$$

6. Show that $S_d(k) = 2 < \cos(ku)^2 > +2 < \cos(ku) >^2 (S(k) - 1)$.
7. Assuming that the moments $< u^2 >$ and $< u^4 >$ are finite, calculate the expansion of $S_d(k)$ to the order k^4. Configurations corresponding to the vanishing structure factor when $k \to 0$, are "super-uniform" (or hyperuniform). Justify this terminology. Hint : What is this limit for a uniform perfect gas.
8. Simulations have been performed for dense granular systems that unveils that the structure factor goes to zero as k when k goes to zero. Why does the simulation require a large number of particles (10^6 particles) in order to show this result ?

   For a liquid close the critical temperature of the liquid-gas transition. The spatial correlation function the behaves as $h(r) \sim r^{-(d-2+\eta)}$ pour $r > r_c$, where η is the anomalous exponent.
9. By using the relationship between the correlation function and the structure factor, show that the structure factor diverge at small wave vectors as k^{-A}, where A is an exponent to be determined

A Glossary

The three dimensional Fourier trasnsform of a function f is defined as

$$\hat{f}(\mathbf{k}) = \int d^3\mathbf{r} f(\mathbf{r}) e^{-i\mathbf{kr}} \tag{16}$$

and the inverse transform is given by

$$f(\mathbf{r}) = \frac{1}{(2\pi)^3} \int d^3\mathbf{k} \hat{f}(\mathbf{k}) e^{i\mathbf{kr}} \tag{17}$$

For a Gaussian function

$$f(\mathbf{r}) = e^{-a\mathbf{r}^2/2} \tag{18}$$

the Fourier transform is

$$\hat{f}(\mathbf{k}) = \left(\frac{2\pi}{a}\right)^{3/2} e^{-\mathbf{k}^2/(2a)} \tag{19}$$

Conversely, if

$$\hat{f}(\mathbf{k}) = e^{-b\mathbf{k}^2/2} \tag{20}$$

the inverse Fourier transform is

$$f(\mathbf{r}) = \left(\frac{1}{2\pi b}\right)^{3/2} e^{-\mathbf{r}^2/(2b)} \tag{21}$$

Some identities for $\delta(\mathbf{r})$

$$\delta(\mathbf{r}) = \frac{1}{(2\pi)^3}\int d^3\mathbf{k} e^{i\mathbf{kr}}, 1 = \int d^3\mathbf{r} e^{i\mathbf{kr}}\delta(\mathbf{r}) \tag{22}$$