1 The Verlet algorithms

To solve the Newton equations of an interacting Hamiltonian system, one needs to have algorithms which keeps constant the total energy of the system.

For the sake of simplicity, one considers the equations of motion of a single particle.

$$\frac{d^2r(t)}{dt^2} = \frac{F}{m} \tag{1}$$

where F is the total force on the particle and m the mass.

1. Show the accuracy of a trajectory of duration T given by a position Verlet algorithm is $O(\Delta t^3)$.
2. Introducing the variable velocity, rewrite the equations of motion as a system of coupled equations. Write a discrete algorithm as the second order of Δt.
3. In order to obtain a closed system of discrete differential equation, show that the right-hand side of velocity evolution can be replaced with $\frac{F(t)+F(t+\Delta t)}{m}$, obtain a closed form of the velocity-Verlet equations
4. By using the velocity Verlet algorithm at time t and $t - \Delta t$, and by eliminating the velocity, obtain the discrete time evolution of the particle. Comment the result

2 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

$$H = \sum_{i=1}^{N} \frac{m\vec{v}^2}{2} + \frac{1}{2}\sum_{i\neq j} u(r_{ij}) \tag{10}$$

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

$$\vec{r}_i(t+\Delta t) = \vec{r}_i(t) + \vec{v}_i(t)\Delta t + \frac{(\Delta t)^2}{2m}\vec{F}_i(t) \tag{11}$$

$$\vec{v}_i(t+\Delta t) = \vec{v}_i(t) + \frac{\Delta t}{2m}(\vec{F}_i(t) + \vec{F}_i(t+\Delta t)) \tag{12}$$

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 Hamiltonian

$$H = \frac{m}{2}\left(\frac{dx}{dt}\right)^2 + \frac{k}{2}x^2 \tag{14}$$

   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 $\Omega_0 = \sqrt{k/m}$.

$$x((n+1)\Delta t) = 2x(n\Delta t) - x((n-1)\Delta t) - \frac{k(\Delta t)^2}{m}x(n\Delta t) \tag{15}$$

4. 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

$$\cos(\Omega_v \Delta t) = 1 - \frac{(\Omega_0 \Delta t)^2}{2}$$

   .

   and one obtains the expected relation.

5. Express the discrete velocity $v(n\Delta t)$ as a function of $x(n\Delta t)$. What happens for $\Omega_0 \Delta t = \sqrt{2}$.
6. 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.
7. Can the total energy $E(n\Delta t)$ reach E_{ex} ?
8. Why does the discretized solution underestimate the kinetic energy ?.