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 $O(\Delta t^3)$.

> **Solution:** The position Verlet algorithm is based on a sum of a time expansion of differential in the future and in the past. This leads to eliminate of the odd terms of the expansion. An elementary step of the algorithm gives an accuracy of $O(\Delta t^4)$. For a complete trajectory, one multiplies by the number of steps such that $N\Delta t = T$, and one obtains a accuracy of the trajectory of $TO(\Delta t^3)$

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.

> **Solution:** The Newton equations become
>
> $$\frac{dr(t)}{dt} = v \tag{2}$$
> $$\frac{dv(t)}{dt} = \frac{F}{m} \tag{3}$$
>
> At the second order
>
> $$r(t + \Delta t) = r(t) + v(t)\Delta t + \frac{F(t)}{2m}(\Delta t)^2 \tag{4}$$
> $$v(t + \Delta t) = = v(t) + \frac{F}{m}\Delta t + \frac{1}{2}\frac{dF(t)}{dt}(\Delta t)^2 \tag{5}$$

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

Solution:

$$r(t+\Delta t) = r(t) + v(t)\Delta t + \frac{F(t)}{2m}(\Delta t)^2 \quad (6)$$

$$v(t+\Delta t) = v(t) + \frac{F(t)+F(t+\Delta t)}{2m}\Delta t \quad (7)$$

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

Solution: One has

$$r(t+\Delta t) = r(t) + v(t)\Delta t + \frac{F(t)}{2m}(\Delta t)^2 \quad (8)$$

$$r(t) = r(t-\Delta t) + v(t-+\Delta t)\Delta t + \frac{F(t+\Delta t)}{2m}(\Delta t)^2 \quad (9)$$

By taking the difference of the two equations and inserting the velocity between $t-\Delta t$ and t, one obtains the position-Verlet algorithm. This means that the trajectories are the same at the fourth order.

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

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

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

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

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

1. Express $\vec{F}_i(t)$ as a function of the interaction potential.

Solution:

$$\vec{F}_i(t) = \nabla_i \sum_{j \neq i} u(r_{ij}) \tag{13}$$

2. Show that the total momentum of the system is conserved along the simulation.

Solution: The total momentum is conserved in a isolated system the third law of Newton gives an complete cancellation of the total force.

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.

Solution: The Box-Muller method provides gaussian random numbers. When N initial velocities are chosen, compute the total velocity and substract $1/N$ times the total velocity in order to have the center of mass of the system at rest.

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

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

.

Solution: Inserting the ansatz in the discrete equation of evolution gives

$$e^{i\Omega_v \Delta t} + e^{-i\Omega_v \Delta t} = 2 - \frac{k(\Omega_0 \Delta t)^2}{m} \tag{16}$$

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 $\Omega_0 \Delta t = \sqrt{2}$.

Solution: From the Verlet algorithm, one has that

$$v(n\Delta t) = \frac{x((n+1)\Delta t) - x((n-1)\Delta t)}{2\Delta t} \tag{17}$$

$$= i\frac{\sin(\Omega_v \Delta t)}{\Delta t} x(n\Delta t) \tag{18}$$

When $\Omega_0 \Delta t = \sqrt{2}$, $\Delta t \Omega_v = \pi/2$, and one obtains that the Verlet pulsaton becomes independent of Ω_0, which is a caveat of the method, when the time step is too large.

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.

Solution: Writing $A = |A|e^{-i\phi}$, one has

$$x(n\Delta t) = |A| \cos(n\Omega_v \Delta t - \phi)$$

and

$$v(n\Delta t) = -|A| \frac{\sin(\Omega_v \Delta t)}{\Delta t} \sin(n\Omega_v \Delta t - \phi)$$

Therefore, the total energy is given by

$$E = \frac{m|A|^2}{2} \left(\Omega_0^2 \cos(n\Omega_v \Delta t - \phi)^2 + \left(\frac{\sin(\Omega_v \Delta t)}{\Delta t} \right)^2 \sin(n\Omega_v \Delta t - \phi)^2 \right) \tag{19}$$

By using that

$$\left(\frac{\sin(\Omega_v \Delta t)}{\Delta t} \right)^2 = \frac{1 - (1 - (\Omega_0 \Delta t)^2/2)^2}{\Delta t^2}$$

one obtains that

$$E = E_{ex} - \frac{m|A|^2}{4} \Omega_0^4 \Delta t^2 \sin(n\Omega_v \Delta t - \phi)^2 \tag{20}$$

where $e_{ex} = \frac{m|A|^2}{2}\Omega_0^2$ Taking the time average of the above equation, one obtains that

$$E_v = E_{ex}(1 - \frac{\Omega_0^2 \Delta t^2}{4})$$

7. Can the total energy $E(n\Delta t)$ reach E_{ex} ?

Solution: The exact total energy is reaches when the sin funtion vanishes, twice per period.

8. Why does the discretized solution underestimate the kinetic energy ?.

Solution: The mean value of the potential energy is exact (even if the period is underestimated) , but the kinetic energy is underestimated. When the kinetic energy cancels, the total energy reaches the exact energy.