1.10 Integration schemes

Exercise Harmonic Oscillators: Symplectic vs.non-symplectic integrators (credit: Prof. E. Carlon)

Compare the performance of two MD integration schemes for a one dimensional harmonic oscillator. The Hamilton's equations of motion are:

$$\begin{cases} \dot{p} &= -\frac{\partial H}{\partial x} &= -kx \\ \dot{x} &= \frac{\partial H}{\partial p} &= p/m \end{cases} \tag{1.35}$$

where the Hamiltonian is given by

$$H = \frac{p^2}{2m} + \frac{kx^2}{2} \tag{1.36}$$

Set for convenience $k = m = 1$.
The first integrator (Euler integrator) we consider is

$$\begin{cases} p(t + \Delta t) = p(t) - x(t)\Delta t \\ x(t + \Delta t) = x(t) + p(t)\Delta t \end{cases} \tag{1.37}$$

The second integrator is also first order, but reads:

$$\begin{cases} p(t + \Delta t) = p(t) - x(t)\Delta t \\ x(t + \Delta t) = x(t) + p(t + \Delta t)\Delta t \end{cases} \tag{1.38}$$

Note that there is only a slight difference between the two.

a) Express Eqs. (1.37) and (1.38) in matrix form

$$\begin{pmatrix} x \\ p \end{pmatrix}_{t+\Delta t} = M \begin{pmatrix} x \\ p \end{pmatrix}_t \tag{1.39}$$

and show that for Eq. (1.37) $\det(M) > 1$ while for Eq. (1.38) $\det(M) = 1$. What does this tells us about the two algorithms and why?

Symplectic integrators do not strictly conserve the Hamiltonian H, but they conserve a so-called *shadow*-Hamiltonian H', which differs from H by terms of order Δt^k. For this reason they do not suffer from long time drift as non-symplectic integrators. Symplectic integrators are also volume preserving. The velocity Verlet scheme is a symplectic integrator (and it is of order $k = 2$). Eq. (1.38) defines the so-called Euler symplectic integrator of order $k = 1$.

b) Show analytically that the symplectic integrator defined by Eq. (1.38) has the following constant of motion (shadow Hamiltonian)

$$H' = H - \frac{px}{2}\Delta t \tag{1.40}$$

c) Take $\Delta t = 10^{-3}$ and $\Delta t = 10^{-2}$ with initial conditions $x(0) = 1, p(0) = 0$. and plot the solutions of Eqs. (1.37) and (1.38) up to time $T = 10$. Compare the relative errors of the two integration schemes to the exact solution of Eq. (1.35). Which of the two integrators is more accurate?

d) For the same values of the parameters given above plot the value of H as a function of t up to time $T = 10$. Plot H' as well for the symplectic integrator. Which of the two integrators has a long time drift in the energy estimate?

Exercise Implement the Velocity Verlet algorithm and another one between: i) Verlet algorithm ii) Beeman algorithm iii) Predictor-corrector algorithm.

Exercise The harmonic oscillator $\#2$:

$$\begin{aligned} \frac{dq}{dt} &= p, \\ \frac{dp}{dt} &= -\omega^2 q. \end{aligned} \tag{1.41}$$

The exact solution of $p(t)$ vs $\omega q(t)$ we get a circular orbit in phase that rotates by an amount of $\omega \Delta t$ at every time step. Considering this system, compare the two algorithms implemented above in terms of i) energy conservation ii) discrepancy with the analytical solution. Verify that the Velocity Verlet is stable for $\omega \Delta t < 2$.