Exercise 02

Numerical integration of differential equations (MD integrators)

Deadline: Please, hand in your solutions by **Thursday, 22 May, 2.15 p.m.**

2.1 Classical harmonic oscillator (6 P)

Consider a point particle of mass m which moves in a one-dimensional potential

$$V(x) \;=\; \frac{1}{2}kx^2\,. \tag{1}$$

where k is a constant (classical harmonic oscillator). The equation of motion is

$$m \cdot \frac{d^2}{dt^2}x(t) \;=\; -\frac{d}{dx}V(x(t)) = -kx(t) \tag{2}$$

To obtain the trajectory of the point particle, one needs to solve this differential equation for $x(t)$. Eq. 2 essentially states that the second derivative of $x(t)$ has to be proportional to $-x(t)$

(a) Verify that $x(t) = A\sin(\omega_0 t + \phi)$ is a solution to eq. 2. How is ω_0 related to k and m? (1 P)

(b) If $x(t) = A\sin(\omega_0 t + \phi)$, what is the equation for $v(t)$? (1 P)

(c) Determine the values of A and ϕ from the initial conditions (1 P)

$$\begin{aligned} x(0) &= 0 \\ v(0) &= 5\,\text{m/s}\,. \end{aligned}$$

(d) What is the period T of the oscillation if k= 0.2 kg/s^2 and m = 5 kg? (1 P)

(e) Plot $x(t)$ and $v(t)$ for these values from $t = 0$ to $t = 100$. (2 P)

2.2 Euler algorithm (10 P)

The equations for the Euler algorithm are

$$\begin{aligned} \mathbf{r}_i(t+\Delta) &= \mathbf{r}_i(t) + \mathbf{v}_i(t)\Delta + \frac{1}{2m_i}\mathbf{F}_i(t)\Delta^2 + \mathcal{O}(\Delta^3) \\ \mathbf{v}_i(t+\Delta) &= \mathbf{v}_i(t) + \frac{1}{m_i}\mathbf{F}_i(t)\Delta + \mathcal{O}(\Delta^2) \end{aligned} \tag{3}$$

(a) Implement the Euler algorithm using the potential in eq. 1. (6 P)

(b) Set k= 0.2 kg/s^2 and m = 5 kg. Use $x(0) = 0$, and $v(0) = 5\,$m/s as starting conditions. Simulate the oscillation with time step $\Delta = 0.1\,T$, $0.01\,T$, and $0.001\,T$, where T is the period of analytical solution (see exercise 2.1.d). The length of each simulation should be $10\,T$. For each simulation, plot $x(t)$ and $v(t)$. (3 P)

(c) Discuss the quality of the algorithm. Consider the amplitude and the period of the oscillation. (1 P)

2.3 Verlet algorithm (10 P)

$$\begin{aligned} \mathbf{r}_i(t+\Delta) &= 2\mathbf{r}_i(t) - \mathbf{r}_i(t-\Delta) + \frac{\mathbf{F}_i(t)}{m_i}\Delta^2 + \mathcal{O}(\Delta^4) \\ \mathbf{v}_i(t) &= \frac{\mathbf{r}_i(t+\Delta) - \mathbf{r}_i(t-\Delta)}{2\Delta} \end{aligned} \tag{4}$$

(a) Implement the Verlet algorithm using the potential in eq. 1. (6 P)

(b) Simulate the oscillation with the same parameters and initial conditions as in 2.2.b.
For each simulation, plot $x(t)$ and $v(t)$. (3 P)

(c) Discuss the quality of the algorithm. Consider the amplitude and the period of the oscillation. (1 P)