Worksheet 1: Integrators

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1 Introduction

In this worksheet we use will be using molecular dynamics simulation to look at the trajectory of a cannonball under the influence of gravity, friction, and wind and at a 2D representation of the solar system. We will be studying the behavior of a few different integrators in the latter simulation.

2 Cannonball

2.1 Simulating a cannonball

In this first exercise we simulate a cannonball in 2D under gravity in the absence of friction. The cannonball has a mass $m = 2.0\,\mathrm{kg}$,we take gravitational acceleration to be $g = 9.81\,\frac{\mathrm{m}}{\mathrm{s}^2}$, the cannonball has initial position $\boldsymbol{x}(0) = \boldsymbol{0}$, and initial velocity $\boldsymbol{v}(0) = \begin{pmatrix} 50 \\ 50 \end{pmatrix} \frac{\mathrm{m}}{\mathrm{s}}$. We will use the simple Euler scheme to integrate or system. This is given by:

$$\boldsymbol{x}(t + \Delta t) = \boldsymbol{x}(t) + \boldsymbol{v}(t)\Delta t \tag{1}$$

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

This is essentially just the Taylor expansion of position and velocity cut off below second order. We implement the simple Euler algorithm in python as follows:

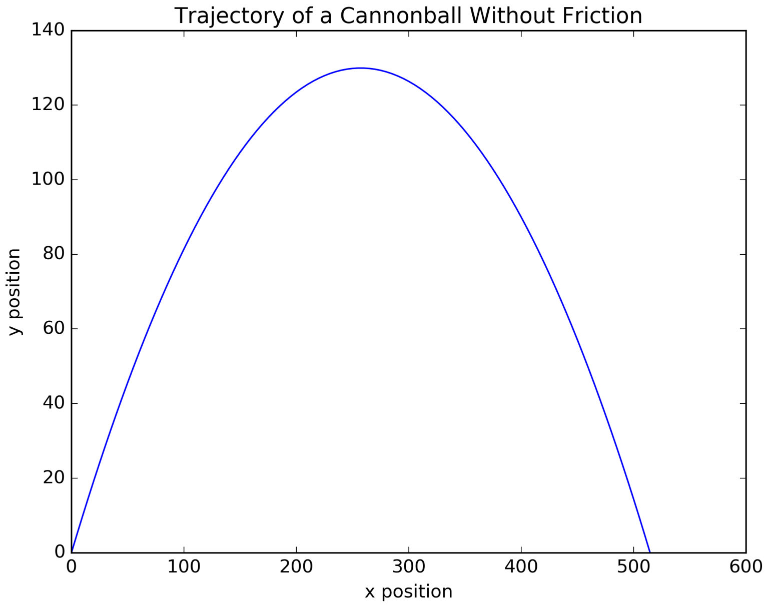

Figure 1: Trajectory of a cannonball with no friction using the simple Euler scheme

```python
def step_euler(x, v, dt):
    f = compute_forces(x)
    x += v*dt
    v += f*dt/m
    return x, v
```

The forces are computed simply with

```python
def compute_forces(x):
    f = np.array([0.0, -m*g])
    return f
```

We integrate until the cannonball reaches the ground. The trajectory can be seen in fig. 1.