Computational Physics: Molecular Dynamics Simulations, Assignment 1

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2025

1. Halley's comet

a) Generalized velocity

It would be prone to error to make simulations with would work with value to the order or 10^{-11}, for the gravitational constant, and values of order 10^{+11}, one astronomical unit. Therefore before anything is done, space will be rescaled by $1AU$ and time by one year ($1Y$), as follows.

$$\begin{cases} r \to & R = \frac{r}{1AU} \\ t \to & T = \frac{t}{1Y} \end{cases}$$

With this, the gravitational acceleration formula can be rewritten

$$\begin{aligned} \frac{d^2r}{dt^2} &= -\frac{GM}{r^3}\hat{r} \\ \frac{d^2R}{dT^2} &= -\frac{(1Y)^2}{(1AU)^3}\frac{GM}{R^3}\hat{R} \\ \frac{d^2R}{dT^2} &= -\Gamma\frac{GM}{R^3}\hat{R} \end{aligned}$$

With $\Gamma \approx 39,39$. The position, velocity, and acceleration of the Verlet algorithm (eqs. (118), (119) from the lecture notes) can be generalized to 2D as follows

$$\begin{cases} \vec{x} = (x, y) \\ \vec{v} = (v_x, v_y) \\ \vec{a} = (a_x, a_y) \end{cases}$$

$$\begin{cases} a_x &= -\Gamma\frac{x}{\sqrt{x^2+y^2}^3} \\ a_y &= -\Gamma\frac{y}{\sqrt{x^2+y^2}^3} \end{cases}$$

These positions and velocities are all rescaled as indicated above, meaning that the initial conditions are as follows $\vec{x}(t=0) = (35.2, 0)$ and $\vec{v}(t=0) = (0, 0.1920952)$

b)

Simulation implemented in jupyter notebook, $dt = 0.01$ (equivalent to 3.6 days). When trying $dt = 0.1$ accumulated error was too big and comet wasn't in orbit for more than 1 period.

c)

2.

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3.