Computational Physics: Molecular Dynamics Simulations, Assignment 1

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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. Symplectic vs.non-symplectic integrators

a)

For the Euler integrator, it can be directly seen from equation (123) from the lecture notes that the Jacobian of the time transformation is

$$M = \begin{pmatrix} 1 & \Delta t \\ -\Delta t & 1 \end{pmatrix}$$

From this we can easily see that $\det(M) = 1 + \Delta t^2 > 1$ for $\Delta t > 0$.
The same can be done for the sympletic integrator from equation (124) of the lecture notes, but an extra step needs to be taken. After rewriting the expression for $q(t + \Delta t)$ as

$$q(t + \Delta t) = q(t) + (p(t) - q(t)\Delta t)\Delta t$$

We can find that the Jacobian of the time transformation for this integrator is.

$$M_s = \begin{pmatrix} 1 - \Delta t^2 & \Delta t \\ -\Delta t & 1 \end{pmatrix}$$

For the sympletic integrator we have that $\det(M_s) = 1 - \Delta t^2 + \Delta t^2 = 1$.

b)

To show that H' is a constant of motion I'll show that $H'(t + \Delta t) = H'(t)$.

$$\begin{aligned}
H'(t+\Delta t) &= \frac{(p(t+\Delta t)^2 + q(t+\Delta t)^2)}{2} - \frac{p(t+\Delta t)q(t+\Delta t)}{2}\Delta t \\
p(t+\Delta t)^2 &= p(t)^2 - 2p(t)q(t)\Delta t + q(t)^2\Delta t^2 \\
q(t+\Delta t)^2 &= p(t)^2\Delta t^2 + 2p(t)q(t)(\Delta t - \Delta t^3) + q(t)^2(1 - \Delta t^2) \\
p(t+\Delta t)^2 + q(t+\Delta t)^2 &= p(t)^2(1 + \Delta t^2) - 2p(t)q(t)\Delta t^3 + q(t)^2(1 - \Delta t^2 + \Delta t^4) \\
p(t+\Delta t)q(t+\Delta t) &= p(t)^2\Delta t + p(t)q(t)(1 - 2\Delta t^2) - q(t)^2(\Delta t - \Delta t^3) \\
&\Rightarrow \\
2H'(t+\Delta t) &= p(t)^2 - p(t)q(t)\Delta t + q(t)^2 \\
&= 2H'(t)
\end{aligned}$$

Therefore it holds that $H' = H - \frac{pq}{2}\Delta t$ is a constant of motion.

c)

SIMULATION $\Rightarrow$ TODO

3.