MM553: Project 1

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N particles in 1 dimension

This problem consists of many particles with a spring-like force that acts on neighboring particles.

1. Hamilton's Equations

To obtain Hamilton's equations for this exercise, we need to analyze the equation of total energy given, as seen in Figure 1.

$$H = E = \sum_{i=1}^{N} \frac{1}{2} p_i^2 + \sum_{\langle i,j \rangle} V(|x_i - x_j|),$$
$$V(|x_i - x_{i+1|}) = \frac{1}{2}(|x_i - x_{i+1}|)^2 + \frac{1}{3}(|x_i - x_{i+1}|)^3 + \frac{1}{4}(|x_i - x_{i+1}|)^4.$$

Figure 1. Equation for total energy of particles.

Since each pair is counted only once, the potential sum of particles can be rewritten as a sum over $N - 1$ elements, as shown in Figure 2. The last element N doesn't have a right pair, so it isn't counted in the sum (x_i has been replaced with q_i to stay consistent with p and q terms).

$$H = E = \sum_{i=1}^{N} \frac{1}{2} p_i^2 + \sum_{\langle i,j \rangle} V(|q_i - q_j|)$$
$$= \frac{1}{2} \sum_{i=1}^{N} p_i^2 + \sum_{i=1}^{N-1} V(|q_i - q_{i+1}|)$$

Figure 2. Rewritten equations for total energy.

When taking the partial derivative with respect to p_i, we obtain

$$\dot{q}_i = \frac{\partial H}{\partial p_i} = \frac{1}{2} \cdot 2p_i = p_i$$

When taking the partial derivative with respect to q_i, we have a trickier operation. Notice how since each pair is counted only once, every particle q_i appears twice in the equation, since its position is accounted for the potential sum of the left neighbor and of the right neighbor. However, notice how q_1 and q_N appear only once, since the first particle only has a right neighbor and thus a right potential force but not left neighbor. The last particle also has no right neighbor, so only the force from the left is accounted for in the sum.

Let $q_L = q_{i-1} - q_i$ be the position difference of the left neighbor and $q_R = q_i - q_{i+1}$ be the position difference of the right neighbor. Thus, the result we obtain is

$$\dot{p}_i = -\frac{\partial H}{\partial q_i} = F(q_L) - F(q_R)$$

$$F(q) = \left(|q| + |q|^2 + |q|^3\right) \cdot sign(q)$$

as seen in Figure 3 and Figure 4.

$$\dot{p}_i = -\frac{\partial H}{\partial q_i} = \frac{-H}{d q_L} \cdot \frac{\partial q_L}{\partial q_i} = \frac{-H}{\partial q_L} \cdot (-1) = \frac{\partial H}{\partial q_L}$$

$$= \frac{\partial}{\partial q_L}\left(\frac{1}{2}|q_L|^2 + \frac{1}{3}|q_L|^3 + \frac{1}{4}|q_L|^4\right)$$

$$= \left(|q_L| + |q_L|^2 + |q_L|^3\right) \cdot sign(q_L) = F(q_L)$$

Figure 3. Negative partial derivative of H with respect to q_i to obtain force from the left.

$$\dot{p}_i = -\frac{\partial H}{\partial q_i} = \frac{-H}{d q_R} \cdot \frac{\partial q_R}{\partial q_i} = \frac{-H}{\partial q_L} \cdot (1)$$

$$= \frac{-\partial}{\partial q_R}\left(\frac{1}{2}|q_R|^2 + \frac{1}{3}|q_R|^3 + \frac{1}{4}|q_R|^4\right)$$

$$= -\left(|q_R| + |q_R|^2 + |q_R|^3\right) \cdot sign(q_R) = -F(q_R)$$

Figure 4. Negative partial derivative of H with respect to q_i to obtain force from the right.

2. Initial conditions

For initial conditions, we choose a value between 100 and 1000 particles for the system and set their initial positions to 0. Additionally, we choose random momenta between -1 and 1 (excluding 0) for each particle.

- Initialize time params, constants, and the initial positions and momenta for each particle.

3. Numerical integration (EC, LF, RK2)

We now implement the rest of the solution in MATLAB. - Define `V` and `F` as the solutions we obtained analytically. - The way these functions manipulate not only the current position, but also the neighboring positions is made possible with a special MATLAB function called `diff()`. This function calculates the difference between elements in a $M \times N$ matrix, and outputs a $M - 1 \times N$ matrix with entries `X(2) - X(1), X(3) - X(2), ... , X(M) - X(M-1)`. - When a formula requires entries $x_i - x_{i+1}$, use `[-diff(X,1,2) , 0]`. - When a formula requires entries $x_{i-1} - x_i$, use `[ 0 , flip(diff(flip(X),1,2)) ]`.

- Define the initial Hamiltonian, and run the 3 integration methods.

Now we can plot the energy over time, as seen in Figure 5.

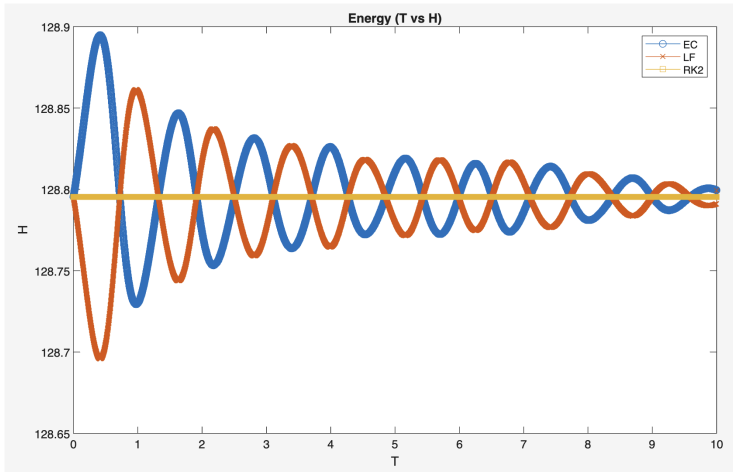


Figure 5. Plot of energy over time for each iteration method.

As we can see, the energy in the system is approximately constant for each method, RK2 making the best approximation out of the 3 integration methods.

4. Average Velocity Squared

To analyze the average velocity squared ($v^2(t)$) of the system, take the sum of momenta squared over all particles and divide it into the number of particles in the system.

```
avg_vel_squared = sum(EC_P'.^2) / n_particles;
```

Now we can analyze how the AVS of the system stabilizes around a specific value over time, as seen in Figure 6. As time passes, the system has time to stabilize and distribute the energy equally across the entire string of particles.

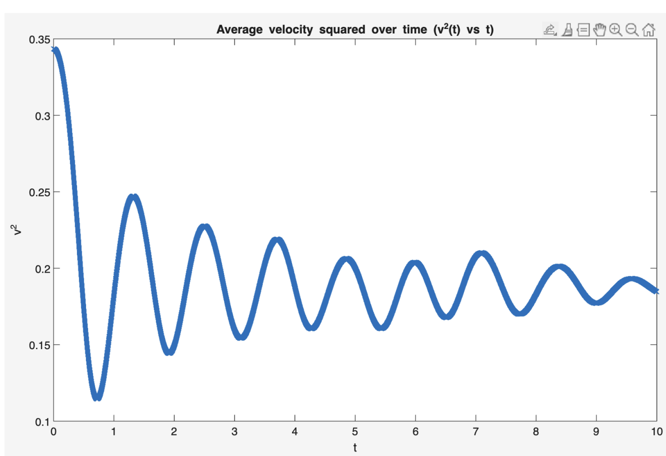


Figure 6. Plot of AVS over time.

5. Histogram of AVS and Maxwell-Boltzmann distribution

When taking a histogram of the velocities at an intermediate time, the system has had enough time to stabilize, and we obtain a normal distribution, as seen in Figure 7.

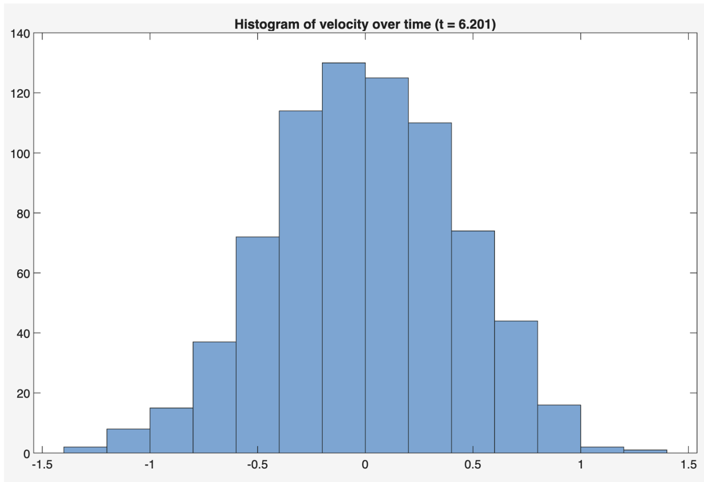


Figure 7. Plot of velocity squared over time.

After enough time, the energy begins to dissipate and equilibrate along the string, and velocities are more spread out, resulting in a normal distribution.

The Maxwell-Boltzmann distribution of the system depicts the probability of finding a particle with a certain velocity with a specific temperature T in the system.

We can estimate the kT value of our system by taking the mean velocity squared and multiplying it by the mass of a particle, which results in a value of around 0.2. Figure 8 shows the histogram of velocities at t=6.201 against the MB distribution formula with the obtained kT value and at the same time step as the histogram.

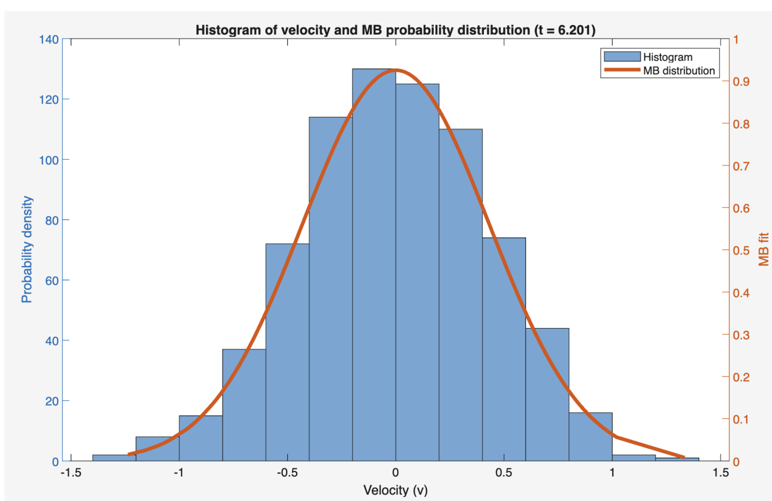


Figure 8. Histogram of velocities against MB fit.

As we can see, both approximations for the velocities at a certain time match up, suggesting that the simulation depicts how particles would behave in real conditions.

Two planets around the sun in 2 dimensions

This problem consists of 2 (or more) planets rotating around the sun.

1. Hamilton's equations

To obtain Hamilton's equations for this exercise, we need to analyze the equation of total energy given, as seen in Figure 8.

$$H = E = \frac{\langle \vec{p}_1, \vec{p}_1 \rangle}{2m_1} + \frac{\langle \vec{p}_2, \vec{p}_2 \rangle}{2m_2} - \frac{Gm_1 M}{r_1} - \frac{Gm_2 M}{r_2}$$

Figure 1. Equation for total energy of planets.

where $r = \sqrt{x_i^2 + y_i^2}$.

When taking partial derivatives for p and q, as seen in Figure 9.

$$H = E = \frac{\langle \vec{p}, \vec{p} \rangle}{2m} - \frac{GmM}{r} = \frac{1}{2m}\left(p_x^2 + p_y^2\right) - GmM \cdot \frac{1}{\sqrt{q_x^2 + q_y^2}}$$

$$\dot{q}_x = \frac{\partial H}{\partial p_x} = \frac{p_x}{m} \qquad \dot{p}_x = \frac{-\partial H}{q_x} = GmM \cdot \left(-\frac{1}{\cancel{2}}\right)\left(q_x^2 + q_y^2\right)^{-3/2} \cdot \cancel{2} q_x$$

$$= -GmM \; q_x \left(q_x^2 + q_y^2\right)^{-3/2} = F_x$$

$$\dot{q}_y = \frac{\partial H}{\partial p_y} = \frac{p_y}{m} \qquad \dot{p}_y = \frac{-\partial H}{\partial q_y} = GmM \cdot \left(\frac{-1}{\cancel{2}}\right)\left(q_x^2 + q_y^2\right)^{-3/2} \cdot \cancel{2} q_y$$

$$= -GmM \cdot q_y \left(q_x^2 + q_y^2\right)^{-3/2} = F_y$$

Figure 9. Hamilton's equations for the system.

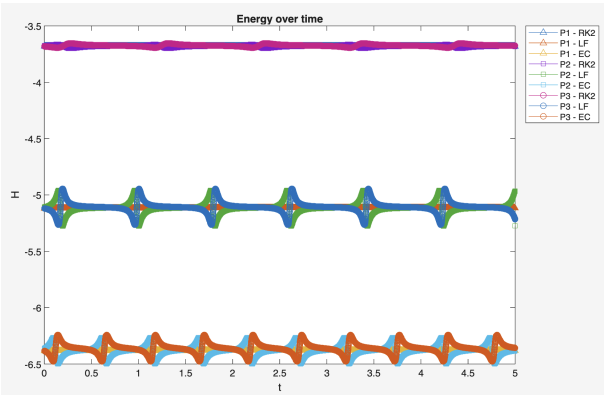
We now have a formula for force applied to the x and y axis, since our p and q are 2D vectors in space. If we wish to add more planets to our system, we can just sum the total energy for each planet to obtain the total Hamiltonian of the system (since each planet orbits independently of the others).

2. Numerical integration (EC, LF, RK2)

We will now implement this analytical result into MATLAB.

- Initialize time parameters.
- Define constants for our system; in this case we will use 3 planets.
- Define `P` and `Q` matrices, which are of size `nstep` $\times$ `nplanets` $\times$ 2. This stores all the information about the system at a certain time, for a certain planet, at a certain coordinate (respectively).
- Define `V` and `F` that we obtained analytically; x and y have been replaced with `q(1)` and `q(2)` respectively.

- Loop over the amount of planets in the system, and obtain the matrices for momenta and positions, using the functions for Euler-Cromer, Leapfrog, and RK2 iteration.
- With these matrices, we can plot the energy over time of each method. It can be seen in Figure 10 and 11 that the total energy of the system remains approximately constant at different levels for each planet.



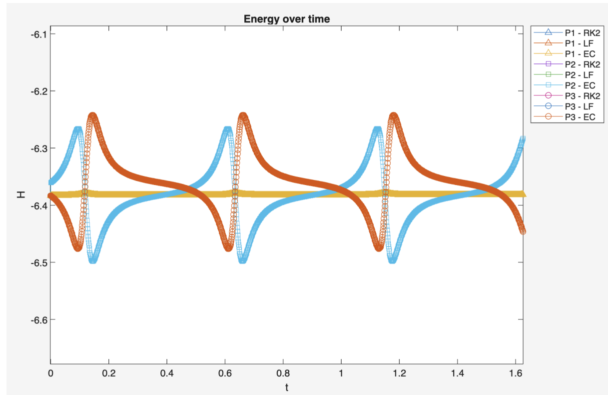
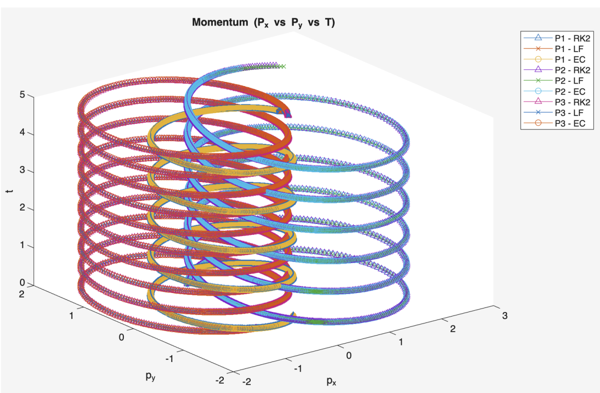


Figure 10. Energy plot over time.

Figure 11. Close up of Planet 3 energy over time.

- We can also plot the momenta and positions over time, as seen in Figure 12 and 13.



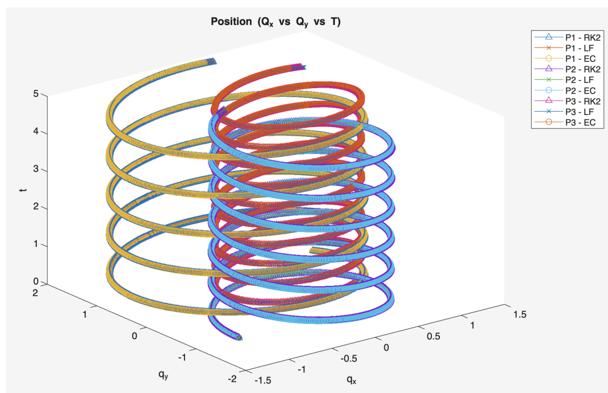


Figure 12. Plot of momenta over time.

Figure 13. Plot of positions over time.

3. Initial conditions

With the initial conditions chosen before, the motion of the planets can be simulated, as shown in Figure 14.

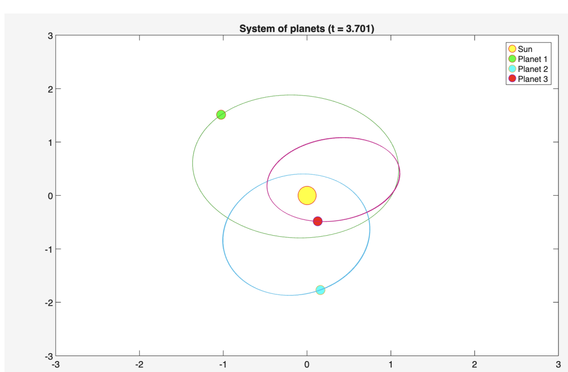


Figure 14. System at `t = 3.701`.

4. Kepler's Third Law

In order to show Kepler's Third Law in our system, we need to obtain a and T for each planet.

a is half of the longest axis of the ellipse formed by the movement of a planet. This is obtained by tracking the euclidean distance r from the origin, and finding the peaks and valleys of its trajectory, as shown in Figure 15.

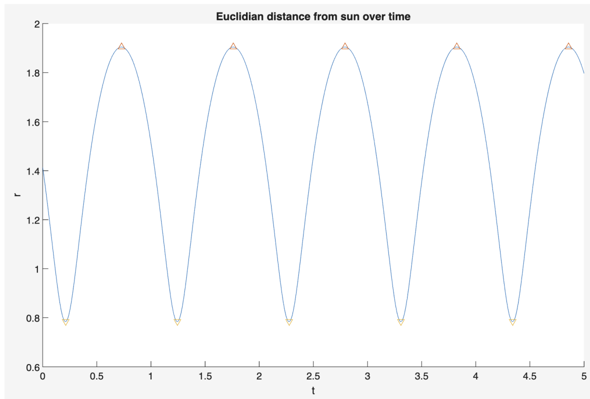


Figure 15. Euclidean distance from the sun over time of Planet 1.

The point furthest from the sun is known as the **aphelion**, and the closest point from the sun is known as the **perihelion**. a can be obtained by taking half of the euclidean distance between these 2 opposing points.

T is the time it takes a planet to perform a full orbit around the sun. Since we know the time indexes at which the peaks and valleys occur and since no energy is lost, these extrema must happen periodically. We can calculate the period T by subtracting any 2 indexes of extrema (here the time between the first 2 valleys was chosen as T, but any other periodic extrema index could've been chosen).

As shown in Figure 16, the ratio a^3/T^2 for all 3 planets is roughly equal, since all 3 objects are orbiting the same primary star.

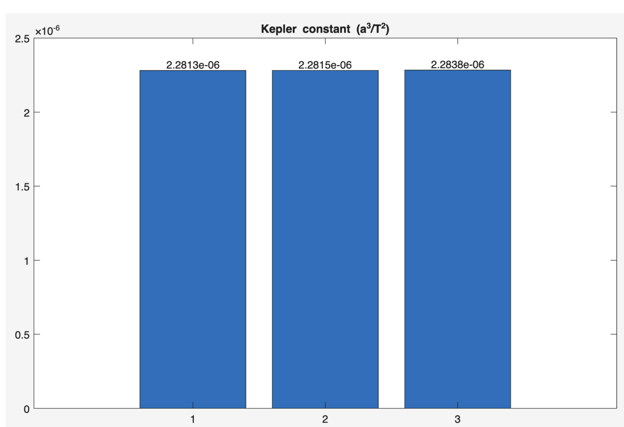


Figure 16. Kepler constant of the 3 planets.