Computational Physics
Exercise Sheet 01

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Code and plots can be found in the zip folder

a)

Newton $f = m\ddot{r}$

Taylor expansion to get next timestep

$$r(t+\Delta t) = r(t) + \dot{r}(t)\Delta t + \frac{1}{2}\ddot{r}(t)\Delta t^2 \quad (1)$$
$$r(t-\Delta t) = r(t) - \dot{r}(t)\Delta t + \frac{1}{2}\ddot{r}(t)\Delta t^2 \quad (2)$$

Adding them

$$r(t+\Delta t) + r(t-\Delta t) = 2r(t) + \ddot{r}(t)\Delta t^2 \leftarrow \text{verlet algorithm}$$

We can show that velocity verlet is the same

good

$$r(t+\Delta t) = r(t) + \dot{r}(t)\Delta t + \frac{1}{2}\ddot{r}(t)\Delta t^2$$
$$\dot{r}(t+\Delta t) = \dot{r}(t) + \frac{1}{2}[\ddot{r}(t) + \ddot{r}(t+\Delta t)]\Delta t$$

→ Second order taylor expansion

$$r(t+2\Delta t) = r(t+\Delta t) + \dot{r}(t+\Delta t)\Delta t + \frac{1}{2}\ddot{r}(t+\Delta t)\Delta t^2$$

adding (1)

$$r(t+2\Delta t) + r(t) = 2r(t+\Delta t) + [\dot{r}(t+\Delta t) - \dot{r}(t)]\Delta t + \frac{1}{2}[\ddot{r}(t+\Delta t) - \ddot{r}(t)]\Delta t^2$$

use $\dot{r}(t+\Delta t) - \dot{r}(t) = \frac{1}{2}[\ddot{r}(t+\Delta t) + \ddot{r}(t)]\Delta t$

and (2)

$$\Rightarrow r(t+2\Delta t) + r(t) = 2r(t+\Delta t) + \ddot{r}(t+\Delta t)\Delta t^2$$

↳ verlet algorithm

Starting conditions vel.-verlet: r_0 and v_0

Verlet: just r_0 and r_1 no velocity necessary.

b) How can I calculate the positions $\vec{r}$?

I have $\vec{r}_0$ and $\dot{\vec{r}}_0 = \vec{v}_0$.

$$V_{ij}(r_{ij}) = -G \frac{M_i M_j}{r_{ij}}$$

Velocity-Verlet algorithm:

$$\vec{r}_i(t+\Delta t) = \vec{r}_i(t) + \vec{v}_i(t)\,\Delta t + \frac{\Delta t^2}{2m_i} \cdot \vec{F}_i(t) + \mathcal{O}(\Delta t^3)$$

$$\vec{v}_i(t+\Delta t) = \vec{v}_i(t) + \frac{\Delta t}{2m_i}\left[\vec{F}_i(t) + \vec{F}_i(t+\Delta t)\right] + \mathcal{O}(\Delta t^3)$$

So I need to calculate the force for each t and $t+\Delta t$.

$$\vec{F}(\vec{r}) = -\nabla V(\vec{r}) = -G \frac{M_i M_j}{|r_{ij}|^3} \vec{r}_{ij}$$

$$\vec{F}_i(\vec{r}(t)) = \sum_{j=1}^{n} -\nabla V_{ij} \quad i \neq j$$

Unit check ✓

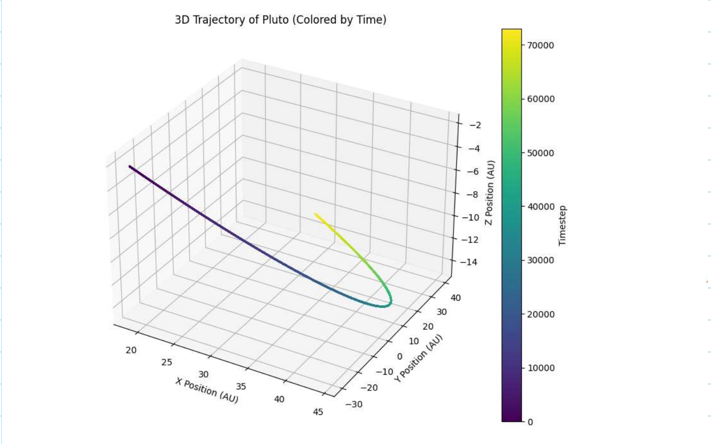
$[v] = \frac{AU}{day}$ $\quad [r] = AU$ $\quad [G] = \frac{m^3}{kg\,s^2}$ $\quad [m] = 10^{29}\,kg$ $\quad 1N = kg\frac{m}{s^2}$

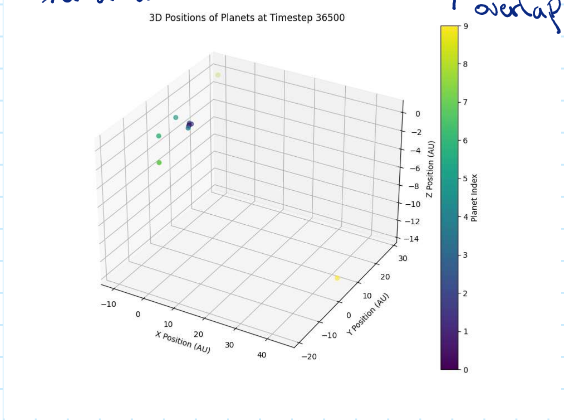
convert $G \Rightarrow \frac{AU^3}{10^{29}kg\ day^2} = \frac{\left(\frac{1}{1.5}10^{11}\,AU\right)^3}{\frac{1}{10^{29}}kg\left(\frac{1}{86400}day\right)^2} \cdot 6{,}67\ 10^{-11}$

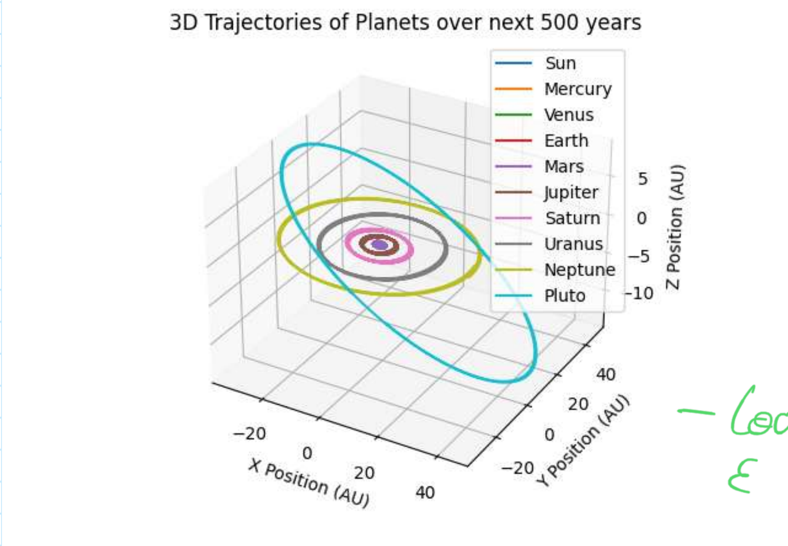
unit check is good practise! Excellent

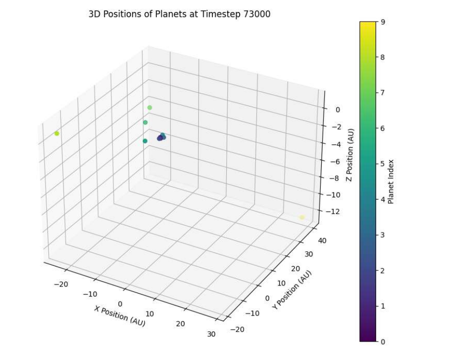
- Where are energy plots for euler / VV ?
You did it, but it is not in this pdf, you dont even comment on it. I almost missed it.

looks better in Ovito
→ and use radius = 0,1 so they dont overlap.









— Looks good. Why is your E so bad then?

Plutos orbital period is 256,5 years. Looks good but how did you get that

c) Verlet algorithm

Again we have mass, positions t=0 and the potential.

$$f_i(t) = \sum_{i\neq j, j=1}^{n} -\nabla V_{ij}$$

$\Rightarrow$ new_pos : $\vec{r}_i(t+\Delta t) = 2\vec{r}_i(t) - \vec{r}_i(t-\Delta t) + \frac{\Delta t}{m_i}\vec{f}_i(t) + O(\Delta t^4)$

vel : $\vec{v}_i(t) = \frac{\vec{r}_i(t+\Delta t) - \vec{r}_i(t-\Delta t)}{2\Delta t} + O(\Delta t^3)$

Where do I get the second set of positions?

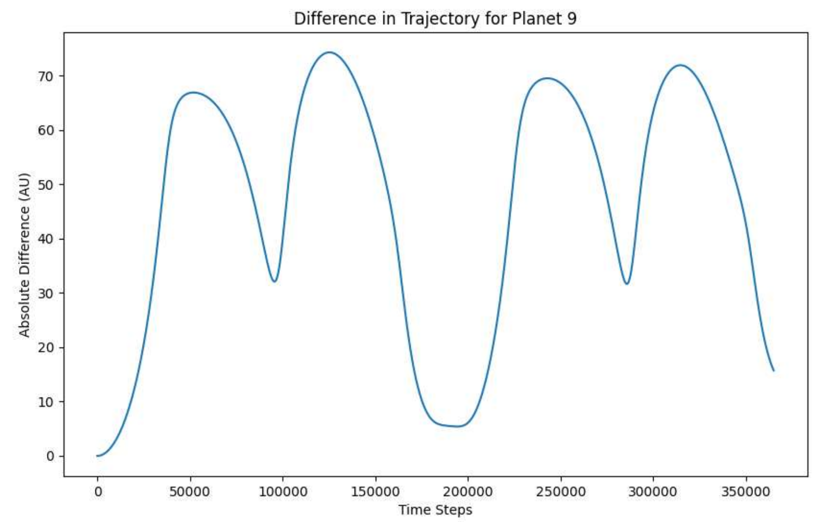
Start with:

$$\vec{r}(2) = 2\vec{r}(1) - \vec{r}(0) + \frac{\Delta t}{m_i}\vec{f}(0)$$

$$v(1) = \frac{\vec{r}(2) - \vec{r}(0)}{2\Delta t}$$

We took the calculated pos from the velocity verlet.

Comparison velocity-verlet and Verlet



For each timestep calculated the $|\vec{r}_{vv}(t) - \vec{r}_v(t)|$

$\mathcal{O}(\Delta t^4)$ from Taylor for Verlet

↳ What does this mean?

The estimated orbital period of Mars is 39,20 years.

How do you calc that?

$t_{orbit\,Mars} \approx 2$ years

d)

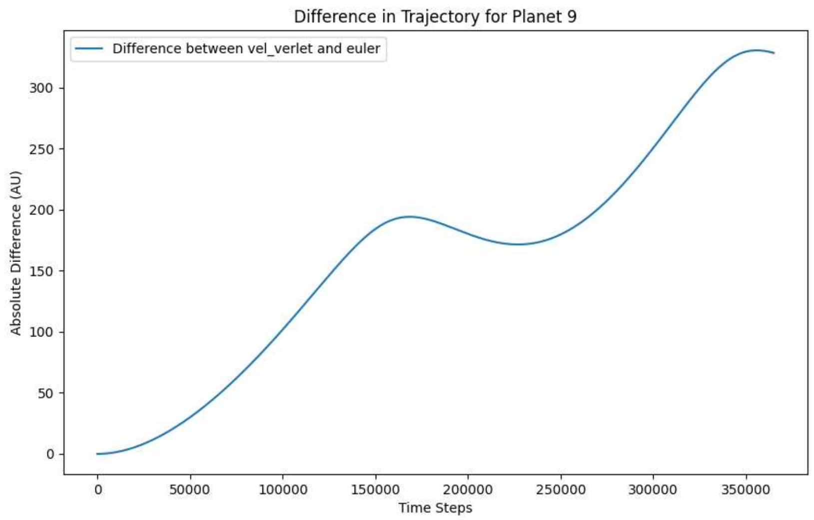
Euler

$$\vec{r}_i(t+\Delta t) = \vec{r}_i(t) + \Delta t \cdot \vec{v}_i(t) + \frac{\Delta t^2}{2m_i}\vec{f}_i(t) + \mathcal{O}(\Delta t^3)$$

← only difference to Velocity Verlet.

$$\vec{v}_i(t+\Delta t) = \vec{v}_i(t) + \frac{\Delta t}{m_i}\vec{f}_i(t) + \mathcal{O}(\Delta t^2)$$

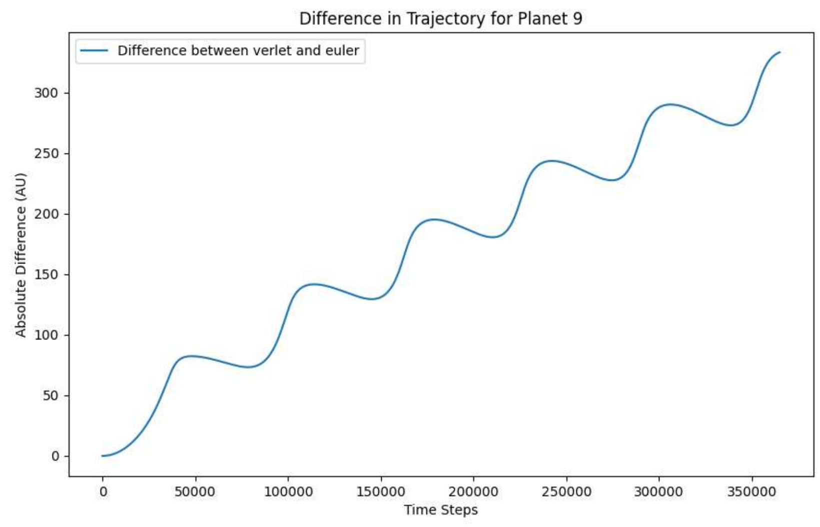
Comparison Euler - Velocity-Verlet



For each timestep calculated the $|\vec{r}_{vv}(t) - \vec{r}_v(t)|$

Accordingly same difference to Verlet. Just like in c)

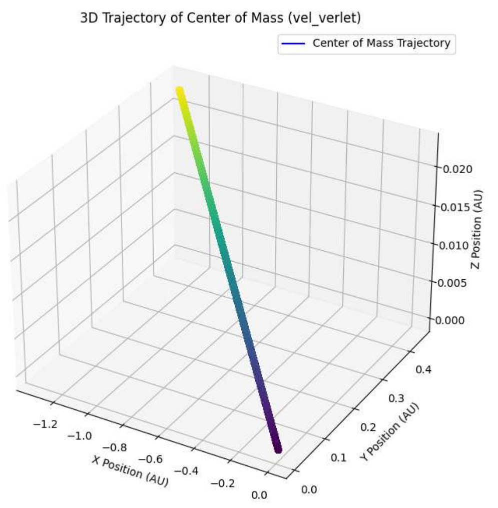
$$E = \sum_i \frac{1}{2} m_i |\vec{v}_i|^2 + \sum_i \sum_{j, j \neq i} V_{ij}$$ $i \in$ Planets with Sun



e) Center of mass

$$\vec{r}_{COM} = \frac{\sum r_i m_i}{\sum m_i}$$

The center of mass is just a straight line. That might cause from the initial dataset. The initial data doesn't come from COM system. Pictures of all simulations can be found in the zip. For all simulations the drift of COM is the same.



$v_{sum} = 0$ so
total momentum $\neq 0$
$\Rightarrow$ COM drifts

f) Not realistic XD

Wikipedia Mercury eccentricity is 0,2056 how did you calc that?

Simulation eccentricity for each simulation $\varepsilon > 0,96$

But just velocity verlet seems the most realistic because every planet stays in the solar system. In the other simulations planets move on a hyperbolic trajectory.

→ See pictures in zip.

Wait... for Verlet your planets leave the solar system?

Code:

- Why is orbit for pluto good, but for Mars off? Discuss!
- In force calc use antisym:
  if you have force from particle A on particle B, so have force particle B on particle A as well
  ↳ Instead of full matrix, just calc half
- Use numba: @njit decorator for forces
  This is a <u>must</u> for ex 2! 1 order of magnitude speedup
- Because you don't state what exactly is happening I can't tell if your force calc works 100% as intended. For VV: ε should be solid, to orbit (both Mars and Pluto) should be good.
  At first glance the code looks fine, but please look into it! From energy: VV looks good
- Dont attach so many files again!
  1 pdf containing all figures, commented, referenced with text + interpretation of the result.
  If you want to attach bonus pictures create a sub folder.
- Structure your report better for next time!