Numerical Method for Ordinary differential equations and Its Application in Physics

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Abstract

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1 Introduction

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2 Examples of ordinary differential problems in physics

2.1 The Earth-Sun system

The Earth-Sun system is a two-body system governs by the gravitational force

$$\vec{F}_G = \frac{GM_\mathrm{S} M_\mathrm{E} \hat{r}}{r^2}, \tag{1}$$

where G is the gravitational constant; M_S and M_E are mass of the Sun and the Earth; $\vec{r}$ is the displacement between them.

Given the fact the Sun is about 10^6 heavier than the Earth, we can safely keep the Sun as the center of mass (C.M.) in this problem. With proper coordinate setup, the orbit of the Earth is co-planer in xy-plane. Using Newton's second law we get the following first-order ordinary differential equations (ODEs) for the Earth

$$\begin{cases} \frac{dx}{dt} = v_x \\ \frac{dx}{dt} = v_x \\ \frac{dv_x}{dt} = -\frac{GM_\mathrm{S} x}{r^3} \\ \frac{dv_y}{dt} = -\frac{GM_\mathrm{S} y}{r^3}. \end{cases} \tag{2}$$

By solving above equations, we can obtain the informations about the Earth's orbit we need.

2.2 Many body problem

In the above Sec. 2.1, we simplify the calculation of the orbit of the Earth by taking into account only it's interaction with the Sun. This simplification is reasonable as the Sun is much heavier than other planets in the solar system.

However, if we want to go a step further to get a more precise description of the Earth's orbit. We have to include distortions from other seven planets as well as the Pluto. We should also abandon our previous static Sun setup but using the real center of mass of the solar system. Until now, we have a new set of ODEs for the Earth

$$\begin{cases} \frac{dx}{dt} = v_x \\ \frac{dy}{dt} = v_y \\ \frac{dv_x}{dt} = \sum_{i=1}^{n} -\frac{GM_i x_i}{r_i^3} \\ \frac{dv_y}{dt} = \sum_{i=1}^{n} -\frac{GM_i y_i}{r_i^3}, \end{cases} \tag{3}$$

where i runs over all other celestial bodies except the Earth itself. Besides the Earth, we have similar sets of ODEs for every celestial body.

By solving these coupled ODEs, we can obtain a full description for the solar system.

3 Numerical methods

3.1 Euler forward method

Suppose a first-order ordinary differential equation

$$\frac{dx}{dt} = f(x, t); \; t \in [t_0, t_1] \tag{4}$$

with a initial value x_0 at time t_0.

In order to solve this problem, we first discretize the region $[t_0, t_1]$ into N subintervals with a step h, so we get the relation

$$h = \frac{t - t_0}{N}. \tag{5}$$

Then, We have discretized $x_i = x(t_i = t_0 + ih)$ where i is a integer between 0 and N.

Using Taylor expansion, we get

$$x_{i+1} = x_i + \frac{dx_i}{dt} h + \frac{d^2 x_i}{dt^2} h^2 + O(h^3), \tag{6}$$

where i goes from 0 to $N - 1$. The Euler forward method truncates at the second term of the above equation. Thus, Eq. 6 becomes

$$\begin{aligned} x_{i+1} &= x_i + \frac{dx_i}{dt} h + O(h^2) \\ &= x_i + f(x_i, t_i) h + O(h^2). \end{aligned} \tag{7}$$

We can see it's a one-step method with a local error $O(h^2)$.

Getting back to the Earth-Sun system, we can formulate Eq. 2 to

$$\begin{cases} x_{i+1} = x_i + v_x^i h \\ y_{i+1} = y_i + v_y^i h \\ v_x^{i+1} = v_x^i - \frac{4\pi^2 x_i}{r_i^3} h \\ v_y^{i+1} = v_y^i - \frac{4\pi^2 y_i}{r_i^3} h. \end{cases} \tag{8}$$

in unit of AU for length, year (yr) for time and M_S for mass. We will keep using these units in our report calculations. Starting from some initial conditions, we can simply solve out time evolution of the

Input: $x_0 = 1$, $y_0 = 0$, $v_x^0 = 0$, $v_y^0 = 2\pi$, $M_{\rm E}$, $M_{\rm S}$, G

Output: $\vec{x}$=(x_0,x_1,...,x_N), $\vec{y}$, $\vec{v}_x$, $\vec{v}_y$, $\vec{E}_k$, $\vec{E}_p$, $\vec{E}$, $\vec{L}_z$

$r = \text{sqrt}(x_0^2{+}y_0^2)$;
// i is deferent time points $t_i = t_0 + ih$;
for $i = 1; i <= N; i++$ **do**
    $x_i = x_{i-1} + v_x^{i-1}h$; $y_i = y_{i-1} + v_y^{i-1}h$;
    $v_x^i = v_x^{i-1} - \frac{4\pi^2 x_{i-1}}{r_{i-1}^3}h$; $v_y^i = v_y^{i-1} - \frac{4\pi^2 y_{i-1}}{r_{i-1}^3}h$;
    $r = \text{sqrt}(x_i^2{+}y_i^2)$;
    // Kinetic energy E_k, Potential energy E_k, Total energy E, Angular momentum in $\hat{z}$ L_z;
    $E_k^i = 0.5M_{\rm E}((v_x^i)^2{+}(v_y^i)^2)$; $E_p^i = -\frac{GM_{\rm E}M_{\rm S}}{r}$;
    $E^i = E_p^i + E_k^i$; $L_z^i = M_{\rm E}(x_i v_y^i - y_i v_x^i)$;
end
return $\vec{x}$, $\vec{y}$, $\vec{v}_x$, $\vec{v}_y$, $\vec{E}_k$, $\vec{E}_p$, $\vec{E}$, $\vec{L}_z$;

Algorithm 1: The Euler forward method for the Earth-Sun system. It initials from a circular orbit.

Earth iteratively. Our implementation of this method with circular orbit initial conditions is shown in Algorithm **??**.

We can see that the Euler forward method is easy to be realized. However, it has a vital defects that it violates the energy conservation and time reversibility. The total energy increases with time in the Euler forward method. That's why we need the Velocity-Verlet method to describe physical systems.

3.2 Velocity-Verlet method

The velocity-Verlet method is widely used in molecular dynamics calculation as it overcomes these defects. It conserves energy with small round-off errors[1].

Staring from the Taylor expansions under same discretization

$$\begin{aligned} x_{i+1} &= x_i + x_i^{(1)}h + x_i^{(2)}h^2 + O(h^3), \\ v_x^{i+1} &= v_x^i + v_x^{i(1)}h + v_x^{i(2)}h^2 + O(h^3), \end{aligned} \tag{9}$$

with a initial value x_0 and v_x^0 at time t_0. We truncate at the third term and evaluate $v_x^{i(2)}h \approx v_x^{i+1(1)} - v_x^{i(1)}$. We can see that velocity-Verlet method is a two-step method with a local error $O(h^3)$

In the Earth-Sun system, with this method, we can formulate Eq. 2 to

$$\begin{cases} x_{i+1} = x_i + v_x^i h - \frac{4\pi^2 x_i}{r_i^3}\frac{h^2}{2} \\ y_{i+1} = y_i + v_y^i h - \frac{4\pi^2 y_i}{r_i^3}\frac{h^2}{2} \\ v_x^{i+1} = v_x^i - (\frac{4\pi^2 x_i}{r_i^3} + \frac{4\pi^2 x_{i+1}}{r_{i+1}^3})\frac{h}{2} \\ v_y^{i+1} = v_y^i - (\frac{4\pi^2 y_i}{r_i^3} + \frac{4\pi^2 y_{i+1}}{r_{i+1}^3})\frac{h}{2}. \end{cases} \tag{10}$$

We show our realization of the velocity-Verlet method in Algorithm **??**. Compared with the Euler forward method, we can see the calculations in this method is more complicated.

3.3 Object oriented code development

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Input: $x_0 = 1$, $y_0 = 0$, $v_x^0 = 0$, $v_y^0 = 2\pi$, M_{E}, M_{S}, G

Output: $\vec{x}$=(x_0,x_1,...,x_N), $\vec{y}$, $\vec{v}_x$, $\vec{v}_y$, $\vec{E}_k$, $\vec{E}_p$, $\vec{E}$, $\vec{L}_z$

$r = \mathrm{sqrt}(x_0^2 + y_0^2)$;

$a_x^0 = \frac{4\pi^2 x_{i-1}}{r_{i-1}^3}$; $a_y^0 = \frac{4\pi^2 y_{i-1}}{r_{i-1}^3}$;

// i is deferent time points $t_i = t_0 + ih$;

for $i = 1; i <= N; i++$ **do**

$\quad x_i = x_{i-1} + v_x^{i-1}h - \frac{a_x^0 h^2}{2}$; $y_i = y_{i-1} + v_y^{i-1}h - \frac{a_y^0 h^2}{2}$;

$\quad r = \mathrm{sqrt}(x_i^2 + y_i^2)$;

$\quad a_x^1 = \frac{4\pi^2 x_i}{r_i^3}$; $a_y^1 = \frac{4\pi^2 y_i}{r_i^3}$;

$\quad v_x^i = v_x^{i-1} - \frac{(a_x^0 + a_x^1)h}{2}h$; $v_y^i = v_y^{i-1} - \frac{(a_y^0 + a_y^1)h}{2}h$;

$\quad a_x^0 = a_x^1$; $a_y^0 = a_x^1$;

$\quad$ // Kinetic energy E_k, Potential energy E_k, Total energy E, Angular momentum in $\hat{z}$ L_z;

$\quad E_k^i = 0.5 M_{\mathrm{E}}((v_x^i)^2 + (v_y^i)^2)$;

$\quad E_p^i = -\frac{GM_{\mathrm{E}}}{r}$; $E^i = E_p^i + E_k^i$;

$\quad L_z^i = M_{\mathrm{E}}(x_i v_y^i - y_i v_x^i)$;

end

return $\vec{x}$, $\vec{y}$, $\vec{v}_x$, $\vec{v}_y$, $\vec{E}_k$, $\vec{E}_p$, $\vec{E}$, $\vec{L}_z$;

Algorithm 2: The Velocity-Verlet method for the Earth-Sun system. It initials from a circular orbit.

4 Results and discussion

4.1 Comparison between two methods

To test the stability of Euler forward (Euler) and the velocity-Verlet (VV) method, we initialize the Earth-Sun system with a circular orbit as stated in Algorithms **??**.

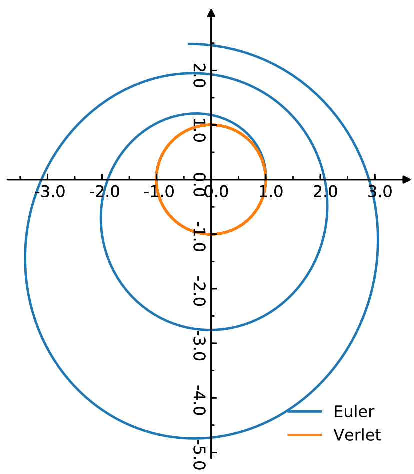
We varies the step size h starting from 0.02 yr to 0.001 yr. The Earth's orbits calculated by these two methods for 10 years are show in Fig. 1. Globally speaking, we see orbits given by the Euler method expand in time. On the other hand, VV methods' orbits keep circular with some tiny fluctuation hardly seen in Fig. 1a. It justifies the our statements in Sec. 3 that the VV method conserves energy but the Euler method increase energy.

For a large step size in Fig. 1a, the Euler method is very unstable. Its orbit deviates from circle both in distance and shape apparently. As the step size becomes smaller, we can see that the Euler method becomes better; as the orbits expand slower and slower from 1a to Fig. 1d. The trends we observed agree with the statement that the error in the Euler method goes down with decreasing h. We can hardly see differences between orbits yielded from the VV method, which indicates the it's stability.

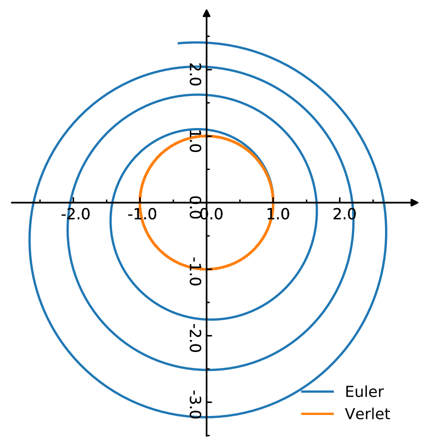
For detailed check and performance comparison, we list distances, energies, angular momentums together with execution times for these two methods in Table 1&2 with precision up to 10^{-6}. As conservation laws predicted by classical mechanics, physical quantities including kinetic, potential, total energies and angular momentum should be conserved in the Earth-Sun system. From these two tables, we can see conservations in the VV method but not in the Euler method. Thus, we can conclude that the VV method is stable and the Euler method is not.

Compared the execution time of two methods, we find the Euler method is faster. Counting the FLOPS from these two algorithms, we find there is about $30N$ for the Euler method and $45N$ for the VV method. It explains speed advantage of the Euler method.

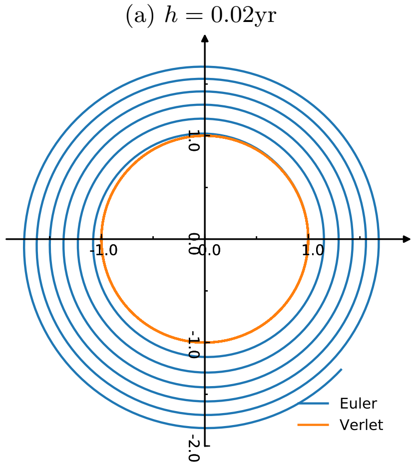
For physically meaningful, we will keep using the VV method in our further calculations.



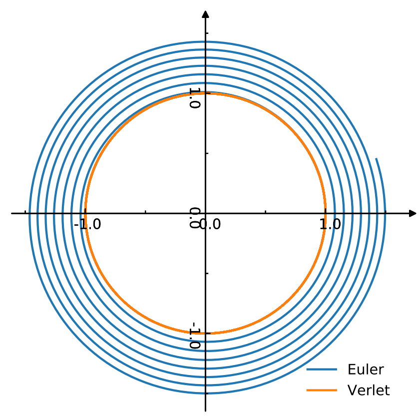
(a) $h = 0.02$yr



(b) $h = 0.01$year



(c) $h = 0.002$year



(d) $h = 0.001$year

Figure 1: Comparison of different step size h of two methods for 10 years.

4.2 Escape velocity from the Sun

In physics, the escape velocity from the Sun is defined as the minimum speed needed for an object to escape from its gravitational influence. An object starts from the Earth with a initial speed v_i. Suppose it can goes to infinity far at which potential energy is zero. At the same time, it has a minimum kinetic energy zero. Due to the energy conservation, we can generalize the formula for the escape velocity

$$\frac{mv_e^2}{2} - GM_{\rm S}m/r = 0 \Longrightarrow v_e = \sqrt{\frac{2GM_{\rm S}}{r}}. \tag{11}$$

We can see from Eq. 11 that the escape velocity v_e is independent of the mass of object. In our unit system $v_e = 2\sqrt{2}\pi$ which larger than the speed of circular v_c a factor of $\sqrt{2}$.

We would like to use a trial and error method to find the escape velocity. In our calculation, we fix the step size $h = 0.001$ and set up a criteria for escape. It is if an object doesn't start to turn back after time t_c, then it be regarded as a successful escape. We initialize our calculation the same as in Algorithm **??** except a different $v_y^0 = 2\pi\alpha$, where α is a constant larger than 1. With $1.3 < \sqrt{2} < 1.5$, we have a

Table 1: The Euler forward method: step size; kinetic energy; potential energy; total energy; angular momentum in z direction, distance from the Sum and execution time from left to the right.

h	E_{kin}	E_{pot}	E_{tot}	L_z	r	execution time (ms)
2.000E-02	3.300E-05	-4.700E-05	-1.400E-05	3.500E-05	2.520E+00	2.500E-02
1.000E-02	2.900E-05	-4.900E-05	-2.000E-05	3.200E-05	2.432E+00	5.000E-02
2.000E-03	3.200E-05	-6.500E-05	-3.300E-05	2.500E-05	1.824E+00	9.400E-02
1.000E-03	4.000E-05	-7.900E-05	-4.000E-05	2.300E-05	1.493E+00	1.680E-01

Table 2: The Velocity-Verlet method: step size; kinetic energy; potential energy; total energy; angular momentum in z direction, distance from the Sum and execution time from left to the right.

h	E_{kin}	E_{pot}	E_{tot}	L_z	r	execution time (ms)
2.000E-02	5.900E-05	-1.180E-04	-1.180E-04	1.900E-05	1.000014	2.600E-02
1.000E-02	5.900E-05	-1.180E-04	-1.180E-04	1.900E-05	1.000E+00	5.600E-02
2.000E-03	5.900E-05	-1.180E-04	-1.180E-04	1.900E-05	1.000E+00	1.840E-01
1.000E-03	5.900E-05	-1.180E-04	-1.180E-04	1.900E-05	1.000E+00	3.350E-01

lower and upper bounds for α where we can start a binary search for v_e.

The results for different t_c are presented in Table 3. From the table, we find $\alpha/\sqrt{2}$ converges to one as increasing t_c. Moreover, the total energy gets closer to zero at the same time. In sum, We would expect v_e and E_tot converge their theoretical value $2\sqrt{2}\pi$ and zero eventually.

4.3 Extension to whole solar system

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4.4 The perihelion precession of Mercury

Historically, the discrepancy between the observed and calculated values of perihelion precession of Mercury were not able to be accounted by classical Newtonian mechanics. Until the introduction of general relativity, the problem was solved. It also labeled as a great success of general relativity. The value results from relativistic correction is about $\delta\varphi \approx 43''$ per century[2]. In order to get this value, we introduce a correction to our gravitational force, so that the force becomes

$$\vec{F}_G = \frac{GM_{\mathrm{S}}M_{\mathrm{M}}\hat{r}}{r^2}\left[1 + \frac{3l^2}{r^2c^2}\right], \tag{12}$$

Table 3: The escape velocity factor $\alpha/\sqrt{2}$ in $v_e = 2\pi\alpha$ and total energy for different t_c.

t_c	$\alpha/\sqrt{2}$	E_{tot}
500	0.998968061	-5.9E-07
1000	0.998418985	-3.7E-07
2000	0.999002447	-2.4E-07
5000	0.999456311	-1.3E-07
10000	0.999655708	-0.8E-07
20000	0.999781297	-0.5E-07
50000	0.999879019	-0.3E-07

Table 4: The perihelion precession angle $\delta\varphi$ of Mercury due to relativistic correction after one century.

h	$\delta\varphi$
5.00E-07	$53.2277''$
2.00E-07	$45.8665''$
1.00E-07	$42.8183''$
5.00E-08	$42.9333''$

where M_{M} is the mass of Mercury, l is $\vec{r} \times \vec{v}$ and c is the speed of light in vacuum.

In our calculation, we use the Mercury mass and new force to calculate the acceleration. The system initials from $x_0 = 0.3075$, $y_0 = 0$, $v_x^0 = 0$ and $v_y^0 = 12.44$. For this elliptical orbit, theoretical calculation gives a period $T_m \approx 0.24073$yr. We also notice for a resolution higher to $1''$, we have to use a very small step size.

Before setting up the step size, we did a rough estimation. The Mercury moves about 420 circles in a century which is about 5.5E08 degrees. To distinguish 1" for a century, we need a step size $h = 100/5.5\text{E}08 \approx 1.84\text{E-}07$. Therefore, $h = 1.0\text{E-}07$ would be a good choice.

We try different h in our calculations and the final results are given in Table 4. The outcomes justify our estimation that the error will less than $1''$ for $h = 1.0\text{E-}07$. Eventually, our calculation gives $\delta\varphi = 42.9333''$ with h smaller to 5.0E-08 which is very close to the theoretical value $43''$.

5 Conclusions

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References

[1] Søren Toxvaerd, Ole J Heilmann, and Jeppe C Dyre. Energy conservation in molecular dynamics simulations of classical systems. *The Journal of chemical physics*, 136(22):224106, 2012.

[2] Wikipedia contributors. Two-body problem in general relativity — wikipedia, the free encyclopedia, 2018. [Online; accessed 1-April-2018].

[3] Morten Hjorth-Jensen. Computational physics lectures: Eigenvalue problems. `https://compphysics.github.io/ComputationalPhysicsMSU/doc/pub/eigvalues/html/eigvalues.html`. Accessed Mar 5, 2018.