Numerical methods
Bachelor in Physics

Practicum 6: Ordinary differential equations with BC

Contact: jeroen.mulkers@uantwerpen.be U.305

1. **The pendulum.** The equation of motion of a pendulum with length L is

$$\frac{d^2\theta}{dt^2} = -\frac{g}{L}\sin\theta,$$

with g as the standard gravity. For small deviations, it holds true that $\sin\theta \approx \theta$. This approximation simplifies the equation to

$$\frac{d^2\theta}{dt^2} = -\frac{g}{L}\theta.$$

Solving this differential equation is easy:

$$\theta(t) = C_1 \cos(2\pi t/T + C_2),$$

The constants C_1 and C_2 can be derived from the initial conditions θ en $\omega = d\theta/dt$. The periodicity is given by $T = 2\pi\sqrt{\frac{L}{g}}$.

Solve numerically the equation of motion of the pendulum without the small-angle approximation. Use Euler's method (make your own implementation or use the file slinger_euler.m). Choose time units $t' = \sqrt{L/g}$. Plot the angle and velocity in function of the time. Plot also the velocity in function of the angle. What do you notice? Do you get a more accurate solution when you use the Euler-Cromer method (see slides)?. What happens when you start with a large initial angle?

Another method which is used to derive the equation of motion is the Verlet integration, which is described below.

Verlet integration. Let's start with the following equations of motion.

$$\frac{d\vec{r}}{dt} = \vec{v}$$
$$\frac{d^2\vec{r}}{dt^2} = \vec{a}.$$

When using the central difference scheme for the first and second derivative, we obtain

$$\frac{\vec{r}_{i+1} - \vec{r}_{i-1}}{2h} + O(h^2) = \vec{v}_i$$
$$\frac{\vec{r}_{i+1} - 2\vec{r}_i + \vec{r}_{i-1}}{h^2} + O(h^2) = \vec{a}_i,$$

with step size h. This can be rewritten to the following scheme

$$\vec{r}_{i+1} = 2\vec{r}_i - \vec{r}_{i-1} + h^2\vec{a}_i + O(h^4) \tag{1}$$
$$\vec{v}_i = \frac{\vec{r}_{i+1} - \vec{r}_{i-1}}{2h} + O(h^2). \tag{2}$$

This method is called 'Verlet integration'. Assume that $\vec{r}_1$ and $\vec{r}_2$ are known, then one can calculate $\vec{r}_3$ with expression (1). Next, one can calculate $\vec{v}_2$ with expression (2). And so on.

However, $\vec{r}_1$ and $\vec{v}_1$ are ussualy known, and $\vec{r}_2$ unknown. You can use Euler's method in the first step to calculate $\vec{r}_2 = \vec{r}_1 + \vec{v}_1 h$, and then proceed with the Verlet integration.

Verlet integration has a small rounding error. Furthermore the computation of the velocity can be skipped if the force depends only on $\vec{r}$. This makes the method ideal for the calculation of paths in many particle simulations, such as in molecular dynamics' simulations.

Write a script (or function file) which uses Verlet integration to solve the equation of motion of the pendulum. Plot again the position and velocity in function of the time. Visualize the phase space of the pendulum by solving the equation of motion for different initial conditions.

2. **The predator-prey model.** The following set of differential equations (which are based on the Volterra equations) model the interaction between a predator and a prey population:

$$\frac{dP}{dt} = K_1 P - CPJ$$
$$\frac{dJ}{dt} = -K_2 J + DPJ$$

with initial conditions $P = P_0$ and $J = J_0$ at $t = 0$. P denotes the size of the prey population (e.g. hares) and J denotes the size of the predator population (e.g. lynx). K_1, K_2, C and D are positive constants. The first equation shows how the prey population change depends on two factors. Firstly, the size of the population increases proportionally to the size of the population itself (they procreate), and secondly, the size of the population will decrease with the amount of encounters between predator and pray, which is proportional to the product of the size of both populations. On the other hand, the size of the predator population will decrease if there are many predators, due to rivalry, and will increase proportionally to the number of encounters between predator and prey (since this means more food for the predators).

The solution of this system of differential equations depends strongly on the values of the constants, and will, in many cases, result in a stable cycle. The determination of the constants is not our task (it's the task of biologists). We will use $K_1 = 2, K_2 = 10, C = 0.001$ and $D = 0.002$. Solve these differential equations with MATLAB's ODE solver `ode45`. Start with a population of 5000 hazes and 100 lynx. Plot the size of the populations in function of the time.

3. **Orbit of comet around the sun.** Consider a small satellite, such as a comet, which rotates around the sun. We will use a Copernican coordinate system with the sun in the origin. Consider only the attractive force of the sun on the comet and neglect all other forces. The force on the comet is

$$\vec{F} = -G\frac{mM}{|\vec{r}|^3}\vec{r},$$

with $\vec{r}$ the position of the comet, m its mass, $M(= 1.99 \times 10^{30}$ kg) the mass of the sun, and $G(= 6.67 \times 10^{11}$ m^3/kg·s^2) the gravitational constant. We will use 1 year as the unit of time, and the astronomical unit for distances (AU $= 1.496 \times 10^{11}$ m), which is equal to the distance between the sun and the earth. Using these units, it holds true that $GM = 4\pi^2 \mathrm{AU}^3/\mathrm{jaar}^2$. We will also use the mass m of the comet as the unit of mass. The mass of the comet is typically $10^{15\pm3}$ kg.

Let's recapitulate some well known results about the orbits of satellites. The total energy of a satellite is

$$E = \frac{1}{2}mv^2 - \frac{GMm}{r}.$$

This total energy is a conserved quantity, just like the angular momentum $\vec{L} = \vec{r} \times m\vec{v}$. The centripetal force will be equal to the attractive force if the orbit is circular.

$$\frac{mv^2}{r} = \frac{GMm}{r^2} \Rightarrow v = \sqrt{GM/r}.$$

E.g. for a circular orbit with $r = 1$ AU, the velocity $v = 2\pi\mathrm{AU/jaar}$ (approximately 30 000 km/h). The total energy is then given by

$$E = -\frac{GMm}{2r}. \tag{3}$$

The large and small axis of the orbit, a and b, are different if the orbit is elliptic. The eccentricity e is defined as

$$e = \sqrt{1 - \frac{b^2}{a^2}}.$$

The eccentricity of the earth is $e = 0.017$, which means that it is almost a perfect sphere. Expression (3) for the total energy holds true for elliptical orbits if we replace r with the large axis a;

$$E = -\frac{GMm}{2a}.$$

For the velocity, we obtain

$$v = \sqrt{GM\left(\frac{2}{r} - \frac{1}{a}\right)}.$$

Finally, we can use the conservation of angular momentum to derive Kepler's law:

$$T = \frac{4\pi^2}{GM}a^3,$$

with T the period of the orbit.

a) The script `orbe.m` calculates the orbit of a comet around the sun using Euler's method. Study this script and visualize the result for a *circular* orbit with radius 1 and time step 0.02 jaar. You will see that the method of Euler is not stable, just like in the example with the pendulum. Do you see this in the plot of the energy?

b) Implement the Euler-Cromer algorithm and check again for a circular orbit.

c) Run the Euler-Cromer algorithm for $r_0 = 1$, $v_0 = \pi$ and $\tau = 0.02$ year. What is happening? What is the meaning of the positive energy?

d) Do you get a better result if you decrease the time step to 0.005 year? Note the improper drift of the orbit. We need an even better method.

For the zealous students (not obligatory):

e) Implement the Runga-Kutta fourth-order method for this problem and study again the orbit and the total energy.

f) Note that the velocity of the comet is at it largest when it is close to the sun. One can expect that it is useful to use a small step size when the comet is near the sun, and a large step size when the comet is far away from the sun. If you make the orbit more elliptic (e.g. use $r_0 = 1, v_0 = \pi/2$), then the Runge-Kutta method will fail for $\tau = 0.005$.

Even for $\tau = 0.0005$, you will notice a drift of the orbit. Choosing an even smaller step size will lead to large computation times. Instead, try to implement the Runga-Kutta method with an adaptive time step in order to increase the accuracy.

4. **The Lorrentz attractor.** The laws of Newton give a deterministic description of the material world. It has long been thought that, in principle, it should be possible to predict the weather by the aid of computers. In the beginning of the sixties, the Dutch mathematician and meteorologist Edward Lorentz[1] thought this assumption was false. He concluded that the weather is intrensically unpredictable. Lorentz formulated a simple model to describe the weather. This model consisted out of 12 non-linear differential equations. He noticed that a chaotic behaviour which was extremely dependent on the initial conditions.

   Later, he introduced a more simple model, with only three variables, which showed the same chaotic behaviour. The model of Lorentz is given by

$$\begin{aligned}
\frac{dx}{dt} &= \sigma(y - x) \\
\frac{dy}{dt} &= rx - y - xz \\
\frac{dz}{dt} &= xy - bz
\end{aligned}$$

   with σ, r and b positive constants (usually, one takes $\sigma = 10$ en $b = 8/3$). For $r > 24.7$, the system exhibits a chaotic behaviour.

   Solve this system by using `ode45`. Plot x, y and z in function of the time. Study the paths in phase space: plot x in function of y, and x in function of z. Compare the results for two, almost identical, initial conditions. Why is the behaviour called 'chaotic'? Study also the effect of a very small r.

   Lorentz called the extreme dependence on the initial conditions, the 'butterfly' effect: a single stroke of a butterfly's wing can have a noticeable impact on the weather.

[1] Not to be confused with Hendrik Lorentz, we all know of the Lorrentz transformation and the Lorentz force.