Methods of Mathematical Physics I: Numerical Analysis 1

IUCAA-NCRA Graduate School

August - September 2012

8 August 2012

To be returned in the class on 17 August 2012

- The deadline for the submission of the solutions of this assignment will be strictly enforced. No credits will be given if the assignment is not returned in time.
- You are free to discuss the solutions with friends, seniors and consult any books. However, you are expected to write the numerical program by yourself. You should understand and be clear about every step in the program. Marks may be reduced if you have not understood what you have written even though the answer and the plots are correct.
- Let me know if you find anything to be unclear or if you think that something is wrong in any of the questions.

Simple Harmonic Oscillator:

Consider a classical simple harmonic oscillator described by the well known ordinary differential equation (ODE)

$$\frac{\mathrm{d}^2x}{\mathrm{d}t^2} = -\omega_0^2 x.$$

It is possible to rescale $t \to \omega_0 t$ such that the equation takes a convenient form

$$\frac{\mathrm{d}^2x}{\mathrm{d}t^2} = -x.$$

Let us say that the initial conditions at $t = 0$ are $v(0) = \dot{x}(0) = v_0,\ x(0) = x_0$. The solution of the above equation is then

$$x(t) = x_0 \cos t + v_0 \sin t.$$

Also, you know that the total energy of the system is conserved:

$$E = \frac{1}{2}\left(v^2 + x^2\right) = \frac{1}{2}\left(v_0^2 + x_0^2\right).$$

For numerical solutions, we need to rewrite the second order ODE as a set of two coupled first order ODEs:

$$\frac{\mathrm{d}v}{\mathrm{d}t} = -x; \qquad \frac{\mathrm{d}x}{\mathrm{d}t} = v.$$

Suppose we know the values of v and x at a time t, then the time at a later instant $t + \Delta t$ can be found by carrying out a Taylor expansion:

$$v(t + \Delta t) = v(t) - x(t)\Delta t; \qquad x(t + \Delta t) = x(t) + v(t)\Delta t.$$

We have ignored terms $\mathcal{O}(\Delta t)^2$ in the above expansion.

Let us now discretize the time axis such that

$$t_i = i\ \Delta t; \qquad i = 0, 1, 2, \ldots$$

Then we can find the values of the position and velocity at a time t_{i+1} using the above Taylor expansion

$$v(t_{i+1}) = v(t_i) - x(t_i)\Delta t; \qquad x(t_{i+1}) = x(t_i) + v(t_i)\Delta t.$$

Since $x(t_0) = x(0) = x_0$ and $v(t_0) = v_0$ are given as initial conditions, the equation can be used for determining the values at successive steps. This method of solving ODEs numerically is known as the **Euler method**.

For definiteness, let us take $x_0 = 0, v_0 = 1$.

1. Take $\Delta t = 0.1$ and solve the system of equations numerically from $t = 0$ to $t = 20$. Plot $x(t)$ and $v(t)$. Also plot the energy $E(t) = (x^2 + v^2)/2$ along with the theoretical value of the conserved energy $E_{\mathrm{theo}} = (x_0^2 + v_0^2)/2$. Find the smallest value of t for which the quantity

$$\delta E \equiv \frac{|E_{\mathrm{theo}} - E(t)|}{E_{\mathrm{theo}}} > 0.2.$$

Note that δE measures the deviation of the numerically evaluated energy from its theoretical value, i.e., it gives an idea about how accurate your calculations are.

[10 marks]

2. Repeat the problem with $\Delta t = 0.01$. What is the smallest value of t where $\delta E > 0.2$?

[5 marks]

You might have realized that the energy of the oscillator computed by the above method is not conserved. This happens because we have ignored higher order terms in the Taylor expansions. Decreasing Δt helps to some extent, however, the program will take longer to complete if we decrease the step size.

A somewhat better method of solving the equations would be to realize that while solving for the new position $x(t+\Delta t)$, we have used the velocity at the instant t. Clearly this is an oversimplification. An improvement would be to use the velocity halfway between, i.e., at $t + \Delta t/2$. We can then change the relevant equations to

$$v(t + \Delta t/2) = v(t - \Delta t/2) - x(t)\Delta t; \quad x(t + \Delta t) = x(t) + v(t + \Delta t/2)\Delta t.$$

One difficulty with this approach is that we require $v(-\Delta t/2)$ to compute $v(\Delta t/2)$, while we are given only $v(0)$. We thus make the approximation $v(-\Delta t/2) = v(0) - x(0)\Delta t/2$. Then the system is solved completely. This method of solving ODEs is known as the **leap-frog method**.

There is still another difficulty with this method: Suppose we want to calculate quantities like the energy E at a given time t. We would require both $x(t)$ and $v(t)$ to compute the energy. Unfortunately, the velocity is calculated only in half steps, i.e., we only have $v(t-\Delta t/2)$ and $v(t+\Delta t/2)$ but not $v(t)$. To avoid this problem, assume $v(t) = v(t-\Delta t/2) - x(t)\Delta t/2$ while calculating $E(t)$.

3. Now, using the leap-frog method, solve the same simple harmonic oscillator problem from $t = 0$ to $t = 20$. Use $\Delta t = 0.1$. Plot $x(t), v(t)$ and $E(t)$ as before. What is the maximum value of δE you get for $0 \le t \le 20$?

[15 marks]

4. **Bonus:** Solve the non-linear oscillator problem

$$\frac{\mathrm{d}^2 x}{\mathrm{d}t^2} = -\sin x$$

using the leap-frog method. Solve for three sets of initial conditions: $\{x(0) = 0.5, v(0) = 0\}$, $\{x(0) = 2.5, v(0) = 0\}$ and $\{x(0) = 3.14, v(0) = 0\}$. Plot $x(t), v(t)$ and $E(t)$ for $0 \le t \le 50$ for the three cases. Also plot the phase space diagram, i.e., the trajectory in the (v, x) space, for the three cases.

Kepler Problem:

The Kepler problem for a body moving under a r^{-2} force is described by the ODE

$$\frac{\mathrm{d}^2 \mathbf{x}}{\mathrm{d}t^2} = -\frac{GM\mathbf{x}}{|\mathbf{x}|^3}.$$

Since the motion is confined to a plane, it is sufficient to work with two-dimensional Cartesian coordinates (x, y). Then the relevant equations are

$$\frac{\mathrm{d}^2 x}{\mathrm{d}t^2} = -\frac{GMx}{r^3}; \quad \frac{\mathrm{d}^2 y}{\mathrm{d}t^2} = -\frac{GMy}{r^3}; \quad r = \sqrt{x^2 + y^2}.$$

As before, we can rescale the coordinates such that $GM = 1$.

5. Solve the Kepler problem using the leap-frog method. Take the initial conditions to be $x(0) = 0.5,\ y(0) = 0.0,\ \dot{x}(0) = 0.0,\ \dot{y}(0) = 1.63$. Take the time interval $\Delta t = 0.1$ and solve the equations till $t = 5$. Plot the motion of the particle in the (x, y) plane. Also plot the energy as a function of t.

[20 marks]

There are more sophisticated methods for solving ODEs accurately and efficiently. They are mostly based on the **Runge-Kutta** method. Nowadays there are routines which are readily available for use. You can learn about these from the book *Numerical Recipes in Fortran 77* by Press, Teukolsky, Vetterling & Flannery (Chapter 16). There are corresponding books on other programming languages as well.