PH 4433/6433 HW 4, due Wednesday Sept. 30

1 ODE solvers

This problem is based on 9.5.4 on pages 205-206. For this homework you will solve the following 2nd order ODE:

$$m\frac{d^2x}{dt^2} = -kx^{p-1}$$

For $p = 2$ this reduces to simple harmonic motion with the solution $x(t) = A\sin(\omega_0 t + \phi)$, $\omega_0 = \sqrt{k/m}$.

1. Take $p = 2$. Pick values of k and m such that the period T of the oscillator is 1.

2. Use 4th order Runge-Kutta to solve this ODE (use program module from class). You will have three source code files:

   (a) deriv.f90 : This contains definitions of parameters (n, k/m, etc). These should be "public" if other modules need to use their value. This file also contains the definition of the ODE itself.

   (b) rk4.f90 : contains the Runge-Kutta code. You will not have to modify this file at all.

   (c) main.f90 : Here you define the solution vector $y(i)$ and set initial conditions. The actual integration of the ODE is a simple loop calling rk4.

   The program is compiled like this: `gfortran -O2 deriv.f90 rk4.f90 main.f90`

3. Solve for several periods of oscillation. Starting with a relatively large step size ($\Delta t \approx T/5$), show how the error varies with t. Make plots of the error versus t (like Fig 9.5) for several values of Δt.

4. Modify the `rk4.f90` module so that it instead uses the 2nd-order Runge-Kutta algorithm. Repeat part (2) with this code.

5. Repeat with the Runge-Kutta-Fehlberg `rk45.f90` code. How does the error vary with time when you give this code a certain error tolerance?

2 Classical Scattering

Based on 9.14, pp 222-225.

In this problem you will solve for the trajectory of a point particle moving in two dimensions, interacting with the following potential function:

$$V(x,y) = x^2y^2e^{-(x^2+y^2)}$$

A plot of $V(x,y)$ is in Fig. 9.8, page 223. You can also view a plot in `gnuplot` with the following commands:

```
set xrange[-1:1]
set yrange[-1:1]
splot x*x*y*y*exp(-(x*x+y*y))
```

The particle is given an initial velocity $\vec{v}_i = v_i \hat{j}$ in the $+y$ direction. The impact parameter b is the initial value of x for the particle. You want to solve for the scattering angle θ after the particle interacts with the potential.

1. Write a program to solve for the motion of the particle using 4th order Runge-Kutta. The ODE in standard form is on page 224; note that for the positive (repulsive) potential, the upper sign in Eq. 9.67 is used. Note that in the text, the y's are numbered from zero, while in the Fortran array they will be numbered from one. In addition to the position of the particle you should calculate its kinetic and potential energies.

2. Take the mass of the particle $m = 0.5$. Take the initial conditions for the particle as

   $y(1) \equiv x = b$

   $y(2) \equiv y = -y_0$

   $y(3) \equiv \frac{dx}{dt} = 0$

   $y(4) \equiv \frac{dy}{dt} = 0.5$

   b is the impact parameter, which you will vary between -1 and 0. y_0 is the initial y position of the particle, which you should choose such that the initial ratio of potential to kinetic energy is very small, around 10^{-10}.

3. Verify that your solution conserves the total energy of the particle. This is a good test that the results are correct.

4. Make some plots of the trajectory $(x,y) = (y(1), y(2))$ for several values of b

5. Calculate the scattering angle θ as a function of b and make a plot of $\theta(b)$ for $-1 < b < 0$. The formula for θ is given on page 224. Note that you must integrate for a large enough time that the particle as left the region near the potential. The text suggests I recommend checking for two conditions before calculating θ:

   (a) PE/KE $< 10^{-10}$ (suggested by text)

   (b) $t > t_0$ This is so the integration proceeds enough that the particle has time to interact.

6. Interpret your results for $\theta(b)$. Does the θ you get for $b = -1$ and $b = 0$ make sense? Try increasing the number of b's you calculate in the intermediate region. You will find very complicated behavior.

7. Try initial y velocities ($y(4)$) of 1.0 and 1.5, plotting $\theta(b)$ for each. What is different in this case?