Assignment XI: Differential Equations

Due 11/21/2016

1. *(6 pts)* **Solution of a Differential Equation**

(a) Writer a computer code to solve the differential equation

$$y'(x) = 2(y+1) \tag{1}$$

in the region $-2 < x < 2$ using Euler's method. Use as initial condition $y(0) = 0$.

Use as step size $h = 0.05$, 0.1, 0.15, and 0.2, and plot your results and the error with respect to the exact solution of the differential equation.

(b) Use a fixed step size $h = 0.1$ and compare your result of the Euler method with the improved Euler method and the 4th order Runge-Kutta method (rk4.f90). Plot your different solutions and the error.

(c) Use the adaptive Runge-Kutta solver from *difsis.f90*. Use as starting value your smallest h from **(a)** and compare the final h the codes uses with the values of h used in **(a)** and **(b)**. Compare the error obtained with the errors from **(a)** and **(b)**.

(d) Solve the differential equation using Picard iteration. Start with the initial guess $y_0(x) = 0$. Use your favorite integration scheme, and plot your iterations $n = 4, 8, 12, 16$ with the exact solution and document the error.

(e) Assess and discuss the errors of your four different algorithms for solving Eq. (1).

2. *(6 pts)* **Classical Coulomb Problem**

The general form of Newton's equation of motion is given as

$$m\frac{d^2\mathbf{r}}{dt^2} = \mathbf{F}(t, \mathbf{r}, \mathbf{v}) \tag{2}$$

with

$$\begin{aligned} \mathbf{r}(t_0) &= \mathbf{r}_0 \\ \mathbf{v}(t_0) &= \mathbf{v}_0 \end{aligned} \tag{3}$$

Consider a particle of mass $m = 1u$ (unified atomic mass units), carrying the elementary charge $q = -e$, which orbits around a fixed charge $Q = e$, located at the origin. The initial position of the particle is at $x_0 = 1\mathring{A}$ and $y_0 = 0$. Its velocity components are $v_{x_0} = 0$ and $v_{y_0} = 4.5\mathring{A}/ps$. The Coulomb force components are given by

$$F_x = K\frac{qQ}{r^2}\frac{x}{r}$$

$$F_y = K\frac{qQ}{r^2}\frac{y}{r}, \tag{4}$$

where $K = e^2/(r\pi = 14.3996517 eV/\AA$.

(a) Propagate the trajectory of the particle up to $t_{max} = 20ps$ using the improved Euler method using a step $h = 0.01$. Plot the time dependence of the particle's x-position and its trajectory. Assess the stability of the orbit, and determine the orbital period.

(b) Repeat **(a)** using the Runge-Kutta method of *rk4.f90*, again with the time step $h = 0.01$. Assess the stability of the two different orbits in **(a)** and **(b)**, explain qualitatively the difference if there is any, and if so, determine the time step h for which the orbit is close to the one in **(b)**.

(c) Plot for both cases the kinetic, potential, and total energies, as well as the particle trajectories. Since you did not explicitly built energy conservation into the solution of the differential equation, checking that the total energy is conserved is a demanding test of the accuracy of your solution. Check if your numerically computed energy is constant at the different time-steps.

(d) Check the long-term *stability* of your solution by plotting

$$\log\left[\frac{|E(t) - E(t=0)|}{E(t=0)}\right] \tag{5}$$

for a large number of cycles. You may get 11 or more places of precision. If you do not, then you may need to decrease the value of h or look for bugs in your program.