PHYS 305: Computational Physics II

Winter 2018

Homework #2

(Due: February 5, 2018)

Each problem is worth 10 points. E-mail your soultions to `steve@physics.drexel.edu` *with a subject including PHYS 305 and the Homework number. The e-mail should have as an attachment a zip (or tar) file containing a PDF document containing all discussion, reasults, and graphs requested, and files containing Python scripts for all programs written.*

1. The general form of a Runge-Kutta scheme (state $n \to n+1$) to solve the ODE

$$\frac{dy}{dx} = f(x, y)$$

is

$$\begin{aligned}
\delta y_0 &= \delta x\, f(x_n,\, y_n) \\
\delta y_1 &= \delta x\, f(x_n + a_1\delta x,\, y_n + b_{10}\delta y_1) \\
\delta y_2 &= \delta x\, f(x_n + a_2\delta x,\, y_n + b_{20}\delta y_0 + b_{21}\delta y_1) \\
&\cdot \\
&\cdot \\
&\cdot \\
\delta y_{s-1} &= \delta x\, f\left(x_n + a_{s-1}\delta x,\, y_n + \sum_{i=0}^{s-2} b_{s-1,i}\,\delta y_i\right) \\
y_{n+1} &= y_n \;+\; \sum_{i=0}^{s-1} c_i \delta y_i
\end{aligned}$$

(see Numerical Recipes, Sec. 16.2). This is not quite the syntax used previously in class or in the book—the count starts at 0 to facilitate translation of the algorithm into Python. The method is defined by s, the number of stages, the offsets a_i and b_{ji}, and the weights c_i.

(a) Implement the following scheme, defined by $s = 6$, $a = (0, 1/5, 3/10, 3/5, 1, 7/8)$, $c = (37/378, 0, 250/621, 125/594, 0, 512/1771)$, and

$$b = \begin{pmatrix}
0 & & & & & \\
1/5 & 0 & & & & \\
3/40 & 9/40 & 0 & & & \\
3/10 & -9/10 & 6/5 & 0 & & \\
-11/54 & 5/2 & -70/27 & 35/27 & 0 & \\
1631/55296 & 175/512 & 575/13824 & 44275/110592 & 253/4096 & 0
\end{pmatrix},$$

where all elements on and above the diagonal are zero.

(b) Apply this integrator to the Duffing oscillator with parameters $\alpha = -2$, $\beta = 1$, $\delta = 0$ (as used in class), with initial conditions $y = 1$ and $y' = 1.5$ at $x = 0$. Integrate the system from $x = 0$ to $x = 20$ with step size $\delta x = 0.01$ and plot (i) the phase portrait (y versus x) and (ii) the energy error $E(x) - E(0)$ as a function of x.

(c) For the same parameters and initial conditions, make a log–log plot of the absolute value of the final energy error $|E(20) - E(0)|$ as a function of δx for $\delta x = 2^{-n}, n = 1, \ldots 13$, and hence determine the order of this scheme.

(d) Run the calculation from $x = 0$ to $x = 20$, and then backwards from $x = 20$ to $x = 0$ and print the values of y and y' at the end. Is the scheme reversible?

2. The general form of a symplectic scheme to solve the conservative second-order dynamical system

$$\begin{aligned}\frac{dx}{dt} &= v\\ \frac{dv}{dt} &= a(x)\end{aligned}$$

is

$$\begin{aligned}v &= v + d_0\, a(x)\, \delta t\\ x &= x + c_0\, v\, \delta t\\ &\ \ \vdots\\ v &= v + d_{s-1}\, a(x)\, \delta t\\ x &= x + c_{s-1}\, v\, \delta t\end{aligned}$$

This generalized "kick–drift" method is defined by s, the number of stages, and the coefficients c_i and d_i.

(a) Implement the following scheme, defined by $s = 4$, $c = (1/r, q/r, q/r, 1/r)$, $d = (0, 2/r, -2p/r, 2/r)$, where $p = 2^{1/3}$, $q = 1 - p$, $r = 4 - 2p$.

(b) Apply this integrator to the Duffing oscillator with parameters $\alpha = -2$, $\beta = 1$, $\delta = 0$ (as used in class), with initial conditions $x = 1$ and $v = 1.5$ at $t = 0$. Integrate the system from $t = 0$ to $t = 20$ with step size $\delta t = 0.01$ and plot (i) the phase portrait (v versus x) and (ii) the energy error $E(t) - E(0)$ as a function of t.

(c) For the same parameters and initial conditions, make a log–log plot of the absolute value of the final energy error $|E(20) - E(0)|$ as a function of δt for $\delta t = 2^{-n}, n = 1, \ldots 13$, and hence determine the order of this scheme.

(d) Run the calculation from $t = 0$ to $t = 20$ with $\delta t = 0.01$, and then backwards from $t = 20$ to $t = 0$ with the same δt, and print the values of x and v at the end. Is the scheme reversible?