PHYS 305: Computational Physics II

Winter 2018

Homework #6

(Due: March 22, 2018, at noon)

Answer three problems. Each is worth 10 points. As usual, e-mail your solutions 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, results, and graphs requested, and files containing Python scripts for all programs written.*

1. A 6th-order symplectic scheme is defined by

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

for $s = 8$, where the eight c and d coefficients are determined as follows:

(a) Define

$$w = (-1.17767998417887,\ 0.235573213359357,\ 0.784513610477560)$$

(with indices running from 0 to 2) and

$$w_{sum} = 1 - 2\sum_{k=0}^{2} w_k$$

(b) Define

$$\begin{aligned} c_0 &= c_7 = \tfrac{1}{2} w_2 \\ c_1 &= c_6 = \tfrac{1}{2}(w_2 + w_1) \\ c_2 &= c_5 = \tfrac{1}{2}(w_1 + w_0) \\ c_3 &= c_4 = \tfrac{1}{2}(w_0 + w_{sum}) \end{aligned}$$

(c) Define

$$\begin{aligned} d_0 &= 0 \\ d_1 &= d_7 = w_2 \\ d_2 &= d_6 = w_1 \\ d_3 &= d_5 = w_0 \\ d_4 &= w_{sum} \end{aligned}$$

(a) Implement this scheme and verify (as in Homework 2, problem 2) that it is 6th order and time reversible. Be careful if you cut and paste w from the PDF, as characters may be silently lost or substituted!

(b) Apply the scheme to the dynamics of a system of $N = 50$ identical particles of total mass 1, initially distributed in a uniform sphere of radius 1 with randomly oriented velocities all of magnitude 0.7 (see Homework 3, problem 3a). Run the system with $G = 1$ and softening parameter $\epsilon = 0.001$ for 20 time units, and find a fixed time step δt such that the energy is conserved to within 10^{-4} by the end of the run. State the value of δt you have found. Do you think variable time steps might be warranted in this case?

(c) Create a duplicate system, place the two clusters in a circular orbit with separation 2 units and circular center of mass speeds of 0.5, and allow the combined system to evolve. How long does it take for the two clusters to merge and settle down into an equilibrium state, as judged by oscillations in the total kinetic energy of the system (see Homework 4, problem 1)? Plot the kinetic, potential, and total energies of the system as a function of time.

2. How does the accuracy of the shooting method depend on the accuracy of the underlying integrator used? Up to now we have simply adopted Runge-Kutta 4 with a fixed step, but the result must depend at some level on our choice of scheme and step Δx. Solve the boundary-value problem

$$y'' + +2y' + y - 10y^2 + 5y^3 \;=\; 0,$$

with $y(0) = 0$, $y(2) = 1$, by shooting from $x = 0$, but this time vary both the integration scheme and the choice of step. Solve the problem in turn using the Midpoint method, Runge-Kutta 4, and the 6th-order Runge-Kutta method introduced in Homework 2, problem 1, using steps $\Delta x = 0.001, 0.01$, and 0.1. Focus on the solution that, for "standard" parameters (Runge-Kutta 4, $\Delta x = 0.01$), has $y'(0)$ between 60 and 70, and do the following for this particular solution.

Use the maximum absolute difference $\Delta(y^{(1)}, y^{(2)}) = \max_n \left(|y_n^{(1)} - y_n^{(2)})|\right)$ as a measure of the deviation between solutions $y^{(1)}(x)$ and $y^{(2)}(x)$, and make a table of the deviation of each scheme from Runge-Kutta 6 with $\Delta x = 0.001$, which we will assume is the best solution. (Is this a good assumption?) Also plot as a function of x the the difference $y(x) - y^{best}(x)$ between each solution and this "best" solution on a single graph. What conclusions can you draw about the choice of integration parameters?

3. The time-independent Schrödinger equation for the hydrogen atom starts off as a complicated three-dimensional partial differential equation for the wavefunction $\psi(\mathbf{r})$. However, as you have seen/will see in Quantum I/II, we can separate the radial and angular behavior by writing

$$\psi(\mathbf{r}) \;=\; R(r)Y_{lm}(\theta, \phi),$$

where Y_{lm} is a spherical harmonic describing the angular part of the solution. In this case the radial equation simplifies to

$$\frac{1}{r^2}\left(r^2 R'\right)' + \left[\frac{2m_e}{\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0 r} + E\right) - \frac{l(l+1)}{r^2}\right] R \;=\; 0,$$

where $R' = dR/dr$.

(a) Make the system non-dimensional by writing $x = r/a_0$, where

$$a_0 \;=\; \frac{4\pi\epsilon_0\hbar^2}{m_e e^2}$$

is the Bohr radius of the atom, and then defining $u = xR$. Show that the equation becomes

$$u'' + \left[z + \frac{2}{x} - \frac{l(l+1)}{x^2}\right] u = 0,$$

where $u' = du/dx$ and $z = 32\pi^2\epsilon_0 E\hbar^2/m_e e^4$ is the dimensionless electron energy.

(b) Use the shooting method to find the first 5 spherically symmetric ($l = 0$) solutions of this equation. You can shoot from $x = 0$ because we know that $u(x) \to 0$ at least as fast as x as $x \to 0$, so the $1/x$ term in the acceleration never becomes singular. Plot the solutions, labeled by their (dimensionless) energies, on the same graph.

4. The matrix method described in class is based on simple second-order differencing of the differential equation

$$y'' + g(x)\, y \;=\; 0,$$

using the expansion

$$y''_n \;=\; \frac{y_{n+1} - 2y_n + y_{n-1}}{\Delta^2} + \mathcal{O}(\Delta^2),$$

leading to the matrix equation

$$y_{n+1} - \Big[2 - \Delta^2 g(x_n)\Big] + y_{n-1} \;=\; r_n,$$

where the matrix corresponds to interior points only and the vector on the right side takes care of the boundary conditions (see class notes). Implementations of a basic boundary-value solver and an eigenvalue solver (assuming boundary conditions $y = 0$ at the ends of the range) can be found on the course web page, as `matrix_ode.py` and `ex7.9.py`. Note that these scripts differ slightly from those presented in class, in that the `numpy` bug leading to their unexpected scaling has been corrected, so please refresh your browser window to make sure you have the proper versions.

The Numerov algorithm improves upon these simple methods. Numerov realized that, since the next term is in fact $\frac{1}{12}\Delta^2 y''''$, it can also be estimated by taking the numerical derivative of the original differential equation. The details can be found in the Wikipedia page linked to the course web page. The result is a remarkably compact fourth-order method that can be applied with essentially no additional work, but leads to substantially more accurate results.

Implement the Numerov algorithm, taking if you wish the online examples as starting points, and answer the following questions:

(a) Apply the simple and Numerov methods to the basic boundary-value problem discussed numerous times in class

$$y'' + y \;=\; 0,$$

with $y(0) = 1, y(1) = 2$. Use the maximum absolute error $\Delta y = \max_n \left(|y_n - y_a(x_n)|\right)$ as a measure of accuracy, where y_a is the analytic solution. Determine how the errors of the two methods scale with Δ by considering systems with $\Delta = 1/N$, for $N = 5, 10, 20, \cdots, 640$.

(b) Show that the eigenvalue problem

$$y'' + g(x)\, y + zy \;=\; 0,$$

with $y(a) = 0, y(b) = 0$, becomes with Numerov a matrix equation of the form

$$Ay + z\,\Delta^2 By = 0$$

and write down the matrices A and B. The problem then reduces to finding the eigenvalues and eigenvectors of the matrix $B^{-1}A$.

Hence solve the following problems relating to the Schrödinger equation, choosing a, b, and N as appropriate:

(i) Find all bound eigenvalues and plot the corresponding eigenfunctions of the finite well system with $U_0 = 50$.

(ii) Find the first 10 bound eigenvalues and plot the corresponding eigenfunctions of the harmonic oscillator with potential $U = x^2$.

(iii) Find all bound eigenvalues and plot the corresponding eigenfunctions of the system with potential $U = -\exp(-\sqrt{|x|})$.