Numerical Engineering Analysis

Homework 4

Due: October 25, class-time

Please complete the following Chapter 4 exercises from the textbook.

Q1. Exercise 1 on page 84.

Q2. Exercise 16 on page 91.

Q3. Exercise 20 on page 94.

Q4. Exercise 25 on page 97-98.

Q5. Exercise 26 on page 98-99.

Note that the shooting method requires a time integrator. Hence, you might use the second-order Runge-Kutta (RK2) integrator or a fourth-order Runge-Kutta (RK4), or you can even use existing ode45 in MATLAB or odeint in python. You can also use ode45 in Exercise 16 (see https://en.wikipedia.org/wiki/Lorenz_system). If it is not stated in the problem description, you can use step size of h=0.01 or h=0.001. These problems will not take too much CPU time.

techniques were discussed in Section 2.5. Finite difference formulas for first and second derivatives can be substituted, for example, in (4.41), and the resulting system of equations can be solved. Alternatively, the differential equation can be transformed, and the resulting equation can be solved using uniform mesh formulas.

EXERCISES

1. Consider the equation

$$y' + (2 + 0.01x^2)y = 0$$
$$y(0) = 4 \quad 0 \leq x \leq 15.$$

   (a) Solve this equation using the following numerical schemes: i) Euler, ii) backward Euler, iii) trapezoidal, iv) second-order Runge–Kutta and v) fourth-order Runge–Kutta. Use $\Delta x = 0.1, 0.5, 1.0$ and compare to the exact solution.
   (b) For each scheme, estimate the maximum Δx for stable solution (over the given domain) and discuss your estimate in terms of results of part (a).

2. A physical phenomenon is governed by the differential equation

$$\frac{dv}{dt} = -0.2v - 2\cos(2t)v^2$$

   subject to the initial condition $v(0) = 1$.

   (a) Solve this equation analytically.
   (b) Write a program to solve the equation for $0 < t \leq 7$ using the Euler explicit scheme with the following time steps: $h = 0.2, 0.05, 0.025, 0.006$. Plot the four numerical solutions along with the exact solution on one graph. Set the x axis from 0 to 7 and the y axis from 0 to 1.4. Discuss your results.
   (c) In practical problems, the exact solution is not always available. To obtain an accurate solution, we keep reducing the time step (usually by a factor of 2) until two consecutive numerical solutions are nearly the same. Assuming that you do not know the exact solution for the present equation, do you think that the solution corresponding to $h = 0.006$ is accurate (to plotting accuracy)? Justify your answer. In case you find it not accurate enough, obtain a better one.

3. Discuss the stability of the real and spurious roots of the second-order Adams–Bashforth method and plot them. How would you characterize the behavior of the spurious root in the right half-plane where the exact solution is unbounded? Show that the stability diagram in Figure 4.10 is the intersection of the regions of stability of both roots.

4. Suppose we use explicit Euler to start the leapfrog method. Obtain expressions for c_1 and c_2 in terms y_0 and λh, in (4.33). Use power series expansions to show that the leading term in the expansion of c_2 is $O(h^2)$. Discuss the power series expansion of c_1.

16. Non-linear differential equations with several degrees of freedom often exhibit chaotic solutions. Chaos is associated with sensitive dependence to initial conditions; however, numerical solutions are often confined to a so-called strange attractor, which attracts solutions resulting from different initial conditions to its vicinity in the phase space. It is the sensitive dependence on initial conditions that makes many physical systems (such as weather patterns) unpredictable, and it is the attractor that does not allow physical parameters to get out of hand (e.g., very high or low temperatures, etc.) An example of a strange attractor is the Lorenz attractor, which results from the solution of the following equations:

$$\frac{dx}{dt} = \sigma(y - x)$$
$$\frac{dy}{dt} = rx - y - xz$$
$$\frac{dz}{dt} = xy - bz.$$

The values of σ and b are usually fixed ($\sigma = 10$ and $b = 8/3$ in this problem) leaving r as the control parameter. For low values of r, the stable solutions are stationary. When r exceeds 24.74, the trajectories in xyz space become irregular orbits about two particular points.

(a) Solve these equations using $r = 20$. Start from point $(x, y, z) = (1, 1, 1)$, and plot the solution trajectory for $0 \le t \le 25$ in the xy, xz, and yz planes. Plot also x, y, and z versus t. Comment on your plots in terms of the previous discussion.

(b) Observe the change in the solution by repeating (a) for $r = 28$. In this case, plot also the trajectory of the solution in the three-dimensional xyz space (let the z axis be in the horizontal plane; you can use the MATLAB command `plot3(z,y,x)` for this). Compare your plots to (a).

(c) Observe the unpredictability at $r = 28$ by overplotting two solutions versus time starting from two initially nearby points: (6, 6, 6) and (6, 6.01, 6).

17. In this problem we will numerically examine vortex dynamics in two dimensions. We assume that viscosity is negligible, the velocity field is solenoidal ($\nabla \cdot \boldsymbol{u} = 0$), and the vortices may be modeled as potential point vortices. Such a system of potential vortices is governed by a simple set of coupled equations:

$$\frac{dx_j}{dt} = -\frac{1}{2\pi} \sum_{\substack{i=1 \\ i \neq j}}^{N} \frac{\omega_i (y_j - y_i)}{r_{ij}^2} \tag{1a}$$

$$\frac{dy_j}{dt} = \frac{1}{2\pi} \sum_{\substack{i=1 \\ i \neq j}}^{N} \frac{\omega_i (x_j - x_i)}{r_{ij}^2} \tag{1b}$$

where (x_j, y_j) is the position of the jth vortex, ω_j is the strength and rotational direction of the jth vortex (positive ω indicates counter-clockwise rotation), with h being the time step.

(a) Determine the coefficients $\omega_1, \omega_2, \beta_0$, and β_1 that would maximize the order of accuracy of the method. Can you name this method?
(b) Applying this method to $y' = \alpha y$, what is the maximum step size h for α pure imaginary?
(c) Applying this method to $y' = \alpha y$, what is the maximum step size h for α real negative?
(d) With the coefficients derived in part (a) draw the stability diagram in the $(h\lambda_R, h\lambda_I)$ plane for this method applied to the model problem $y' = \lambda y$.

20. The following scheme has been proposed for solving $y' = f(y)$:

$$
\begin{aligned}
y^* &= y_n + \gamma_1 h f(y_n) \\
y^{**} &= y^* + \gamma_2 h f(y^*) + \omega_2 h f(y_n) \\
y_{n+1} &= y^{**} + \gamma_3 h f(y^{**}) + \omega_3 h f(y^*)
\end{aligned}
$$

where

$$\gamma_1 = 8/15, \qquad \gamma_2 = 5/12, \qquad \gamma_3 = 3/4, \qquad \omega_2 = -17/60, \qquad \omega_3 = -5/12,$$

with h being the time step.

(a) Give a word description of the method in terms used in this chapter.
(b) What is the order of accuracy of this method?
(c) Applying this method to $y' = \alpha y$, what is the maximum step size h for α pure imaginary and for α negative real?
(d) Draw a stability diagram in the $(h\lambda_R, h\lambda_I)$ plane for this method applied to the model problem $y' = \lambda y$.

21. Chemical reactions often give rise to stiff systems of coupled rate equations. The time history of a reaction of the following form:

$$
\begin{aligned}
&\mathrm{A}_1 \rightarrow \mathrm{A}_2 \\
&\mathrm{A}_2 + \mathrm{A}_3 \rightarrow \mathrm{A}_1 + \mathrm{A}_3 \\
&2\mathrm{A}_2 \rightarrow 2\mathrm{A}_3
\end{aligned}
$$

is governed by the following rate equations

$$
\begin{aligned}
\dot{C}_1 &= -k_1 C_1 + k_2 C_2 C_3 \\
\dot{C}_2 &= k_1 C_1 - k_2 C_2 C_3 - 2k_3 C_2^2 \\
\dot{C}_3 &= 2k_3 C_2^2
\end{aligned}
$$

where k_1, k_2, and k_3 are reaction rate constants given as

$$k_1 = 0.04, \qquad k_2 = 10.0, \qquad k_3 = 1.5 \times 10^3,$$

and the C_i are the concentrations of species A_i. Initially, $C_1(0) = 0.9$, $C_2(0) = 0.1$, and $C_3(0) = 0$.

(a) What is the analytical steady state solution? Note that these equations should conserve mass, that is, $C_1 + C_2 + C_3 = 1$.

equations in

$$\phi = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix} = \begin{bmatrix} y \\ y' \\ y'' \\ y''' \end{bmatrix}.$$

The general solution can be written as

$$\phi = \psi + \sum_{i=1}^{4} c_i \boldsymbol{u}^{(i)}$$

where ψ is the particular solution obtained by shooting with homogeneous conditions. The $\boldsymbol{u}^{(i)}$ are the solutions of the homogeneous equation with initial conditions $\boldsymbol{e}_i$, where the $\boldsymbol{e}_i$ are the Cartesian unit vectors in four dimensions. Show that only three "shots" are necessary to solve the problem and that one only needs to solve a 2×2 system of equations to get c_3 and c_4. In addition, explain why with this procedure only one shot will be necessary for each additional P that may be used.

25. The goal of this problem is to compute the self-similar velocity profile of a compressible viscous flow. The flow is initiated as two adjacent parallel streams that mix as they evolve. After some manipulation and a similarity transformation, the thin shear layer equations (the boundary layer equations) may be written as the third-order ordinary differential equation:

$$f''' + ff'' = 0 \tag{1}$$

where $f = f(\eta)$, η being the similarity variable. The velocity is given by $f' = u/U_1$, U_1 being the dimensional velocity of the high-speed fluid. U_2 is the dimensional velocity of the low-speed fluid. The boundary conditions are

$$f(0) = 0 \qquad f'(\infty) = 1 \qquad f'(-\infty) = \frac{U_2}{U_1}.$$

This problem is more difficult than the flat-plate boundary layer example in the text because the boundary conditions are specified at three different locations. A very accurate solution, however, may be calculated if you shoot in the following manner:

(a) Guess values for $f'(0)$ and $f''(0)$. These, with the given boundary condition $f(0) = 0$, specify three necessary conditions for advancing the solution numerically from $\eta = 0$. Choose $f'(0) = (U_1 + U_2)/(2U_1)$, the average of the two streams.

(b) Shoot to $\eta = \infty$. (For the purposes of this problem ∞ is 10. This can be shown to be sufficient by asymptotic analysis of the equations.)

(c) Now here's where we get around the fact that we have a three-point boundary value problem. We observe that $g(a\eta) = f(\eta)/a$ also satisfies Equation (1). If we choose $a = f'(10)$, which was obtained in (b), the equation recast in g and the corresponding boundary conditions at zero and ∞ are satisfied.

(d) Now take the initial guesses, divide by a and solve for the lower half of the shear layer in the g variable. You have $g(0) = 0$, $g'(0) = f'(0)/a$, and

$g''(0) = f''(0)/a$ giving the required initial condition for advancing the solution in g from $\eta = 0$ to $\eta = -10$.

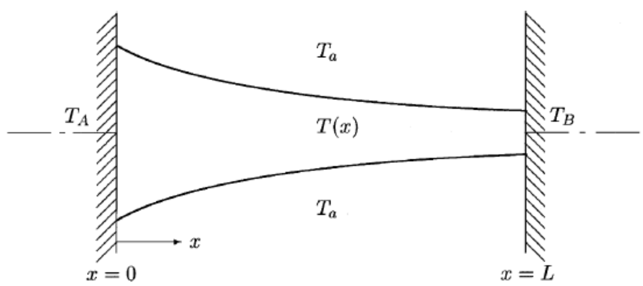
(e) Compare the value of $g'(-10)$ to the boundary condition $f'(-\infty) = U_2/U_1$. Use this difference in a secant method iteration specifying new values of $f''(0)$ until $g'(-10) = U_2/U_1$ is within some error tolerance.

As iteration proceeds, fixing $g'(-10)$ to the boundary condition for $f'(-10)$ in (e) forces a to approach 1 thus making $g \approx f$, the solution. However, a will not actually reach 1, because we do not allow our $f'(0)$ guess to vary. The solution for g, though accurate, may be further refined using step (f).

(f) Use your final value for $g'(0)$ as the fixed $f'(0)$ value in a new iteration. Repeat until you have converged to $a = 1$ and evaluate.

Take $U_1 = 1.0$ and $U_2 = 0.5$, solve, and plot $f'(\eta)$. What was your final value of a? Use an accurate ODE solver for the shooting. (First reproduce the Blasius boundary layer results given in Example 4.9 in the text. Once that is setup, then try the shear layer.) How different is the solution after (f) than before with $f'(0) = (U_1 + U_2)/(2U_1)$?

26. The diagram shows a body of conical section fabricated from stainless steel immersed in air at a temperature $T_a = 0$. It is of circular cross section that varies with x. The large end is located at $x = 0$ and is held at temperature $T_A = 5$. The small end is located at $x = L = 2$ and is held at $T_B = 4$.



Conservation of energy can be used to develop a heat balance equation at any cross section of the body. When the body is not insulated along its length and the system is at a steady state, its temperature satisfies the following ODE:

$$\frac{d^2T}{dx^2} + a(x)\frac{dT}{dx} + b(x)T = f(x), \tag{1}$$

where $a(x)$, $b(x)$, and $f(x)$ are functions of the cross-sectional area, heat transfer coefficients, and the heat sinks inside the body. In the present example, they are given by

$$a(x) = -\frac{x+3}{x+1}, \qquad b(x) = \frac{x+3}{(x+1)^2}, \quad \text{and} \quad f(x) = 2(x+1) + 3b(x).$$

(a) In this part, we want to solve (1) using the shooting method.

(i) Convert the second-order differential equation (1) to a system of 2 first-order differential equations.

(ii) Use the shooting method to solve the system in (i). Plot the temperature distribution along the body.

(iii) If the body is insulated at the $x = L$ end, the boundary condition becomes $dT/dx = 0$. In this case use the shooting method to find $T(x)$ and in particular the temperature at $x = L$. Plot the temperature distribution along the body.

(b) We now want to solve (1) directly by approximating the derivatives with finite difference approximations. The interval from $x = 0$ to $x = L$ is discretized using N points (including the boundary points):

$$x_j = \frac{j-1}{N-1}L \quad j = 1, 2, \ldots, N.$$

The temperature at point j is denoted by T_j.

(i) Discretize the differential equation (1) using the central difference formulas for the second and first derivatives. The discretized equation is valid for $j = 2, 3, \ldots, N-1$ and therefore yields $N-2$ equations for the unknowns $T_1, T_2, \ldots, T_N$.

(ii) Obtain two additional equations from the boundary conditions ($T_A = 5$ and $T_B = 4$) and write the system of equations in matrix form $AT = f$. Solve this system with $N = 21$. Plot the temperature using symbols on the same plot of part (a)(ii).

27. *Mixed boundary conditions.*
With the implementation of boundary conditions in boundary value problems, it is important to preserve the structure of the matrix created by the interior stencil. This often facilitates the solution of the resulting linear equations. Consider the problem in Section 4.11.2 with a mixed boundary condition:

$$ay(0) + by'(0) = g$$

(a) Use the technique suggested in Section 4.11.2 to implement this boundary condition for the problem given by (4.41) and find the new entries in the first row of the matrix.

(b) Alternatively, introduce a ghost point y_{-1} whose value is unknown. Using the equation for the boundary condition and the differential equation evaluated at the point $j = 0$, eliminate y_{-1} to obtain an equation solely in terms of y_0 and y_1. What are the entries in the first row of the matrix?

28. Consider the following eigenvalue problem:

$$\frac{\partial^2 \phi}{\partial x^2} + k^2 f(x)\phi = 0,$$

with the boundary conditions $\phi(0) = \phi(1) = 0$. k is the eigenvalue and ϕ is the eigenfunction. $f(x)$ is given and known to vary between 0.5 and 1.0. We would like to find positive real values of k that would allow nonzero solutions of the problem.

(a) If one wants to use the shooting method to solve this problem, how should the ODE system be set up? What initial condition(s) should be used? What