INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI

DEPARTMENT OF MATHEMATICS

MA 322: SCIENTIFIC COMPUTING

Semester–II, Academic Year 2022-23

Some Practice Problems

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1. Show that $x = -t^2/4$ and $x = 1 - t$ are solutions of the initial-value problem (IVP)

$$2x' = \sqrt{t^2 + 4x} - t, \tag{1}$$
$$x(2) = -1. \tag{2}$$

Does this contradict the Picard's theorem for existence and uniqueness of solutions of an IVP? Justify your answer. Solve the above IVP using your favorite numerical method to solve IVP and compare your result with the closed form solutions mentioned above.

2. The following initial-value problem (IVP)

$$x' = t^2 + e^x \qquad x(0) = 0$$

has a unique solution in the interval $|t| \leq 0.351$ (Verify!). Solve the IVP using fourth-order Adams-Bashforth-Multon method for $0 \leq t \leq 0.5$. Comments on the solution for $t > 0.351$.

3. Solve the following IVP

$$x''' - \sin(x') + e^t x' + 2t\cos x = 25, \tag{3}$$
$$x(0) = 5 \quad x'(0) = 3 \quad x''(0) = 7. \tag{4}$$

4. Solve the following autonomous IVP

$$x''' + 2x'' - x' - 2x = e^t, \tag{5}$$
$$x(8) = 3 \quad x'(8) = 2 \quad x''(8) = 1. \tag{6}$$

numerically.

5. Write

$$y'' + yz = 0 \qquad y(0) = 1 \qquad y'(0) = 0 \tag{7}$$
$$z' + 2yz = 4 \qquad z(0) = 3 \tag{8}$$

as a system of first-oder equations with initial conditions. Solve the resultant IVP.

6. Derive the fifth-order Adams-Bashforth and Adams-Multon methods.

7. Derive the third-order Runge-Kutta (RK) method.

8. Show that the local truncation error of the modified Euler method

$$x(t+h) = x(t) + hf\left(t + \frac{1}{2}h, x(t) + \frac{1}{2}hf(t, x(t))\right)$$

is $\mathbf{O}(h^3)$. Determin $m \geq 1$ such that $\tau = \mathbf{O}(h^m)$.

9. Prove that when the fourth-order RK method is applied to the problem $x' = \lambda x$, the formula for advancing this solution will be

$$x(t+h) = \left[1 + h\lambda + \frac{1}{2}h^2\lambda^2 + \frac{1}{6}h^3\lambda^+ \frac{1}{24}h^4\lambda^4\right] x(t).$$

Hence, determine the range of stability of the method.

10. The specific volume of a super-heated steam is listed in steam tables for various temperatures. For example, at a pressure of 3000 lb/in^2:

T (°F)	v (ft^3/lb$_m$)
700	0.0977
720	0.12184
740	0.14060
760	0.15509
780	0.16643

Use first- through fourth-order polynomial interpolation to estimate v at $T = 750$°F. Interpret your results.

11. The Redlich-Kwong equation of state is given by

$$p = \frac{RT}{v-b} - \frac{a}{v(v+b)\sqrt{T}},$$

where R = the gas constant [= 0.518 kJ/(kg K)], T = absolute temperature (K), p = absolute pressure (kPa), and v = the specific volume of a kg of gas (m^3/kg). The parameters a and b are calculated by

$$a = \frac{0.427R^2T_c^{2.5}}{p_c}, \qquad b = 0.0866R\frac{T_c}{p_c},$$

where p_c = critical pressure (kPa) and T_c = critical temperature (K). You are asked to determine the amount of methane fuel (p_c = 4580 kPa and T_c = 191 K) that can be held in a 3-m^3 tank at a temperature of -50°C with a pressure of 65,000 kPa. Use the bisection method of your choice to calculate v and then determine the mass of methane contained in the tank.

12. Develop a fixed point iteration scheme to find the root of any given number X. Also find the root using Newton's method.

13. The Manning equation may be written for a rectangular open channel as:

$$Q = \frac{\sqrt{S}(BH)^{5/3}}{n(B+2H)^{2/3}}$$

where Q is the flow rate (m^3/s), S is the slope (m/m), H is the depth (m) and n is the Mannin roughness coefficient. Solve the above equation for H, when $Q = 5$, $S = 0.0002$, $B = 20$ and $n = 0.03$, using the Newton's method.

14. Use Newton's method to find the root of the equation: $e^{-0.5x}(4 - x) - 2 = 0$. Try different initial guesses and see to which root(s) do the iterations converge.

15. Determine the roots of the simultaneous non-linear equations:

$$\begin{aligned}(x-4)^2 + (y-4)^2 &= 5 \\ x^2 + y^2 &= 16\end{aligned}$$

using the Newton's method. Can you take an initial guess such that $x_0 = y_0$? Explain.

16. Solve the equation $f(x) \equiv -2x^6 - 1.5x^4 + 10x + 2 = 0$ using the Secant Method. Try the initial guess $x_{-1} = 0$ and $x_0 = 1$.

17. Determine the lowest positive root of $f(x) \equiv 7e^{-x}\sin(x) - 1 = 0$. Start with initial guesses, $x_{-1} = 0.5$ and $x_0 = 0.4$.

18. Develop a computer program to solve the following set of $2n$ non-linear algebraic equations using Newton's method, for the unknowns $\mathbf{y} = [c_1,\ x_1,\ c_2,\ x_2,\ ...,\ c_n,\ x_n]^T$.

$$f_k(\mathbf{y}) \equiv \sum_{j=1}^{n} c_j x_j^{k-1} - \int_{-1}^{1} t^{k-1}\mathrm{d}t = 0, \qquad k = 1,\ 2,\ ...,\ 2n$$

Report your solutions for $n = 2,\ 3$ and 4. These equations naturally arise while applying Gauss quadrature to approximately compute integrals.

19. Perform the following integrals using the Trapezoidal and the Simpson's 1/3 rule, for various values of the arguments (x, y, etc.) of your choice:

$$\begin{aligned}
&\text{(a)} \qquad I(y) = \int_{-\infty}^{y} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right)\mathrm{d}x \\
&\text{(b)} \qquad Ei(x) = \int_{x}^{\infty} \frac{e^{-x}}{x}\mathrm{d}x \\
&\text{(c)} \qquad Si(z) = \int_{0}^{z} \frac{\sin(t)}{t}\mathrm{d}t
\end{aligned}$$

20. The outflow concentration from a reactor is measured at discrete times over a 24-hr period and the values are as follows:

t (hr.)	0	1	5.5	10	12	14	16	18	20	24
c, (mg/l)	1	1.5	2.3	2.1	4	5	5.5	5	3	1.2

The outflow rate in m^3/s may be computed using the relation:

$$Q(t) = 20 + 10\sin\left\{\frac{2\pi}{24}(t-10)\right\}$$

where t is in seconds. Compute the average concentration leaving the reactor over the 24-hr. period. The avg. concentration is defined as:

$$\bar{c} = \frac{\int_0^t \mathrm{d}t' Q(t')c(t')}{\int_0^t \mathrm{d}t' Q(t')}$$

21. It is suspected that the high amounts of tannin in mature oak leaves inhibit the growth of the winter moth (*Operophtera bromata L., Geometridae*) larvae that extensively damage these trees in certain years. The following table (Table 1) lists the average weight of two samples of larvae at times in the first 28 days after birth.

Day	0	6	10	13	17	20	28
Sample 1 average weight (mg)	6.67	17.33	42.67	37.33	30.10	29.31	28.74
Sample 1 average weight (mg)	6.67	16.11	18.89	15.00	10.56	9.44	8.89

Table 1: Average weight of oak leaves (two samples)

The first sample was reared on young oak leaves, whereas the second sample was reared on mature leaves from the same tree.

(a) Use Lagrange interpolation to approximate the average weight on days 12 and 16 for each sample.

(b) Find an approximate maximum average weight for each sample by determining the maximum.

22. Recall that the velocity of the free falling parachutist with linear drag can be computed analytically as

$$v(t) = \frac{gm}{c}(1 - e^{-(c/m)t}),$$

where $v(t)$ is velocity (m/s), t is time (s), $g = 9.81$ m/s^2, m is mass (kg), c is linear drag coefficient (kg/s). Use Composite Simpson's $\frac{1}{3}$-rd integration rule to compute how far the jumper travels during the first 8 seconds of free fall given $m = 80$ kg and $c = 10$ kg/s. Compute the answer to $|\varepsilon_a| < 0.1\%$.

23. You measure the voltage drop V across a resistor for a number of different values of current i. The results are

i	V
0.25	20.45
0.75	20.6
1.25	0.70
1.5	1.88
2.0	6.0

Use second- through fourth-order polynomial interpolation (both Newton divided difference and Lagrange interpolation) to estimate the voltage drop for $i = 1.15$. Use $x_0 = 0.25$ as the base point for the linear interpolation. Interpret your results.

24. Bacteria growing in a batch reactor utilize a soluble food source (substrate) as depicted in Fig 1. The uptake of the substrate is represented by a logistic model with Michaelis-Menten limitation. Death of the bacteria produces detritus which is subsequently converted to the substrate by hydrolysis. In addition, the bacteria also excrete

some substrate directly. Death, hydrolysis and excretion are all simulated as first-order reactions. Mass balances can be written as

$$\begin{aligned}
\frac{\mathrm{d}X}{\mathrm{d}t} &= \mu_{\max}\Big(1-\frac{X}{K}\Big)\Big(\frac{S}{K_s+S}\Big)X - k_d X - k_e X \\
\frac{\mathrm{d}C}{\mathrm{d}t} &= k_d X - k_h C \\
\frac{\mathrm{d}S}{\mathrm{d}t} &= k_e X + k_h C - \mu_{\max}\Big(1-\frac{X}{K}\Big)\Big(\frac{S}{K_s+S}\Big)X
\end{aligned}$$

where X, C, and S = the concentrations [mg/L] of bacteria, detritus, and substrate, respectively; $\mu_{\max}$ = maximum growth rate [/d], K = the logistic carrying capacity [mg/L]; K_s = the Michaelis-Menten half-saturation constant [mg/L], k_d = death rate [/d]; k_e = excretion rate [/d]; and k_h = hydrolysis rate [/d]. Simulate the concentrations from $t = 0$ to 100 d, given the initial conditions $X(0) = 1$ mg/L, $S(0) = 100$ mg/L, and $C(0) = 0$ mg/L. Employ the following parameters in your calculation: $\mu_{\max} = 10$/d, $K = 10$ mg/L, $K_s = 10$ mg/L, $k_d = 0.1$/d, $k_e = 0.1$/d, and $k_h = 0.1$/d.

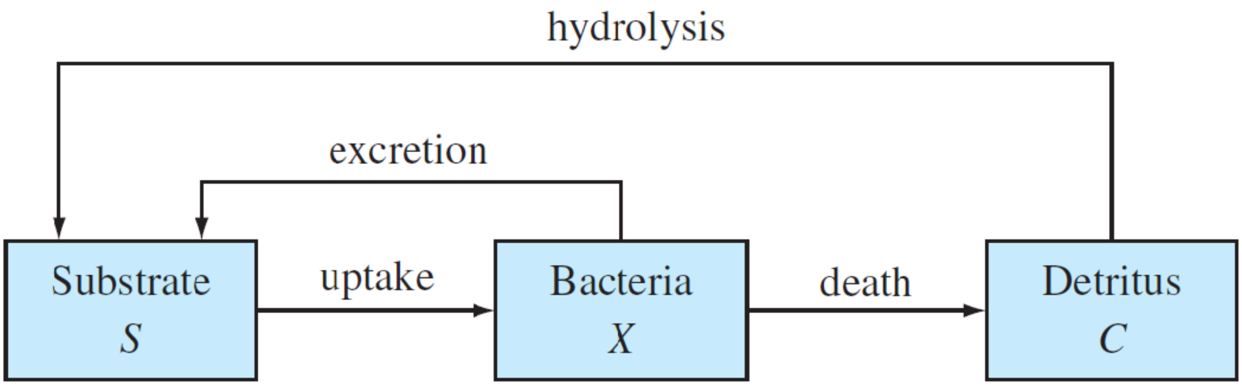


Figure 1:

25. Solve the Lorenz equations:

$$\begin{aligned}
\frac{\mathrm{d}x}{\mathrm{d}t} &= -\sigma x + \sigma y \\
\frac{\mathrm{d}y}{\mathrm{d}t} &= rx - y - xz \\
\frac{\mathrm{d}z}{\mathrm{d}t} &= -bz + xy
\end{aligned}$$

using the fourth-order RK method for $\sigma = 10$, $b = 2.666667$, $r = 28$, and initial conditions of $x = y = z = 5$. In all cases use single-precision variables and a step size of 0.1 and simulate from $t = 0$ to 20. Develop phase-plane plots (A phase-plan representation is useful in discerning the underlying structure of a mathematical model. Rather than plotting x, y and z versus t, we can plot x versus y and x versus z. These plots illustrate the way that the state variables (x and y, and x and y) interact, and are referred to as a phase-plane representations.).

26. Epidemiology is the study of progression of a disease in a population. While there are many models available, the Kermack-McKendrick SIR model is one of the simplest ones, which tracks the number of people infected by a contagious virus in a closed population. It assumes a fixed population size (i.e., negligible births and deaths as compared to the entire population due to disease, or other natural causes), incubation period of the infectious agent is instantaneous, and duration of infectivity is the same as the length of the disease. It also assumes a completely homogeneous population with no age, spatial, or social structure. The resulting equations are as follows:

$$\frac{\mathrm{d}S}{\mathrm{d}t} = -\beta S(t)I(t)$$

$$\frac{\mathrm{d}I}{\mathrm{d}t} = \beta S(t)I(t) - \gamma I(t)$$

$$\frac{\mathrm{d}R}{\mathrm{d}t} = \gamma I(t)$$

where $S(t)$ is the susceptible population, $I(t)$ is the infected population and $R(t)$ is the number of people to have recovered from the disease and developed immunity - all of these are normalized and unitless quantities. On the other hand, β is the infectivity and γ is the recovery rate. The key element in a disease progression is the quantity, $R_0 = \beta S(t)/\gamma$, which essentially indicates (see the second equation) on average how many people are infected by a single infected individual. If $R_0 < 1$, the infections decay over time; if $R_0 > 1$, no. of infections grow. Solve the above equations subject to $S(0) = 1$, $I(0) = 10^{-6}$ and $R(0) = 0$ using the 4-th order RK method, for various choices of β and γ. Make plots of S, I, R and R_0 with t.

27. The basic differential equation of the elastic curve for a uniformly loaded beam (Fig. 2) is given as

$$EI\frac{\mathrm{d}^2y}{\mathrm{d}x^2} = \frac{wLx}{2} - \frac{wx^2}{2}$$

where E = the modulus of elasticity and I = the moment of inertia. Solve for the deflection of the beam using

   (a) the finite-difference approach ($\Delta x = 2$ ft) and

   (b) the shooting method.

   The following parameter values apply: $E = 30,000$ ksi, $I = 800$ in^4, $w = 1$ kip/ft, $L = 10$ ft. Compare your numerical results to the analytical solution,

$$y = \frac{wLx^3}{12EI} - \frac{wx^4}{24EI} - \frac{wL^3x}{24EI}.$$

28. The temperature distribution in a tapered canonical cooling fin (see Fig. 3) is described by the following differential equation, which has been nondimensionallized

$$\frac{\mathrm{d}^2u}{\mathrm{d}x^2} + \left(\frac{2}{x}\right)\left(\frac{\mathrm{d}u}{\mathrm{d}x} - pu\right) = 0,$$

where u = temperature ($0 \le u \le 1$), x = axial distance ($0 \le x \le 1$), and p is a nondimensional parameter that describes the heat transfer and geometry

$$p = \frac{hL}{k}\sqrt{1 + \frac{4}{2m^2}},$$

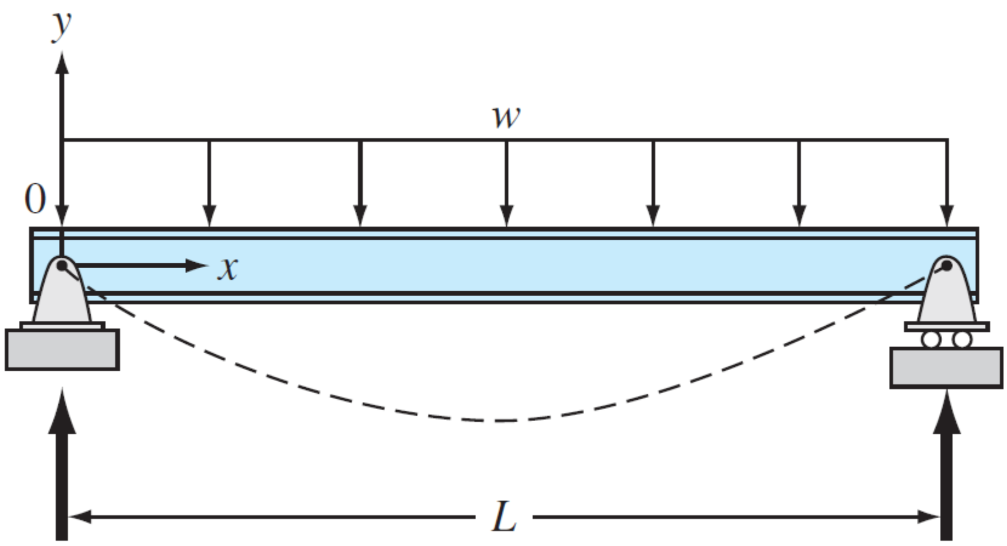


Figure 2:

where h = a heat transfer coefficient, k = thermal conductivity, L = the length or height of the cone, and m = slope of the cone wall. The equation has the boundary conditions

$$u(x = 0) = 0, \quad u(x = 1) = 1.$$

Solve this equation for the temperature distribution using finite difference methods. Use second-order accurate finite difference analogues for the derivatives. Write a computer program to obtain the solution and plot temperature versus axial distance for various values of $p = 10, 20, 50$, and 100.

29. The steady-state height of the water table in a one-dimensional, unconfined groundwater aquifer (Fig. 4) can be modeled with the following second-order ODE,

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(Kh\frac{\mathrm{d}h}{\mathrm{d}x}\right) + N = 0,$$

where x = distance [m], K = hydraulic conductivity [m/d], h = height of the water table [m], and N =infiltration rate [m/d]. Solve for the height of the water table for $x = 0$ to 1000 m where $h(0) = 10$ m and $h(1000) = 5$ m. Use the following parameters for the calculation: $K = 1$ m/d and $N = 0.0001$ m/d. Obtain your solution with

(a) the shooting method, and

(b) the finite-difference method ($\Delta x = 100$ m).

30. A rod subject to an axial load will be deformed, as shown in the stress-strain curve (see figure 5). The area under the curve from zero stress out to the point of rupture is called the modulus of toughness of the material. It provides a measure of the energy per unit volume required to cause the material to rupture. As such, it is representative of the material's ability to withstand an impact load. Use Trapezoidal method to compute the modulus of toughness for the shown stress-strain curve.

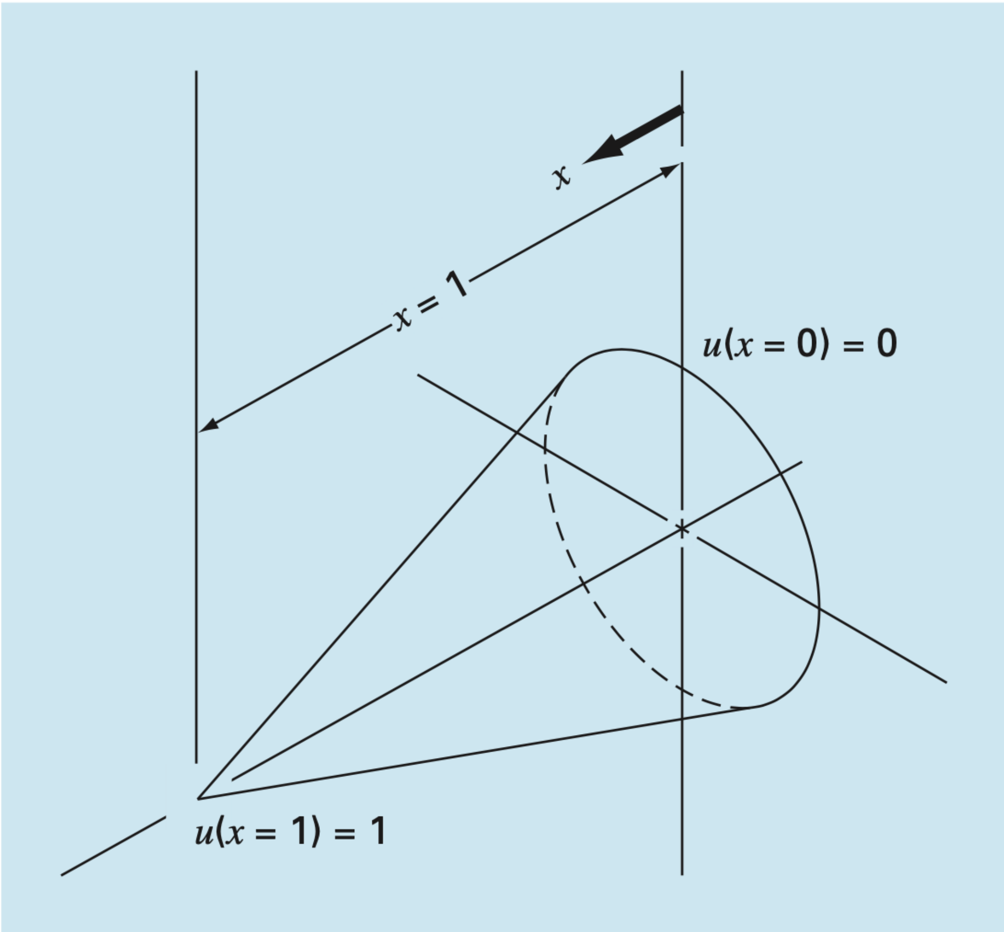


Figure 3:

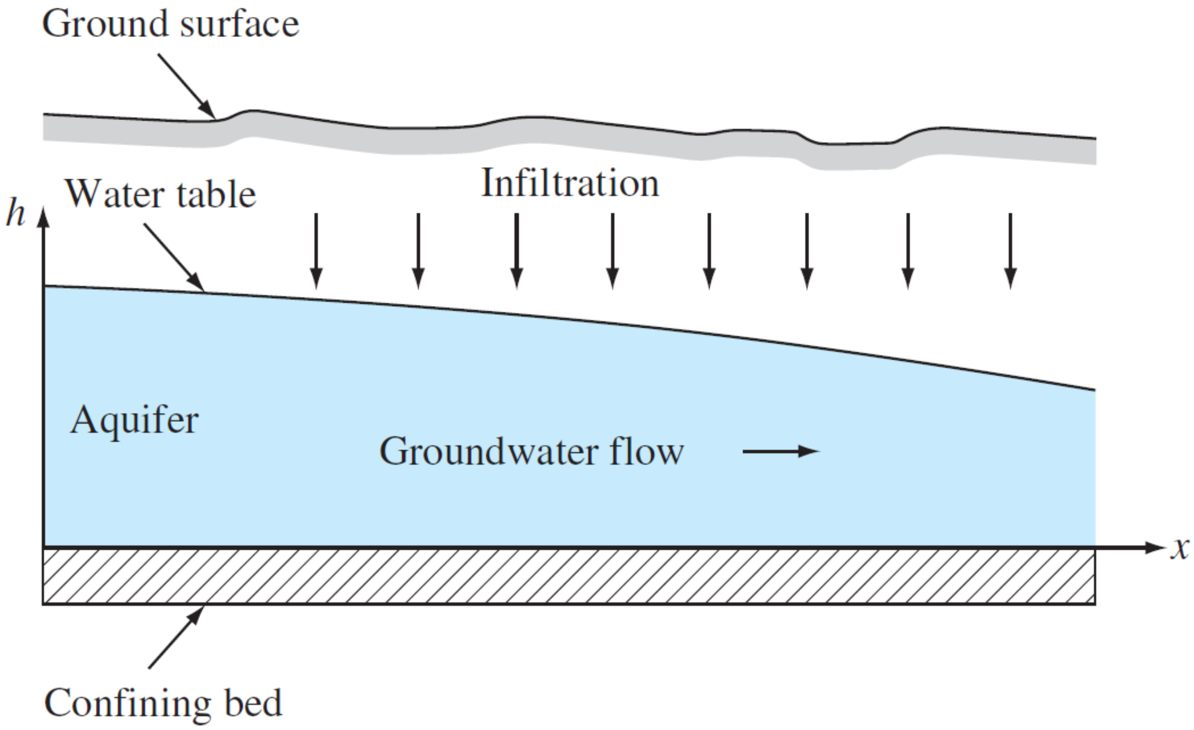
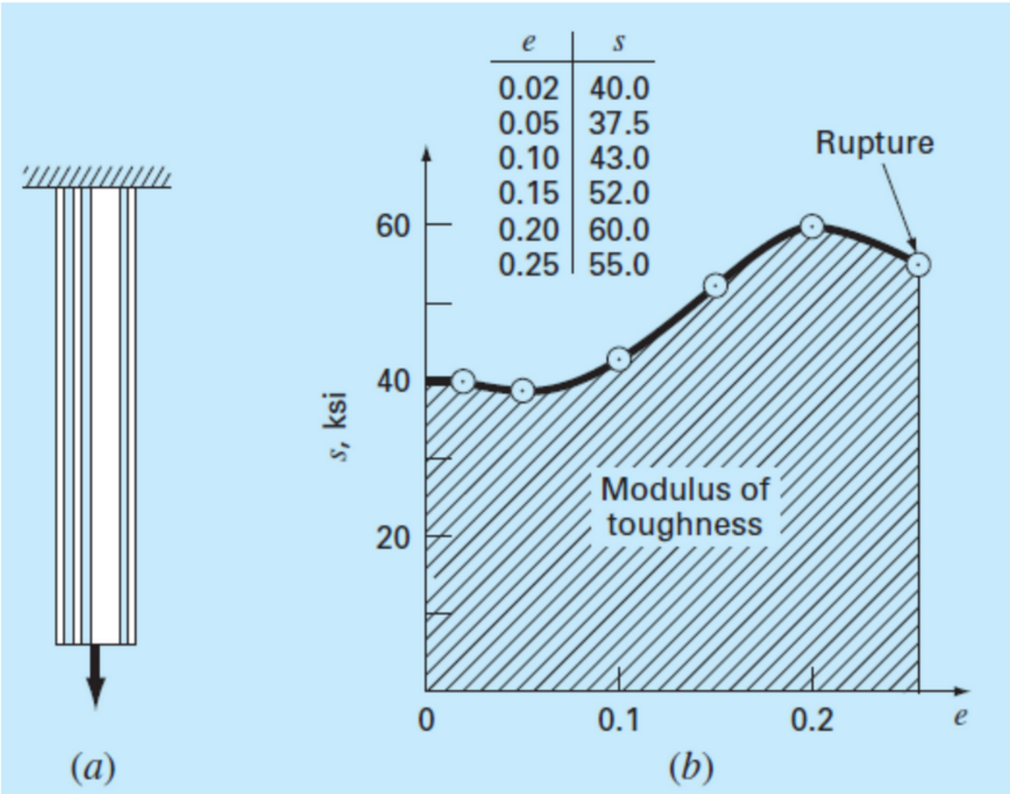

Ground surface
Water table
Infiltration
h
Aquifer
Groundwater flow
x
Confining bed

Figure 4:



(a)
e
s
0.02 40.0
0.05 37.5
0.10 43.0
0.15 52.0
0.20 60.0
0.25 55.0
Rupture
60
40
20
s, ksi
Modulus of toughness
0
0.1
0.2
e
(b)

Figure 5:

31. The differential equation for the velocity of a bungee jumper is different depending on whether the jumper has fallen to a distance where the cord is fully extended and begins to stretch. Thus, if the distance fallen is less than the cord length, the jumper is only subject to gravitational and drag forces. Once the cord begins to stretch, the spring and dampening forces of the cord must also be included. These two conditions can be expressed by the following equations:

$$\frac{\mathrm{d}v}{\mathrm{d}t} = \begin{cases} g - \mathrm{sgn}(v)\frac{c_d}{m}v^2, & x \leq L \\ g - \mathrm{sgn}(v)\frac{c_d}{m}v^2 - \frac{k}{m}(x-L) - \frac{\gamma}{m}v, & x > L \end{cases},$$

where v is velocity (m/s), t is time (s), g is gravitational constant (9.81 m/s^2), $\mathrm{sgn}(x)$ is a function that returns -1, 0, 1 for negative, zero, and positive x, respectively, c_d is second-order drag coefficient (kg/m), m is mass (kg), k is cord spring constant (N/m), γ is cord dampening coefficient (Ns/m), and L cord length (m). Determine the position and velocity of the jumper given the following parameters: $L = 30$ m, $m = 68.1$ kg, $c_d = 0.25$ kg/m, $k = 40$ N/m, and $\gamma = 8$ kg/s. Perform the computation from $t = 0$ to 50 s and assume that the initial conditions are: $x(0) = v(0) = 0$.

You are required to write a computer program implementing the following methods: (1) Euler Method; (2) Heun's Method; (3) Midpoint method; (4) Fourth order Runge-Kutta method. You should compare the performance (accuracy, time step requirements, ease of implementation, computation time etc.) of these methods.

32. The steady-state distribution of temperature on a heated plate can be modelled by the Laplacian equation,

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$$

If the plate is represented by a series of nodes (see the figure below), convert the partial differential equation at each node into algebraic equation using a suitable numerical method. Use the Gauss-Seidel method to solve for the temperature of the nodes shown in Fig. 6.

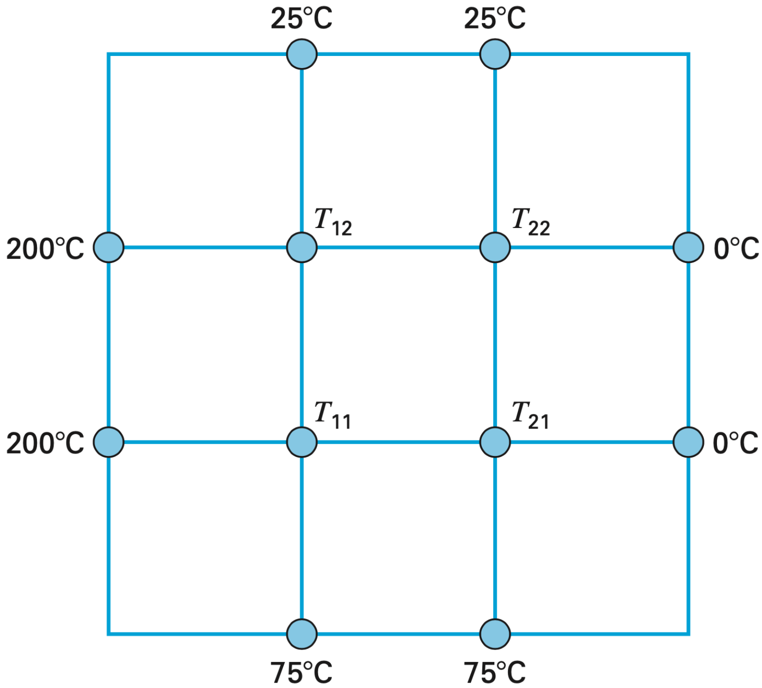


Figure 6: