Final Exam
Administered: Tuesday, December 7, 2021
10:30 AM – 12:45 PM
40 points

Problem 1. (14 points)

Consider a one-dimensional problem in the x direction in which a mass is attached to a dashpot and spring in series, anchored to a fixed point.

The equation of motion for the particle is

$$ma = F_{dashpot} + F_{spring} \tag{1}$$

where m is the mass of the particle, a is the acceleration of the particle. $F_{dashpot}$ is the force exerted by the dashpot,

$$F_{dashpot} = -cv \tag{2}$$

where c is a constant associated with the dashpot and v is the velocity of the particle. F_{spring} is the force of the spring,

$$F_{spring} = -kx \tag{3}$$

where k is a constant associated with the dashpot and x is the position of the particle.

The velocity is the first derivative of the position and the acceleration is the second derivative.

$$v = \frac{dx}{dt} \tag{4}$$

$$a = \frac{d^2x}{dt^2} \tag{5}$$

where t is time. Substituting equations (2) through (5) into equation (1) yields

$$\frac{d^2x}{dt^2} = -\frac{c}{m}\frac{dx}{dt} - \frac{k}{m}x \tag{6}$$

Consider a system with initial position of the particle, $x_o = 1.5$ m, and initial velocity of the particle, $v_o = 0.0$ m/s. Numerical values of the system constants are $m = 1.0$ kg, $c = 0.5$ N·s/m and $k = 1.0$ N/m. Perform the following tasks.

(a) Convert the second order ODE in equation (6) to a system of first order ODEs.
(b) Is this an initial value problem or a boundary value problem?
(c) What numerical technique will you use to solve this system of first order ODEs?
(d) Plot the system of ODEs from time = 0 to time =10.0 s.
(e) Report the particle position and velocity at time =10.0 s.
(f) Numerically verify that your result in (e) is accurate.
(g) By running a longer simulation, estimate the final particle position and velocity when the system comes to rest.

Problem 2. (8 points)
The longest relaxation time of a polymer can be measured through an auto-correlation function (acf) of the polymer end-to-end distance.

$$acf = c \cdot exp\left(-\frac{t}{\tau}\right) \tag{1}$$

where t is time (sec), τ is relaxation time (sec) and c is a prefactor. The acf is dimensionless.

For the acf vs t data given in the file, http://utkstair.org/clausius/docs/mse301/data/xm4p02_f21.txt, perform the following tasks. In this data file, the first column is time and the second column contains the values of the acf.

(a) Identify all variables, $y = mx + b$, when equation (1) is linearized.
(b) Report the best value of τ and c.
(c) Report the standard deviations of τ and c.
(d) Report the measure of fit.

Problem 3. (8 points)

In the data of a spectroscopy experiment two peaks are measured. The first peak corresponds to the abundance of compound A and the second peak corresponds to the abundance of compound B. The signal data is given in the file, http://utkstair.org/clausius/docs/mse301/data/xm4p03_f21.txt. In this data file, the first column is x, the second column contains the values of the peak 1 signal, and the third column contains the values of the peak 2 signal. perform the following tasks.

(a) What is the appropriate numerical method to integrate these signals?
(b) Find the integral of the first peak.
(c) Find the integral of the second peak.
(d) Find the relative abundance of compound A with respect to compound B.

Problem 4. (10 points)
Consider a mixture where the volume of the mixture, V_{mix}, is given by the sum of the pure component molar volumes, V_i, weighted by the mole fraction, x_i.

$$V_{mix} = \sum_{i=1}^{n_c} x_i V_i \tag{1}$$

where n_c is the number of components. The enthalpy of the mixture, H_{mix}, is nonideal,

$$H_{mix} = \sum_{i=1}^{n_c} \sum_{j \geq i}^{n_c} (2 - \delta_{ij}) \Omega_{ij} x_i x_j \tag{2.a}$$

where δ_{ij} is the Kronecker delta function and is 1 for $i = j$ and 0 for $i \neq j$. For a three-component mixture, this equation becomes

$$\begin{aligned} H_{mix} = \Omega_{AA} x_A x_A &+ 2\Omega_{AB} x_A x_B + 2\Omega_{AC} x_A x_C \\ &+ \Omega_{BB} x_B x_B \quad + 2\Omega_{BC} x_B x_C \\ &\qquad\qquad\qquad + \Omega_{CC} x_C x_C \end{aligned} \tag{2.b}$$

(This is one equation split into three lines for ease in reading.) The mixing parameters, $\Omega_{ij} = \sqrt{H_i H_j}$, where H_i and H_j are the pure component enthalpies. As a reminder, the sum of the mole fractions is unity.

$$1 = \sum_{i=1}^{n_c} x_i \tag{3}$$

The molar volumes and enthalpies of the pure components and mixtures are given below.

component	A	B	C	mixture
molar volume (liter/mol)	18	14	12	16.0
enthalpy (kJ/mol)	41	64	52	50.0

(a) Is this system of algebraic equations linear or nonlinear? (2 pts)
(b) What is the appropriate method to solve this system of algebraic equations? (2 pts)
(c) Determine the composition of this mixture. Show reasoning and method. (6 pts)