Advanced Numerical Analysis for Chemical Engineering
Mid-Term Examination -2 (2 hrs.)

1. Consider the following equation arising in a least square estimation problem

$$\mathbf{e} = \mathbf{b} - \mathbf{A}\boldsymbol{\theta}$$

$$\mathbf{A} = \begin{bmatrix} -1 & 1 \\ 0 & -1 \\ -1 & 0 \\ 0 & -1 \\ 1 & 0 \end{bmatrix} \quad ; \quad \mathbf{b} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

   (a) Find estimate of $\boldsymbol{\theta} = \begin{bmatrix} \alpha_1 & \alpha_2 \end{bmatrix}^T$ such that $\phi = \mathbf{e}^T\mathbf{e}$ is minimized with respect to $\boldsymbol{\theta}$. (*4 points*)

   (b) Find components of vector $\mathbf{b}$ in the column space $\mathbf{A}$ and in the left null space of $\mathbf{A}$, respectively. (*3 points*)

   (c) Let $L_2[0,1]$ represent the set of square integrable continuous functions on interval $0 \leq z \leq 1$ and let the inner product of any functions $f(z), g(z) \in L_2[0,1]$ be defined as follows

$$\langle f(z), g(z) \rangle = \int_0^1 z(1-z) f(z) g(z) dz$$

   Given a set of two linearly independent vectors, $f_1(z) = 1$ and $f_2(z) = z$, find orthonormal set of vectors $e_1(z)$ and $e_2(z)$ using the Gram-Schmidt process. (*5 points*)

2. **Prblem Discretization**

   (a) Consider a packed bed reactor with jacket temperature cooling. It is assumed that an exothermic gas phase reaction $A \rightarrow B$ is carried out in the reactor and the reaction is of zero order. The steady state behavior of the system is described by the following set of coupled ODEs

$$\frac{du}{dz} = \alpha(v-u) - \beta(u-T)$$

$$\frac{d^2v}{dz^2} = B(v-u) + C(v-T) - A\exp\left(\frac{\eta v}{v+1}\right)$$

$$u(0) = 0 \; ; \; \left[\frac{dv}{dz}\right]_{z=0} = 0 \quad \text{and} \quad \left[\frac{dv}{dz}\right]_{z=1} = 0$$

where u and v represent dimensionless gas temperature and catalyst packing temperature, respectively. Here, $(\alpha, \beta, \eta, A, B, C)$ represent dimensionless model parameters and T represents scaled wall temperature (which is assumed to be known *a-priori*). Discretize the above set of ODE-BVP using the method of orthogonal collocations. Use two internal grid points at (0.21132, 0.78868) for discretization. What is the degree of freedom (no. of variables - no. of equations) for the resulting set of equations? (*7 points*)

Note: **S** *and* **T** *matrices for two internal collocation points at (0.21132, 0.78868) are as follows*

$$\mathbf{S} = \begin{bmatrix} -7 & 8.2 & -2.2 & 0 \\ -2.7 & 1.7 & 1.7 & -0.7 \\ 0.7 & -1.7 & -1.7 & 2.7 \\ -1 & 2.2 & -8.2 & 7 \end{bmatrix} \quad ; \quad \mathbf{T} = \begin{bmatrix} 24 & -37.2 & 25.2 & -12 \\ 16.4 & -24 & 12 & -4.4 \\ -4.4 & 12 & -24 & 16.4 \\ -12 & 25.2 & -37.2 & 24 \end{bmatrix}$$

(b) Consider PDE describing concentration dynamics in a TRAM.

$$\frac{\partial C}{\partial t} = (1+\alpha C)\frac{\partial^2 C}{\partial z^2} + \alpha\left(\frac{\partial C}{\partial z}\right)^2 \qquad (0 < z < 1, \quad 0 > t)$$

$$I.C. \; : \; C(z,0) = 1 + 0.2z$$

$$B.C.1(at\ z = 0) : C(0,t) = 1 \quad ; \quad B.C.2(at\ z = 0) : \frac{\partial C(1,t)}{\partial z} = 0$$

It is desired to discretize the above PDE in space and convert it to a set of ODE-IVP using the finite difference method. The grid points are selected as follows

$$z_0 = 0, z_1 = 0.1, z_2 = 0.3, z_3 = 0.7, z_4 = 1$$

Using these grid points, derive the set of ODEs that approximate the TRAM dynamics and specify appropriate initial conditions. (*6 points*)

Note: *Expressions for approximating the first and the second derivatives are as follows*

$$\frac{du(z_i)}{dz} \approx \frac{u_{i+1} - u_i}{\Delta z_i + \Delta z_{i-1}}$$

$$\frac{d^2u(z_i)}{dz^2} \approx \frac{2}{\Delta z_i + \Delta z_{i-1}}\left[\frac{u_{i+1} - u_i}{\Delta z_i} - \frac{u_i - u_{i-1}}{\Delta z_{i-1}}\right]$$

where $\Delta z_i = z_{i+1} - z_i$.