Advanced Numerical Analysis for Chemical Engineering
Quiz-2 (1 hrs.)

1. 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

$$
\begin{aligned}
\frac{du}{dz} &= \alpha(v-u) - \beta(u-T) \\
\frac{d^2v}{dz^2} &= B(v-u) + C(v-T) - A\exp\left(\frac{\eta v}{v+1}\right) \\
u(0) &= 0 \;\; ; \;\; \left[\frac{dv}{dz}\right]_{z=0} = 0 \quad \text{and} \quad \left[\frac{dv}{dz}\right]_{z=1} = 0
\end{aligned}
$$

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?

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

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

2. Consider PDE describing concentration dynamics in a TRAM.

$$
\begin{aligned}
\frac{\partial C}{\partial t} &= (1+\alpha C)\frac{\partial^2 C}{\partial z^2} + \alpha\left(\frac{\partial C}{\partial z}\right)^2 \qquad (0 < z < 1, \;\; 0 > t) \\
I.C. &: \; C(z,0) = 1 + 0.2z \\
B.C.1(at\ z &= 0) : C(0,t) = 1 \quad ; \quad B.C.2(at\ z = 0) : \frac{\partial C(1,t)}{\partial z} = 0
\end{aligned}
$$

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.

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