dvanced Numerical Analysis for Chemical Engineering
Programming Quiz C (2 hrs 30 minutes)

Problem: Solve the given ODE-IVP using the specified method.

System: Catalytic Converter

The behavior of a catalytic converter in automative exhausts, in which CO, NO and O_2 react on irridium and rhodium catalyst, is given by followin ODE-IVPs

$$\begin{aligned}
\frac{dx_1}{d\tau} &= KR(1-x_1)(1-x_2) + (S-R)(1-x_1)\,x_3 \\
\frac{dx_2}{d\tau} &= K(1-x_1)(1-x_2) \\
\frac{dx_3}{d\tau} &= -(1-x_1)x_3 \\
K &= 2 \quad ; \quad R = 0.33 \quad ; \quad S = 0.33
\end{aligned}$$

where x_1, x_2 and x_3 represent conversions of CO, NO and O_2, respectively, and τ represents dimensionless reactor length. Integrate the above set of equations starting from initial condition

$$\mathbf{x}(0) = \begin{bmatrix} 0 & 0 & 1 \end{bmatrix}$$

from $\tau = 0$ to $\tau = 5$ with integration step size $h = 0.05$. Plot $x_1(\tau)$ v/s τ, $x_2(\tau)$ v/s τ and $x_3(\tau)$ v/s τ in three separate figures.

Integration Method

Given ODE-IVP

$$\frac{d\mathbf{x}}{dt} = \mathbf{F}(\mathbf{x}, t) \tag{1}$$

$$\mathbf{x}(0) \quad : \quad \text{Initial Condition} \tag{2}$$

where $\mathbf{x} \in R^n$ and $F(\mathbf{x}, t)$ is a $n \times 1$ function vector.

Notation:

$$\begin{aligned}
\mathbf{x}(n-i) &= \mathbf{x}(t_n - ih) \\
\mathbf{F}(n-i) &\equiv \mathbf{F}\left[\mathbf{x}(t_n - ih), (t_n - ih)\right] \\
i &= -1, 0, 1, ...p
\end{aligned}$$

Gear's (**non iterative)** Predictor-Corrector Algorithm:

Gear's four step Predictor

$$\mathbf{z}(n+1) = \frac{1}{3}\left[-10\mathbf{x}(n) + 18\mathbf{x}(n-1) - 6\mathbf{x}(n-2) + \mathbf{x}(n-3)\right] + 4h\,\mathbf{F}(n)$$

Gear's 4-step Corrector

$$\mathbf{x}(n+1) = \frac{1}{25}\left[48\mathbf{x}(n) - 36\mathbf{x}(n-1) + 16\mathbf{x}(n-2) - 3\mathbf{x}(n-3)\right] + \frac{12}{25}h\,\mathbf{F}(\mathbf{z}(n+1))$$

Note: *Start integration from $n = 4$ and initially assume that*

$$\mathbf{x}(3) = \mathbf{x}(2) = \mathbf{x}(1) = \mathbf{x}(0)$$