Advanced Numerical Analysis for Chemical Engineering
Programming Quiz A (2 hrs 30 minutes)

Integration Method: Nystrom Predictor Corrector (Non-Iterative Form)

Given ODE-IVP

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

$$\mathbf{x}(0) = \mathbf{x}_0 \quad (2)$$

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

Notation:

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

Develop generic program for the following Adam's Predictor-Corrector Algorithm

Nystrom three step Predictor :

$$\mathbf{x}(n+1) = \mathbf{x}(n-1) + \frac{h}{3}\left[7\mathbf{F}(n) - 2\mathbf{F}(n-1) + \mathbf{F}(n-2)\right]$$

Nystrom three step Corrector :

$$\mathbf{x}(n+1) = \mathbf{x}(n-1) + \frac{h}{3}\left[\mathbf{F}(n+1) + 4\mathbf{F}(n) - \mathbf{F}(n-1)\right]$$

Note: *For predictor - corrector methods, assume that state* $\mathbf{x}(t) = \mathbf{x}(0)$ *for time* $t \leq 0$. *Also, develop a non-iterative version, which involves prediction step followed by only one correction step.*

Problem: CSTR with exothermic reversible reaction

A first order exhothermic reversible reaction $A \rightleftarrows B$ is acrried out in a CSTR. The dynamics of this system is given by followin ODE-IVPs

$$\begin{aligned} \frac{dx_1}{dt} &= -0.16\frac{x_1}{x_3}u_1 + k_1(1 - x_1) - k_2 x_1 \\ \frac{dx_2}{dt} &= 0.16\frac{u_1}{x_3}(u_2 - x_2) + 5\left[k_1(1 - x_1) - k_2 x_1\right] \\ \frac{dx_3}{dt} &= 0.16u_1 - 0.4\sqrt{x_3} \\ k1 &= 3 \times 10^5 \exp(-5000/x_2) \quad ; \quad k2 = 6 \times 10^7 \exp(-7500/x_2) \\ u_1 &= 1.2 \quad ; \quad u_2 = 430 \end{aligned}$$

where x_1, x_2 and x_3 represent conversions of conversion of A, reactor temperature and reactor level, respectively. Integrate the above system of equations starting from initial state

$$\mathbf{x}(0) = \begin{bmatrix} 0.5088 & 435.6 & 0.16 \end{bmatrix}$$

from $t = 0$ to $t = 6$ with integration step size $h = 0.1$. Plot $x_1(t)$ v/s time, $x_2(t)$ v/s time and $x_3(t)$ v/s time in three separate figures.