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

Given ODE-IVP

\[ \frac{dx}{dt} = F(x, t) \]
\[ x(0) = x_0 \]

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

Notation:

\[ x(n-i) = x(t_n - ih) \]
\[ F(n-i) \equiv F[x(t_n - ih), (t_n - ih)] \]
\[ i = -1, 0, 1, \ldots, p \]

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

Nystrom three step Predictor:

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

Nystrom three step Corrector:

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

Note: For predictor - corrector methods, assume that state \( x(t) = x(0) \) 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 exothermic reversible reaction \( A \rightleftharpoons B \) is carried out in a CSTR. The dynamics of this system is given by followin ODE-IVPs

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

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

\[ x(0) = [ 0.5088 \quad 435.6 \quad 0.16 ] \]

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.