CHBE 553, Assignment 2 (Newton's method for coupled nonlinear equations)

Consider two reactions in a batch reactor:

$$2A + B \Leftrightarrow C, \text{ with equilibrium constant } K_1 = \frac{C_c}{C_A^2 C_B} = 5 \times 10^{-4},$$

$$A + D \Leftrightarrow C, \text{ with equilibrium constant } K_2 = \frac{C_c}{C_A C_D} = 4 \times 10^{-2}.$$

The initial concentrations are:

$$C_{A,0} = 40 \text{ kmol/m}^3,\ C_{B,0} = 15 \text{ kmol/m}^3,\ C_{C,0} = 0,\ C_{D,0} = 10 \text{ kmol/m}^3.$$

Calculate the equilibrium conversion of the two reactions.

* **Hint**: let the conversion be x_1 and x_2 for the two reactions, then the equilibrium concentrations for the reactants are:

$$C_A = C_{A,0} - 2x_1 C_{B,0} - x_2 C_{D,0}, \qquad C_B = C_{B,0} - x_1 C_{B,0},$$

$$C_C = C_{C,0} + x_1 C_{B,0} + x_2 C_{D,0}, \qquad C_D = C_{D,0} - x_2 C_{D,0}.$$

From these, the two equilibrium constants provide two nonlinear equations for the two unknowns.

Write a general Newton's iteration module for n coupled equations with n unknowns, and then apply it to solve the problem here. Consider using numerical differentiation in constructing the Jacobian. You may use any of the direct and iterative methods for solving the linear system, and may use canned Fortran routines or MatLab functions.