ChE 505
Final Exam (100 points)
Advanced Mathematics for Engineers
Administered: 8:00-10:00 A.M. Saturday December 9, 2000
(Two problems, one on each side of this page.)

Problem 1. (50 points)

When we dealt with the numerical solution to parabolic PDEs, we split the study up into linear and nonlinear problems. With linear problems, we used a Crank-Nicholson method, which allowed us to calculate a Jacobian and perform one matrix inversion in order to solve the entire problem at all positions and times in one fell swoop. With nonlinear problems, we used a Runge-Kutta type method, where we did not require any linear algebra, but instead looped through time, advancing one time-step each pass through the loop.

When we dealt with ODEs, we ignored treating the linear problem individually and just used the Runge-Kutta type solution to solve both linear and nonlinear ODEs. However, an analogous linear method could have been used to solve ODEs. Outline the procedure to solve a linear ODE at all times with a single matrix inversion. Consider this single linear ODE:

$$\frac{dy}{dx} = ay + bx + c \tag{1}$$

$$y(x = x_o) = y_o \tag{2}$$

You are asked to solve over the range $x_o \le x \le x_f$ using n_x intervals.
Use the forward finite difference formula:

$$\frac{dy}{dx} \approx \frac{y_{j+1} - y_j}{\Delta x} \tag{3}$$

Use a second-order method, namely

$$\frac{y_{j+1} - y_j}{\Delta x} = \frac{1}{2}\left[K_j + K_{j+1}\right] \tag{4}$$

where K_j is the right hand side of equation (1) evaluated at (x_j, y_j).
In outlining your procedure,

(a) provide an algorithm.
(b) provide the generic equation, which you will end up solving.
(c) show the first and second row of the matrix
(d) comment on the structure and bandwidth of the matrix.
(e) point out any loops in the algorithm.
(f) comment on convergence.
(g) comment on stability. What can make the program crash?

Problem 2. (50 points)

Consider an isothermal batch reactor containing monomer molecules. The monomers and polymers can react to form longer polymers of length i, P_i. For example, P_6, can be created by these reactions

$$P_5 + P_1 \to P_6, \qquad P_4 + P_2 \to P_6, \qquad \text{and} \qquad 2P_3 \to P_6$$

Also, P_6, can be consumed by these reactions

$$P_6 + P_1 \to P_7, \qquad P_6 + P_2 \to P_8, \qquad \text{and generally} \quad P_6 + P_{n-6} \to P_n$$

A mole balance can be written for the number of moles of a polymer of length i, P_i, for every value of i:

accumulation = in - out + generation - consumption

$$\frac{dP_i}{dt} = 0 - 0 + \sum_{j=1}^{i/2} k_f(i-j,j)P_{i-j}P_j - \sum_{n=i+1}^{\infty} k_f(i,n-i)P_iP_{n-i} \tag{2.1}$$

where $k_f(i-j,j)$ is a reaction rate constant which is a function of the length of the two reactants, P_{i-j} and P_j.

Assume you have a smooth function that describes $k_f(i-j,j)$ as a function of its two arguments (i,j) from (1,1) to $(n_{max}-i,i)$ where is $n_{max} = 10^6$.

The reactor is initially filled with 100% monomer, P_1.

Using the model in equation (2.1), answer the following questions:

(a) What sort of equations do you have? (ODE, PDE, AE, IE)?
(b) Are the equations linear or nonlinear?
(c) How many equations do you have?
(d) What technique would you use to solve this problem?
(e) What problems would you expect to encounter using this technique?

Since the summation in the mole balance (2.1) is over a large range ($n_{max} = 10^6$), we could approximate the sum with an integral and assume that P_i is a continuous function over i. The mole balance becomes:

$$\frac{dP(x)}{dt} = \int_{y=1}^{x/2} k_f(x-y,y)P(x-y)P(y)dy - \int_{n=x}^{n_{max}} k_f(x,n-x)P(x)P(n-x)dn \tag{2.2}$$

Answer questions (a) through (e) for equation (2.2).