

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:

$$\frac{dy}{dx} = ay + bx + c \quad (1)$$

$$y(x = x_0) = y_0 \quad (2)$$

You are asked to solve over the range  $x_0 \leq x \leq x_f$  using  $n_x$  intervals.

Use the forward finite difference formula:

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

Use a second-order method, namely

$$\frac{y_{j+1} - y_j}{\Delta x} = \frac{1}{2} [K_j + K_{j+1}] \quad (4)$$

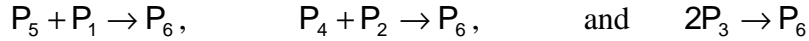
where  $K_j$  is the right hand side of equation (1) evaluated at  $(x_j, y_j)$ .

In outlining your procedure,

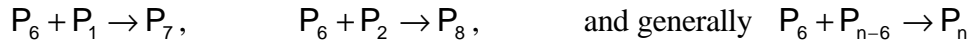
- (a) provide an algorithm.
- (b) provide the generic equation, which you will end up solving.
- (c) show the first and second row of the matrix
- (d) comment on the structure and bandwidth of the matrix.
- (e) point out any loops in the algorithm.
- (f) comment on convergence.
- (g) comment on stability.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



Also,  $P_6$ , can be consumed by these reactions



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

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

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:

- What sort of equations do you have? (ODE, PDE, AE, IE)?
- Are the equations linear or nonlinear?
- How many equations do you have?
- What technique would you use to solve this problem?
- 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:

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

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