CBE 20258 Numerical and Statistical Analysis

Algorithm Problem Set 7

due in class Thursday, 4/21
(or in the box by 4pm Friday…)

Problem 1. Systems of Equations:

The velocity profile due to a heated wire (this is one of the experiments in senior lab) is governed by the pair of coupled non-linear ODE's given below. Write down the equivalent set of first order coupled ODE's.

$$f''' = -g + \frac{1}{Pr}\left[\frac{1}{5}(f')^2 - \frac{3}{5} f f''\right]$$

and

$$g' = \frac{-3}{5} f g$$

For those of you who are interested, f ' is the dimensionless vertical velocity (f is the streamfunction) and g is the dimensionless temperature. Pr is the Prandtl number, a constant determined by the fluid used in the experiment.

For this problem, write down the equivalent set of first order coupled ODE's identifying all the dependent variables.

Problem 2. Integration Error: You are integrating the non-linear ODE:

$$\frac{dy}{dt} = -3y^2 \quad ; \; y(0) = 1$$

This actually has the simple solution:

$$y = \frac{1}{1+3t}$$

a. Using a step size of ½, integrate this ODE from 0 to 1 using the Euler Method.

b. Using the same step size, integrate it using the Backward Euler Method.

c. Which integration procedure is more accurate and why? What are the stability intervals (maximum step size) for each method?

Problem 3. Boundary Conditions:

Often we need to estimate the derivative of a function at a boundary in order to satisfy boundary conditions. Suppose we have function evaluations at node locations as given below:

x	y
0	y_0
h	y_1
2h	y_2

Two approximations are in common use, the low order algorithm:

$$\left.\frac{dy}{dx}\right|_{x=0} \approx \frac{1}{h}\left(y_1 - y_0\right)$$

and the higher order algorithm:

$$\left.\frac{dy}{dx}\right|_{x=0} \approx \frac{1}{2h}\left(4y_1 - 3y_0 - y_2\right)$$

By using a Taylor series expansion, calculate the error in each of these rules.

Problem 4. Determining the Critical Mass of an Atomic Bomb:

While the details are complicated, of course, fundamentally the determination of the critical mass necessary for an atomic explosion (first solved as a part of the Manhattan Project during WWII) involves the solution of an autocatalytic partial differential equation given below:

$$\frac{\partial \phi}{\partial t} = D\nabla^2 \phi + k\phi \quad ; \quad \left.\phi\right|_{t=0} = 1 \quad ; \quad \left.\phi\right|_{\partial D=0} = 0$$

where D is the diffusion coefficient (resulting from neutron scattering from inert species) and k is a measure of volumetric neutron production due to bombardment of a fissile nuclei. Here we examine the explosion of a cubical mass of length a in each direction. It is convenient to render all lengths dimensionless with respect to a, time dimensionless with respect to the diffusion time scale a^2/D, and (dividing through) we get a dimensionless production rate of $\lambda = ka^2/D$. Your goal is to determine the critical value of λ which makes the cubical mass blow up!

While an analytical solution of this problem is possible, it is *very* simple to just simulate the diffusion and production process using Monte Carlo. The key is to populate the cube (with a dimensionless size of one in each direction) with N_0 tracers distributed at random. At each time step dt the tracers are given a normally distributed random kick of standard deviation $(2\,D\,dt)^{1/2}$ in each direction (just $(2\,dt^*)^{1/2}$ in dimensionless form). In addition, if a random number uniformly distributed between zero and one (for each tracer) is less than k dt (or λ dt* in dimensionless form), that tracer is "twinned", simulating a fission event. Tracers escaping the box are removed from the list (N decreases) and tracers produced are added to the list (N increases). Keeping track of $N(t)/N_0$ yields the total concentration.

OK, now for the problem: write a short code (adapting the tutorial code is fine, if you like, but it may be simpler to start fresh) which does the simulation described above and determine the value of λ which causes the cube to blow up. Plot up $N(t^*)/N_0$ as a function of t* for λ a bit above and below this value (put both on the same graph) to demonstrate the dynamics of the process.