Physics 218 – Spring, '07 - Assignment #5 – The Diffusion Equation

Overview: A large class of physical systems are described by differential equations that have more than one independent variable. At the beginning of the semester, we developed methods for solving coupled, ordinary differential equations (ODEs), but in those systems there was only one independent variable, time. Now we look at one method for solving "partial differential equations" (PDEs) that depend on both position and time, independently.

The equation we will simulate is the one dimensional "diffusion equation,"

$$\frac{\partial T(x,t)}{\partial t} = D\frac{\partial^2 T(x,t)}{\partial x^2},$$

where we will take *T(x,t)* to be the temperature of some object and *D* is a constant called the "thermal diffusivity" of the material that makes up the object. (We could equally well have modeled the diffusion of a chemical by letting *T(x,y)* represent the concentration of some chemical and *D* be the constant "diffusivity" of the chemical species inside the material that makes up the object.) Don't be intimidated by the $\partial/\partial x$ notation instead of the usual d/dx notation. It still means take a derivative, just that when you take the derivative with respect to *x*, say, you should treat the other independent variable, *t*, as a constant.

As will be discussed in class, we will make Euler-like approximations for the derivatives. We adopt the notation that $T^n{}_i$ represents the temperature at location $i\Delta x$ and at time $n\Delta t$. Then, in the FTCS scheme

$$T^{n+1}{}_i = T^n{}_i + \frac{D\Delta t}{\Delta x^2}\left(T^n{}_{i+1} + T^n{}_{i-1} - 2T^n{}_i\right).$$

As with ODEs, you must supply PDEs with initial conditions. In this case, you need to supply $T^0{}_i$ for **all** locations *i.* Then the FTCS scheme can produce all later values for *T*. You must also specify what happens at the boundaries of the system. Some possibilities are: a) Fixed temperature, *i.e.,* you specify a temperature at the boundary and don't change it. b) "No flux" or insulating boundaries. This involves setting the *x* derivative of *T* to zero at the boundaries and keeping it zero at all times. c) Periodic boundaries. If you have locations represented by *i=0, 1, 2,…(N-1)* then you treat *i=N* to be the same point as *i=0*. This is often used to simulate infinite systems (and is an easy one to implement).

One can show that the FTCS scheme is unstable unless $D\Delta t/\Delta x^2 < 1/2$.

Product 5.1: We are first going to simulate a one dimensional metal "bar." The bar has length 1 and has a thermal diffusivity of 1. At time *t=0* the temperature at *i=0* is 1 and this remains fixed. At time *t=0*, the temperature at all other locations in 0. At *i=(N-1)* impose a no-flux boundary condition. Start with *N=40*. Create an animation that shows how the temperature profile evolves over time. Stop when the temperature is essentially uniform over the whole bar. About how much time has gone by? For your report, document the conditions you used and include some plots of temperature as a function of position at illustrative values of time.

Product 5.2: Let's have some fun with IDL's visualization tools. Now assume that our bar is two dimensional with width 1. Change notation slightly, so that $T^n{}_{i,j}$ represents the temperature at time $n\Delta t$ and location $x = i\Delta x$ and $y = j\Delta x$. For this section, just use the code for Product 5.1 and set the temperature at all values of *j* to be the same as at *j=0,* maybe even after you have done the calculation. Find a couple of ways in IDL to display the temperature data. For example, a contour plot or a surface plot. The iTools widgets might be useful. Include some nice illustrations in your report.

Product 5.3: Now let's do the second dimension right. 1) Implement no-flux boundary conditions in the *y* direction. 2) At *i=0* only have fixed temperature boundary conditions (with *T=1)* for a length of *y=0.1* centered at *y=0.5.* At other values of *y* implement no-flux boundary conditions at *i=0.* 3) Change the FTCS scheme to:

$$T^{n+1}{}_{i,j} = T^n{}_{i,j} + \frac{D\Delta t}{\Delta x^2}\left(T^n{}_{i+1,j} + T^n{}_{i-1,j} + T^n{}_{i,j+1} + T^n{}_{i,j-1} - 4T^n{}_{i,j}\right)$$

Make some nice images and/or movies of the resultant temperature field.

Project ideas: a) How about moving to 3D? b) Devise your own problem, perhaps a real-world problem where not every parameter is 1. c) An unconditionally stable PDE integration scheme is called the Crank-Nicholson method. It would be a real challenge, but implementing that algorithm would make a worthwhile project.