Parabolic PDEs — the Diffusion Equation

The diffusion equation, or heat equation, is, in general, and in three dimensions,

$$\frac{\partial\phi}{\partial t} = k\nabla^2\phi + f,$$

where k is the diffusivity, f the source and t the time. Both k and f are, in general, functions of position and time. The equation is telling us that ϕ diffuses out from regions where there is more ϕ than the average of the surroundings or where ϕ is being 'created' towards regions where there is less or where it is being absorbed. This applies to things such as heat or chemical concentrations.

For numerical purposes, we look only at a simplified case; we take k to be constant, and it might as well be 1 [scaling time if necessary], we take f to be zero [no supply of heat, or whatever] and we assume the one-dimensional case [eg, heat diffusion in a rod]. So the equation becomes

$$\frac{\partial\phi}{\partial t} = \frac{\partial^2\phi}{\partial x^2}.$$

This PDE is usually an initial-value problem in t and a boundary-value problem in x. As a heat problem, you can think of ϕ as temperature, so we have a rod that has been heated in a particular way so that some parts are hot and others cold, and is then left to its own devices at $t = 0$. In x, the more usual conditions are either that it's a very long rod, with 'nothing happening' at infinity, and we want to know how the heat diffuses along the rod — as heat is conserved, less and less will happen as time goes on and the heat gets more spread out and more feeble — or that the ends of the rod are maintained at specific temperatures — in which case the ends will absorb/emit heat, and the rod will finish up with a uniform temperature gradient.

Again, for the sake of a specific problem, we assume that $\phi = 0$ at $x = 0$ and at $x = 1$, both for all t [ends of the rod held in ice, for example]. So whatever the initial distribution of ϕ, we should find $\phi \to 0$ as $t \to \infty$. The more general cases are not numerically [more] interesting, though of course they may be of practical interest.

OK, first attempt. Why not treat this more-or-less like an elliptic PDE? Take strips of width h in the x-direction, and replace

$$\frac{\partial^2 \phi}{\partial x^2} \approx \frac{u_{i-1,j} - 2u_{i,j} + u_{i+1,j}}{h^2},$$

where $u_{i,j}$ is our approximate value of ϕ at $x = hi$ and $t = kj$ for some time-step k. Then we can approximate

$$\frac{\partial \phi}{\partial t} \approx \frac{u_{i,j+1} - u_{i,j}}{k},$$

so that the PDE becomes

$$u_{i,j+1} \approx u_{i,j} + kh^{-2}(u_{i-1,j} - 2u_{i,j} + u_{i+1,j}).$$

Now, all the $u_{i,0}$ are known from the initial conditions, so we can use this equation to find all the $u_{i,1}$, then all the $u_{i,2}$, and so on, stepping up through time.

Note that this method is rather like Euler's method; we could, and probably should, replace the crude approximation to $\frac{\partial \phi}{\partial t}$ by some sort of Modified Euler or Runge–Kutta scheme. But that turns out not to be the point. Also note that we are not now being given $\nabla^2 \phi$, but are using it in the time-step, so we can expect cancellation errors if we take h too small. But that turns out not to be the point either.

Example

We take the initial ϕ at $t = 0$ to be $\sin \pi x$ [which is zero at $x = 0$ and $x = 1$]. Then the exact solution is $\phi = e^{-\pi^2 t} \sin \pi x$, so that, for example, at $t = 1$, $x = 0.5$, $\phi = e^{-\pi^2} \approx 0.00005172$. [The small value might ring alarm bells, but that turns out not to be the problem either.] We choose some values for h and k more-or-less at random, and use the above scheme to find the approximation to ϕ For example,

$$h = 0.1, \quad k = 0.025, \quad u_{5,40} \approx -8 \times 10^{20}.$$

Oops. Well, that *is* [at least partly] a problem of taking 'only' 40 time steps, and the fairly rapid transient behaviour is not being tracked. Try

$$h = 0.1, \quad k = 0.01, \quad u_{5,100} \approx -2 \times 10^{29}.$$

Oops. Try

$$h = 0.1, \quad k = 0.001, \quad u_{5,1000} \approx 0.00005344$$

Well, that's not at all bad [and we can expect Runge – Kutta to do better]. Now we know that 1000 time steps are necessary, let's try to make the x-approximation better:

$$h = 1/24, \quad k = 0.001, \quad u_{12,1000} \approx 2 \times 10^{95};$$

$$h = 1/24, \quad k = 0.0001, \quad u_{12,10000} \approx 0.00005220.$$

We have two instabilities. The more obvious is the partial instability caused by the transient decay term; in this case, we needed to track something like e^{-10}, so we needed time-steps significantly smaller than 0.1. But there is also an instability caused by interference with the space derivative; note the factor k/h^2 in the equations for u. We need *also* k to be significantly less than h^2. The more we refine the space terms, the much, much more we have to refine the time terms.

This stability problem makes the above scheme impractical. Using Runge – Kutta improves the accuracy when the process is stable, but does nothing when it's unstable. Curing this is beyond the scope of this module; basically, we have to tie in space derivatives at $j+1$ as well as at j so that we can produce an equation for $u_{i,j+1}$ that does not have large terms on the RHS. But the consequence is that the equation *also* involves $u_{i-1,j+1}$ and $u_{i+1,j+1}$, so we get lots of simultaneous equations for each time step, and, as usual, matrices to invert to solve them. But you only need enough time steps to solve the transient behaviour. Look up the Crank – Nicolson method if you ever have to do this in real life.

This particular PDE in this form can be solved exactly by separation of variables and Fourier analysis of the starting ϕ. But note that if there are significant Fourier terms of high frequency, these correspond to very rapidly-decaying transients, and we are back to partial instabilities caused by the problem. To get good solutions, you always need space and time steps that adequately reflect physical reality [even when that is transient].

Hyperbolic PDEs —the Wave Equation

As previously noted, this is

$$\frac{\partial^2 \phi}{\partial t^2} = c^2 \frac{\partial^2 \phi}{\partial x^2},$$

with c [often, but not necessarily, constant] the speed of sound [or light, or water waves]. Why hyperbolic? If we make the substitutions [with c constant] $u = x + ct$, $v = x - ct$, then we find

$$\frac{\partial^2 \phi}{\partial u \partial v} = 0,$$

$$\phi = f(u) + g(v) = f(x + ct) + g(x - ct),$$

with f and g arbitrary functions, to be found from the boundary conditions. So the lines of constant $x + ct$, $x - ct$ play a key role in the solution. If we think of the PDE as a quadratic equation [algebraic rather than differential], then it turns out that these characteristic lines are like a generalised form of asymptote; when these are real, the equation is 'like' a hyperbola, if they are real but coincide it is 'like' a parabola, if they are imaginary it is 'like' an ellipse. We could have solved the Laplace equation similarly, to get $\phi = f(x + \mathrm{i}y) + g(x - \mathrm{i}y)$ [which is not necessarily, but is sometimes, helpful].

Unsurprisingly, we will want to solve wave equations numerically by the same general ideas of dividing into strips, and we will find the same sorts of instability; and some new ones, this time quite physical, because if we try to make things happen faster than the speed of sound, we get shock waves in real life and numerical problems from these.