Numerical Solution of the Diffusion Equation

Let's consider the numerical solution of diffusive problems. The diffusion equation is

$$\frac{\partial u}{\partial t} = D\nabla^2 u.$$

We will keep the problem as simple as possible by looking at a problem with D constant and just one spatial dimension:

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}\,.$$

As with any numerical integration, we start by discretizing the system — that is, determining the solution only at J particular positions x_j, and at certain times t_n, defined by

$$\begin{aligned} x_j &= x_0 + j\Delta x, \quad j = 0, \dots J-1\,, \\ t_n &= t_0 + n\Delta t, \quad n = 0, 1, \dots\,, \end{aligned}$$

(where Δx and Δt are assumed constant), and we define

$$u_j^n = u(x_j, t_n)$$

(the superscript n is conventional). We then difference the equation in the usual way: write the time derivative as

$$\left.\frac{\partial u}{\partial t}\right|_j^n \approx \frac{u_j^{n+1} - u_j^n}{\Delta t}$$

(forward differencing in time), and the space derivative as

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_j^n \approx \frac{\frac{u_{j+1}^n - u_j^n}{\Delta x} - \frac{u_j^n - u_{j-1}^n}{\Delta x}}{\Delta x} = \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta x^2}$$

(centered differencing in space). Substituting these expressions into the differential equation, we find

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = D\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta x^2}\,.$$

If all quantities with a superscript n (the state of the system at time t) are regarded as 'known", we can easily solve this equation for the unknown "$n+1$" quantities:

$$u_j^{n+1} = u_j^n + \alpha(u_{j+1}^n - 2u_j^n + u_{j-1}^n)\,,$$

where $\alpha = D\Delta t/\Delta x^2$.

This is a simple FTCS explicit differencing integration scheme for the diffusion problem. Now let's see how it works! Exercise 9.1 asks us to propagate the fundamental solution

$$u(x,t) = \frac{1}{\sqrt{4\pi D t}}\; e^{-x^2/4Dt}$$

forward in time from $t = 1$ to $t = 10$ — that is, we choose as initial conditions the solution at $t = 1$, then integrate it numerically to $t = 10$, and compare with the analytic solution.

Note as usual that the above equation only holds for "interior" points, with $j = 1, \dots, J-2$, because of the "$j-1$" and "$j+1$" references. The values of u_0 and u_{J-1} must be provided as boundary conditions—in this case we will just set $u = 0$ at the boundaries.