Numerical Solution of the Diffusion Equation in Spherical Co-ordinates via the Crank-Nicholson Method

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The diffusion equation in spherical polar co-ordinates is:

$$\frac{\partial c}{\partial t} = \frac{2D}{r}\frac{\partial c}{\partial r} + D\frac{\partial^2 c}{\partial r^2} \tag{1}$$

With initial condition:

$$c(0,r) = c_0(r) \tag{2}$$

and boundary conditions:

$$\left.\frac{\partial c}{\partial r}\right|_{r=0} = 0, \quad \left.\frac{\partial c}{\partial r}\right|_{r=R} = f(t) \tag{3}$$

The following discretisation for the derivatives are taken:

$$\frac{\partial c}{\partial t} \approx \frac{c_{i+1,j} - c_{i,j}}{\delta t}, \quad \frac{\partial c}{\partial r} \approx \frac{c_{i,j+1} - c_{i,j-1}}{2\delta r}, \quad \frac{\partial^2 c}{\partial r^2} \approx \frac{c_{i,j+1} - 2c_{i,j} + c_{i,j-1}}{\delta r^2} \tag{4}$$

Typically the radial component is split into N equal pieces, so $1 \leqslant j \leqslant N$ The Crank-Nicholson method takes the average of the solution over the two sequential times, and so:

$$\begin{aligned}\frac{c_{i+1,j} - c_{i,j}}{\delta t} = \frac{D}{2}\Bigg(&\frac{c_{i+1,j+1} - c_{i+1,j-1}}{2r_j\delta r} + \frac{c_{i+1,j+1} - 2c_{i+1,j} + c_{i+1,j-1}}{\delta r^2} + \\ &+ \frac{c_{i,j+1} - c_{i,j-1}}{2r_j\delta r} + \frac{c_{i,j+1} - 2c_{i,j} + c_{i,j-1}}{\delta r^2}\Bigg)\end{aligned} \tag{5}$$

This can be rearranged into the following form:

$$\begin{aligned}&\left(\frac{D\delta t}{4r_j\delta r} + \frac{D\delta t}{2\delta r^2}\right)c_{i+1,j+1} - \left(1 + \frac{D\delta t}{\delta r^2}\right)c_{i+1,j} + \left(\frac{D\delta t}{2\delta r^2} - \frac{D\delta t}{4r_r\delta r}\right)c_{i+1,j-1} = \\ &-\left(\frac{D\delta t}{4r_j\delta r} + \frac{D\delta t}{\delta r^2}\right)c_{i,j+1} + \left(\frac{D\delta t}{\delta r^2} - 1\right)c_{i,j} - \left(\frac{D\delta t}{2\delta r^2} - \frac{D\delta t}{4r_j\delta r}\right)c_{i,j-1}\end{aligned} \tag{6}$$

This is a tridiagonal matrix equation which can be solved easily. In order to incorporate the boundary conditions into the finite difference scheme, the values of the derivative are required on the boundary. In order to do this, write:

$$\frac{\partial c}{\partial r} = \alpha c(0) + \beta c(\delta r) + \gamma c(2\delta r) \tag{7}$$

Using Taylor's series, the above can be expanded as:

$$\left.\frac{\partial c}{\partial r}\right|_{r=0} = (\alpha+\beta+\gamma)c(0) + (\beta\delta r + 2\gamma\delta r)c'(0) + (\beta\delta r^2/2 + 2\gamma\delta r^2)c''(0) \tag{8}$$

This leads to three linear equations:

$$\alpha+\beta+\gamma = 0, \quad \beta\delta r + 2\gamma\delta r = 1, \quad \frac{\beta\delta r^2}{2} + 2\gamma\delta r^2 = 0 \tag{9}$$

The solution of which is:

$$\alpha = -\frac{3}{2\delta r}, \quad \beta = \frac{2}{\delta r}, \quad \gamma = -\frac{1}{2\delta r} \tag{10}$$

so:

$$\left.\frac{\partial c}{\partial r}\right|_{r=0} \approx \frac{-3c(0) + 4c(\delta r) - c(2\delta r)}{2\delta r} \tag{11}$$

Similarly, the condition on the boundary $r = R$ can be written as:

$$\left.\frac{\partial c}{\partial r}\right|_{r=R} = \alpha c(R) + \beta c(R-\delta r) + \gamma c(R - 2\delta r) \tag{12}$$

The same process can be carried out to show that:

$$\left.\frac{\partial c}{\partial r}\right|_{r=R} \approx \frac{3c(R) - 4c(r-\delta r) + c(R-2\delta r)}{2\delta r} \tag{13}$$

The system of equations (5) is solved for $2 \leqslant j \leqslant N-1$. For simplicity set:

$$s_1 = \frac{D\delta t}{2\delta r^2}, \quad s_2 = \frac{D\delta t}{4\delta r} \tag{14}$$

For $j = 2$, the first equation becomes:

$$(s_1 + s_2 r_2^{-1})c_{i+1,3} - (1+2s_1)c_{i+1,2} + (s_1 - s_2 r_2^{-1})c_{i+1,1} = -(s_1 + s_2 r_2^{-1})c_{i,3} + \\ + (2s_1 - 1)c_{i,2} + (s_1 - s_2 r_2^{-1})c_{i,1} \tag{15}$$

The problem becomes, how to deal with the $c_{i+1,1}$ term. For this the boundary condition at $r = 0$ is used in the form:

$$\frac{-3c(0) + 4c(\delta r) - c(2\delta r)}{2\delta r} = 0 \Rightarrow c_{i+1,1} = \frac{4c_{i+1,2} - c_{i+1,3}}{3} \tag{16}$$

This can be substituted into (15) to get:

$$\frac{1}{3}(2s_1 + 4s_2r_2^{-1})c_{i+1,2} - \frac{1}{3}(3 + 2s_1 + 4s_2r_2^{-1})c_{i+1,3} = -(s_1 + s_2r_2^{-1})c_{i,3} + \\ + (2s_1 - 1)c_{i,2} + (s_1 - s_2r_2^{-1})c_{i,1} \quad (17)$$

Equation (5) for $j = N - 1$ is:

$$(s_1+s_2r_{N-1}^{-1})c_{i+1,N}-(1+2s_1)c_{i+1,N-1}+(s_1-s_2r_{N-1}^{-1})c_{i+1,N-2} = -(s_1+s_2r_{N-1}^{-1})c_{i,N}+ \\ + (2s_1 - 1)c_{i,N-1} + (s_1 - s_2r_{N-1}^{-1})c_{i,N-2} \quad (18)$$

The boundary condition at $r = R$ is:

$$\frac{3c(R) - 4c(r - \delta r) + c(R - 2\delta r)}{2\delta r} = f(t) \Rightarrow c_{i+1,N} = \frac{1}{3}\left(4c_{i+1,N-1} - c_{i+1,N-2} + 2\delta r f(t_{i+1})\right) \quad (19)$$

Just as before the $c_{i+1,N}$ term can be substituted for to yield:

$$-\frac{1}{3}(2s_1-4s_2r_{N-1}^{-1}+3)c_{i+1,N-1}+\frac{1}{3}(2s_1-4s_2r_{N-1}^{-1})c_{i+1,N-2} = -(s_1+s_2r_{N-1}^{-1})c_{i,N}+ \\ + (2s_1 - 1)c_{i.N-1} - (s_1 - s_2r_{N-1}^{-1})c_{i,N-2} - \frac{2\delta r}{3}(s_1 + s_2r_{N-1}^{-1})f(t_{i+1}) \quad (20)$$

To sum up, the solution to the spherical diffusion equation with given initial/boundary conditions is given by the solution of a tridiagonal matrix equation with first row ($j = 2$) is given by:

$$\frac{1}{3}(2s_1 + 4s_2r_2^{-1})c_{i+1,2} - \frac{1}{3}(3 + 2s_1 + 4s_2r_2^{-1})c_{i+1,3} = -(s_1 + s_2r_2^{-1})c_{i,3} + \\ + (2s_1 - 1)c_{i,2} + (s_1 - s_2r_2^{-1})c_{i,1} \quad (21)$$

for $3 \leqslant j \leqslant N - 2$:

$$(s_1 + s_2r_j^{-1})c_{i+1,j+1} - (1 + 2s_2)c_{i+1,j} + (s_1 - s_2r_j^{-1})c_{i+1,j-1} = \\ - (s_1 + s_2r_j^{-1})c_{i,j+1} + (2s_1 - 1)c_{i,j} + (s_1 - s_2r_j^{-1})c_{i,j-1} \quad (22)$$

for $j = N - 1$:

$$-\frac{1}{3}(2s_1-4s_2r_{N-1}^{-1}+3)c_{i+1,N-1}+\frac{1}{3}(2s_1-4s_2r_{N-1}^{-1})c_{i+1,N-2} = -(s_1+s_2r_{N-1}^{-1})c_{i,N}+ \\ + (2s_1 - 1)c_{i.N-1} - (s_1 - s_2r_{N-1}^{-1})c_{i,N-2} - \frac{2\delta r}{3}(s_1 + s_2r_{N-1}^{-1})f(t_{i+1}) \quad (23)$$