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

Mat Hunt

The diffusion equation in spherical polar co-ordinates is:

$$\frac{\partial c}{\partial t} = \frac{D}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial c}{\partial r}\right) \tag{1}$$

With initial condition:

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

and boundary conditions:

$$\left.\frac{\partial c}{\partial r}\right|_{r=0} = 0, \quad \left.\frac{\partial c}{\partial r}\right|_{r=1} = f(t) \tag{3}$$

1 Main Stencil

Initially denote $\xi = \partial_r c$ and note that:

$$\left.\frac{\partial}{\partial r}(r^2\xi)\right|_{r=r_i} = \frac{r_i^{+2}\xi_{i+\frac{1}{2}} - r_i^{-2}\xi_{i-\frac{1}{2}}}{\delta r} \tag{4}$$

where $r_i^{\pm} = r_i \pm \delta r/2$. We also note that:

$$\xi_{i+\frac{1}{2}} = \left.\frac{\partial c}{\partial r}\right|_{r=r_i+\frac{\delta r}{2}} = \frac{c_{i,j+1} - c_{i,j}}{\delta r} \quad \xi_{i-\frac{1}{2}} = \left.\frac{\partial c}{\partial r}\right|_{r=r_i-\frac{\delta r}{2}} = \frac{c_{i,j} - c_{i,j-1}}{\delta r} \tag{5}$$

Then we have:

$$\left.\frac{\partial}{\partial r}\left(r^2\frac{\partial c}{\partial r}\right)\right|_{r=r_i} = \frac{1}{\delta r^2}(r_j^{+2}c_{i,j+1} - (r_j^{+2} + r_i^{-2})c_{i,j} + r_j^{-2}c_{i,j-1}) \tag{6}$$

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:

$$\frac{c_{i+1,j}-c_{i,j}}{\delta t}=\frac{D}{r_i^2}\left[\frac{1}{\delta r^2}(r_j^{+2}c_{i+1,j+1}-(r_j^{+2}+r_j^{-2})c_{i+1,j}+r_j^{-2}c_{i+1,j-1})+\right.$$
$$\left.+\frac{1}{\delta r^2}(r_j^{+2}c_{i,j+1}-(r_j^{+2}+r_j^{-2})c_{i,j}+r_j^{-2}c_{i,j-1})\right] \quad (7)$$

This can be rearranged into the following form:

$$sr_j^{+2}c_{i+1,j+1}-(r_j^2+s(r_j^{+2}+r_j^{-2}))c_{i+1,j}+sr_j^{-2}c_{i+1,j-1}=$$
$$=-(sr_j^{+2}c_{i,j+1}-(r_j^2-s(r_j^{+2}+r_j^{-2}))c_{i,j}+sr_j^{-2}c_{i,j-1}) \quad (8)$$

where $s=D\delta t/(2\delta r)$. This is a tridiagonal matrix equation which can be solved easily.

2 Incorporating the Boundary Conditions

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 set $j=0$ for the boundary condition at $r=0$ and $j=N$ for the boundary condition at $r=1$. Considering the boundary condition at $r=0$, write:

$$sr_0^{+2}c_{i+1,1}-(r_0^2+s(r_0^{+2}+r_0^{-2}))c_{i+1,0}+sr_j^{-2}c_{i+1,-1}=$$
$$=-(sr_0^{+2}c_{i,1}-(r_0^2-s(r_0^{+2}+r_0^{-2}))c_{i,0}+sr_0^{-2}c_{i,-1}) \quad (9)$$

We see that $r_0=0$, and $r_0^{+2}=r_0^{-2}=\delta r^2$. To deal with $j=-1$, use the boundary condition:

$$\frac{c_{i,1}-c_{i,-1}}{2\delta r}=0\Rightarrow c_{i,-1}=c_{i,1} \quad (10)$$

This makes the stencil reduce to:

$$c_{i+1,1}-c_{i+1,0}=-(c_{i,1}-c_{i,0}) \quad (11)$$

The boundary condition at $r=1$ is a little more complicated, the stencil is:

$$sr_N^{+2}c_{i+1,N+1}-(r_N^2+s(r_N^{+2}+r_N^{-2}))c_{i+1,N}+sr_N^{-2}c_{i+1,N-1}=$$
$$=-(sr_N^{+2}c_{i,N+1}-(r_N^2-s(r_N^{+2}+r_N^{-2}))c_{i,N}+sr_N^{-2}c_{i,N-1}) \quad (12)$$

To deal with the $N+1$ term, we use the boundary condition:

$$\frac{c_{i,N+1}-c_{i,N-1}}{2\delta r}=f(t_i)=f_i\Rightarrow c_{i,N+1}=c_{1,N-1}+2f_i\delta r \quad (13)$$

The boundary condition then becomes:

$$\begin{aligned} &-(r_N^2+s(r_N^{+2}+r_N^{-2}))c_{i+1,N}+s(r_N^{-2}+r_N^{+2})c_{i+1,N-1}= \\ &=-((r_N^2-s(r_N^{+2}+r_N^{-2}))c_{i,N}+s(r_N^{-2}+r_N^{+2})c_{i,N-1})-2dr_N^{+2}(f_{i+1}-f_i)\delta r \end{aligned} \tag{14}$$

This results in the system of linear equations:

$$A\mathbf{c}^{i+1}=-B\mathbf{c}^i+\mathbf{d} \tag{15}$$

For $N=5$, the matrices are given by:

$$A=\begin{pmatrix} -1 & 1 & 0 & 0 & 0 \\ sr_1^{-2} & -(r_1^2+s(r_1^{+2}+r_1^{-2})) & sr_1^{+2} & 0 & 0 \\ 0 & sr_2^{-2} & -(r_2^2+s(r_2^{+2}+r_2^{-2})) & sr_2^{+2} & 0 \\ 0 & 0 & sr_3^{-2} & -(r_3^2+s(r_3^{+2}+r_3^{-2})) & sr_3^{+2} \\ 0 & 0 & 0 & s(r_4^{+2}+r_4^{-2}) & \alpha \end{pmatrix}$$

where $\alpha=-(r_4^2+s(r_4^{+2}+r_4^{-2}))$

$$B=\begin{pmatrix} -1 & 1 & 0 & 0 & 0 \\ sr_1^{-2} & -(r_1^2-s(r_1^{+2}+r_1^{-2})) & sr_1^{+2} & 0 & 0 \\ 0 & sr_2^{-2} & -(r_2^2-s(r_2^{+2}+r_2^{-2})) & sr_2^{+2} & 0 \\ 0 & 0 & sr_3^{-2} & -(r_3^2-s(r_3^{+2}+r_3^{-2})) & sr_3^{+2} \\ 0 & 0 & 0 & s(r_4^{+2}+r_4^{-2}) & \beta \end{pmatrix}$$

Where $\beta=-(r_4^4-s(r_4^{+2}+r_4^{-2}))$. Finally the vector $\mathbf{b}$ can be written as:

$$\mathbf{d}=\begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 2sr_4^{+2}(f_i-f_{i+1})\delta r \end{pmatrix}$$

This completes the set up of the numerical solution of the PDE.

3 Implementation of Method in MATLAB

Suppose we wish to solve the equation for $t\in[0,1]$, we have $r\in[0,1]$, if we want N_t intervals in the time variable and N_r intervals in the radial variable.

```
t=linspace(0,1,N_t);
r=linspace(0,1,N_r);
dt=t(2);dr=r(2);
r_plus=r+0.5*dr;
r_minus=r-0.5*dr;
```

The next part is we define the value for D and therefore s:

```
D=0.01;s=D*dt/(2*dr^2);
```

Defining the initial and boundary conditions:

```
c_0=2*ones(1,N_r);
f=0.5*sqrt(t).*exp(-5*t);
```

The next part we define the solution matrix c, A and B. It will be easier to define vectors and then insert them into the matrices A and B.

```
c=zeros(N_t,N_r);
d=zeros(N_r,1);
a_plus=s*r_plus(1:end-1).^2;
a_minus=s*r_minus(1:end-1).^2;
a=-(r.^2+s*(r_plus.^2+r_minus.^2));
b=-(r.^2-s*(r_plus.^2+r_minus.^2));
c(1,:)=c_0;
A=diag(a_plus,1)+diag(a)+diag(a_minus,-1);
B=diag(a_plus,1)+diag(b)+diag(a_minus,-1);
```

For the next part, we should compensate for the boundary conditions

```
A(1,1)=-1;A(1,2)=1;
B(1,1)=-1;B(1,2)=1;
A(N_r,N_r-1)=s*(r_plus(N_r)^2+r_minus(N_r)^2);
B(N_r,N_r-1)=s*(r_plus(N_r)^2+r_minus(N_r)^2);
```

The only other thing to do is for a for loop to compute the solution:

```
for␣i=2:N_t
d(end)=2*s*dr*r_plus(N_r)^2*(f(i-1)-f(i));
v=-B*c(i-1,:)'+d;
u=A\v;
c(i,:)=u';
end
```

Then plot the results:

```
for␣i=1:N_t
plot(r,c(i,:));
axis([0␣1␣0␣2]);
pause(0.05)
end
```