APL321: Introduction to Computational Fluid Dynamics

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1. SPATIAL DISCRETIZATION:

The first order upwind scheme (UDS) is used to discretize the convective term while the second order central differencing scheme (CDS) is used for the diffusive term. Thus, the first order spatial derivative of $c_{i,j}$ w.r.t x at (x_i, y_j) using UDS is given by:

$$\left. \frac{\partial c}{\partial x} \right|_{i,j} = \frac{c_{i,j} - c_{i-1,j}}{\Delta x} \tag{1}$$

The Laplacian of $c_{i,j}$ at (x_i, y_j) using CDS gives:

$$\nabla^2 c|_{i,j} = \left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2}\right)_{i,j} = \frac{c_{i+1,j} + c_{i-1,j} - 2c_{i,j}}{(\Delta x)^2} + \frac{c_{i,j+1} + c_{i,j-1} - 2c_{i,j}}{(\Delta y)^2}$$
(2)

TIME STEPPING SCHEME:

• Fully Implicit Backward Euler Scheme - The discretized equation using this scheme for the diffusive term for $c_{i,j}^n$ at (x_i, y_j, t_n) is given by:

$$\frac{c_{i,j}^{n+1} - c_{i,j}^{n}}{\Delta t} + U(y_j) \frac{c_{i,j}^{n+1} - c_{i-1,j}^{n+1}}{\Delta x} = D \left[\frac{c_{i+1,j}^{n+1} + c_{i-1,j}^{n+1} - 2c_{i,j}^{n+1}}{(\Delta x)^2} + \frac{c_{i,j+1}^{n+1} + c_{i,j-1}^{n+1} - 2c_{i,j}^{n+1}}{(\Delta y)^2} \right]$$
(3)

• Crank Nicolson Scheme - The discretized equation using this time stepping scheme for $c_{i,j}^n$ at (x_i, y_j, t_n) is given by:

$$\frac{c_{i,j}^{n+1} - c_{i,j}^{n}}{\Delta t} + U(y_{j}) \frac{c_{i,j}^{n+1} - c_{i-1,j}^{n+1}}{\Delta x} = \frac{D}{2} \left[\frac{c_{i+1,j}^{n} + c_{i-1,j}^{n} - 2c_{i,j}^{n}}{(\Delta x)^{2}} + \frac{c_{i+1,j}^{n+1} + c_{i-1,j}^{n+1} - 2c_{i,j}^{n+1}}{(\Delta x)^{2}} + \frac{c_{i,j+1}^{n+1} + c_{i,j-1}^{n} - 2c_{i,j}^{n}}{(\Delta y)^{2}} + \frac{c_{i,j+1}^{n+1} + c_{i,j-1}^{n+1} - 2c_{i,j}^{n+1}}{(\Delta y)^{2}} \right]$$

2. • Fully Implicit Backward Euler Scheme - Equation 3 when rearranged gives:

$$\left(\frac{1}{\Delta t} + \frac{U(y_j)}{\Delta x} + \frac{2D}{(\Delta x)^2} + \frac{2D}{(\Delta y)^2}\right) c_{i,j}^{n+1} - \frac{D}{(\Delta x)^2} c_{i+1,j}^{n+1} - \frac{D}{(\Delta y)^2} c_{i,j+1}^{n+1} - \left(\frac{U(y_j)}{\Delta x} + \frac{D}{(\Delta x)^2}\right) c_{i-1,j}^{n+1} - \frac{D}{(\Delta y)^2} c_{i,j-1}^{n+1} = \frac{1}{\Delta t} c_{i,j}^{n}$$

This equation takes the form:

$$A_P c_P + A_E c_E + A_N c_N + A_W c_W + A_S c_S = Q_P \tag{4}$$

where.

$$A_{E} = -\frac{D}{(\Delta x)^{2}}; A_{N} = -\frac{D}{(\Delta y)^{2}}; A_{W} = -\left(\frac{U(y_{j})}{\Delta x} + \frac{D}{(\Delta x)^{2}}\right); A_{S} = -\frac{D}{(\Delta y)^{2}}$$

$$A_{P} = \left(\frac{1}{\Delta t} + \frac{U(y_{j})}{\Delta x} + \frac{2D}{(\Delta x)^{2}} + \frac{2D}{(\Delta y)^{2}}\right); Q_{P} = \frac{1}{\Delta t}c_{i,j}^{n}$$

• Crank Nicolson Scheme - When rearranged, the equation derived above gives:

$$\left(\frac{1}{\Delta t} + \frac{U(y_j)}{\Delta x} + \frac{D}{(\Delta x)^2} + \frac{D}{(\Delta y)^2} \right) c_{i,j}^{n+1} - \frac{D}{2(\Delta x)^2} c_{i+1,j}^{n+1} - \frac{D}{2(\Delta y)^2} c_{i,j+1}^{n+1} - \left(\frac{U(y_j)}{\Delta x} + \frac{D}{2(\Delta x)^2} \right) c_{i,j}^{n+1} - \frac{D}{2(\Delta y)^2} c_{i,j+1}^{n+1} - \left(\frac{U(y_j)}{\Delta x} + \frac{D}{2(\Delta x)^2} \right) c_{i,j}^{n+1} - \frac{D}{2(\Delta y)^2} c_{i,j+1}^{n+1} - \left(\frac{U(y_j)}{\Delta x} + \frac{D}{2(\Delta x)^2} \right) c_{i,j+1}^{n+1} - \frac{D}{2(\Delta y)^2} c_{i,j+1}^{n+1} - \left(\frac{U(y_j)}{\Delta x} + \frac{D}{2(\Delta x)^2} \right) c_{i,j+1}^{n+1} - \left(\frac{U(y_j)}{\Delta x} + \frac{D}{2(\Delta x)^2} \right) c_{i,j+1}^{n+1} - \left(\frac{U(y_j)}{\Delta x} + \frac{D}{2(\Delta x)^2} \right) c_{i,j+1}^{n+1} - \left(\frac{U(y_j)}{\Delta x} + \frac{D}{2(\Delta x)^2} \right) c_{i,j+1}^{n+1} - \left(\frac{U(y_j)}{\Delta x} + \frac{D}{2(\Delta x)^2} \right) c_{i,j+1}^{n+1} - \left(\frac{U(y_j)}{\Delta x} + \frac{D}{2(\Delta x)^2} \right) c_{i,j+1}^{n+1} - \left(\frac{U(y_j)}{\Delta x} + \frac{D}{2(\Delta x)^2} \right) c_{i,j+1}^{n+1} - \left(\frac{U(y_j)}{\Delta x} + \frac{D}{2(\Delta x)^2} \right) c_{i,j+1}^{n+1} - \left(\frac{U(y_j)}{\Delta x} + \frac{D}{2(\Delta x)^2} \right) c_{i,j+1}^{n+1} - \left(\frac{U(y_j)}{\Delta x} + \frac{D}{2(\Delta x)^2} \right) c_{i,j+1}^{n+1} - \left(\frac{U(y_j)}{\Delta x} + \frac{D}{2(\Delta x)^2} \right) c_{i,j+1}^{n+1} - \left(\frac{U(y_j)}{\Delta x} + \frac{D}{2(\Delta x)^2} \right) c_{i,j+1}^{n+1} - \left(\frac{U(y_j)}{\Delta x} + \frac{D}{2(\Delta x)^2} \right) c_{i,j+1}^{n+1} - \left(\frac{U(y_j)}{\Delta x} + \frac{D}{2(\Delta x)^2} \right) c_{i,j+1}^{n+1} - \left(\frac{U(y_j)}{\Delta x} + \frac{D}{2(\Delta x)^2} \right) c_{i,j+1}^{n+1} - \left(\frac{U(y_j)}{\Delta x} + \frac{D}{2(\Delta x)^2} \right) c_{i,j+1}^{n+1} - \left(\frac{U(y_j)}{\Delta x} + \frac{D}{2(\Delta x)^2} \right) c_{i,j+1}^{n+1} - \left(\frac{U(y_j)}{\Delta x} + \frac{D}{2(\Delta x)^2} \right) c_{i,j+1}^{n+1} - \left(\frac{U(y_j)}{\Delta x} + \frac{D}{2(\Delta x)^2} \right) c_{i,j+1}^{n+1} - \left(\frac{U(y_j)}{\Delta x} + \frac{D}{2(\Delta x)^2} \right) c_{i,j+1}^{n+1} - \left(\frac{U(y_j)}{\Delta x} + \frac{D}{2(\Delta x)^2} \right) c_{i,j+1}^{n+1} - \left(\frac{U(y_j)}{\Delta x} + \frac{D}{2(\Delta x)^2} \right) c_{i,j+1}^{n+1} - \left(\frac{U(y_j)}{\Delta x} + \frac{D}{2(\Delta x)^2} \right) c_{i,j+1}^{n+1} - \left(\frac{U(y_j)}{\Delta x} + \frac{D}{2(\Delta x)^2} \right) c_{i,j+1}^{n+1} - \left(\frac{U(y_j)}{\Delta x} + \frac{D}{2(\Delta x)^2} \right) c_{i,j+1}^{n+1} - \left(\frac{U(y_j)}{\Delta x} + \frac{D}{2(\Delta x)^2} \right) c_{i,j+1}^{n+1} - \left(\frac{U(y_j)}{\Delta x} + \frac{D}{2(\Delta x)^2} \right) c_{i,j+1}^{n+1} - \left(\frac{U(y_j)}{\Delta x} + \frac{D}{2(\Delta x)^2} \right) c_{i,j+1}^{n+1} - \left(\frac{U(y_j)}{\Delta x} + \frac{D}{2(\Delta x)^2} \right) c_{i,j+1}^{n+1} - \left(\frac{U(y_$$

where

$$A_{E} = -\frac{D}{2(\Delta x)^{2}}; A_{N} = -\frac{D}{2(\Delta y)^{2}}; A_{W} = -\left(\frac{U(y_{j})}{\Delta x} + \frac{D}{2(\Delta x)^{2}}\right); A_{S} = -\frac{D}{2(\Delta y)^{2}}$$

$$A_{P} = \left(\frac{1}{\Delta t} + \frac{U(y_{j})}{\Delta x} + \frac{D}{(\Delta x)^{2}} + \frac{D}{(\Delta y)^{2}}\right);$$

$$Q_{P} = \left(\frac{1}{\Delta t} - \frac{D}{(\Delta x)^{2}} - \frac{D}{(\Delta y)^{2}}\right)c_{i,j}^{n} + \frac{D}{2}\left(\frac{c_{i+1,j}^{n} + c_{i-1,j}^{n}}{(\Delta x)^{2}} + \frac{c_{i,j+1}^{n} + c_{i,j-1}^{n}}{(\Delta y)^{2}}\right)$$

Note that the above equations and coefficients are only valid for interior nodes. There will be slight modifications to these values for the boundary nodes according to the boundary conditions.

WEST BOUNDARY

Since c=0 for all points on the western boundary at all times, $\frac{\partial c}{\partial t}=0$, $\frac{\partial c}{\partial x}=0$, $\frac{\partial c}{\partial y}=0$, $\frac{\partial^2 c}{\partial x^2}=0$, $\frac{\partial^2 c}{\partial y^2}=0$. All the coefficients become 0 except for A_P which changes to $A_P\to 1$.

NORTH BOUNDARY

The boundary condition specified is Neumann with $\frac{\partial c}{\partial y} = 0$ at all times. Using first order approximation, we can say that $c_{i,N_y+1}^n = c_{i,N_y}^n$

EAST BOUNDARY

The boundary condition specified is Neumann with $\frac{\partial c}{\partial x} = 0$ at all times. Using first order approximation, we can say that $c_{N_x+1,j}^n = c_{N_x,j}^n$

SOUTH BOUNDARY

The boundary condition specified is Neumann with $\frac{\partial c}{\partial y} = 0$ at all times. Using first order approximation, we can say that $c_{i,1}^n = c_{i,2}^n$

3. The isocontours for the concentration field c(x,y) at time, t = 500 sec using Schemes 1 and 2 are given below:

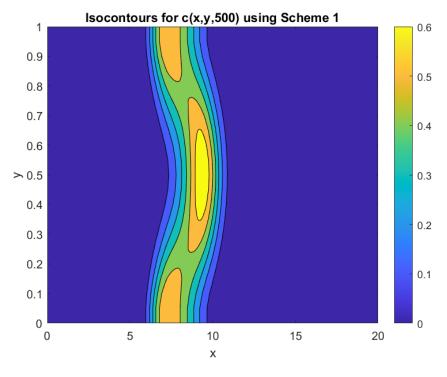


Figure 1: Isocontours for c using Scheme 1

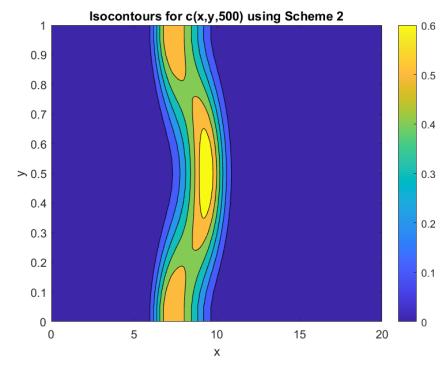


Figure 2: Isocontours for c using Scheme 1

There are no significant differences between the isocontours produced by the two schemes. This suggests that both the schemes are reasonably accurate and good to use for this problem.

4. The concentration field c at $y = \frac{Ly}{2}$ at time t = 500 sec for both the schemes are given by:

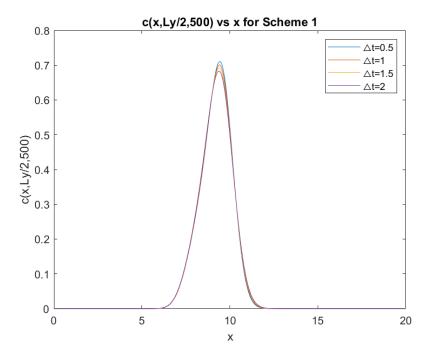


Figure 3: c(x, Ly/2, 500) for Scheme 1

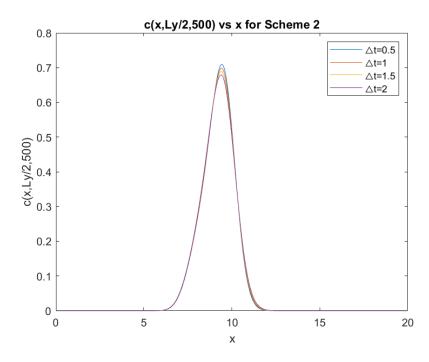


Figure 4: c(x, Ly/2, 500) for Scheme 2

We can see that, in both schemes, as the time step increases, the peak of the curve slightly shifts downwards. This suggests that as we increase the time step value, the solution converges to values different from the exact solution and the error keeps increasing.