PDE's Discussed

- **Laplace Equation**

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0$$

- **Discretization**

$$\frac{\phi_{i-1,j} - 2\phi_{i,j} + \phi_{i+1,j}}{\Delta x^2} + \frac{\phi_{i,j-1} - 2\phi_{i,j} + \phi_{i,j+1}}{\Delta y^2} = 0$$

PDE's Discussed

- **Advection-Diffusion Equation**

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = D\frac{\partial^2 c}{\partial x^2}$$

- Explicit:

$$\frac{c_i^{n+1} - c_i^n}{\Delta t^n} + u_i^n \frac{c_{i+1}^n - c_{i-1}^n}{2\Delta x_i} = D_i^n \frac{c_{i+1}^n - 2c_i^n + c_{i-1}^n}{\Delta x_i^2}$$

- Time-weighted (μ)

$$(1-\mu)\left(-\frac{u\Delta t}{2\Delta x} - \frac{D\Delta t}{\Delta x^2}\right)c_{i-1}^{n+1} + \left(1 + \frac{2(1-\mu)D\Delta t}{\Delta x^2}\right)c_i^{n+1} + (1-\mu)\left(\frac{u\Delta t}{2\Delta x} - \frac{D\Delta t}{\Delta x^2}\right)c_{i+1}^{n+1} =$$

$$\mu\left(\frac{u\Delta t}{2\Delta x} + \frac{D\Delta t}{\Delta x^2}\right)c_{i-1}^n + \left(1 - \frac{2\mu D\Delta t}{\Delta x^2}\right)c_i^n + \mu\left(-\frac{u\Delta t}{2\Delta x} + \frac{D\Delta t}{\Delta x^2}\right)c_{i+1}^n$$

PDE's Discussed

- **Wave Equation**

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

- **Explicit:**

$$\frac{\phi_i^{n-1} - 2\phi_i^n + \phi_i^{n+1}}{\Delta t^2} = u^2 \frac{\phi_{i-1}^n - 2\phi_i^n + \phi_{i+1}^n}{\Delta x^2}$$

- **Implicit:**

$$\frac{\phi_i^{n-1} - 2\phi_i^n + \phi_i^{n+1}}{\Delta t^2} = u^2 \left[\frac{1}{4} \frac{\phi_{i-1}^{n-1} - 2\phi_i^{n-1} + \phi_{i+1}^{n-1}}{\Delta x^2} + \frac{1}{2} \frac{\phi_{i-1}^n - 2\phi_i^n + \phi_{i+1}^n}{\Delta x^2} + \frac{1}{4} \frac{\phi_{i-1}^{n+1} - 2\phi_i^{n+1} + \phi_{i+1}^{n+1}}{\Delta x^2} \right]$$

PDE's Discussed

- **2-D transient diffusion**

$$\frac{\partial c}{\partial t} = D\left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2}\right)$$

- **Explicit:**

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

- **Implicit:**

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

Truncation Error and Stability

- Similar to what was done for ODE
- Truncation error is obtained by comparing the discretized “difference form” with the Taylor’s series
- Stability is obtained by looking at the amplification
- Covered very briefly here and for very simple cases

Truncation Error : Laplace Equation

$$\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}=0 \qquad \frac{\phi_{i-1,j}-2\phi_{i,j}+\phi_{i+1,j}}{\Delta x^2}+\frac{\phi_{i,j-1}-2\phi_{i,j}+\phi_{i,j+1}}{\Delta y^2}=0$$

- Need the Taylor's series expansions

$$\phi_{i\pm1,j}=\left[\phi\pm\Delta x\frac{\partial\phi}{\partial x}+\frac{\Delta x^2}{2!}\frac{\partial^2\phi}{\partial x^2}\pm\frac{\Delta x^3}{3!}\frac{\partial^3\phi}{\partial x^3}+\frac{\Delta x^4}{4!}\frac{\partial^4\phi}{\partial x^4}+\ldots\right]_{i,j}$$

$$\phi_{i,j\pm1}=\left[\phi\pm\Delta y\frac{\partial\phi}{\partial y}+\frac{\Delta y^2}{2!}\frac{\partial^2\phi}{\partial y^2}\pm\frac{\Delta y^3}{3!}\frac{\partial^3\phi}{\partial y^3}+\frac{\Delta y^4}{4!}\frac{\partial^4\phi}{\partial y^4}+\ldots\right]_{i,j}$$

- Not needed here, but for later use:

$$\phi_{i+1,j+1}=\left[\phi+\Delta x\frac{\partial\phi}{\partial x}+\Delta y\frac{\partial\phi}{\partial y}+\frac{1}{2!}\left(\Delta x\frac{\partial}{\partial x}+\Delta y\frac{\partial}{\partial y}\right)^2\phi+\frac{1}{3!}\left(\Delta x\frac{\partial}{\partial x}+\Delta y\frac{\partial}{\partial y}\right)^3\phi\ldots\right]_{i,j}$$

Truncation Error : Laplace Equation

- Difference equation at i,j

$$\frac{\phi_{i-1,j}-2\phi_{i,j}+\phi_{i+1,j}}{\Delta x^2}+\frac{\phi_{i,j-1}-2\phi_{i,j}+\phi_{i,j+1}}{\Delta y^2}=0$$

$$\frac{\partial^2\phi}{\partial x^2}+\frac{\Delta x^2}{12}\frac{\partial^4\phi}{\partial x^4}+\ldots+\frac{\partial^2\phi}{\partial y^2}+\frac{\Delta y^2}{12}\frac{\partial^4\phi}{\partial y^4}+\ldots=0$$

$$\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}=-\frac{\Delta x^2}{12}\frac{\partial^4\phi}{\partial x^4}-\frac{\Delta y^2}{12}\frac{\partial^4\phi}{\partial y^4}+\ldots$$

- Truncation Error: (T.V. – Approx Value) of $\nabla^2\phi$

$$\frac{\Delta x^2}{12}\frac{\partial^4\phi}{\partial x^4}+\frac{\Delta y^2}{12}\frac{\partial^4\phi}{\partial y^4}+\ldots$$

- Second order in both x and y, as expected

Truncation Error : Diffusion Equation

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

- Time-weighted scheme:

$$-(1-\mu)\frac{D\Delta t}{\Delta x^2}c_{i-1}^{n+1} + \left(1+\frac{2(1-\mu)D\Delta t}{\Delta x^2}\right)c_i^{n+1} - (1-\mu)\frac{D\Delta t}{\Delta x^2}c_{i+1}^{n+1} =$$

$$\mu\frac{D\Delta t}{\Delta x^2}c_{i-1}^{n} + \left(1-\frac{2\mu D\Delta t}{\Delta x^2}\right)c_i^{n} + \mu\frac{D\Delta t}{\Delta x^2}c_{i+1}^{n}$$

- Use the Taylor's series expansions (similar to the Laplace equation with i,j, now we have i for space and n for time). We will now need the i±1,n+1 expressions also.

Truncation Error : Diffusion Equation

- Difference equation at i,n simplifies to

$$\frac{\partial c}{\partial t} - D\frac{\partial^2 c}{\partial x^2} = -\frac{\Delta t}{2}\frac{\partial^2 c}{\partial t^2} + (1-\mu)\Delta t D\frac{\partial^3 c}{\partial t\,\partial x^2}$$

$$-\frac{\Delta t^2}{6}\frac{\partial^3 c}{\partial t^3} + (1-\mu)\frac{\Delta t^2}{2}D\frac{\partial^4 c}{\partial t^2\,\partial x^2}$$

$$+D\frac{\Delta x^2}{12}\frac{\partial^4 c}{\partial x^4} + \ldots$$

- Truncation Error: Negative of the r.h.s
- First order in t and Second order in x, as expected (forward difference in time and central in space)

Truncation Error : Diffusion Equation

- If we look at O(Δt) term: $\frac{\Delta t}{2}\frac{\partial^2 c}{\partial t^2}-(1-\mu)\Delta t D\frac{\partial^3 c}{\partial t\,\partial x^2}$
- And use the original PDE, we get the term as

$$\Delta t\left(\mu-\frac{1}{2}\right)\frac{\partial^2 c}{\partial t^2}\ \text{since}\ \frac{\partial^2 c}{\partial t^2}=\frac{\partial}{\partial t}\frac{\partial c}{\partial t}=D\frac{\partial^3 c}{\partial t\,\partial x^2}$$

- This implies that the scheme is second-order accurate in time also, if we use μ=1/2
- Another possibility is to choose the step size in such a way as to make the lowest order error vanish

Truncation Error : Diffusion Equation

- The lowest order term is $\Delta t\left(\mu-\frac{1}{2}\right)\frac{\partial^2 c}{\partial t^2}-D\frac{\Delta x^2}{12}\frac{\partial^4 c}{\partial x^4}$

- Again, the original PDE is used to get

$$\frac{\partial^2 c}{\partial t^2}=\frac{\partial}{\partial t}\left(D\frac{\partial^2 c}{\partial x^2}\right)=D\frac{\partial^2}{\partial x^2}\frac{\partial c}{\partial t}=D^2\frac{\partial^4 c}{\partial x^4}$$

- And the term becomes $\left[D^2\Delta t\left(\mu-\frac{1}{2}\right)-D\frac{\Delta x^2}{12}\right]\frac{\partial^4 c}{\partial x^4}$

- Which may me made to vanish by choosing

$\frac{D\Delta t}{\Delta x^2}=\frac{1}{12\left(\mu-\frac{1}{2}\right)}$ (naturally, works only for μ>1/2 could use explicit, μ=1)

Truncation Error : Pure advection

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = 0$$

- Explicit scheme, with central difference:

$$c_i^{n+1} = \frac{u\Delta t}{2\Delta x}c_{i-1}^n + c_i^n - \frac{u\Delta t}{2\Delta x}c_{i+1}^n$$

- Using Taylor's series (and replacing all time derivatives by spatial derivatives):

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = -\frac{u^2\Delta t}{2}\frac{\partial^2 c}{\partial x^2} + \left(\frac{u^3\Delta t^2}{6} - \frac{u\Delta x^2}{6}\right)\frac{\partial^3 c}{\partial x^3} + \ldots$$

- First order in time and second in space

Truncation Error : Pure advection

- Physically unrealistic
- Because, concentration at node i is being affected by the "downstream" node, i+1
- Upstream or upwind scheme (e.g., for +ive u):

$$\left.\frac{\partial c}{\partial x}\right|_i^n = \frac{c_i^n - c_{i-1}^n}{\Delta x} \Rightarrow c_i^{n+1} = \frac{u\Delta t}{\Delta x} c_{i-1}^n + \left(1 - \frac{u\Delta t}{\Delta x}\right) c_i^n$$

- Truncation Error:

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = \left(\frac{u\Delta x}{2} - \frac{u^2\Delta t}{2}\right)\frac{\partial^2 c}{\partial x^2} + \left(\frac{u\Delta x^2}{6} + \frac{u^3\Delta t^2}{6}\right)\frac{\partial^3 c}{\partial x^3} + \ldots$$

- First order in time and space. Second order if the Courant number is 1 ($u\Delta t/\Delta x=1$)

Stability Analysis

- Matrix method: Similar to the one used for ODE, applied to semi-discretization
- von Neumann method: Based on separation of variables and Fourier series, applied to full discretization
- The amplification at each step should be less than or equal to 1

Stability Analysis: Matrix method

- The PDE is converted to ODE of the form

$$\frac{d\{\phi\}}{dt} = [A]\{\phi\}$$

- Where $\{\phi\}$ is the vector of nodal values
- As discussed earlier for ODE, the largest eigenvalue of A should be ≤1 for stability
- Diffusion equation, $L=m\Delta x$, Dirichlet B.C.

$$\frac{d\phi_i}{dt} = D\frac{\phi_{i-1} - 2\phi_i + \phi_{i+1}}{\Delta x^2}$$

- **A** will be a tridiagonal matrix, size m−1

Stability Analysis: Matrix method

$$A = \begin{bmatrix} -\frac{2D}{\Delta x^2} & \frac{D}{\Delta x^2} & & & \\ \frac{D}{\Delta x^2} & -\frac{2D}{\Delta x^2} & \frac{D}{\Delta x^2} & & \\ & \frac{D}{\Delta x^2} & -\frac{2D}{\Delta x^2} & \frac{D}{\Delta x^2} & \\ . & . & . & . & . \\ & & & \frac{D}{\Delta x^2} & -\frac{2D}{\Delta x^2} \end{bmatrix}$$

- To find the m−1 eigenvalues of **A**, we write $A=-(D/\Delta x^2)$ B, find the Eigenvalues of B, and multiply with $-(D/\Delta x^2)$

Stability Analysis: Matrix method

$$B = \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ . & . & . & . & . \\ & & & -1 & 2 \end{bmatrix} \Rightarrow \begin{bmatrix} 2-\lambda & -1 & & & \\ -1 & 2-\lambda & -1 & & \\ & -1 & 2-\lambda & -1 & \\ . & . & . & . & . \\ & & & -1 & 2-\lambda \end{bmatrix} \begin{Bmatrix} z_1 \\ z_2 \\ z_3 \\ . \\ z_{m-1} \end{Bmatrix} = 0$$

- λ is obtained by solving the linear recursive relationship

$$-z_{k-1} + (2-\lambda)z_k - z_{k+1} = 0 \quad \text{for } k = 1,2,\ldots,m-1$$

- with the condition that $z_0 = z_m = 0$

Stability Analysis: Matrix method

- Using a ratio r of consecutive terms, and writing $z_{k+1}=rz_k$, or, equivalently, $z_k=r^k$,

$$-1+(2-\lambda)r-r^2=0$$

- The solutions are: $r_{1,2}=\dfrac{2-\lambda\pm\sqrt{\lambda^2-4\lambda}}{2}$

- Therefore, the general solution of the recursive equation $-z_{k-1}+(2-\lambda)z_k-z_{k+1}=0$

is $z_k=c_1r_1^k+c_2r_2^k$ for $k=0,1,2,\ldots,m$

Stability Analysis: Matrix method

$$z_k = c_1 r_1^k + c_2 r_2^k \quad \text{for } k = 0,1,2,\ldots,m$$

- Using $z_0=0$, $c_2=-c_1$ => $z_k = c\left(r_1^k - r_2^k\right)$
- Using $z_m=0$, $r_1^m - r_2^m = 0$
- Write $r_{1,2} = \dfrac{2-\lambda \pm \sqrt{\lambda^2 - 4\lambda}}{2}$ as $e^{\pm i\theta}$

$$\cos\theta = \frac{2-\lambda}{2} \text{ and } \sin\theta = \frac{\sqrt{4\lambda - \lambda^2}}{2}$$

- We get $\sin m\theta = 0 = \sin j\pi$

Stability Analysis: Matrix method

- Resulting in the eigenvalues of B as:

$$\lambda_j = 2 - 2\cos\frac{j\pi}{m} \;;\; j = 1,2,\ldots,m-1$$

- The largest magnitude will be for j=m-1, and is approximately 4
- The eigenvalues of A are obtained on multiplying by $-(D/\Delta x^2)$
- Stabilty limit is given by $|\lambda_{max}\Delta t| \leq \mathbf{2}$
- $D\Delta t/\Delta x^2 \leq \mathbf{1/2}$

Stability Analysis: von Neumann method

- The solution is assumed to be of the form

$$\phi = \sum_{k=-\infty}^{\infty} T_k(t) X_k(x)$$

- Assume the function could be represented using a Fourier series with $X_k(x) = e^{ikx}$
- As discussed earlier, the magnification, i.e., $T_k(t_{n+1})/T_k(t_n)$, should be ≤1 for all k to have stable solution
- Again consider the Diffusion equation

Stability Analysis: von Neumann method

- The explicit form is

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = D\,\frac{\phi_{i-1}^n - 2\phi_i^n + \phi_{i+1}^n}{\Delta x^2}$$

- Using variable-separated form, for any k:

$$\frac{T_k^{t+\Delta t} - T_k^t}{\Delta t} e^{ikx} = D T_k^t\,\frac{e^{ik(x-\Delta x)} - 2e^{ikx} + e^{ik(x+\Delta x)}}{\Delta x^2}$$

- The amplification is

$$\sigma = \left|\frac{T_k^{t+\Delta t}}{T_k^t}\right| = \left|1 + \frac{D\Delta t}{\Delta x^2}\left(e^{-ik\Delta x} - 2 + e^{ik\Delta x}\right)\right|$$

Stability Analysis: von Neumann method

- Amplification for any "wave number" k

$$\sigma = \left| 1 + \frac{2D\Delta t}{\Delta x^2}(\cos k\Delta x - 1) \right|$$

- Most critical for cos=−1

$$\left| 1 - \frac{4D\Delta t}{\Delta x^2} \right| \le 1$$

- Which again results in $D\Delta t/\Delta x^2$ $\mathbf{\leq 1/2}$


The End