LECTURE 11

NUMERICAL SOLUTION OF THE TRANSIENT DIFFUSION EQUATION USING THE FINITE DIFFERENCE (FD) METHOD

- Solve the p.d.e.

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

- Initial conditions (i.c.'s)

$$u(x, t=t_o) = u*_o(x)$$

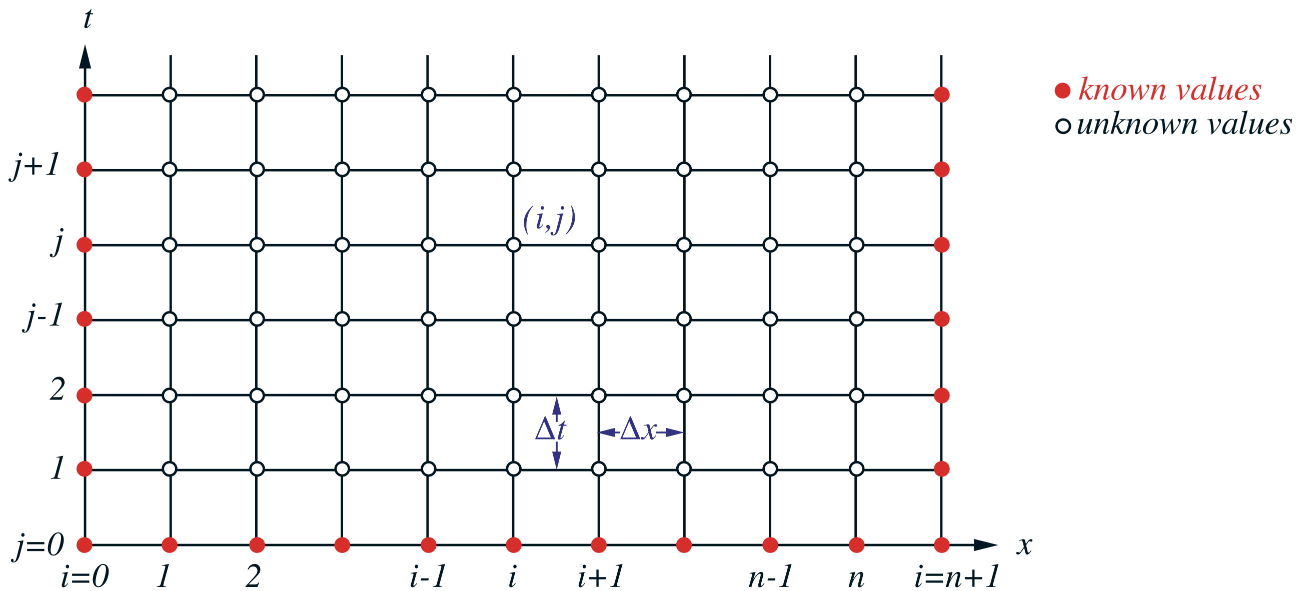
- Boundary conditions (b.c.'s)

$$u(x=x_1, t) = u_1^{**}(t) \qquad u(x=x_2, t) = u_2^{**}(t)$$

- Notes
  - We can also specify derivative b.c.'s but we must have at least one functional value b.c. for uniqueness.
  - This p.d.e. is classified as a parabolic type p.d.e.
  - The equation can represent heat conduction and mass diffusion.

Explicit Solution Procedure

- Evaluate the p.d.e. at point (i, j) $\quad$ (i = spatial index and j = temporal index)



- Let's use a forward difference approximation to evaluate $\frac{\partial u}{\partial t}$ at i, j:

$$\left.\frac{\partial u}{\partial t}\right|_{i,j} = \frac{u_{i,j+1} - u_{i,j}}{\Delta t} \qquad O(\Delta t) \text{ accurate}$$

- Use a central difference approximation to evaluate $\frac{\partial^2 u}{\partial x^2}$ at i, j:

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_{i,j} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{(\Delta x)^2} \qquad O(\Delta x)^2 \text{ accurate}$$

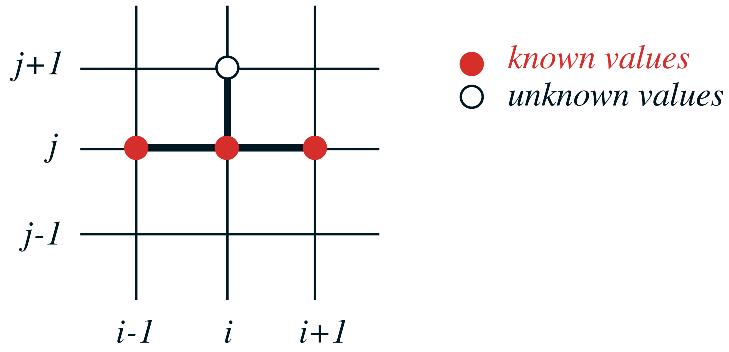
- Substituting into the p.d.e.:

$$\frac{1}{\Delta t}(u_{i,j+1} - u_{i,j}) = \frac{D}{(\Delta x)^2}(u_{i+1,j} - 2u_{i,j} + u_{i-1,j})$$

- Solving for unknown $u_{i,j+1}$ represents the solution at the i^{th} node and the $(j+1)^{th}$ time level.

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

- Notes on solving the discrete approximations to the p.d.e.
    - Let's examine the FD molecule:



- One discrete equation can be written for each node (such that the number of unknowns equals the number of equations)
- We can compute unknown nodal values of u at the new time level directly from values of the previous time level (i.e. they are not coupled at the new time level). The order in which the computations are performed in ***space*** does not matter since the values at the new time level are entirely dependent on values at previous time levels.
- *Explicit Formula - one unknown pivotal (or nodal) value is directly expressed in terms of known pivotal values.*

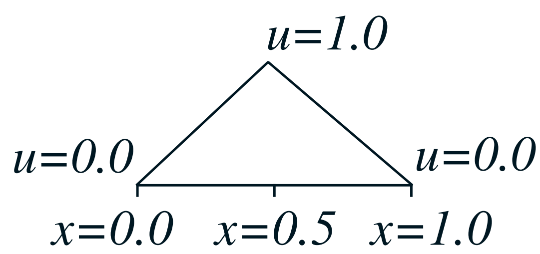
- Notes on time marching and accuracy
  - ***The process advancing from a known time level(s) to the unknown time level is called "time marching".***
  - The solution is known at time level j, starting with the initial conditions at $j = 0$.
  - This explicit solution to the transient diffusion equation is $O(\Delta t)$ accurate in time and $O(\Delta x^2)$ accurate in space.
- Notes on stability
  - ***<u>Stability</u> relates to the unstable amplification or stable damping of the range of wavelength components which comprise a numerical solution. An unstable solution increases until we have reached numerical overflow on the computer performing the calculations.***
  - The major shortcoming of explicit methods is stability.
  - This particular explicit difference solution becomes unstable when:

$$\frac{D\Delta t}{(\Delta x)^2} > \frac{1}{2} \quad \Rightarrow \quad \Delta t > \frac{1}{2}\frac{(\Delta x)^2}{D}$$

  - Therefore there are restrictions on the time step size in order to have a stable solution! Thus this solution is ***conditionally stable***.

Example of heat conduction in a rod

- Specified initial conditions



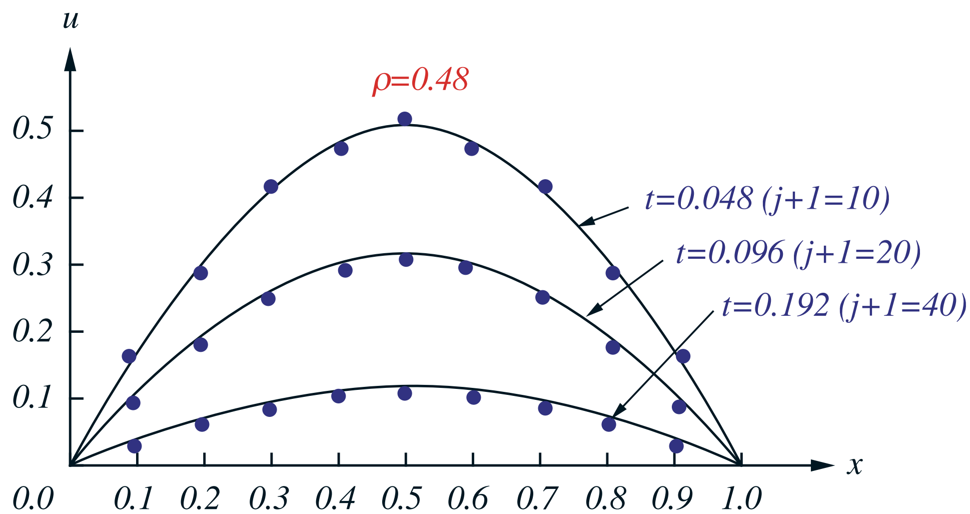
- Boundary conditions

$$u(x = 0, t) = 0 \qquad u(x = 1, t) = 0$$

- Steady state analytical solution

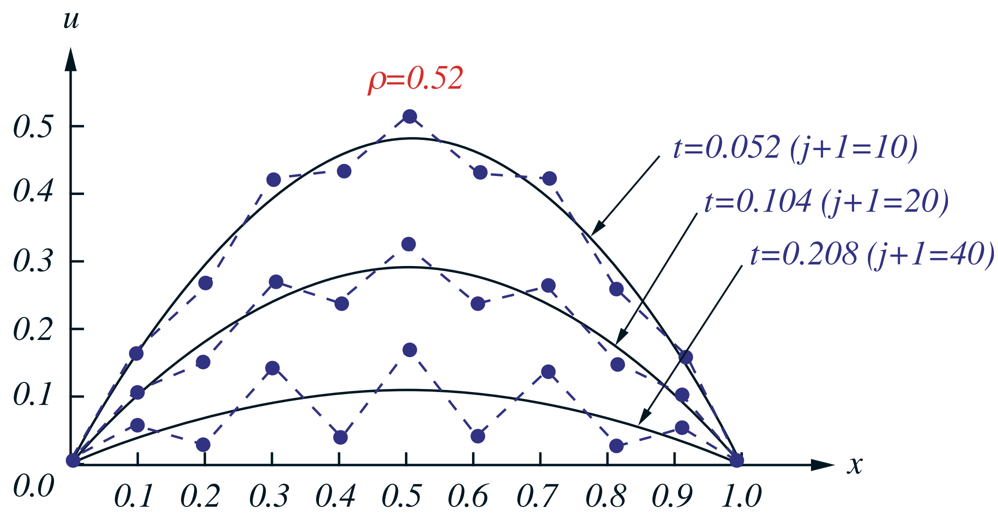
$$u(x, t) = 0 \quad \text{as} \quad t \rightarrow \infty$$

- Letting $\rho = \frac{D\Delta t}{\Delta x^2} = 0.48$ results in a stable numerical solution



- Solution is stable and remains stable as $t \to \infty$

- Letting $\rho = \frac{D\Delta t}{\Delta x^2} = 0.52$ results in an unstable numerical solution



- Notes on instabilities
  - The most rapid unstable growth appears to be for wavelength components in the solution which are on the order of $2 \cdot \Delta x$
  - The amplitudes of the short wavelength solution components experience unbounded growth in the case $\rho = 0.52$

General Notes on Instabilities

- The solution becomes unstable when the coefficient of the $u_{i,j}$ term in the FD formula becomes negative.
- Instabilities have wavelengths on the order of the grid size and amplitudes which increase ***very*** rapidly! Therefore the finer the grid, the smaller the wavelength.
- The amplitude of the solution can grow exponentially.
- Δt required for stability is smaller than that required to keep truncation errors to reasonable values.
- Δx must be kept "reasonably" small for accuracy.

Implicit Solution Procedure

- Evaluate the p.d.e. at the point $(i, j+1)$.
- Use a backward difference approximation for $\frac{\partial u}{\partial t}$ at $(i, j+1)$

$$\left.\frac{\partial u}{\partial t}\right|_{i,j+1} = \frac{u_{i,j+1} - u_{i,j}}{\Delta t}$$

- Use a central difference for $\frac{\partial^2 u}{\partial x^2}$ at $(i, j+1)$

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_{i,j+1} = \frac{1}{\Delta x^2}[u_{i+1,j+1} - 2u_{i,j+1} + u_{i-1,j+1}]$$

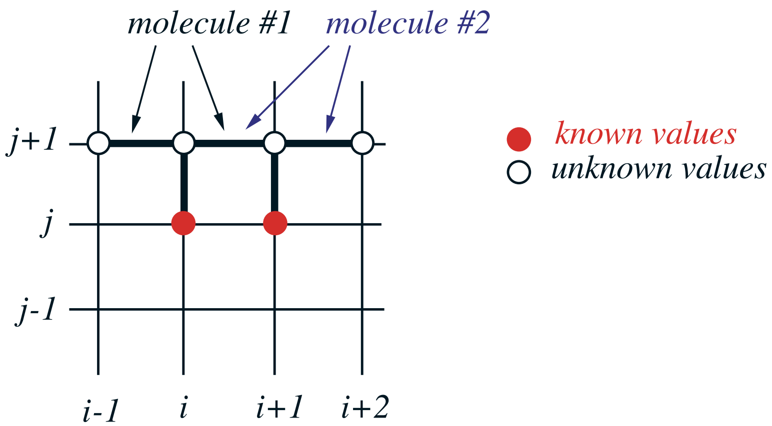
- Substituting into the p.d.e.:

$$\frac{1}{\Delta t}[u_{i,j+1} - u_{i,j}] = \frac{D}{(\Delta x)^2}[u_{i+1,j+1} - 2u_{i,j+1} + u_{i-1,j+1}]$$

- Re-arrange such that unknown values appear on the left hand side of the equation:

$$u_{i-1,j+1} - \left(2 + \frac{(\Delta x)^2}{\Delta t D}\right)u_{i,j+1} + u_{i+1,j+1} = \frac{-(\Delta x)^2}{\Delta t D}u_{i,j}$$

- Notes on Implicit Solution to the transient diffusion equation
  - $u_{i-1, j+1}$, $u_{i, j+1}$, $u_{i+1, j+1}$ are the unknown values.
  - $u_{i, j}$ is the only known value.
  - FD molecule for this representation:



  - Equations for adjacent nodes will be dependent on adjacent values!!
  - ***We can no longer "explicitly" solve for each unknown value independently but must solve for all unknowns simultaneously as a set of linear equations → "Implicit solution"***

- We generate a system of n equations ($n+2$ nodes - 2 b.c.'s). One equation for each unknown value.

- In matrix form:

$$\begin{bmatrix} \alpha & 1 & & & & & & \\ 1 & \alpha & 1 & & & & & \\ & 1 & \alpha & 1 & & & & \\ & & \cdot & \cdot & \cdot & & & \\ & & & \cdot & \cdot & \cdot & & \\ & & & & \cdot & \cdot & \cdot & \\ & & & & & 1 & \alpha & 1 \\ & & & & & & 1 & \alpha \end{bmatrix} \begin{bmatrix} u_{j+1,1} \\ u_{j+1,2} \\ u_{j+1,3} \\ \cdot \\ \cdot \\ \cdot \\ u_{j+1,n-1} \\ u_{j+1,n} \end{bmatrix} = \begin{bmatrix} Au_{j,1} - u^{**}{}_1\big|_{j+1} \\ Au_{j,2} \\ \cdot \\ \cdot \\ \cdot \\ Au_{j,n-1} \\ Au_{j,n} - u^{**}{}_2\big|_{j+1} \end{bmatrix}$$

where $\alpha = -\left(2 + \frac{(\Delta x)^2}{D\Delta t}\right)$ and $A = -\frac{(\Delta x)^2}{D\Delta t}$

- Notes on simultaneous equation solution
  - The matrix is always diagonally dominant, and there are therefore no roundoff error problems in the solution of this system of simultaneous equations. Solve this tri-diagonal, symmetric set of equations by a Gauss-elimination type procedure.
  - If Δx, Δt, D are constants we do not need to re-set and triangularize the matrix at every time step, otherwise we must re-set and re-solve the matrix every Δt.
  - To solve this system of equations requires $O(n)$ operations, the same order is required for an explicit formulation. This however changes for 2D and 3D problems!!
- Implicit methods are ***unconditionally stable*** (i.e. the method is stable for all values of Δt and Δx).
- There are ***still accuracy limitations*** on both Δt and Δx (which are required to limit truncation error!). Δt can be many times larger for an implicit scheme than for an explicit scheme (10 to 100 times), leading to computational savings.
- Truncation order of implicit and explicit methods is the same (order $(\Delta x)^2$ in space and order Δt in time). However the actual error will vary due to the coefficients of the truncation terms.

Crank-Nicolson Implicit (C-N) Method

- Evaluate time derivative at point (i, j) using a forward difference (or at point $i, j+1$ using a backward difference).

- Evaluate the 2nd spatial derivative using the average of the central difference expressions at (i, j) and $(i, j+1)$.

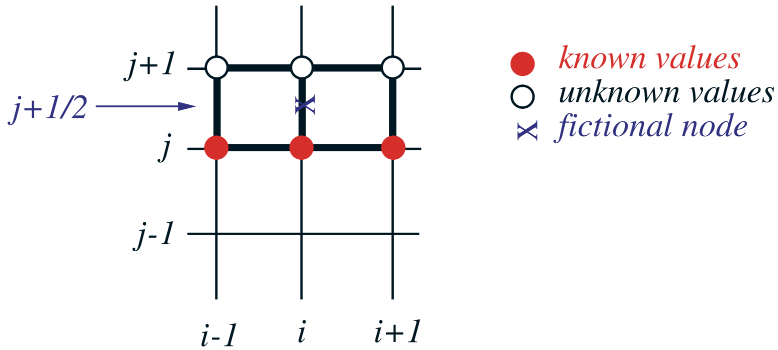
- Applying these two steps to the transient diffusion equation leads to:

$$\frac{1}{\Delta t}[u_{i,j+1} - u_{i,j}] = \frac{D}{(\Delta x)^2}\ \frac{1}{2}[(u_{i+1,j+1} - 2u_{i,j+1} + u_{i-1,j+1}) + (u_{i+1,j} - 2u_{i,j} + u_{i-1,j})]$$

- Arranging knowns and unknowns:

$$\boldsymbol{u_{i-1,j+1} - \left[2 + \frac{2(\Delta x)^2}{\Delta t D}\right]u_{i,j+1} + u_{i+1,j+1} = -u_{i-1,j} + \left[2 - \frac{2(\Delta x)^2}{\Delta t D}\right]u_{i,j} - u_{i+1,j}}$$

- The FD molecule for this solution:

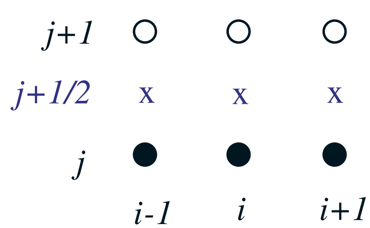


- ***Since the unknowns are coupled (at the new time level), the method is implicit!***

- This C-N solution to the transient diffusion equation is $O(\Delta t^2)$ accurate in time and $O(\Delta x^2)$ accurate in space.

- Stability of the C-N solution to the transient diffusion equation is unconditional for all Δt.

- An alternative interpretation of the C-N solution is to estimate the p.d.e. at $\left(i, j+\frac{1}{2}\right)$:
  - The time derivative term can be thought of as being a central representation of $\frac{\partial u}{\partial t}$ at $\left(i, j+\frac{1}{2}\right)$.
  - The 2nd spatial derivative may be thought of as being a central representation of $\frac{\partial u^2}{\partial x^2}$ at $\left(i, j+\frac{1}{2}\right)$.
  - Values of $u_{i-1, j+\frac{1}{2}}$, $u_{i, j+\frac{1}{2}}$ and $u_{i+1, j+\frac{1}{2}}$ are then estimated using values at full nodes with an interpolation procedure.
  - Defining full and intermediate nodes as:



- We can interpret the C-N solution as:

$$\frac{\partial u_{i,j+1/2}}{\partial t} = D\frac{\partial u^2{}_{i,j+1/2}}{\partial x^2}$$

$$\Rightarrow$$

$$\frac{u_{i,j+1} - u_{i,j}}{\Delta t} = D\left(\frac{u_{i+1,j+1/2} - 2u_{i,j+1/2} + u_{i-1,j+1/2}}{\Delta x^2}\right)$$

- Now we can use linear interpolation:

$$u_{i+1,j+1/2} = \frac{1}{2}(u_{i+1,j+1} + u_{i+1,j})$$

$$u_{i,j+1/2} = \frac{1}{2}(u_{i,j+1} + u_{i,j})$$

$$u_{i-1,j+1/2} = \frac{1}{2}(u_{i-1,j+1} + u_{i-1,j})$$

- Substituting leads to:

$$\mathbf{\frac{1}{\Delta t}[u_{i,j+1} - u_{i,j}] = \frac{D}{(\Delta x)^2}\ \frac{1}{2}[(u_{i+1,j+1} - 2u_{i,j+1} + u_{i-1,j+1}) + (u_{i+1,j} - 2u_{i,j} + u_{i-1,j})]}$$

Weighted Average Approximation

$$\frac{1}{\Delta t}(u_{i,j+1} - u_{i,j}) = \frac{D}{\Delta x^2}[\theta(u_{i+1,j+1} - 2u_{i,j+1} + u_{i-1,j+1}) + (1-\theta)(u_{i+1,j} - 2u_{i,j} + u_{i-1,j})]$$

- θ = degree of implicitness
  - $\theta = 0 \quad \rightarrow$ Explicit solution
  - $\theta = \frac{1}{2} \quad \rightarrow$ Crank-Nicolson solution
  - $\theta = 1 \quad \rightarrow$ Implicit (backward difference) solution
- Stability:
  - Unconditionally stable for $\frac{1}{2} \le \theta \le 1$,
  - Conditionally stable for $0 \le \theta \le \frac{1}{2}$. *Instability occurs if* $\frac{D\Delta t}{(\Delta x)^2} > \frac{1}{2(1-2\theta)}$