ME-704 –CMTFE
Solution of Transport Equation

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Transport Equation-I

- We have now seen how to handle Parabolic Elliptic and Hyperbolic equations
- Hyperbolic equations are best solved by forward marching MOC
- However, MOC programming is tedious in forward mode
- The backward marching is somewhat similar to finite difference methods
- Many schemes exist, we saw only a few for convection equation

Transport Equation-II

- Now we shall go towards solving Navier-Stokes(NS) Equations
- First we will look at the transport equation, which is a model equation for NS equations

$$T_t + uT_x = \alpha T_{xx}$$

- If u = 0, the above classifies as parabolic equation, which did not have any discontinuity in space direction
- If $\alpha = 0$, then it classifies as hyperbolic, which has a strong directional bias

Transport Equation-III

- Transport equation, though strictly will have no discontinuity because of physical diffusion present, can have a strong directional bias depending on the relative strengths of diffusion and convection
- This is characterised by Peclet Number given by

$$P = \frac{uL}{\alpha} = \frac{Convection}{Diffusion}$$

- We will begin with the linear transport equation called the Burgers equation, where u and α are constants

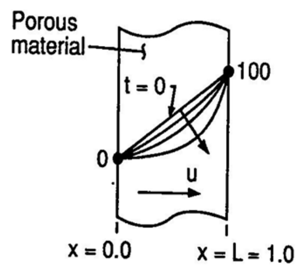
Burger's Equation-I

$\overline{T}_t + u\,\overline{T}_x = \alpha\,\overline{T}_{xx} \;\rightarrow\; \overline{T}(x,t)$

$u = 0.1\ \text{cm/s} \quad \text{and} \quad \alpha = 0.01\ \text{cm}^2/\text{s}$

$\overline{T}(0.0,t) = 0.0 \quad \text{and} \quad \overline{T}(1.0,t) = 100.0\ \text{C}$

$\overline{T}(x,0.0) = 100.0\,x, \quad 0.0 \le x \le 1.0$



Analytical Solution-I

The exact solution is given by:

$$\overline{T}(x,t) = 100\left(\frac{e^{(Px/L)} - 1}{e^{P} - 1} - \frac{4\pi\, e^{(Px/2L)} \sinh(P/2)}{e^{P} - 1} \sum_{m=1}^{\infty} A_m + 2\pi\, e^{(Px/2L)} \sum_{m=1}^{\infty} B_m \right)$$

where the Peclet (Reynolds) number is defined as

$P = uL/\alpha$ **Peclet (Reynolds)number**

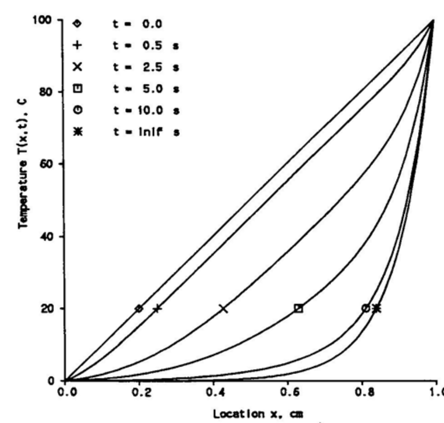
Analytical Solution-II

$$A_m = (-1)^m \left(\frac{m}{\beta_m}\right) \sin\left(\frac{m\pi x}{L}\right) e^{-\lambda_m t}$$

$$B_m = \left((-1)^{m+1} \left(\frac{m}{\beta_m}\right) \left(1 + \frac{P}{\beta_m}\right) e^{-P/2} + \frac{m P}{\beta_m^2} \right) \sin\left(\frac{m\pi x}{L}\right) e^{-\lambda_m t}$$

$$\beta_m = \left(\frac{P}{2}\right)^2 + (m\pi)^2 \quad \text{and} \quad \lambda_m = \frac{u^2}{4\alpha} + \frac{m^2 \pi^2 \alpha}{L^2} = \frac{\alpha \beta_m}{L^2}$$

Analytical Solution-III



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Analytical Solution-IV

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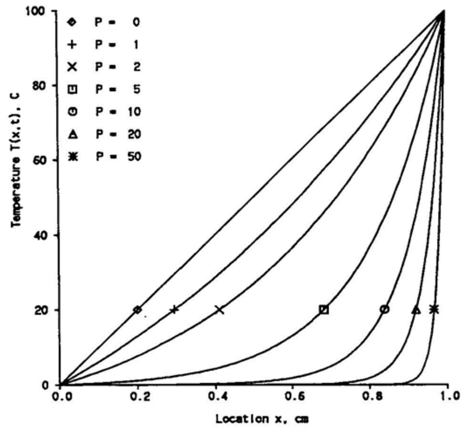

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FTCS - I

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$$\left.\frac{\partial T}{\partial t}\right|_i^n = \frac{T_i^{n+1} - T_i^n}{\Delta t} \qquad \left.\frac{\partial T}{\partial x}\right|_i^n = \frac{T_{i+1}^n - T_{i-1}^n}{2\Delta x} \qquad \left.\frac{\partial^2 T}{\partial x^2}\right|_i^n = \frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{\Delta x^2}$$

- Nodal Equation becomes

$$T_i^{n+1} = T_i^n - \frac{C}{2}(T_{i+1}^n - T_{i-1}^n) + D(T_{i+1}^n - 2T_i^n + T_{i-1}^n)$$

where $C = \frac{u\Delta t}{\Delta x}$ $D = \frac{\alpha \Delta t}{\Delta x^2}$

- Consistency Analysis

$$T_t + uT_x = \alpha T_{xx} - \frac{1}{2}u^2 \Delta t T_{xx} - \left(\frac{1}{6}u\Delta x^2 - u\alpha\Delta t + \frac{1}{3}u^3\Delta t^2\right) T_{xxx} + HOT$$

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FTCS - II

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- Hirt's Stability $\alpha - \frac{1}{2}u^2\Delta t \geq 0 \quad \Rightarrow \frac{u^2 \Delta t}{2\alpha} \leq 1 \quad \Rightarrow \frac{C^2}{2D} \leq 1$
- Von-Neumann $C^2 \leq 2D \leq 1$
- Definition of Cell Peclet (Reynolds) Number $R = \frac{C}{D}$

$$C^2 \leq 2D \quad \Rightarrow \frac{C^2}{D} \leq 2 \quad \Rightarrow R \leq \frac{2}{C}$$

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FTCS - III

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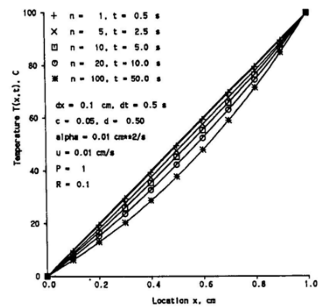
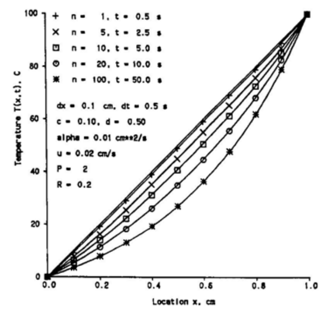
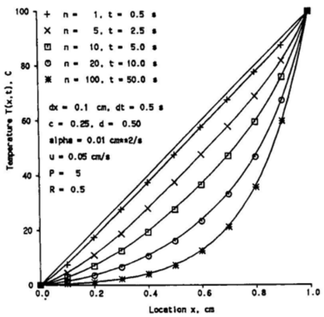
- We look at increasing P for the problem
- C < 1, R < 2/C in every case so as to not violate stability

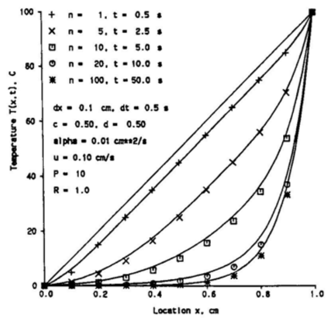




FTCS - IV

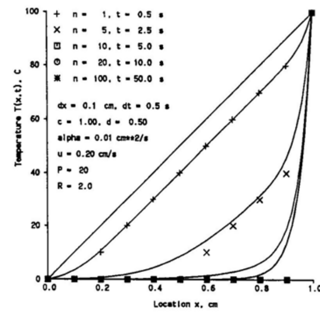
- As P increases, the accuracy deteriorates, Still predictions are OK

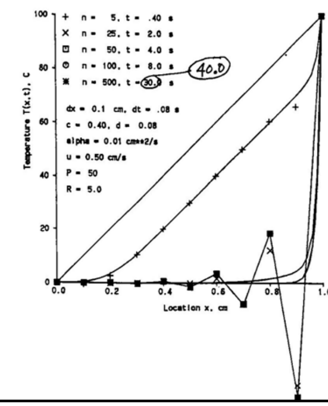




FTCS - V

- At P = 20, the time step is too high to be accurate
- As R goes more than 2 there is a major problem





FTCS - VI

- At P = 20, R = 2/C, there was no stability issue
- At P = 50, R < 2/C, yet there appears to be a unstable like situation, though stability is not violated
- If we rewrite the nodal equation, we can understand the issue

$$T_i^{n+1} = T_i^n - \frac{C}{2}(T_{i+1}^n - T_{i-1}^n) + D(T_{i+1}^n - 2T_i^n + T_{i-1}^n)$$
$$= \left(D - \frac{C}{2}\right)T_{i+1}^n - 2DT_i^n + \left(D + \frac{C}{2}\right)T_{i-1}^n$$
$$= D\left(1 - \frac{R}{2}\right)T_{i+1}^n - 2DT_i^n + D\left(1 + \frac{R}{2}\right)T_{i-1}^n$$

- Note that the coefficient of the first term becomes negative for R > 2

FTCS - VII

- This is called an overshoot problem
- This can be understood by considering a simple example of weighted average

$$T = \alpha T_1 + (1-\alpha)T_2$$

- For the case of say T_1 = 100 and T_2 = 150, we can construct the following table

α	T
0.5	125
0.3	135
0.1	145
0	150
-0.1	155
-0.3	165
-0.5	175

- Notice that the value of weighted average exceeds the two extremum values. Thus when we have negative weights, we will end up with unphysical solutions

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First Order Upwind Scheme - I

$$\left.\frac{\partial T}{\partial t}\right|_i^n = \frac{T_i^{n+1} - T_i^n}{\Delta t} \quad \left.\frac{\partial T}{\partial x}\right|_i^n = \frac{T_i^n - T_{i-1}^n}{\Delta x} \text{ for } u>0, \quad \left.\frac{\partial^2 T}{\partial x^2}\right|_i^n = \frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{\Delta x^2}$$

- Nodal Equation becomes

$$T_i^{n+1} = T_i^n - C(T_i^n - T_{i-1}^n) + D(T_{i+1}^n - 2T_i^n + T_{i-1}^n)$$

$$T_i^{n+1} = DT_{i+1}^n + (1 - C - 2D)T_i^n + (C + D)T_{i+1}^n$$

- Consistency Analysis gives

$$T_t + uT_x = \alpha T_{xx} + \left(0.5u\Delta x - 0.5u^2\Delta t\right) T_{xx} + HOT$$ Consistent

$$= \alpha T_{xx} - 0.5u^2\Delta t T_{xx} + \left(0.5u\Delta x\right) T_{xx} + HOT$$

Same as that of FTCS | Additional

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First Order Upwind Scheme - II

$$\alpha_{effective} = \alpha - 0.5u^2\Delta t + 0.5u\Delta x$$

$$= \alpha - \alpha 0.5\frac{u\Delta t}{\Delta x}\frac{u\Delta x}{\alpha} + \alpha 0.5\frac{u\Delta x}{\alpha}$$

$$= \alpha(1 - 0.5CR + 0.5R)$$

$$= \alpha(1 + 0.5R(1 - C))$$

- For C = 1, the numerical diffusion is equal to physical diffusion, where as for large R, with C<1, the numerical diffusion is large
- Von-Neumann $C^2 \le C + 2D \le 1$

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- It may be observed that as C+2D <1, there is no negative coefficients and hence no overshoot problem for R > 2.
- Thus the method is first order accurate in space and time, is diffusive except for C = 1, consistent and conditionally stable.
- Many of the CFD works on analysis of Convection and Diffusion in large engineering systems use this method, in spite of its limitations.

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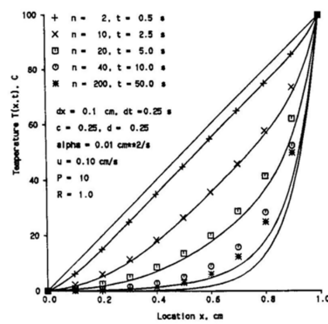
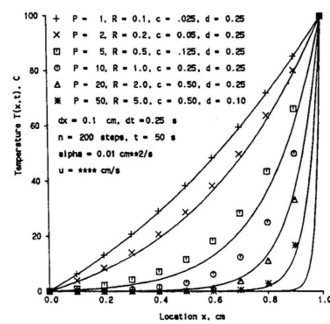
First Order Upwind





Second Order Upwind Scheme -I

- One interesting way of eliminating the extra diffusion by using the third order backward difference for the convective term and central difference for the diffusive. This scheme is called the Leonard Scheme

$$\left.\frac{\partial T}{\partial t}\right|_i^n = \frac{T_i^{n+1} - T_i^n}{\Delta t} \qquad \left.\frac{\partial T}{\partial x}\right|_i^n = \frac{2T_{i+1}^n + 3T_i^n - 6T_{i-1}^n + T_{i-2}^n}{6\Delta x} - \frac{1}{12}T_{xxxx}\Delta x^3$$

for u>0

$$\left.\frac{\partial^2 T}{\partial x^2}\right|_i^n = \frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{\Delta x^2}$$

Second Order Upwind Scheme -II

- The finite difference form of the transport equation may be written as

$$T_i^{n+1} = T_i^n - \frac{C}{6}\left(2T_{i+1}^n + 3T_i^n - 6T_{i-1}^n + T_{i-2}^n\right) + D\left(T_{i+1}^n - 2T_i^n + T_{i-1}^n\right)$$

- Consistency Analysis gives

$$T_t + uT_x = \alpha T_{xx} - 0.5u^2\Delta t T_{xx} + \left(u\alpha\Delta t - \frac{1}{3}u^3\Delta t^2\right)T_{xxx} + HOT$$

- This implies that we can turn off numerical diffusion by decreasing Δt to a sufficiently small value
- Method is $O(\Delta t, \Delta x^2)$

Second Order Upwind Scheme - II

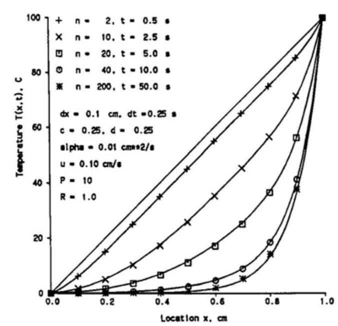
- Von-Neumann

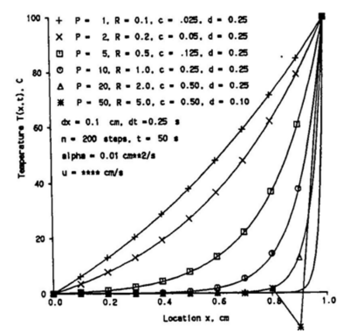
$$G = 1 - 0.5C - 2D + (\tfrac{2}{3}C + 2D)Cos\,\theta - \tfrac{1}{6}Cos\,2\theta$$
$$+ I\left(-\tfrac{4}{3}CSin\,\theta + \tfrac{1}{6}CSin\,2\theta\right)$$

- The expression is messy, but condition for stability can be obtained graphically. Will be shown at the end of the lecture
- The method cannot be applied for the second node and a first order method may have to be invoked.
- Suffers from an overshoot problem at high R

$$T_i^{n+1} = (D - \tfrac{C}{3})T_{i+1}^n + (1 - 2D - \tfrac{C}{2})T_i^n + (C + D)T_{i-1}^n - \tfrac{C}{6}T_{i-2}^n$$

Second Order Upwind





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MacCormack Scheme-I

- Both Lax and Lax-Wendroff Schemes are unconditionally unstable for transport equation
- However, MacCormack Scheme is extremely good to turn off numerical diffusion
- It also has the higher stability limits in comparison with other methods
- We will look at the basis for the scheme
- It has two steps, but utilises explicit methods for both predictor and corrector steps
- The predictor step uses a forward difference for the convective term and central difference for diffusion term

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MacCormack Scheme-II

- Predictor Scheme

$\left.\frac{\partial T}{\partial t}\right|_i^n = \frac{T_i^{n+1} - T_i^n}{\Delta t}$ $\left.\frac{\partial T}{\partial x}\right|_i^n = \frac{T_{i+1}^n - T_i^n}{\Delta x}$ for u>0, $\left.\frac{\partial^2 T}{\partial x^2}\right|_i^n = \frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{\Delta x^2}$

- Nodal Equation becomes

$$\overline{T}_i^{n+1} = T_i^n - C(T_{i+1}^n - T_i^n) + D(T_{i+1}^n - 2T_i^n + T_{i-1}^n)$$

$$\overline{T}_i^{n+1} = DT_{i-1}^n + (1 + C - 2D)T_i^n + (-C + D)T_{i+1}^n$$

- The corrector step uses the same concept, but takes these terms to be an average of the values at n and n+1 level

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MacCormack Scheme-III

- Corrector Scheme

$\left.\frac{\partial T}{\partial t}\right|_i^n = \frac{T_i^{n+1} - T_i^n}{\Delta t}$ $\left.\frac{\partial T}{\partial x}\right|_i^n = 0.5\frac{T_{i+1}^n - T_i^n}{\Delta x} + 0.5\frac{\overline{T}_i^{n+1} - \overline{T}_{i-1}^{n+1}}{\Delta x}$ for u>0,

$$\left.\frac{\partial^2 T}{\partial x^2}\right|_i^n = 0.5\left(\frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{\Delta x^2} + \frac{\overline{T}_{i+1}^{n+1} - 2\overline{T}_i^{n+1} + \overline{T}_{i-1}^{n+1}}{\Delta x^2}\right)$$

- Nodal Equation becomes

$$T_i^{n+1} = T_i^n - \tfrac{C}{2}(T_{i+1}^n - T_i^n + \overline{T}_i^{n+1} - \overline{T}_{i-1}^{n+1}) + \tfrac{D}{2}(T_{i+1}^n - 2T_i^n + T_{i-1}^n) + \tfrac{D}{2}(\overline{T}_{i+1}^{n+1} - 2\overline{T}_i^{n+1} + \overline{T}_{i-1}^{n+1})$$

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MacCormack Scheme-IV

$$T_i^{n+1} = T_i^n - \tfrac{C}{2}(T_{i+1}^n - T_i^n + \overline{T}_i^{n+1} - \overline{T}_{i-1}^{n+1}) + \tfrac{D}{2}(T_{i+1}^n - 2T_i^n + T_{i-1}^n) + \tfrac{D}{2}(\overline{T}_{i+1}^{n+1} - 2\overline{T}_i^{n+1} + \overline{T}_{i-1}^{n+1})$$

- By using the predictor equation for each of the predicted term in the above equation, we can write,

$$T_i^{n+1} = A^* T_{i-2}^n + B^* T_{i-1}^n + C^* T_i^n + D^* T_{i+1}^n + E^* T_{i+2}^n$$

Where, $A^* = 0.5CD + 0.5D^2$, $B^* = 0.5C + D - CD + 0.5C^2 - 2D^2$,
$C^* = 1 - 2D - C^2 + 3D^2$, $D^* = -0.5C + D + CD + 0.5C^2 - 2D^2$,
$E^* = -0.5CD + 0.5D^2$

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MacCormack Scheme-V

- Consistency Analysis gives

Consistent

$$T_t + uT_x = \alpha T_{xx} - \frac{1}{6}\left(u\Delta x^2 - u^3\Delta t^2\right) T_{xxx} +$$
$$\left(\tfrac{1}{12}\alpha\Delta x^2 - \tfrac{1}{8}u^2\Delta x^2\Delta t - \tfrac{1}{2}\alpha u^2\Delta t^2 + \tfrac{1}{8}u^4\Delta t^3\right) T_{xxxx} + HOT$$

- Method is $O(\Delta t^2, \Delta x^2)$
- Less diffusive as leading diffusion term is of fourth order
- Conditionally Stable for about C ≤ 0.85, D ≤ 0.5. The exact stability bound is given later after Von Numann expression is given in next slide

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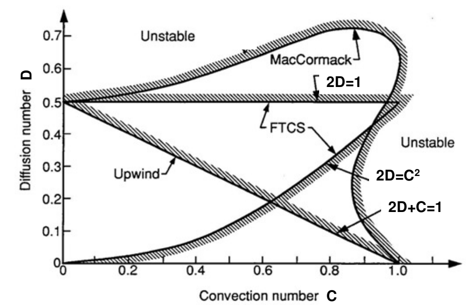
MacCormack Scheme-VI

- Von-Neumann

$$G = C^* + (B^* + D^*)Cos\,\theta + (A^* + E^*)Cos\,2\theta$$
$$+ I\left((D^* - B^*)Sin\,\theta + (E^* - A^*)Sin\,2\theta\right)$$



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Backward-Time Centered-Space Method - I

$$\left.\frac{\partial T}{\partial t}\right|_i^{n+1} = \frac{T_i^{n+1} - T_i^n}{\Delta t} \qquad \left.\frac{\partial T}{\partial x}\right|_i^{n+1} = \frac{T_{i+1}^{n+1} - T_{i-1}^{n+1}}{2\Delta x} \qquad \left.\frac{\partial^2 T}{\partial x^2}\right|_i^{n+1} = \frac{T_{i+1}^{n+1} - 2T_i^{n+1} + T_{i-1}^{n+1}}{\Delta x^2}$$

- Nodal Equation becomes

$$T_i^{n+1} - T_i^n + \frac{C}{2}(T_{i+1}^{n+1} - T_{i-1}^{n+1}) - D(T_{i+1}^{n+1} - 2T_i^{n+1} - T_{i-1}^{n+1}) = 0$$

$$\Rightarrow \left(\frac{C}{2} - D\right)T_{i+1}^{n+1} + (1 + 2D)T_i^{n+1} - \left(\frac{C}{2} + D\right)T_{i-1}^{n+1} = T_i^n$$

- Can Solve by TDMA

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Backward-Time Centered-Space Method - II

- Consistency Analysis gives

$$T_t + uT_x = \left(\alpha + \frac{1}{2}u^2\Delta t\right)T_{xx} - \left(u\alpha\Delta t + \frac{1}{6}u\Delta x^2 + \frac{1}{3}u^3\Delta t^2\right) T_{xxx} + HOT$$

Diffusive Dispersive

- Method is $O(\Delta t, \Delta x^2)$
- Von Neumann analysis $G = \dfrac{1}{1 + 2D(1 - \cos\,\theta) + ICSin\,\theta}$
- Unconditionally stable
- Suffers from Overshoot problem at High R

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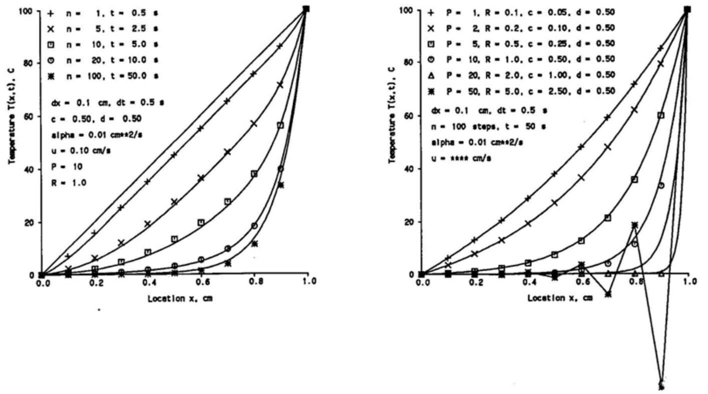
Backward-Time Centered-Space Method - III



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Crank Nicholson Method - I

$$\left.\frac{\partial T}{\partial t}\right|_i^{n+0.5} = \frac{T_i^{n+1} - T_i^n}{\Delta t} \qquad \left.\frac{\partial T}{\partial x}\right|_i^{n+0.5} = 0.5\left(\frac{T_{i+1}^{n+1} - T_{i-1}^{n+1}}{2\Delta x} + \frac{T_{i+1}^{n} - T_{i-1}^{n}}{2\Delta x}\right)$$

$$\left.\frac{\partial^2 T}{\partial x^2}\right|_i^{n+0.5} = 0.5\left(\frac{T_{i+1}^{n+1} - 2T_i^{n+1} + T_{i-1}^{n+1}}{\Delta x^2} + \frac{T_{i+1}^{n} - 2T_i^{n} + T_{i-1}^{n}}{\Delta x^2}\right)$$

- Nodal Equation becomes

$$\left(\frac{C}{2} - D\right)T_{i+1}^{n+1} - 2(1+D)T_i^{n+1} - \left(\frac{C}{2} + D\right)T_{i-1}^{n+1} =$$
$$-\left(\frac{C}{2} - D\right)T_{i+1}^{n} + 2(1-D)T_i^{n} + \left(\frac{C}{2} + D\right)T_{i-1}^{n}$$

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Crank Nicholson Method - II

- Consistency Analysis gives

$$T_t + uT_x = (\alpha)T_{xx} - \left(\frac{1}{6}u\Delta x^2 + \frac{1}{12}u^3\Delta t^2\right)T_{xxx} + HOT$$

Dispersive

- Method is $O(\Delta t^2, \Delta x^2)$
- Von Neumann analysis $G = \dfrac{1 - D(1-\cos\theta) - I\,\frac{C}{2}\,Sin\,\theta}{1 + D(1-\cos\theta) + I\,\frac{C}{2}\,Sin\,\theta}$
- Unconditionally stable
- Suffers from Overshoot problem at High R

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Crank Nicholson Method - III