ME 704

Computational Methods in Thermal and Fluids Engineering

KNI-9 Solution of Parabolic Equations

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Parabolic Equation-I

- One of the most common Parabolic equation is the 1-D Unsteady Heat Equation

$$\frac{1}{\alpha}\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} + \frac{q'''}{k}$$

- Considering x and t as independent variables, if we compare with the general second order differential equations, we can conclude that

$$Af_{xx} + Bf_{xt} + Cf_{tt} + Df_x + Ef_t + F = 0$$

$B = 0$ $C = 0$

- This implies that B^2-4AC = 0
- The equation is parabolic

Parabolic Equation-II

- To appreciate the nature of this equation a little better, we move back to the characteristic equation basics
- In matrix form, we can write

$$\begin{bmatrix} A & 0 & 0 \\ dx & dt & 0 \\ 0 & dx & dt \end{bmatrix} \begin{Bmatrix} f_{xx} \\ f_{xt} \\ f_{tt} \end{Bmatrix} = \begin{Bmatrix} -Ef_t - F \\ d(f_x) \\ d(f_t) \end{Bmatrix}$$

- The characteristic direction would be obtained from

$$\begin{vmatrix} A & 0 & 0 \\ dx & dt & 0 \\ 0 & dx & dt \end{vmatrix} = 0 \quad \Rightarrow Adt^2 = 0 \quad \Rightarrow dt = 0$$

t = constant

Parabolic Equation-III

- Discontinuities can exist along t = constant
- We can interpret this as there can be discontinuities at the initial condition
- Further, the speed of propagation along the characteristic direction given by

$$\frac{1}{u} = \frac{dt}{dx} = 0 \Rightarrow u = \infty$$

- This implies that signals propagate along t=C at infinite speed
- This can be interpreted in a manner that if the boundary value is time dependent, its impact inside the domain will propagate with infinite speed!

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Parabolic Equation-IV

- Further, there cannot be any discontinuities in the spatial direction and the variation will be smooth
- Some of the concepts will be exploited as we go along
- We will now consider the solutions for the case of no source term for simplicity. However, its presence is not going to affect the quality of our discussion
- Similarly, we will keep the discussion for the Dirichlet boundary condition, while we can follow the discussion for the Neumann case in a manner similar to the discussions on ODE solutions

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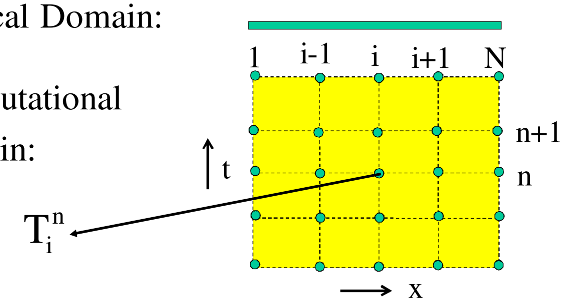
Notations

Governing Equation: $\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$

Physical Domain:

Computational Domain:



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FTCS Method-I

- One of the FDM approximation is

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

- This leads to the nodal equation

$$T_i^{n+1} = T_i^n + \frac{\alpha \Delta t}{\Delta x^2}(T_{i+1}^n - 2T_i^n + T_{i-1}^n)$$

- This method is called explicit method, as the values at T_i^{n+1} are readily obtained explicitly, once the initial and boundary conditions are known

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FTCS Method-II

- We had shown earlier that this method has a stability limit given by $D \le 0.5$, where $D = \frac{\alpha \Delta t}{\Delta x^2}$
- If we need accurate results, we need more sapatial resolution, and this implies small Δx. This will limit Δt to be small and takes more computational time
- Note that halving Δx would call for decreasing Δt by a factor of 4! and this is worse as we move to 2D and 3D

FTCS Method-III

- We had shown earlier that the consistency analysis leads to

$$T_i^n + \left.\frac{\partial T}{\partial t}\right|_i^n \Delta t + \left.\frac{\partial^2 T}{\partial t^2}\right|_i^n \frac{\Delta t^2}{2!} + O(\Delta t^3) =$$

$$T_i^n + \alpha\Delta t\left(\left.\frac{\partial^2 T}{\partial x^2}\right|_i^n + 2\left.\frac{\partial^4 T}{\partial x^4}\right|_i^n \frac{\Delta x^2}{4!} + O(\Delta x^4)\right)$$

$$\frac{\partial T}{\partial t} = \alpha\frac{\partial^2 T}{\partial x^2} + \alpha\Delta t\left(\frac{\partial^4 T}{\partial x^4}\frac{\Delta x^2}{12} - \frac{\partial^2 T}{\partial t^2}\frac{\Delta t}{2\alpha} + O(\Delta t^2, \Delta x^4)\right)$$

- We had also pointed out earlier that the time derivative can be converted into space derivative by the use of governing equation

FTCS Method-IV

- In this particular case, we can write

$$T_{tt} = (T_t)_t = (\alpha T_{xx})_t = (\alpha T_t)_{xx} = (\alpha(\alpha T_{xx}))_x = \alpha^2 T_{xxxx}$$

- Substituting this in the previous equation, we get,

$$\frac{\partial T}{\partial t} = \alpha\frac{\partial^2 T}{\partial x^2} + \alpha\left(\frac{\partial^4 T}{\partial x^4}\frac{\Delta x^2}{12} - \alpha^2\frac{\partial^4 T}{\partial x^4}\frac{\Delta t}{2\alpha} + O(\Delta t^2, \Delta x^4)\right)$$

$$\Rightarrow \frac{\partial T}{\partial t} = \alpha\frac{\partial^2 T}{\partial x^2} + \alpha\frac{\partial^4 T}{\partial x^4}\left(\frac{\Delta x^2}{12} - \alpha\frac{\Delta t}{2}\right) + O(\Delta t^2, \Delta x^4)$$

- If we make the term in the bracket equal to zero, we will get a **higher order accurate** method

$$\frac{\Delta x^2}{12} - \alpha\frac{\Delta t}{2} = 0 \Rightarrow \alpha\frac{\Delta t}{\Delta x^2} = \frac{1}{6}$$

D = 1/6

BTCS Method-I

- Also called Fully Implicit Method

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

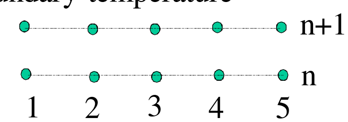
- This leads to the nodal equation

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} = \alpha\frac{T_{i+1}^{n+1} - 2T_i^{n+1} + T_{i-1}^{n+1}}{\Delta x^2}$$

$$T_{i+1}^{n+1}\left(-\frac{\alpha\Delta t}{\Delta x^2}\right) + T_i^{n+1}\left(1 + \frac{2\alpha\Delta t}{\Delta x^2}\right) + T_{i-1}^{n+1}\left(-\frac{\alpha\Delta t}{\Delta x^2}\right) = T_i^n$$

BTCS Method-II

- For the simple case of boundary temperature known



$$\begin{bmatrix} 1 & 0 & & & \\ -\frac{\alpha\Delta t}{\Delta x^2} & 1+\frac{2\alpha\Delta t}{\Delta x^2} & -\frac{\alpha\Delta t}{\Delta x^2} & & \\ & -\frac{\alpha\Delta t}{\Delta x^2} & 1+\frac{2\alpha\Delta t}{\Delta x^2} & -\frac{\alpha\Delta t}{\Delta x^2} & \\ & & -\frac{\alpha\Delta t}{\Delta x^2} & 1+\frac{2\alpha\Delta t}{\Delta x^2} & -\frac{\alpha\Delta t}{\Delta x^2} \\ & & & 0 & 1 \end{bmatrix} \begin{Bmatrix} T_1^{n+1} \\ T_2^{n+1} \\ T_3^{n+1} \\ T_4^{n+1} \\ T_5^{n+1} \end{Bmatrix} = \begin{Bmatrix} T_1^{n+1} \\ T_2^{n} \\ T_3^{n} \\ T_4^{n} \\ T_5^{n+1} \end{Bmatrix}$$

- The matrix can be solved by TDMA

BTCS Method-III

- Consistency analysis gives

$$T_t = \alpha T_{xx} + \left(\frac{1}{2}\alpha^2 \Delta t + \frac{1}{12}\alpha^2 \Delta x^2\right) T_{xxxx} + HOT$$

- von Neumann Stability method gives

$$G = \left(\frac{1}{1 + 2D(1 - \cos\theta)}\right)$$

Since $|G| \le 1$ it is unconditionally stable

Crank Nicholson Method-I

- Defining $\left.\frac{\partial T}{\partial t}\right|_i^n = \frac{T_i^{n+1} - T_i^n}{\Delta t}$ and

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

- The above gives the nodal equation as

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

- Consistency analysis gives

$$T_t = \alpha T_{xx} + \left(\frac{1}{12}\alpha^2 \Delta x^2\right) T_{xxxx} + O\left(\Delta t^2, \Delta x^4\right)$$

Crank Nicholson Method-II

- von Neumann Stability method gives

$$G = \left(\frac{1 - 2D\sin^2\left(\frac{\theta}{2}\right)}{1 + 2D\sin^2\left(\frac{\theta}{2}\right)}\right)$$

- Since $|G| \le 1$ it is unconditionally stable

Theta Method

- Defining $\left.\frac{\partial T}{\partial t}\right|_i^n = \frac{T_i^{n+1} - T_i^n}{\Delta t}$ and

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

- The above gives the nodal equation as

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

Theta Method (Cont'd)

- Consistency analysis gives

$$T_t = \alpha T_{xx} + \left(\left(\theta - \frac{1}{2}\right)\alpha^2 \Delta t + \frac{1}{12}\alpha^2 \Delta x^2\right) T_{xxxx} +$$
$$+ \left[\left(\theta^2 - \theta + \frac{1}{3}\right)\alpha^3 \Delta t^2 + \frac{1}{6}\left(\theta - \frac{1}{2}\right)\alpha^2 \Delta t \Delta x^2 + \frac{1}{360}\alpha \Delta x^4\right] T_{xxxxxx}$$

- For $\theta = 0.5$ the method is $O(\Delta t^2, \Delta x^2)$
- For $\theta = \left(\frac{1}{2} - \frac{\Delta x^2}{12\alpha \Delta t}\right)$ the method is $O(\Delta t^2, \Delta x^4)$
- For $\theta = \left(\frac{1}{2} - \frac{\Delta x^2}{12\alpha \Delta t}\right)$ and $\frac{\alpha \Delta t}{\Delta x^2} = \frac{1}{\sqrt{20}}$ the method is $O(\Delta t^2, \Delta x^6)$

DuFort-Frankel Scheme-I

- Before moving to multi-dimensional equation it is useful to look at an unconditionally stable explicit scheme.
- If one attempts to get a CTCS scheme, given by

Defining $\left.\frac{\partial T}{\partial t}\right|_i^n = \frac{T_i^{n+1} - T_i^{n-1}}{2\Delta t} + O(\Delta t^2)$ and

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

- The method turns out to be unconditionally unstable

DuFort-Frankel Scheme-II

- If the scheme is modified as

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

- The nodal equation for the diffusion equation becomes

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

DuFort-Frankel Scheme-III

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

- Consistency analysis gives

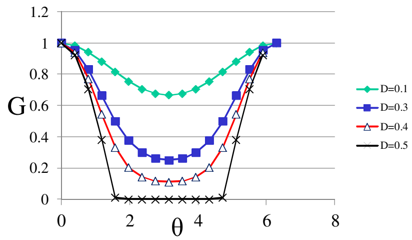
$$T_t = \alpha T_{xx} + \left(\frac{1}{12}\alpha^2 \Delta x^2 - \alpha^3 \frac{\Delta t^2}{\Delta x^2}\right) T_{xxxx} + O\left(\Delta t^2, \Delta x^4, \frac{\Delta t^4}{\Delta x^4}\right)$$

- Inconsistent
- Can get higher order accuracy by choosing $\frac{\alpha \Delta t}{\Delta x^2} = \frac{1}{\sqrt{12}}$
- Stability Analysis gives

$$G = \left(\frac{2D\cos\theta \pm \sqrt{1 - 4D^2 \sin^2\theta}}{1+2D}\right)$$

DuFort-Frankel Scheme-IV

- For D < 0.5, the term under the square root is always positive. The variation of G with θ can be plotted



- For D > 0.5, the term under the square root is imaginary and we can write G as

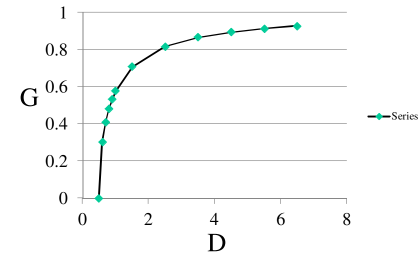
$$G = \left(\frac{2D\cos\theta \pm I\sqrt{4D^2 Sin^2\theta - 1}}{1+2D} \right)$$

DuFort-Frankel Scheme-V

- The magnitude of G can be written as

$$|G| = \left(\frac{\sqrt{4D^2\cos^2\theta + 4D^2 Sin^2\theta - 1}}{1+2D} \right)$$

$$|G| = \left(\frac{\sqrt{4D^2 - 1}}{1+2D} \right)$$



- Unconditionally stable

Multi-Dimensional Equations

Governing Equation: $$\frac{\partial T}{\partial t} = \alpha \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right)$$

- ❑ FTCS method $$\left.\frac{\partial T}{\partial t}\right|_i^n = \frac{T_{i,j}^{n+1} - T_{i,j}^n}{\Delta t}$$

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

- ❑ Nodal Equation for the above scheme shall be

$$T_{i,j}^{n+1} = T_{i,j}^n + D_x\left(T_{i+1,j}^n - 2T_{i,j}^n + T_{i-1,j}^n\right) + D_y\left(T_{i,j+1}^n - 2T_{i,j}^n + T_{i,j-1}^n\right)$$

$D_x = \frac{\alpha\Delta t}{\Delta x^2},\ D_y = \frac{\alpha\Delta t}{\Delta y^2}$ ❑ Conditionally Stable $D_x + D_y \le 0.5$

Crank Nicholson Scheme

- ❑ Crank Nicholson Scheme $$\frac{\partial T}{\partial t} = \frac{T_{i,j}^{n+1} - T_{i,j}^n}{\Delta t}$$

$$\frac{\partial^2 T}{\partial x^2} = \frac{1}{2}\left(\frac{T_{i+1,j}^n - 2T_{i,j}^n + T_{i-1,j}^n}{\Delta x^2} + \frac{T_{i+1,j}^{n+1} - 2T_{i,j}^{n+1} + T_{i-1,j}^{n+1}}{\Delta x^2} \right) = \frac{1}{2}\delta_x^2\left(T_{i,j}^n + T_{i,j}^{n+1}\right)$$

$$\frac{\partial^2 T}{\partial y^2} = \frac{1}{2}\left(\frac{T_{i,j+1}^n - 2T_{i,j}^n + T_{i,j-1}^n}{\Delta y^2} + \frac{T_{i,j+1}^{n+1} - 2T_{i,j}^{n+1} + T_{i,j-1}^{n+1}}{\Delta y^2} \right) = \frac{1}{2}\delta_y^2\left(T_{i,j}^n + T_{i,j}^{n+1}\right)$$

- ❑ Nodal Equation for the above scheme shall be

$$T_{i,j}^{n+1} = T_{i,j}^n + \frac{\alpha\Delta t}{2}\left(\delta_x^2 + \delta_x^2\right)\left(T_{i,j}^n + T_{i,j}^{n+1}\right)$$

- ❑ Unconditionally Stable, but will need a banded solver and is not usually done.

Alternating Direction Implicit

- In order to exploit TDMA, ADI schemes were evolved, called fractional step method

$$\frac{T_{i,j}^{n+0.5} - T_{i,j}^{n}}{\Delta t/2} = \alpha\left(\delta_x^2 T_{i,j}^{n+0.5} + \delta_y^2 T_{i,j}^{n}\right)$$

$$\frac{T_{i,j}^{n+1} - T_{i,j}^{n+0.5}}{\Delta t/2} = \alpha\left(\delta_x^2 T_{i,j}^{n+0.5} + \delta_y^2 T_{i,j}^{n+1}\right)$$

- Unconditionally stable in 2D. But extension to 3D does not produce an unconditionally stable method.

Alternating Direction Implicit

- For 3-D, ADI based on Crank-Nicholson method that is unconditionally stable has been worked developed. The method proceeds in 3 steps.

$$T^{*} - T^{n} = \alpha\Delta t\left[\frac{\delta_x^2}{2}\left\{T^{*} + T^{n}\right\} + \left(\delta_y^2 T^{n}\right) + \left(\delta_z^2 T^{n}\right)\right]$$

$$T^{**} - T^{n} = \alpha\Delta t\left[\left(\frac{\delta_x^2}{2}\left\{T^{*} + T^{n}\right\}\right) + \left(\frac{\delta_y^2}{2}\left\{T^{**} + T^{n}\right\}\right) + \left(\delta_z^2 T^{n}\right)\right]$$

$$T_{i,j}^{n+1} - T_{i,j}^{n} = \alpha\Delta t\left[\left(\frac{\delta_x^2}{2}\left\{T^{*} + T^{n}\right\}\right) + \left(\frac{\delta_y^2}{2}\left\{T^{**} + T^{n}\right\}\right) + \left(\frac{\delta_z^2}{2}\left\{T^{n+1} + T^{n}\right\}\right)\right]$$

Index i , j, k dropped for convenience