ME 704

Computational Methods in Thermal and Fluids Engineering

Classification, Consistency and Numerical Errors

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Concept of Characteristics-I

- Consider a simple PDE called the convection equation given by

$$\frac{\partial T}{\partial t} + u\frac{\partial T}{\partial x} = 0 \quad (1) \qquad u = \text{constant}$$

- Let the initial condition at t = 0, T(0,x) be F (x)
- The analytical solution at any given T(t,x) = F (x-ut)
- This can be verified as follows. On substitution, of the solution into the LHS of the PDE we get,

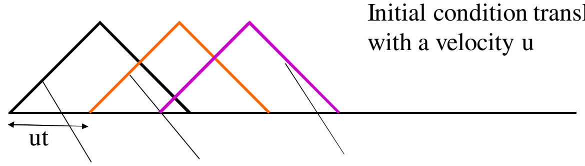
$$\left.\frac{dF}{dx}\right|_{(x-ut)}\frac{\partial(x-ut)}{\partial t} + u\left.\frac{dF}{dx}\right|_{(x-ut)}\frac{\partial(x-ut)}{\partial x}$$

$$\left.\frac{dF}{dx}\right|_{(x-ut)}(-u) + u\left.\frac{dF}{dx}\right|_{(x-ut)} \qquad \text{Hence OK}$$

Concept of Characteristics-II

- To appreciate the solution graphically let us refer to the figure shown below

Initial condition translates with a velocity u



Initial Condition After time t_1 After time t_2

- Since T = T(x,t), using chain rule assuming continuity of T, we can write

$$dT = \frac{\partial T}{\partial t}dt + \frac{\partial T}{\partial x}dx \quad (2)$$

Concept of Characteristics-III

- Eqs. (1) and (2) can be viewed as two simultaneous equations for the partial derivatives as given by

$$\begin{bmatrix} 1 & u \\ dt & dx \end{bmatrix}\begin{Bmatrix} T_t \\ T_x \end{Bmatrix} = \begin{Bmatrix} 0 \\ dT \end{Bmatrix}$$

- For unique solutions of T_t and T_x the necessary condition is

$$\begin{vmatrix} 1 & u \\ dt & dx \end{vmatrix} \neq 0$$

- Discontinuities in the slopes are possible, if

$$\begin{vmatrix} 1 & u \\ dt & dx \end{vmatrix} = 0 \quad \text{Or when} \quad \frac{dt}{dx} = \frac{1}{u} \quad (3)$$

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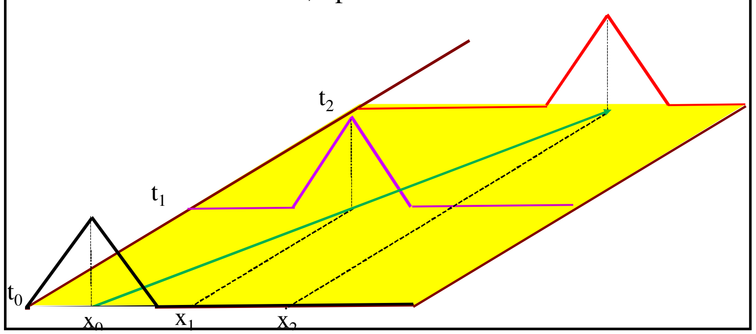
Concept of Characteristics-IV

- Eq. (3) when separated and integrated with an initial condition of $x = x_0$ at $t = t_0$ will give,

  $$x = x_0 + u(t - t_0) \quad (4)$$

- The state of fluid in t,x plane can be visualised as follows



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Concept of Characteristics-V

- From the previous slide, we have realized that Eq. (2) and its integrated form in Eq. (4) describes the path along which the discontinuities can propagate
- This is called the **Characteristic Direction**
- The speed of propagation of the discontinuity is given by

  $$\frac{dx}{dt} = \frac{u}{1} = u$$

- Equations that have real characteristic direction are called **Hyperbolic Equations** (Propagation type)
- Thus, convection equation is a hyperbolic equation

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Concept of Characteristics-VI

- If instead of Eq. (1), if we would have had the governing equation as

  $$A\frac{\partial T}{\partial t} + B\frac{\partial T}{\partial x} = 0$$

- By analogy, the characteristic direction would have been by

  $$\frac{dx}{dt} = \frac{B}{A} = -\frac{\partial T}{\partial t} \Big/ \frac{\partial T}{\partial x} = \lambda$$

  Usually denoted by λ

- Thus, λ is obtained by solving the equation

  $$B - \lambda A = 0 \quad (5)$$

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Concept of Characteristics-VII

- Now we will extend it to a set of first order equations
- The motivation arises from the fact that compressible flows are governed by this type of equations
- We shall start from the most general form. It is convenient to work with the matrix notation

  $$\begin{bmatrix} a_1 & a_2 \\ b_1 & b_2 \end{bmatrix} \frac{\partial}{\partial t}\begin{Bmatrix} f \\ g \end{Bmatrix} + \begin{bmatrix} a_3 & a_4 \\ b_3 & b_4 \end{bmatrix} \frac{\partial}{\partial x}\begin{Bmatrix} f \\ g \end{Bmatrix} = \begin{Bmatrix} a_5 \\ b_5 \end{Bmatrix}$$

  $$[A]\frac{\partial}{\partial t}\begin{Bmatrix} f \\ g \end{Bmatrix} + [B]\frac{\partial}{\partial x}\begin{Bmatrix} f \\ g \end{Bmatrix} = \{S\}$$

- If we compare this with our example for one variable, the equation is identical except for the fact that the coefficients A and B are now matrices and the variable T has become a vector f and g

Concept of Characteristics-VIII

- The characteristic directions in this case is given by solving

$$\frac{dx}{dt} = -\frac{\partial \begin{Bmatrix} f \\ g \end{Bmatrix} \Big/ \partial t}{\partial \begin{Bmatrix} f \\ g \end{Bmatrix} \Big/ \partial x} = \frac{[B]}{[A]} = \lambda$$

$$Or \quad [B] - \lambda [A] = 0$$

Concept of Characteristics-IX

- To consider a concrete example, we shall take a set called the water hammer equation given by the set

$$\frac{1}{a^2}\frac{\partial p}{\partial t} + \frac{u}{a^2}\frac{\partial p}{\partial x} + \rho\frac{\partial u}{\partial x} = 0 \qquad \text{Mass Balance}$$

$$\rho\frac{\partial u}{\partial t} + \rho u\frac{\partial u}{\partial x} + \frac{\partial p}{\partial x} = 0 \qquad \text{Momentum Balance}$$

- The above two equations can be recast as

$$\begin{bmatrix} 0 & \frac{1}{a^2} \\ \rho & 0 \end{bmatrix} \frac{\partial}{\partial t}\begin{Bmatrix} u \\ p \end{Bmatrix} + \begin{bmatrix} \rho & \frac{u}{a^2} \\ \rho u & 1 \end{bmatrix} \frac{\partial}{\partial x}\begin{Bmatrix} u \\ p \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \end{Bmatrix}$$

Concept of Characteristics-X

$$[B] - \lambda [A] = 0$$

$$\Rightarrow \begin{bmatrix} \rho & \frac{u}{a^2} \\ \rho u & 1 \end{bmatrix} - \lambda \begin{bmatrix} 0 & \frac{1}{a^2} \\ \rho & 0 \end{bmatrix} = 0$$

$$\Rightarrow \begin{bmatrix} \rho & \frac{u-\lambda}{a^2} \\ \rho(u-\lambda) & 1 \end{bmatrix} = 0 \qquad \Rightarrow \rho = \rho\frac{(u-\lambda)^2}{a^2}$$

$$\Rightarrow (u-\lambda) = \pm a \qquad \Rightarrow \lambda = u \pm a = \frac{dx}{dt}$$

Thus the set is hyperbolic

- In general, the first order set in TFE are hyperbolic equations and we shall look at their solutions later

Concept of Characteristics-XI

- We can now extend this to second order PDEs. Consider a general second order equation

$$Af_{xx} + Bf_{xy} + Cf_{yy} + Df_x + Ef_y + F = 0$$

- Also by chain rule we can write.

$$d(f_x) = f_{xx}dx + f_{xy}dy$$

$$d(f_y) = f_{yx}dx + f_{yy}dy$$

- In matrix form, we can write

$$\begin{bmatrix} A & B & C \\ dx & dy & 0 \\ 0 & dx & dy \end{bmatrix} \begin{Bmatrix} f_{xx} \\ f_{xy} \\ f_{yy} \end{Bmatrix} = \begin{Bmatrix} -Df_x - Ef_y - F \\ d(f_x) \\ d(f_y) \end{Bmatrix}$$

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Concept of Characteristics-XII

- For multiple solutions for f_{xx}, f_{xy} and f_{yy}

$$\begin{vmatrix} A & B & C \\ dx & dy & 0 \\ 0 & dx & dy \end{vmatrix} = 0$$

$$\Rightarrow Ady^2 - Bdxdy + Cdx^2 = 0$$

$$\Rightarrow A\left(\frac{dy}{dx}\right)^2 - B\frac{dy}{dx} + C = 0$$

$$\Rightarrow \frac{dy}{dx} = \frac{B \pm \sqrt{B^2 - 4AC}}{2A}$$

- The nature of characteristic direction will depend on the nature of discriminant

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Concept of Characteristics-XIII

$For \quad B^2 - 4AC > 0$ Roots real, hence **Hyperbolic**

$For \quad B^2 - 4AC = 0$ Roots real, but repeated **Parabolic**

$For \quad B^2 - 4AC < 0$ Roots imaginary, hence **Elliptic**

- We shall get to more details when we solve them later

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Consistency-I

- A finite difference scheme solving a given PDE is said to be consistent, if when Δt and Δx are allowed to approach zero, the approximate solution will approach the exact solution of the PDE
- Consistency of a scheme can be checked by application of Taylor series
- Let us consider an example for illustration

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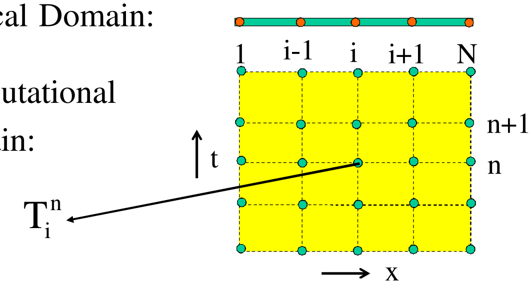
Consistency-II

Consider transient conduction in a rod

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

Physical Domain:

Computational Domain:



Consistency-III

- One of the FDM approximation is FTCS

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

- This leads to the nodal equation

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

Consistency-IV

- Using Taylor series, we can write the following:

$$T_i^{n+1} = T_i^n + \left.\frac{\partial T}{\partial t}\right|_i^n \Delta t + \left.\frac{\partial^2 T}{\partial t^2}\right|_i^n \frac{\Delta t^2}{2!} + \left.\frac{\partial^3 T}{\partial t^3}\right|_i^n \frac{\Delta t^3}{3!} + \text{HOT}$$

- Similarly, we can write

$$T_{i\pm 1}^n = T_i^n \pm \left.\frac{\partial T}{\partial x}\right|_i^n \Delta x + \left.\frac{\partial^2 T}{\partial x^2}\right|_i^n \frac{\Delta x^2}{2!} \pm \left.\frac{\partial^3 T}{\partial x^3}\right|_i^n \frac{\Delta x^3}{3!} + \text{HOT}$$

- The above can be modified as

$$\frac{T_{i+1}^n + T_{i-1}^n - 2T_i^n}{\Delta x^2} = 2\left.\frac{\partial^2 T}{\partial x^2}\right|_i^n \frac{1}{2!} + 2\left.\frac{\partial^4 T}{\partial x^4}\right|_i^n \frac{\Delta x^2}{4!} + \text{HOT}$$

Consistency-V

- Substituting these in our nodal equation, we get

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

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

- Cancelling T_i^n from both sides and then dividing both sides by Δt and finally allowing Δt and Δx approach 0, we get the exact original equation hence consistent

Consistency-VI

For finite values of Δt and Δx we are actually solving a different PDE. This is called Modified PDE or MPDE

The equation in the previous slide can be written as

$$\frac{\partial T}{\partial t} + O(\Delta t) = \alpha \frac{\partial^2 T}{\partial x^2} + O(\Delta x^2)$$

The **leading truncation error** for the approximation used is also included.

Thus, the scheme is said to be **First order accurate in time and Second order accurate in space**.

Inconsistency (an example)-I

- Consider, Convection Equation $\dfrac{\partial T}{\partial t} + u\dfrac{\partial T}{\partial x} = 0$
- FTCS scheme does not work
- Modelling by Lax Scheme

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

- Nodal Equation becomes

$$\frac{T_i^{n+1} - 0.5\left(T_{i+1}^n + T_{i-1}^n\right)}{\Delta t} + \frac{u(T_{i+1}^n - T_{i-1}^n)}{2\Delta x} = 0$$

$$T_i^{n+1} = 0.5\left(T_{i+1}^n + T_{i-1}^n\right) - \frac{u\Delta t}{2\Delta x}(T_{i+1}^n - T_{i-1}^n) \qquad (6)$$

Inconsistency (an example)-II

- From Taylor Series, we get

$$T_{i\pm1}^n = T_i^n \pm \left.\frac{\partial T}{\partial x}\right|_i^n \Delta x + \left.\frac{\partial^2 T}{\partial x^2}\right|_i^n \frac{\Delta x^2}{2!} \pm \left.\frac{\partial^3 T}{\partial x^3}\right|_i^n \frac{\Delta x^3}{3!} + \text{HOT}$$

$$\Rightarrow T_{i+1}^n - T_{i-1}^n = 2\left.\frac{\partial T}{\partial x}\right|_i^n \Delta x + 2\left.\frac{\partial^3 T}{\partial x^3}\right|_i^n \frac{\Delta x^3}{3!} + HOT$$

$$And \quad T_{i+1}^n + T_{i-1}^n = 2T_i^n + 2\left.\frac{\partial^2 T}{\partial x^2}\right|_i^n \frac{\Delta x^2}{2!} + O(\Delta x^4)$$

- Plugging the above in Eq. (6), we get

$$\cancel{T_i^n} + T_t\big|_i^n \Delta t + T_{tt}\big|_i^n \frac{\Delta t^2}{2} + O\left(\Delta t^3\right) = \cancel{T_i^n} + T_{xx}\big|_i^n \frac{\Delta x^2}{2} - \frac{u\Delta t}{\Delta x}\left(T_x\big|_i^n \Delta x + O(\Delta x^3)\right) \qquad (7)$$

Inconsistency (an example)-III

$$\Rightarrow T_t\big|_i^n + O(\Delta t) + u\left(T_x\big|_i^n + O(\Delta x^2)\right) = T_{xx}\big|_i^n \frac{\Delta x^2}{2\Delta t}$$

- Hence, as Δt and Δx tend to zero, the RHS does not go to zero due the inconsistent term on the RHS
- It is interesting to note that as we reduce Δt to zero for a fixed Δx, the errors build, while for a given Δt, as we reduce Δx, the errors diminish and the method can behave consistently

Inconsistency (Cont'd)

- We note that we get an indeterminate quantity, which depends on how the ratio of Δt and Δx approaches a limit
- For most propagation equations, we can convert higher order time derivatives into space derivatives
- For example, if we consider convection equation

$$T_{tt} = (T_t)_t = (-uT_x)_t = (-uT_t)_x = (-u(-uT_x))_x = u^2 T_{xx}$$

- Thus, Eq. (7) can be written as

$$T_t + uT_x = 0.5\frac{\Delta x^2}{\Delta t}T_{xx} - 0.5\Delta t\, u^2 T_{xx} + \text{HOT}$$

- Note that in MPDE given above, RHS has only spatial derivatives. This will be used later in analysing errors

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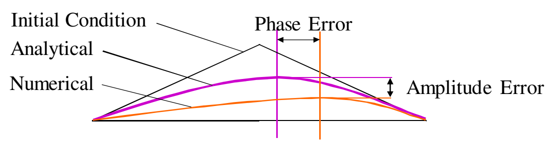
Concepts in Numerical Errors

- Consider, Transport Equation $\dfrac{\partial T}{\partial t} + u\dfrac{\partial T}{\partial x} = \alpha\dfrac{\partial^2 T}{\partial x^2}$



- Causes: Spurious derivatives introduced due to truncation error
- Terminology: Numerical Diffusion
  Numerical Dispersion

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Behaviour of Error

- Consider $\dfrac{\partial T}{\partial t} = \alpha\dfrac{\partial^2 T}{\partial x^2}$
- Let error ε be defined as $\varepsilon = T_{numerical} - \overline{T}_{exact}$
- Numerical Solution actually solves for

$$\frac{\partial(\overline{T}+\varepsilon)}{\partial t} = \alpha\frac{\partial^2(\overline{T}+\varepsilon)}{\partial x^2}$$

$$\Rightarrow \cancel{\frac{\partial(\overline{T})}{\partial t}} + \frac{\partial(\varepsilon)}{\partial t} = \alpha\left(\cancel{\frac{\partial^2(\overline{T})}{\partial x^2}} + \frac{\partial^2(\varepsilon)}{\partial x^2}\right)$$

- The above implies that the error equation is identical to the original governing equation
- For problems with boundary values specified, error at boundaries will be zero

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Analytical Solution of Linear PDE

- Consider $\dfrac{\partial T}{\partial t} = \alpha\dfrac{\partial^2 T}{\partial x^2}$ with $T(0,x) = \mathrm{Sin}\left(\frac{\pi x}{L}\right)$
  and $T(t,0) = T(t,L) = 0$
- Let Solution be of the form $T(t,x) = \hat{\varepsilon}\, e^{st} e^{ikx}$

$$\Rightarrow T_t = \hat{\varepsilon} s\, e^{st} e^{ikx} = sT \qquad T_{xx} = \hat{\varepsilon}(ik)^2 e^{st} e^{ikx} = -k^2 T$$

- Substituting these in Gov. Eq., we get $s = -\alpha k^2$
- Thus, $T(t,x) = \hat{\varepsilon} e^{-\alpha k^2 t} e^{ikx}$
- From initial condition we get, $T(0,x) = \hat{\varepsilon} e^{ikx} = \mathrm{Sin}\left(\frac{\pi x}{L}\right)$
- By comparison, we can state that: $\hat{\varepsilon} = 1,\ k = \left(\frac{\pi}{L}\right)$ and only imaginary part to be used
- Thus the solution is $T(t,x) = e^{-\alpha\left(\frac{\pi}{L}\right)^2 t}\,\mathrm{Sin}\left(\frac{\pi x}{L}\right)$

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Analysis of Error Propagation

- Consider general purpose MPDE of the error equation

$$\frac{\partial(\varepsilon)}{\partial t} = \sum_{m=1}^{\infty} A_{2m}\frac{\partial^{2m}(\varepsilon)}{\partial x^{2m}} + \sum_{m=0}^{\infty} A_{2m+1}\frac{\partial^{2m+1}(\varepsilon)}{\partial x^{2m+1}}$$

- Substituting $\varepsilon = \hat{\varepsilon}\, e^{st} e^{ikx}$ we get

$$s\cancel{\varepsilon} = \cancel{\varepsilon}\sum_{m=1}^{\infty} A_{2m} k^{2m}(-1)^m + \cancel{\varepsilon}\sum_{m=0}^{\infty} A_{2m+1} k^{2m+1}(-1)^m i$$

- In general, writing $s = \sigma + i\omega$ we get

$$\sigma = \sum_{m=1}^{\infty} A_{2m} k^{2m}(-1)^m \quad \text{and} \quad \omega = \sum_{m=0}^{\infty} A_{2m+1} k^{2m+1}(-1)^m$$

Error Propagation (Cont'd)

- Substituting σ and ω in assumed form of Solution we get $\varepsilon(t,x) = \hat{\varepsilon}\, e^{\sigma t} e^{i(kx+\omega t)}$

$$\Rightarrow \varepsilon(t+\Delta t, x) = \hat{\varepsilon}\, e^{\sigma(t+\Delta t)} e^{i(kx+\omega(t+\Delta t))}$$

- Defining error amplification, G as,

$$G = \frac{\varepsilon(t+\Delta t, x)}{\varepsilon(t,x)} = e^{\sigma\Delta t} e^{i\omega\Delta t)}$$

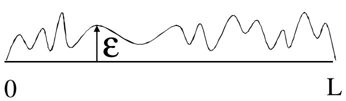
$$\Rightarrow |G| = e^{\sigma\Delta t} \text{ and } \phi = \omega\Delta t$$

- Note that amplitude growth of error is from σ which is determined by coefficient of even derivatives and the phase error is from ω which is determined by coefficient of odd derivatives

Stability Analysis

- If the magnitude of error amplification is greater than 1, then, error will explode
- It will be seen that most explicit methods employed for obtaining the solution tend to explode, when time step is too large.
- von Neumann stability analysis method is a simple and effective tool to identify the constraints on the time step

von Neumann Stability Analysis



- Consider an arbitrary error distribution as shown
- From Fourier theory, we can decompose the error as

$$\varepsilon(x) = \frac{a_0}{2} + \sum_{m=1}^{\infty} a_m \cos\left(\frac{m\pi x}{L}\right) + \sum_{m=1}^{\infty} b_m \sin\left(\frac{m\pi x}{L}\right)$$

- The above can be rewritten as

$$= \frac{a_0}{2} + \sum_{m=1}^{\infty} c_m e^{I\frac{m\pi x}{L}} + \sum_{m=1}^{\infty} c_{-m} e^{-I\frac{m\pi x}{L}}$$

von Neumann Analysis (Cont'd)

- where $c_m = \dfrac{a_m - Ib_m}{2}, \; + c_{-m} = \dfrac{a_m + Ib_m}{2}$ and $I = \sqrt{-1}$
- The equation can be compactly written as

$$\varepsilon(x) = \sum_{m=-\infty}^{\infty} c_m e^{I\frac{m\pi x}{L}}$$

- Stability would imply that none of the Fourier component would grow.
- It is illustrative to show the procedure with an example

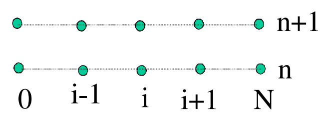
von Neumann Analysis (Example)

- Consider $\dfrac{\partial T}{\partial t} = \alpha \dfrac{\partial^2 T}{\partial x^2} \Rightarrow \dfrac{\partial \varepsilon}{\partial t} = \alpha \dfrac{\partial^2 \varepsilon}{\partial x^2}$
- Let the finite difference equation be

$$\varepsilon_i^{n+1} = \varepsilon_i^n + D(\varepsilon_{i+1}^n - 2\varepsilon_i^n + \varepsilon_{i-1}^n) \quad \text{where} \quad D = \frac{\alpha \Delta t}{\Delta x^2}$$

- Consider a Fourier component $\varepsilon_i^n = c_m e^{I\frac{m\pi x}{L}}$
- Since $x = i\,\Delta x$, $\varepsilon_i^n = c_m e^{I\frac{im\pi\Delta x}{L}} = c_m e^{Ii\theta_m}$

where $\theta_m = \frac{m\pi\Delta x}{L}$



Example (Cont'd)

- Thus, $\varepsilon_i^n = c_m e^{Ii\theta_m}$, $\varepsilon_{i\pm1}^n = c_m e^{I(i\pm1)\theta_m}$, $\varepsilon_i^{n+1} = G\varepsilon_i^n$
- Substitution of the above in the finite difference Eq.,

$$G\cancel{c_m e^{Ii\theta_m}} = \cancel{c_m e^{Ii\theta_m}} + D\cancel{c_m e^{Ii\theta_m}}\left(e^{\theta_m} - 2 + e^{-\theta_m}\right)$$

$$\Rightarrow \quad G = 1 + D(2\cos\theta_m - 2) = 1 + 2D(\cos\theta_m - 1)$$

- For stability $|G| \le 1 \quad \Rightarrow \quad -1 \le G \le 1$

Example (Cont'd)

$G \le 1$	$-1 \le G$
$1 + 2D(\cos\theta_m - 1) \le 1$	$-1 \le 1 + 2D(\cos\theta_m - 1)$
$2D(\cos\theta_m - 1) \le 0$	$-2 \le 2D(\cos\theta_m - 1)$
$D \ge 0$	$D \le \dfrac{1}{(1 - \cos\theta_m)}$
	smallest value $\Rightarrow D \le 0.5$

- Thus for stability there is an upper bound on Δt