§4. Parabolic PDE's: unsteady heat equation

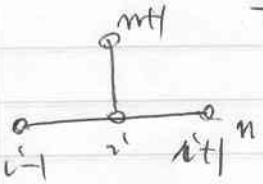
Heat conduction or mass diffusion

$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T = \begin{cases} \alpha \, \partial^2 T / \partial x^2 & 1D \\ \alpha \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) & 2D \end{cases}$$

Take 1D as example.

① Central differencing in x + forward differencing in t:

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



$$T_i^{n+1} - T_i^{n} = \frac{\alpha \Delta t}{\Delta x^2} \underbrace{\left(T_{i+1}^n - 2T_i^n + T_{i-1}^n \right)}_{\text{Explicit scheme.}}$$

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

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

Numerical implementation, numerically stable for $c = 0.45$, but unstable for $c = 0.55$. Why?

(Numerical results depicted on next pages)

② von Neumann stability analysis:

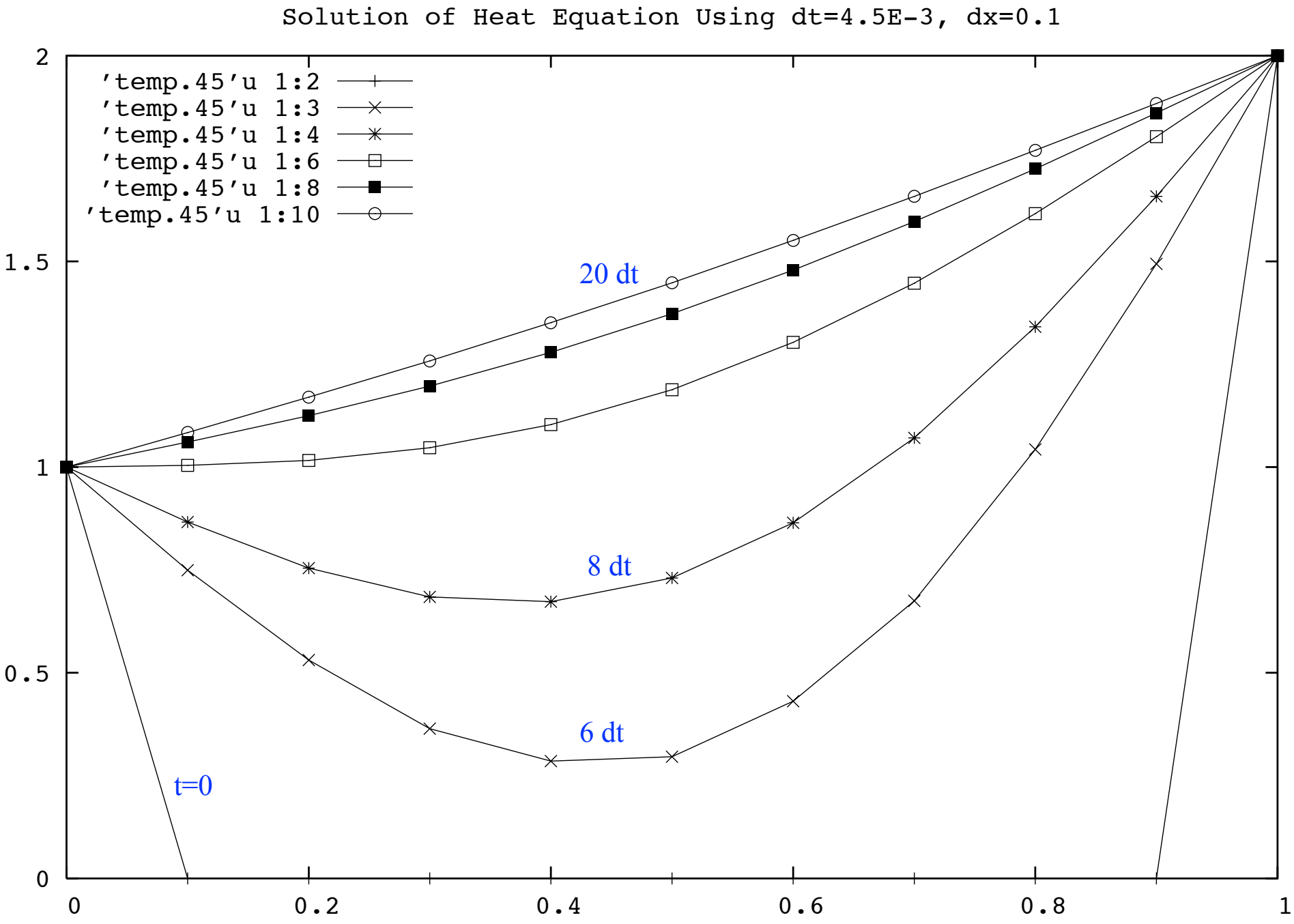
How error propagates from one time step to next.

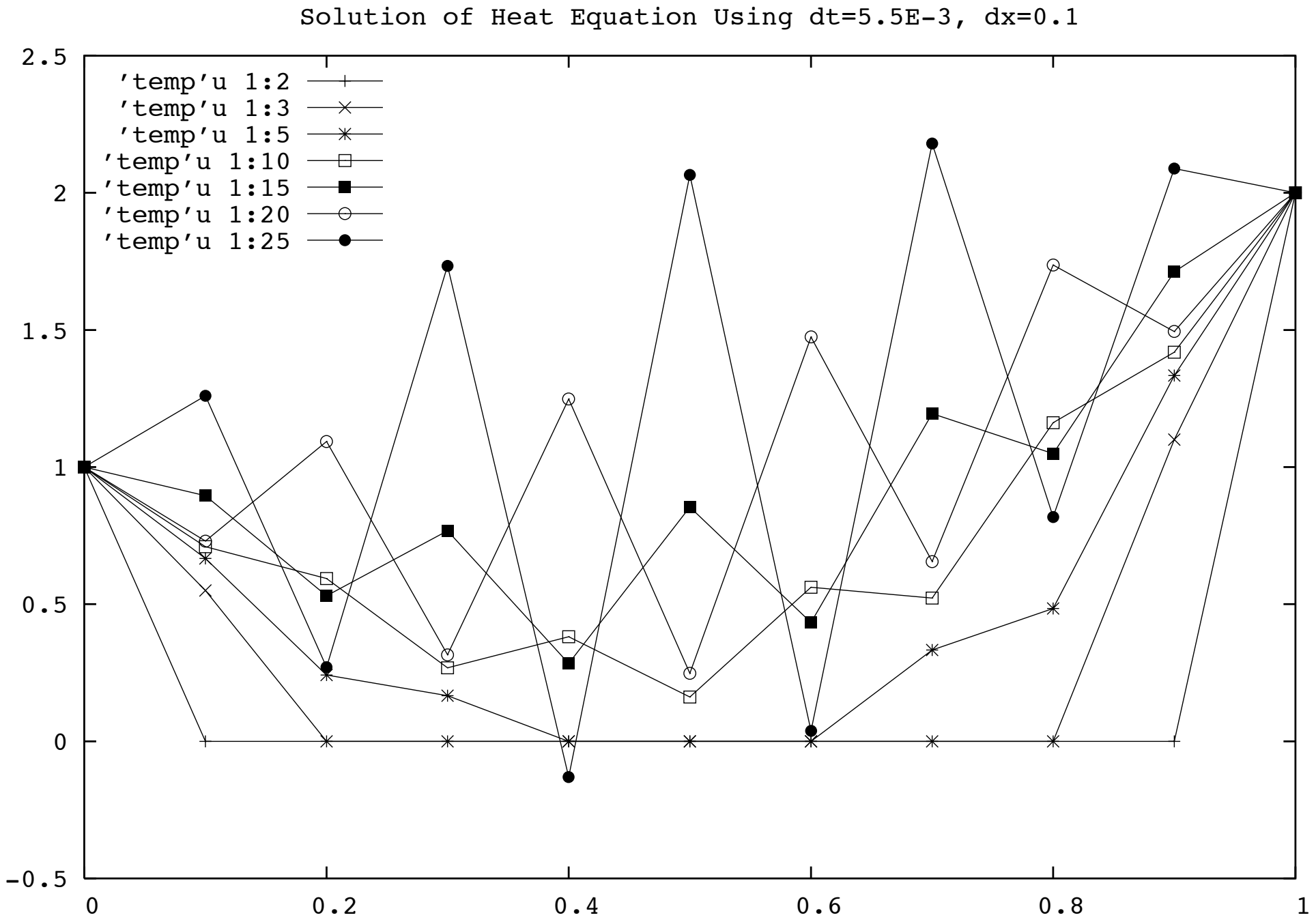
$$T_i^{n+1} = c\, T_{i+1}^n + c\, T_{i-1}^n + (1-2c)\, T_i^n$$

$$\bar{T}_i^{n+1} = c\, \bar{T}_i^n + c\, \bar{T}_{i-1}^n + (1-2c)\, \bar{T}_i^n$$

(What about truncation error?)

$$\Rightarrow \varepsilon_i^{n+1} = c\, \varepsilon_i^n + c\, \varepsilon_{i-1}^n + (1-2c)\, \varepsilon_i^n$$


Solution of Heat Equation Using dt=4.5E-3, dx=0.1
'temp.45'u 1:2
'temp.45'u 1:3
'temp.45'u 1:4
'temp.45'u 1:6
'temp.45'u 1:8
'temp.45'u 1:10
20 dt
8 dt
6 dt
t=0
0
0.5
1
1.5
2
0
0.2
0.4
0.6
0.8
1


Solution of Heat Equation Using dt=5.5E-3, dx=0.1
'temp'u 1:2
'temp'u 1:3
'temp'u 1:5
'temp'u 1:10
'temp'u 1:15
'temp'u 1:20
'temp'u 1:25
2.5
2
1.5
1
0.5
0
-0.5
0
0.2
0.4
0.6
0.8
1

Do Fourier expansion of error: $\epsilon_i^n = \sum_{k=0}^{\infty} \xi_k^n e^{ikx_i}$
and look at one mode $\xi^n e^{ikx}$:

$$\xi^{n+1} e^{ikx_i} = c\,\xi^n (e^{ikx_{i-1}} + e^{ikx_{i+1}}) + (1-2c)\xi^n e^{ikx_i}$$

"amplification factor" $\left\{ \dfrac{\xi^{n+1}}{\xi^n} = c(e^{-ik\Delta x} + e^{ik\Delta x}) + (1-2c) \right.$

$$= 2c\cos(k\Delta x) + (1-2c) = 1 - 2c(1-\cos k\Delta x)$$

cf. "positivity rule" on p. 396 of Constantinides & Mostofi.

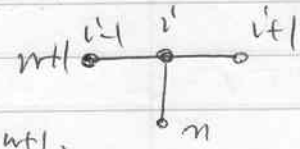
$$= 1 - 4c\sin^2\left(\frac{k\Delta x}{2}\right)$$

Stability: $\left|\dfrac{\xi^{n+1}}{\xi^n}\right| < 1$; $\quad -1 < 1 - 4c\sin^2\dfrac{k\Delta x}{2} < 1$

Or: $c\sin^2\dfrac{k\Delta x}{2} < \dfrac{1}{2}$. Largest $\sin^2\dfrac{k\Delta x}{2}$ is for wave number $k = \dfrac{\pi}{\Delta x} \Rightarrow c < \dfrac{1}{2}$ for stability!

A restriction on time step!

③ Implicit method:



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

Does the von Neumann analysis work for nonlinear equations?

$$c\,T_{i+1}^{n+1} + c\,T_{i-1}^{n+1} - (1+2c)\,T_i^{n+1} = -T_i^n$$

Tridiagonal system with Dirichlet B.C.:

$$\begin{pmatrix} -(1+2c) & c & 0 & \cdots & 0 \\ c & -(1+2c) & c & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & \ddots & c \\ 0 & \cdots & & c & -(1+2c) \end{pmatrix} \begin{pmatrix} T_2 \\ T_3 \\ \vdots \\ \vdots \\ T_{N-1} \end{pmatrix} = \begin{pmatrix} -T_2^n - cT_a \\ -T_3^n \\ \vdots \\ -T_{N-2}^n \\ -T_{N-1}^n - cT_b \end{pmatrix}$$

How about stability? Always stable, for any Δt.
But mind the accuracy $O(\Delta t, \Delta x^2)$!

Von Neumann analysis:

$$\xi^{n+1}\left[c\left(e^{ik\Delta x}+e^{-ik\Delta x}\right)-(1+2c)\right]=-\xi^{n}$$

$$\frac{\xi^{n+1}}{\xi^{n}}=\left[(1+2c)-2c\cos k\Delta x\right]^{-1}=\frac{1}{1+4c\sin^2\frac{k\Delta x}{2}}$$

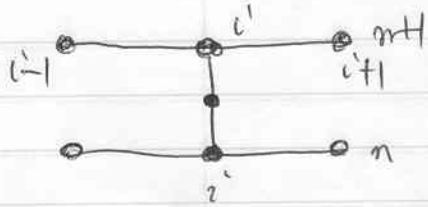
$$<1.$$

Alway stable.

Could choose any Δt. But mind accuracy:

$O(\Delta t, \Delta x^2)$.

④ Crank–Nicolson



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

$$\left.\frac{\partial^2 T}{\partial x^2}\right|_{n+\frac{1}{2}}=\frac{1}{2}\left(\left.\frac{\partial^2 T}{\partial x^2}\right|_{n}+\left.\frac{\partial^2 T}{\partial x^2}\right|_{n+1}\right)+O(\Delta x^2)$$

$$=\frac{1}{2}\left[\frac{T_{i+1}^{n}-2T_i^{n}+T_{i-1}^{n}}{\Delta x^2}+\frac{T_{i+1}^{n+1}-2T_i^{n+1}+T_{i-1}^{n+1}}{\Delta x^2}\right]$$

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

Again tridiagonal system. Thomas scheme.

Stability: $\xi^{n+1}\left[2\cos k\Delta x-2\left(1+\frac{1}{c}\right)\right]=-\xi^{n}\left[2\cos k\Delta x-2\left(1-\frac{1}{c}\right)\right]$

$$\frac{\xi^{n+1}}{\xi^{n}}=-\frac{1-\cos k\Delta x-\frac{1}{c}}{1-\cos k\Delta x+\frac{1}{c}}=-1+\frac{2/c}{1-\cos k\Delta x+1/c}$$

$$=-1+\frac{2}{1+2c\sin^2\frac{k\Delta x}{2}}\ ;\quad -1<\frac{\xi^{n+1}}{\xi^{n}}<1\Rightarrow\frac{1}{1+2c\sin^2\frac{k\Delta x}{2}}<1$$

Always satisfied.

(alternating direction

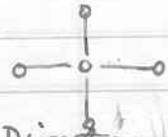
(5) How about 2D problem, implicit method)

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

If we follow forward differencing for $\frac{\partial T}{\partial t}$, central for $\nabla^2 T^{n+1}$, we'll end up with a system similar to the Poisson equation (elliptic). In fact, iterative solutions of a steady state problem is similar to time evolution.

Here is a nice method to keep the implicit nature (conditionally stable), and simplifies the solution procedure: divide and conquer!

Separate the coupling in the two dimensions. Take 2 half steps, each allowing coupling in one Direction.

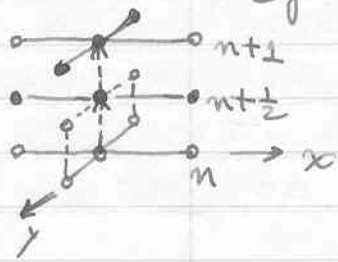


$$\frac{\partial T}{\partial t} = \alpha\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right)$$

$$\frac{T_{i,j}^{n+\frac{1}{2}} - T_{i,j}}{\Delta t/2} = \alpha\left[\frac{T_{i+1,j}^{n+\frac{1}{2}} - 2T_{i,j}^{n+\frac{1}{2}} + T_{i-1,j}^{n+\frac{1}{2}}}{\Delta x^2} + \frac{T_{i,j-1}^{n} - 2T_{i,j}^{n} + T_{i,j+1}^{n}}{\Delta y^2}\right]$$

$$\frac{T_{i,j}^{n+1} - T_{i,j}^{n+\frac{1}{2}}}{\Delta t/2} = \alpha\left[\frac{T_{i+1,j}^{n+\frac{1}{2}} - 2T_{i,j}^{n+\frac{1}{2}} + T_{i-1,j}^{n+\frac{1}{2}}}{\Delta x^2} + \frac{T_{i,j-1}^{n+1} - 2T_{i,j}^{n+1} + T_{i,j+1}^{n+1}}{\Delta y^2}\right]$$

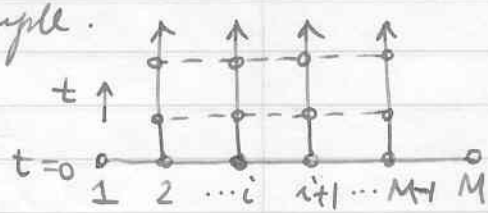
Alternating direction implicit.



- Unconditionally stable
- $O(\Delta t^2, \Delta x^2)$ accurate
- Each half step involves a tridiagonal matrix → Thomas algorithm.
  (book-keeping: reordering unknowns.)

⑥ Method of lines.

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} \quad \text{as an example.}$$



Discretize $\frac{\partial^2 T}{\partial x^2}$ only, but leave $\partial T/\partial t$ as is:

$$\left\{ \frac{\partial T_i}{\partial t} = \alpha\left(T_{i-1} - 2T_i + T_{i+1}\right)/\Delta^2 \quad i = 2, \cdots, M-1 \right.$$

Linear 1st order ODE for $T_i, (i = 2, \cdots, M-1)$. Becomes nonlinear if original equation is nonlinear.

Use ODE method to solve I.V.P.: Runge-Kutta or predictor-corrector scheme.