CHAPTER 4.

Difference Method for Parabolic PDE.

Consider the IBVP.

$$\begin{cases} u_t = \sigma u_{xx}, & 0<x<1, \quad t>0, \\ u(x,0) = \phi(x), & 0 \le x \le 1, \\ u(0,t) = f(t), \quad u(1,t) = g(t), & t>0. \end{cases} \qquad (1)$$

FT-CS. Scheme

$$\begin{cases} U_j^{n+1} = r U_{j-1}^n + (1-2r) U_j^n + r U_{j+1}^n, & j = 1,2,\dots,J-1, \\ & n>0. \\ U_j^0 = \phi(x_j) = \phi(j\Delta x) & \\ U_0^n = f(t_n) = f(n\Delta t), \quad U_J^n = g(n\Delta t). & \end{cases} \qquad (2)$$

$$r \equiv \sigma \Delta t / \Delta x^2.$$

For homogeneous B.C.'s. $f(t) \equiv 0$, $g(t) \equiv 0$

we have proved FT-CS converges
FT-CS Stable in $\|\cdot\|_\infty$

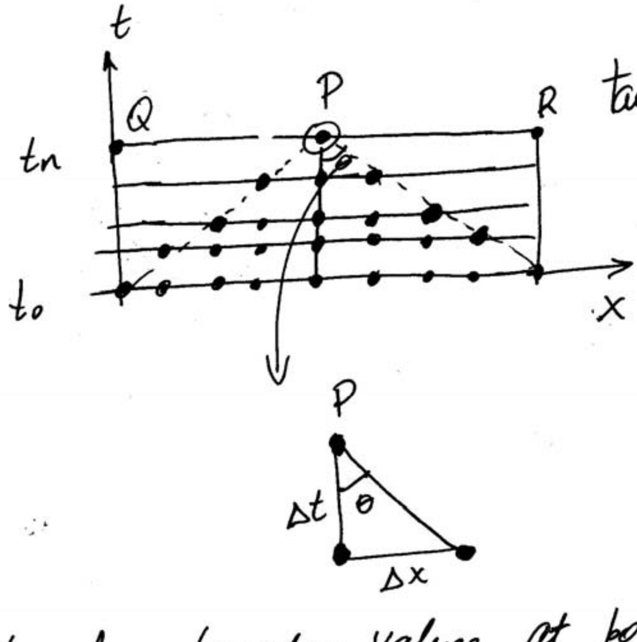
if $0 < r \le 1/2$. , $r = \sigma \dfrac{\Delta t}{\Delta x^2}$

$$\Rightarrow \Delta t = \frac{r \Delta x^2}{\sigma}$$

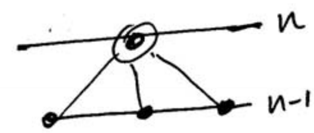
The condition $r \le 1/2$ impose limitations on the choice of Δt.

How can we define numerical schemes for our IBVP with less limitation on the choice of Δt?

<u>Idea</u>: Domain of dependence for num. sch. (2)



$$\tan\theta = \frac{\Delta x}{\Delta t}$$



Obviously, boundary values at points Q and R at level n don't enter into the computation of P at level n.

From PDE theory, we know that Solution at point P certainly depends on boundary data at Q and R.

From the previous graph, we conclude that the angle θ Should be $\pi/2$ (or close to it) for Q and R to enter into the Computation at P.

In chapter 2, we perform two experiments depending on **r** values for FT-CS Scheme.

a) $r = 10^{-1}$ Num. scheme was stable and converges $\Delta x = 0.1$, $\Delta t = 10^{-3}$, $\sigma = 1$

b) $r = 1$ Num. sch. unstable. $\Delta x = 0.1$, $\Delta t = 10^{-2}$, $\sigma = 1$.

$r = \dfrac{\sigma \Delta t}{\Delta x^2}$

$\Rightarrow \dfrac{\Delta x}{\Delta t} = \dfrac{\sigma}{r \Delta x}$

In (a) $\theta = \tan^{-1}\left(\dfrac{\Delta x}{\Delta t}\right) = \tan^{-1}\left(\dfrac{\sigma}{r\Delta x}\right)$

$r = 10^{-1}$

$$\theta = \tan^{-1}\left(\frac{1}{10^{-1}10^{-1}}\right) = \tan^{-1}(100) \simeq 1.56 \simeq \pi/2$$

In (b) $r = 1$

$$\theta = \tan^{-1}\left(\frac{1}{1 \times 10^{-1}}\right) = \tan^{-1}(10) \simeq 1.47 < \pi/2$$

The previous analysis motivates the construction of implicit schemes. For implicit schemes, the solution at P will involve all the other unknowns at the same time level, and it will also include the boundary conditions at Q and R.

<u>Example:</u> BT-CS at the point (x_j, t_{n+1})

$$(u_t)_j^{n+1} = \sigma\,(u_{xx})_j^{n+1}$$

approx. by
$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \sigma\,\frac{U_{j-1}^{n+1} - 2U_j^{n+1} + U_{j+1}^{n+1}}{\Delta x^2}$$

$j = 1, 2, .., J-1$

Also called backward-Euler method.

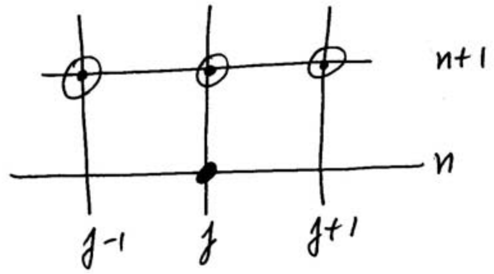
It can be written as

$$\boxed{-r\,U_{j-1}^{n+1} + (1+2r)\,U_j^{n+1} - r\,U_{j+1}^{n+1} = U_j^n,} \quad j = 1, 2, \dots, J-1 \qquad (4.1)$$

For our IBVP (1), we also know

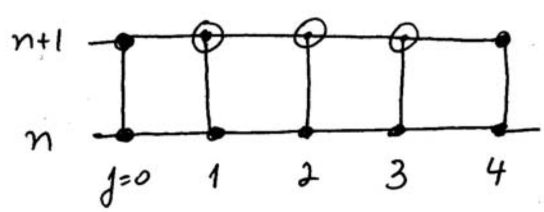
$$U_0^{n+1} = f(t_{n+1}) = f^{n+1}; \quad U_J^{n+1} = g^{n+1}$$

Computational stencil:



Obviously, for a given j equ. (4.1) is not enough. A system of equations needs to be solved at every time level $n+1$.

In particular, if $J=4$



We have a system of 3 equs. to be solved simultaneously. In fact,

$$j=1, \quad -r\,U_0^{n+1} + (1-2r)\,U_1^{n+1} - r\,U_2^{n+1} = U_1^n$$

$$j=2, \quad -r\,U_1^{n+1} + (1-2r)\,U_2^{n+1} - r\,U_3^{n+1} = U_2^n$$

$$j=3, \quad -r\,U_2^{n+1} + (1-2r)\,U_3^{n+1} - r\,U_4^{n+1} = U_3^n$$

B.C's $\quad U_0^{n+1} = f^{n+1}, \qquad U_4^{n+1} = g^{n+1}$

The above System can be written in matrix form as

$$\begin{pmatrix} 1-2r & -r & 0 \\ -r & 1-2r & r \\ 0 & -r & 1-2r \end{pmatrix} \begin{pmatrix} U_1^{n+1} \\ U_2^{n+1} \\ U_3^{n+1} \end{pmatrix} = \begin{pmatrix} U_1^{n} \\ U_2^{n} \\ U_3^{n} \end{pmatrix} + r \begin{pmatrix} \overset{=f^{n+1}}{U_0^{n+1}} \\ 0 \\ \underset{=g^{n+1}}{U_4^{n+1}} \end{pmatrix}$$

Since this implicit scheme involves the B.C to compute all the unknowns at level t_{n+1}, we expect better stability properties.

We can take a more general point of view and combine BT-CS at (x_j, t_{n+1}) with FT-CS at (x_j, t_n) in what is called weigthed average

BT-CS at (x_j, t_{n+1}) $$\left[\frac{U_j^{n+1} - U_j^n}{\Delta t} = \sigma \frac{\overbrace{U_{j+1}^{n+1} - 2U_j^{n+1} + U_{j-1}^{n+1}}^{\delta^2 U_j^{n+1}}}{\Delta x^2}\right] * \theta$$

FT-CS at (x_j, t_n) $$\left[\frac{U_j^{n+1} - U_j^n}{\Delta t} = \sigma \frac{\overbrace{U_{j+1}^{n} - 2U_j^{n} + U_{j-1}^{n}}^{\delta^2 U_j^{n}}}{\Delta x^2}\right] * (1-\theta)$$

$0 \le \theta \le 1$.

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \sigma \frac{\theta \delta^2 U_j^{n+1} + (1-\theta)\delta^2 U_j^n}{\Delta x^2} \qquad (7.1)$$

Clearly, if $\theta = 0$ in (7.1) we obtain the explicit FT-CS scheme.

if $\theta = 1$ in (7.1) we obtain the euler implicit BT-CS scheme.

(7.1) can also be written as

$$\boxed{\begin{aligned} -r\theta U_{j-1}^{n+1} + (1+2r\theta) U_j^{n+1} - r\theta U_{j+1}^{n+1} &= \\ = r(1-\theta) U_{j-1}^n + [1 - 2r(1-\theta)] U_j^n + r(1-\theta) U_{j+1}^n, \end{aligned}} \qquad (7.2)$$

$j = 1, 2, \dots, J-1$

$U_0^{n+1} = f^{n+1}, \quad U_J^{n+1} = g^{n+1}$.

(7.1) Can be written as

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \sigma\theta \frac{U_{j+1}^{n+1} - 2U_j^{n+1} + U_{j-1}^{n+1}}{\Delta x^2} + \sigma(1-\theta)\frac{U_{j+1}^n - 2U_j^n + U_{j-1}^n}{\Delta x^2}$$

$$\Rightarrow \quad U_j^{n+1} - \theta r\left(U_{j+1}^{n+1} + U_{j-1}^{n+1}\right) + 2\theta r U_j^{n+1} = \cdots$$

$$\Rightarrow \quad -r\theta U_{j-1}^{n+1} + (1+2\theta r)U_j^{n+1} - r\theta U_{j+1}^{n+1} = \cdots$$

$$j = 1, 2, \ldots, J-1$$

$$j=1 \quad \underbrace{-r\theta U_0^{n+1}}_{=-r\theta f^{n+1}} + (1+2r\theta)U_1^{n+1} - r\theta U_2^{n+1} =$$

$$= \underbrace{r(1-\theta)U_0^{n}}_{=r(1-\theta)f^n} + \big(1-2r(1-\theta)\big)U_1^{n} + r(1-\theta)U_2^{n}$$

$$j=2 \quad -r\theta U_1^{n+1} + (1+2r\theta)U_2^{n+1} - r\theta U_3^{n+1} = \cdots$$

$$\vdots$$

$$j=J-1 \quad -r\theta U_{J-2}^{n+1} + (1+2r\theta)U_{J-1}^{n+1} \underbrace{-r\theta U_J^{n}}_{=-r\theta g^{n+1}} = r(1-\theta)U_{J-2}^{n}$$

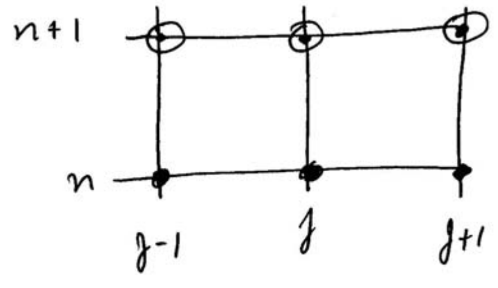
$$+ \big(1-2r(1-\theta)\big)U_{J-1}^{n} + \underbrace{r(1-\theta)U_J^{n}}_{=r(1-\theta)g^n}$$

$$\therefore \left(\begin{bmatrix} 1 & & & 0 \\ & 1 & & \\ & & \ddots & \\ 0 & & & 1 \end{bmatrix} + r\theta \begin{bmatrix} 2 & -1 & 0 & 0 & \cdots & 0 \\ -1 & 2 & -1 & 0 & \cdots & 0 \\ & \ddots & \ddots & \ddots & & \\ & & & \ddots & \ddots & \\ & & & -1 & 2 & -1 \\ & & & & -1 & 2 \end{bmatrix} \right) \begin{bmatrix} U_1^{n+1} \\ U_2^{n+1} \\ \vdots \\ U_{J-1}^{n+1} \end{bmatrix} =$$

$$= \left(\begin{bmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{bmatrix} + r(1-\theta) \begin{bmatrix} -2 & 1 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 \\ & \ddots & \ddots & \ddots & & \\ & & & \ddots & \ddots & 1 \\ & & & & 1 & -2 \end{bmatrix} \right) \begin{bmatrix} U_1^{n} \\ U_2^{n} \\ \vdots \\ U_{J-1}^{n} \end{bmatrix} + r \begin{bmatrix} \theta f^{n+1} + (1-\theta) f^n \\ 0 \\ \vdots \\ 0 \\ \theta g^{n+1} + (1-\theta) g^n \end{bmatrix}$$

which can be written as (7.2) in page 8.

For $\theta \in (0,1)$ the computational stencil looks like



(7.2) in matrix form is also a tridiag. non-homogeneous system for $\theta \in (0,1)$. In fact,

$$\boxed{\left[I - r\theta C\right]\vec{U}^{n+1} = \left[I + r(1-\theta)C\right]\vec{U}^{n} + r\vec{f}^{n},} \quad (8.1)$$

where

$$\vec{U}^{n} = \begin{bmatrix} U_1^n \\ U_2^n \\ U_3^n \\ \vdots \\ U_{J-1}^n \end{bmatrix}, \quad C = \begin{bmatrix} -2 & 1 & 0 & \cdots & 0 \\ 1 & -2 & 1 & \cdots & 0 \\ & \ddots & \ddots & \ddots & 1 \\ 0 & & & 1 & -2 \end{bmatrix}$$

$$\vec{f}^{n} = \begin{bmatrix} \theta f^{n+1} + (1-\theta) f^{n} \\ 0 \\ \vdots \\ 0 \\ \theta g^{n+1} + (1-\theta) g^{n} \end{bmatrix}$$

CRANK- NICHOLSON

An important particular scheme from the family of weighted average scheme (7.2) is obtained when $\theta = 1/2$. This is called Crank-Nicholson's scheme.

$$\boxed{-\frac{r}{2} U_{j-1}^{n+1} + (1+r) U_j^{n+1} - \frac{r}{2} U_{j+1}^{n+1} = \frac{r}{2} U_{j-1}^{n} + (1-r) U_j^{n} + \frac{r}{2} U_{j+1}^{n}} \qquad (8'.1)$$

$j = 1, 2, \ldots, J-1.$

An alternative way to obtain (8'.1) is by using centered difference in time approximations for U_t at the point $(x_j, t_{n+1/2})$ and also using centered difference in space approximations for U_{xx} at $(x_j, t_{n+1/2})$. In fact, $\boxed{(U_t)_j^{n+1/2} = K\,(U_{xx})_j^{n+1/2}}$

CT- CS at $(x_j, t_{n+1/2})$. with time step size $\frac{\Delta t}{2}$

$$\frac{U_j^{n+1} - U_j^{n}}{2\left(\frac{\Delta t}{2}\right)} = K\,\frac{U_{j+1}^{n+1/2} - 2U_j^{n+1/2} + U_{j-1}^{n+1/2}}{(\Delta x)^2}$$

In fact,

CT – CS at $(x_j, t_{n+1/2})$, with time step $\frac{\Delta t}{2}$.

$$\frac{u_j^{n+1} - u_j^n}{\cancel{2}\left(\frac{\Delta t}{\cancel{2}}\right)} = K \; \frac{u_{j+1}^{n+1/2} - 2u_j^{n+1/2} + u_{j-1}^{n+1/2}}{\Delta x^2}$$

$$\underline{\underline{\text{Using Average in time}}} \quad \frac{\dfrac{u_{j+1}^{n+1} + u_{j+1}^{n}}{2} - 2\,\dfrac{u_j^{n+1} + u_j^{n}}{2} \quad \dfrac{u_{j-1}^{n+1} + u_{j-1}^{n}}{2}}{\Delta x^2}$$

$$= \frac{K}{2}\left[\frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{\Delta x^2} + \frac{u_{j+1}^{n} - 2u_j^{n} + u_{j-1}^{n}}{\Delta x^2}\right]$$

If $r = K\dfrac{\Delta t}{\Delta x^2}$

$$\Rightarrow \quad u_j^{n+1} - u_j^n = \frac{r}{2}\left[u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1} + u_{j+1}^{n} - 2u_j^{n} + u_{j-1}^{n}\right]$$

$$\Rightarrow \quad \boxed{-\frac{r}{2}u_{j-1}^{n+1} + (1+r)\,u_j^{n+1} - \frac{r}{2}u_{j-i}^{n+1} = \frac{r}{2}u_{j-1}^{n} + (1-r)\,u_j^{n} + \frac{r}{2}u_{j+1}^{n}}$$

Same as (8.1)

(8.1) is a tridiagonal system. there is a faster way to solve it than naive Gauss elimination.

In general, for

$$A\vec{x} = \vec{f}. \quad , \qquad A_{n\times n}.$$

$$A = \begin{pmatrix} a_1 & c_1 & & & & \\ b_2 & a_2 & c_2 & & 0 & \\ & \ddots & \ddots & \ddots & & \\ & & & & & \\ & 0 & & b_{N-1} & a_{N-1} & c_{n-1} \\ & & & & b_N & a_N \end{pmatrix}$$

Assuming than pivoting is not necessary

A can be factored as

$$A = LU$$

Where L : Lower

U : upper

$$L = \begin{pmatrix} 1 & & & \\ l_2 & 1 & & \\ & l_3 & 1 & \\ & & \ddots & \ddots \\ & & & l_N & 1 \end{pmatrix}, \quad U = \begin{pmatrix} u_1 & v_1 & & & \\ & u_2 & v_2 & & \\ & & \ddots & \ddots & \\ & & & u_{N-1} & v_{N-1} \\ & & & & u_N \end{pmatrix}$$

The entries for L and U can be computed directly for $A = LU$.

$$\begin{pmatrix} a_1 & c_1 & & \\ b_2 & a_2 & c_2 & \\ & & \ddots & \\ & & b_N & a_N \end{pmatrix} = \begin{pmatrix} u_1 & v_1 & & \\ l_2 u_1 & l_2 v_1 + u_2 & v_2 & \\ & & & \\ & & l_N u_{N-1} & l_N v_{N-1} + u_N \end{pmatrix}$$

Therefore,

$$u_1 = a_1, \quad v_1 = c_1$$

$$l_2 = b_2/u_1$$

$$u_2 = a_2 - l_2 v_1$$

$$v_2 = c_2$$

In general,

$u_1 = a_1$
$v_1 = c_1$
$j = 2, 3 \dots, N$
 $l_j = b_j / u_{j-1}$
 $u_j = a_j - l_j v_{j-1}$
 $v_j = c_j$
end.

Once the entries of L and U have been determined, the system

$$A\vec{x} = \vec{f} \quad \text{or} \quad LU\vec{x} = \vec{f}$$

can be solved in two steps

$$U\vec{x} = \vec{y}$$
$$L(U\vec{x}) = L\vec{y} = \vec{f}$$

First, we solve

$$L\vec{y} = \vec{f}$$

by forward substitution. Then, we solve

$$U\vec{x} = \vec{y}$$

using backward substitution.

See tridiag. algorithm in book.

(I) FACTORIZATION.

(II) Forward- and Backward Substitution.

Stability of weighted average scheme.

Using Von Neumann method

$$U_j^n = \sum_{k=0}^{J-1} A_k^n \, w_j^k , \qquad w_j^k = e^{i 2\pi j/J}$$

Assuming initial conditions are periodic in x of period 2π.

Now, Subst. in the Num. scheme. leads to

$$\sum_{k=0}^{J-1} \Big[A_k^{n+1} \left(-r\theta e^{-i2\pi k/J} + 1 + 2r\theta - r\theta e^{i2\pi k/J} \right) -$$

$$- A_k^n \left(r(1-\theta) e^{-i2\pi k/J} + 1 - 2r(1-\theta) + r(1-\theta) e^{i2\pi k/J} \right) \Big] w_j^k = 0$$

Since $-e^{-i2\pi k/J} - e^{i2\pi k/J} = -2\cos(2\pi k/J)$

and $e^{-i2\pi k/J} + e^{i2\pi k/J} = 2\cos(2\pi k/J)$

Then, using orthogonality of w_j^k's

$$A_k^{n+1} = M_k A_k^n , \qquad \text{where} \quad \boxed{M_k = 1 - \frac{2r\left(1-\cos(2\pi k/J)\right)}{1+2r\theta\left(1-\cos(2\pi k/J)\right)}}$$

Or

$$M_K = 1 - \frac{4r \sin^2(K\pi/J)}{1 + 4r\theta \sin^2(K\pi/J)}$$

$$A_k^{n+1} = M_k A^n \Rightarrow \underline{A_K^n = (M_K)^n A_K^0}$$

Since we know that the Soln. for a periodic initial Value problem for Heat Cond. should decay in time, we will ask

$$|M_K| \leq 1$$

i.e.,

$$-1 \leq 1 - \frac{4r \sin^2(\,)}{1 + 4r\theta \sin^2(\,)} \leq 1$$

rhs always satisfied.

lhs. is equivalent to

$$\frac{4r \sin^2(\,)}{1 + 4r\theta \sin^2(\,)} \leq 2$$

$$\Rightarrow 4r \sin^2(\,) \leq 2 + 8r\theta \sin^2(\,)$$

$$\Rightarrow 2r \sin^2(\,) \leq 1 + 4r\theta \sin^2(\,) \Rightarrow \boxed{2r(1-2\theta)\sin^2(\,) \leq 1}$$

for all K

then the Condition Should be

$$2r(1-2\theta) \le 1$$

(I) for $0 \le \theta < 1/2$

$1-2\theta > 0 \quad \Rightarrow \quad r \le \dfrac{1}{2(1-2\theta)}$

rmk: Notice that for $\theta = 0$, $r \le 1/2$ explicit scheme.

(II) for $1/2 \le \theta \le 1$ (implicit schemes) $\Rightarrow 1-2\theta \le 0$

$$\Rightarrow \quad 2r(1-2\theta) \le 1, \quad \text{for all } r$$

It means Weighted Scheme is stable for any choice of Δt and Δx. It's said that the Scheme is <u>unconditionally stable</u>.