Consider the IBVP.

\[
\begin{aligned}
U_t &= \sigma U_{xx}, \quad 0 < x < 1, \quad t > 0, \\
U(x, 0) &= \phi(x), \quad 0 \leq x \leq 1, \\
U(0, t) &= f(t), \quad U(1, t) = g(t), \quad t > 0.
\end{aligned}
\]  

\tag{1}

**FT-CS Scheme**

\[
\begin{aligned}
U_{j}^{n+1} &= r U_{j-1}^{n} + (1 - 2r) U_{j}^{n} + r U_{j+1}^{n}, \quad j = 1, 2, \ldots, J-1, \\
U_{j}^{0} &= \phi(x_{j}) = \phi(j \Delta x), \\
U_{0}^{n} &= f(t_{n}) = f(n \Delta t), \quad U_{j}^{n} = g(n \Delta t). \\
\end{aligned}
\]  

\tag{2}

\( r = \frac{\sigma \Delta t}{\Delta x^2} \).

For homogeneous B.C.s. \( f(t) \equiv 0, \quad g(t) \equiv 0 \)

we have proved **FT-CS converges**

\textbf{FT-CS Stable in II.IIIo}

\[ 0 < r \leq \frac{1}{2} \]

\[ r = \frac{\sigma \Delta t}{\Delta x^2} \]

\[ \Rightarrow \Delta t = \frac{r \Delta x^2}{\sigma} \]
The condition \( R \leq \frac{1}{2} \) impose limitations on the choice of \( \Delta t \).

How can we define numerical schemes for our IBVP with less limitation on the choice of \( \Delta t \)?

**Idea:** Domain of dependence for num. sch. (2)

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 $\Theta$ 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.

\[ \Delta x = 0.1, \quad \Delta t = 10^{-3}, \quad \sigma = 1 \]

b) $r = 1$, Num. scheme unstable.

\[ \Delta x = 0.1, \quad \Delta t = 10^{-2}, \quad \sigma = 1. \]

In (a) $r = 10^{-1}$

\[ \Theta = \tan^{-1} \left( \frac{\Delta x}{\Delta t} \right) = \tan^{-1} \left( \frac{\sigma}{r \Delta x} \right) \]

\[ \Rightarrow \frac{\Delta x}{\Delta t} = \frac{\sigma}{r \Delta x} \]

In (b) $r = 1$

\[ \Theta = \tan^{-1} \left( \frac{1}{10 \times 10^{-1}} \right) = \tan^{-1} (100) \approx 1.56 \approx \pi/2 \]

\[ \Theta = \tan^{-1} \left( \frac{1}{1 \times 10^{-1}} \right) = \tan^{-1} (10) \approx 1.47 < \pi/2 \]
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 \( R \).

**Example:** BT-CS at the point \( (x_j, t_{nn}) \)

\[
(\Delta t)^{n+1} = \sigma \left( U_{xx}\right)^{n+1}_j
\]

Approx. by

\[
\frac{U_j^{n+1} - U_j^n}{\Delta t} = \sigma \frac{U_{j-1}^{n+1} - 2U_j^{n+1} + U_{j+1}^{n+1}}{\Delta x^2}
\]

Also called backward-Euler method.

It can be written as

\[
-\gamma U_{j+1}^{n+1} + (1 + 2\gamma) U_j^{n+1} - \gamma U_{j-1}^{n+1} = U_j^n \quad \rightarrow \quad (4.1)
\]

For our IBVP (1), we also know

\[
U_0^{n+1} = f(t_{nn}) = f^{n+1}, \quad U_j^{n+1} = g^{n+1}
\]
Computational stencil:

\[ \begin{array}{c}
  \text{\textbullet} \\
  n+1 \\
  j_1 \quad j \quad j+1 \\
  n \\
  j-1 \\
  \end{array} \]

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

In particular, if \( J=4 \)

\[ \begin{array}{c}
  \text{\textbullet} \\
  n+1 \\
  n \\
  j=0 \quad 1 \quad 2 \quad 3 \quad 4 \\
  \end{array} \]

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

\[ \begin{align*}
  &j=1, \quad -r \, U_j^{n+1} + (1-2r) \, U_j^{n} - r \, U_{j+1}^{n} = U_j^{n} \\
  &j=2, \quad -r \, U_j^{n+1} + (1-2r) \, U_j^{n} - r \, U_{j+1}^{n} = U_j^{n} \\
  &j=3, \quad -r \, U_j^{n+1} + (1-2r) \, U_j^{n} - r \, U_{j+1}^{n} = U_j^{n}
\end{align*} \]
B.C's

\[ U_{0}^{n+1} = f^{n+1}, \quad U_{4}^{n+1} = g^{n+1} \]

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}
0 \\
0 \\
0
\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 weighted average.
\[
\text{BT-CS at } (x_j, t^n): \quad \frac{U_j^{n+1} - U_j^n}{\Delta t} = \sigma \left( \frac{U_{j+1}^{n+1} - 2U_j^{n+1} + U_{j-1}^{n+1}}{\Delta x^2} \right) \cdot \theta \Rightarrow \Delta^2 U_j^{n+1} \\
\text{FT-CS at } (x_j, t^n): \quad \frac{U_j^{n+1} - U_j^n}{\Delta t} = \sigma \left( \frac{U_{j+1}^n - 2U_j^n + U_{j-1}^n}{\Delta x^2} \right) \cdot (1-\theta) \Rightarrow \Delta^2 U_j^n
\]

\[
\frac{U_j^{n+1} - U_j^n}{\Delta t} = \sigma \left( \frac{\theta \Delta^2 U_j^{n+1} + (1-\theta) \Delta^2 U_j^n}{\Delta x^2} \right), \quad 0 \leq \theta \leq 1. \tag{7.1}
\]

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

\[
-\theta r \gamma_j^{n+1} + (1+\theta r) \gamma_j^{n+1} - \theta r \gamma_j^{n+1} = 0 \tag{7.2}
\]

\[
= r (1-\theta) \gamma_{j+1}^n + [1-r(1-\theta)] \gamma_j^n + r (1-\theta) \gamma_{j-1}^n, \quad j = 1, 2, \ldots, J-1
\]

\[
U_j^{n+1} = f^{n+1}, \quad U_j^{n+1} = g^{n+1}.
\]
(7.1) can be written as

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

\[
\Rightarrow \quad U_j^{n+1} = \theta r (U_{j+1}^{n+1} + U_{j-1}^{n+1}) + 2(1-\theta) U_j^n = \ldots \ldots
\]

\[
\Rightarrow -r \sigma U_{j-1}^{n+1} + (1+2\sigma)U_j^n - r \sigma U_{j+1}^{n+1} = \ldots \ldots
\]

\[
\Rightarrow \quad g = 1, 2, \ldots, J-1
\]
\[ j = 1 \]
\[ -2 \sigma \mathcal{U}_1^{n+1} + (1 + 2 \sigma \epsilon) \mathcal{U}_1^n - \sigma \mathcal{U}_2^n = \]
\[ = \sigma \mathcal{U}_0^n \mathcal{R}(\nu \epsilon) \mathcal{F}_m^n + \sigma \mathcal{R}(\nu \epsilon) \mathcal{U}_1^n + \sigma (\nu \epsilon) \mathcal{U}_2^n \]

\[ j = 2 \]
\[ -2 \sigma \mathcal{U}_1^{n+1} + (1 + 2 \sigma \epsilon) \mathcal{U}_2^n - \sigma \mathcal{U}_3^n = \]
\[ = -\sigma \mathcal{R}(\nu \epsilon) \mathcal{F}_m^n \]

\[ j = J - 1 \]
\[ -2 \sigma \mathcal{U}_J^{n+1} + (1 + 2 \sigma \epsilon) \mathcal{U}_J^n - \sigma \mathcal{R}(\nu \epsilon) \mathcal{F}_m^n \]
\[ = \sigma \mathcal{R}(\nu \epsilon) \mathcal{U}_J^n + \sigma (\nu \epsilon) \mathcal{U}_J^n \]
\[ + (1 - 2 \nu \epsilon) \mathcal{U}_J^{n+1} + \sigma (\nu \epsilon) \mathcal{U}_J^n \]

\[ \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} + \sigma \epsilon \begin{bmatrix} 2 & -1 & 0 & \ldots & 0 \\ -1 & 2 & -1 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \vdots & \vdots & \vdots & 2 & -1 \\ \vdots & \vdots & \vdots & \vdots & 1 \end{bmatrix} \]

\[ \begin{bmatrix} \mathcal{U}_1^{n+1} \\ \mathcal{U}_2^{n+1} \\ \mathcal{U}_J^{n+1} \end{bmatrix} = \begin{bmatrix} \mathcal{U}_1^n \\ \mathcal{U}_2^n \\ \mathcal{U}_J^n \end{bmatrix} + \mathcal{R}(\nu \epsilon) \mathcal{F}_m^n 
\]

where \( \mathcal{F}_m^n \) can be written as \((7.3)\) in page 8.
For $\theta \in (0, 1)$ the computational stencil looks like

\[
\begin{array}{ccc}
  n+1 & & \\
  & \bullet & \\
  n & & \\
  & \bullet & \\
  j-1 & j & j+1
\end{array}
\]

Equation (7.2) in matrix form is also a tridiagonal system for $\theta \in (0, 1)$. In fact,

\[
[I - \rho \theta C] \hat{U}^{n+1} = [I + \gamma (1 - \theta) \gamma] \hat{U}^n + \gamma \hat{f}^n \tag{8.1}
\]

where

\[
\hat{U}^n = \begin{bmatrix}
  U_1^n \\
  U_2^n \\
  \vdots \\
  U_{N-1}^n \\
  U_N^n
\end{bmatrix}, \quad
C = \begin{bmatrix}
  -2 & 1 & 0 & \cdots & 0 \\
  1 & -2 & 1 & \cdots & 0 \\
  \vdots & \vdots & \vdots & \ddots & \vdots \\
  0 & \cdots & 1 & -2 & 1 \\
  \end{bmatrix}, \quad
\hat{f}^n = \begin{bmatrix}
  \theta f_1^{n+1} + (1 - \theta) f_1^n \\
  \vdots \\
  \theta g_1^{n+1} + (1 - \theta) g_1^n \\
  \end{bmatrix}
\]
An important particular scheme from the family of weighted average scheme (7.2) is obtained when $\theta = \frac{1}{2}$. This is called Crank-Nicholson's scheme.

\[
\frac{r}{2} U_{j-1}^{n+1} + (1+r) U_j^{n+1} - \frac{r}{2} U_{j+1}^{n+1} = \frac{r}{2} U_{j-1}^n + (1-r) U_j^n + \frac{r}{2} U_{j+1}^n
\]

\(j = 2, \ldots, J-1.\)

An alternative way to obtain (8.1) is by using centered difference in time approximations for $U_t$ at the point $(x_j, t_{n+\frac{1}{2}})$ and also using centered difference in space approximations for $U_{xx}$ at $(x_j, t_{n+\frac{1}{2}}).$ In fact, \(U_j^{n+\frac{1}{2}} = k (U_{xx})^{n+\frac{1}{2}}\). CTS at $(x_j, t_{n+\frac{1}{2}})$ with step size $\Delta t$.

\[
\frac{U_j^{n+1} - U_j^n}{\frac{\Delta t}{2}} = k \frac{U_{j+1}^{n+\frac{1}{2}} - 2U_j^{n+\frac{1}{2}} + U_{j-1}^{n+\frac{1}{2}}}{(\Delta x)^2}
\]
In fact, CT-CS at \((x_j, t_{n+1})\), with time step \(\Delta t\)

\[
\frac{U_j^{n+1} - U_j^n}{2 (\Delta t)} = K \frac{U_{j+1}^{n+1} - 2U_j^{n+1} + U_{j-1}^{n+1}}{\Delta x^2} - 2 \frac{U_j^{n} + U_j^n}{2} + \frac{U_{j+1}^{n} + U_{j-1}^{n}}{2}
\]

Using average in time:

\[
= K \frac{1}{2} \left[ \frac{U_{j+1}^{n+1} - 2U_j^{n+1} + U_{j-1}^{n+1}}{\Delta x^2} + \frac{U_{j+1}^{n} + U_{j-1}^{n}}{2} \right]
\]

If \( r = K \frac{\Delta t}{\Delta x^2} \)

\[
U_j^{n+1} - U_j^n = \frac{r}{2} \left[ U_{j+1}^{n+1} - 2U_j^{n+1} + U_{j-1}^{n+1} + U_{j+1}^{n} - 2U_j^{n} + U_{j-1}^{n} \right]
\]

\[
-\frac{r}{2} U_{j-1}^{n+1} + (1+r) U_j^n - \frac{r}{2} U_{j+1}^{n+1} = \frac{r}{2} U_{j-1}^{n} + (1-r) U_j^n + \frac{r}{2} U_{j+1}^{n}
\]

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

$$A\hat{x} = \tilde{f}, \quad A_{nn}$$

$$A = \begin{pmatrix}
  a_1 & c_1 & & \\
  b_2 & a_2 & c_2 & \\
  & b_3 & a_3 & c_3 \\
  & & \ddots & \ddots & \ddots \\
  & & & b_{n-1} & a_{n-1} & c_{n-1} \\
  & & & & b_n & a_n & \end{pmatrix}$$

Assuming that pivoting is not necessary

$A$ can be factored as

$$A = LU$$

Where $L$: Lower

$U$: Upper

$$L = \begin{pmatrix}
  1 & & & & & \\
  l_2 & 1 & & & & \\
  & l_3 & 1 & & & \\
  & & \ddots & \ddots & & \\
  & & & l_{n-1} & 1 & \\
  & & & & l_n & 1
\end{pmatrix}, \quad U = \begin{pmatrix}
  U_1 & V_1 & & & & \\
  & U_2 & V_2 & & & \\
  & & \ddots & \ddots & & \\
  & & & \ddots & V_{n-1} & \\
  & & & & U_{n-1} & V_{n-1} \\
  & & & & & U_n
\end{pmatrix}$$
The entries for \( L \) and \( U \) can be computed directly for \( A = LU \).

\[
\begin{pmatrix}
a_1 & c_1 \\
b_2 & a_2 & c_2 \\
\vdots & & \ddots & \ddots \\
b_N & \cdots & \cdots & a_N
\end{pmatrix}
= 
\begin{pmatrix}
u_1 & v_1 \\
l_2u_1 & l_2v_1 + u_2 & v_2 \\
\vdots & & \ddots & \ddots \\
l_Nu_{N-1} + u_N
\end{pmatrix}
\]

Therefore, \( u_1 = a_1, \ v_1 = c_1 \)
\( l_2 = b_2 / u_1 \)
\( u_2 = a_2 - l_2v_1 \)
\( v_2 = c_2 \)

In general,
\( u_j = a_j \)
\( v_j = c_j \)
\( j = 2, 3, \ldots, N \)
\( l_j = b_j / u_{j-1} \)
\( u_j = a_j - l_jv_{j-1} \)
\( v_j = c_j \)
edn.
Once the entries of $L$ and $U$ have been determined, the system

\[ A \tilde{x} = \tilde{f} \quad \text{or} \quad LU \hat{x} = \hat{f} \]

Can be solved in two steps

\[ U \hat{x} = \hat{y} \]
\[ L(U \hat{x}) = L \hat{y} = \hat{f} \]

First, we solve

\[ L \hat{y} = \hat{f} \]

by forward substitution. Then, we solve

\[ U \hat{x} = \hat{y} \]

Using backward substitution.

See triag. Algorithm in book.

(1) Factorization.

(II) Forward- and Backward Substitution.
Stability of weighted average scheme.

Using Von Neumann method

\[ U_j^n = \sum_{k=0}^{J-1} A_k^n w_j^k, \quad w_j^k = e^{i \frac{2 \pi j}{J}} \]

Assuming initial conditions are periodic in $x$ of period $2\pi$.

Now, Substitute in the Num. scheme. leads to

\[ \sum_{k=0}^{J-1} \left[ A_{k+1}^n \left(-r \sigma e^{-i \frac{2 \pi k}{J}} + 1 + 2r - r \sigma e^{i \frac{2 \pi k}{J}} \right) - A_k^n \left(r(1-\theta) e^{-i \frac{2 \pi k}{J}} + 1 - 2r(1-\theta) + r(1-\theta) e^{i \frac{2 \pi k}{J}} \right) \right] w_j^k = 0 \]

Since $e^{-i \frac{2 \pi k}{J}} - e^{i \frac{2 \pi k}{J}} = -2 \cos\left(\frac{2 \pi k}{J}\right)$

And $e^{-i \frac{2 \pi k}{J}} + e^{i \frac{2 \pi k}{J}} = 2 \cos\left(\frac{2 \pi k}{J}\right)$

Then, using orthogonality of $w_j^k$'s

\[ A_{k+1}^n = M_k A_k^n \]

Where

\[ M_k = 1 - \frac{2r \left(1 - \cos\left(\frac{2 \pi k}{J}\right)\right)}{1 + 2r(1-\cos\left(\frac{2 \pi k}{J}\right))} \]
\[ M_k = 1 - \frac{4r \sin^2(k \pi / 3)}{1 + 4r \theta \sin^2(k \pi / 3)} \]

\[ A_k''' = M_k A_k'' \quad \Rightarrow \quad A_k'' = (M_k)^n A_k \]

Since we know that the soln. for a periodic initial value problem for Heat cond. should decay \( k \) twice, we will ask \( |M_k| \leq 1 \)

i.e.,

\[ -1 \leq 1 - \frac{4r \sin^2(\cdot)}{1 + 4r \theta \sin^2(\cdot)} \leq 1 \]

RHS always satisfied.

LHS is equivalent to

\[ \frac{4r \sin^2(\cdot)}{1 + 4r \theta \sin^2(\cdot)} \leq 2 \]

\[ 4r \sin^2(\cdot) \leq 2 + 8r \theta \sin^2(\cdot) \]

\[ 2r \sin^2(\cdot) \leq 1 + 4r \theta \sin^2(\cdot) \quad \Rightarrow \quad 2r (1 - 2\theta) \sin^2(\cdot) \leq 1 \]

for all \( k \)
Then the condition should be

$$2v(1-2\theta) \leq 1$$

\[\text{(I) for } 0 \leq \theta < \frac{1}{2} \quad \Rightarrow \quad v \leq \frac{1}{2(1-2\theta)}\]

Remark: Notice that for $\theta = 0$, $v \leq \frac{1}{2}$ explicit scheme.

\[\text{(II) for } \frac{1}{2} \leq \theta \leq 1 \quad \Rightarrow \quad 1-2\theta \leq 0\]

\[\Rightarrow \quad 2v(1-2\theta) \leq 1, \quad \text{for all } v\]

It means weighted scheme is stable for any choice of $\Delta t$ and $\Delta x$. It's said that the scheme is unconditionally stable.