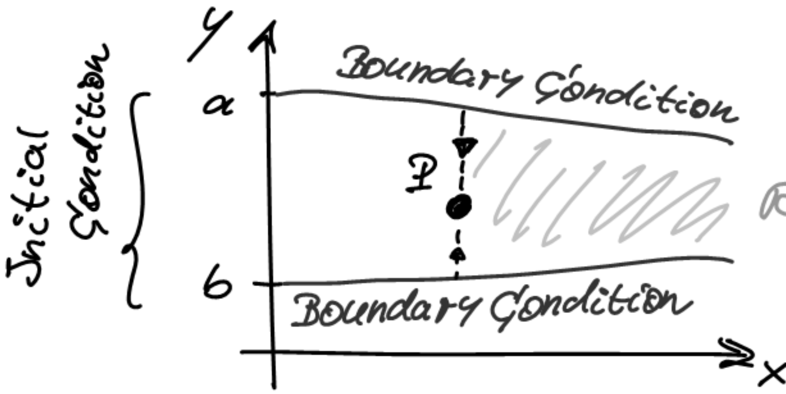
Integration of Linear Parabolic Equations

- Parabolic PDEs ⟶ 1 real characteristic



Infinite speed along characteristics

- Solution @ P influenced by Initial- and Boundary Conditions

- In this case, solution is marched in x-direction.
  $\Longrightarrow$ x is time-like.

- Parabolic equations represent diffusion phenomena such as heat conduction and viscous effects spreading away from a wall.

Example: "Heat Conduction"

$$\boxed{\frac{\partial T}{\partial t} = -\alpha \frac{\partial^2 u}{\partial x^2}}$$

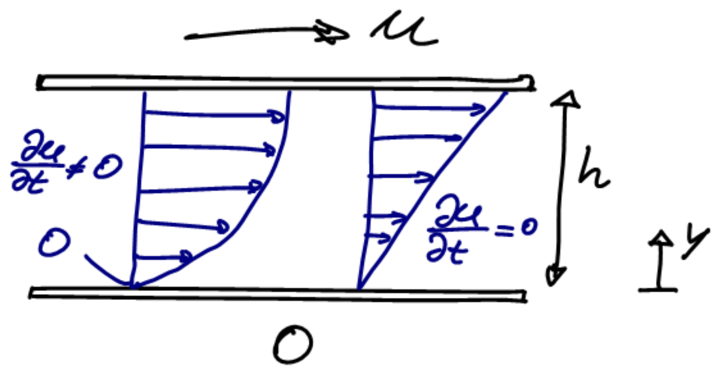
→ One-Dimensional heat conduction in a cooling fin.

Example: "Couette Flow"

$$\boxed{\frac{\partial u}{\partial t} = \nu \frac{\partial^2 u}{\partial y^2}} \quad ; \quad t \geq 0 \, , \; 0 \leq y \leq h \qquad (1)$$

→ Incompressible viscous flow between two plates

$\nu \hat{=}$ Kinematic Viscosity of the fluid



→ Initial condition:

$$\boxed{u(y,0) = 0} \quad ; \quad 0 \leq y \leq h \qquad (2)$$

→ Boundary conditions:

$$\boxed{\begin{cases} u(0,t) = 0 \\ u(h,t) = U \end{cases}} \quad ; \; t \geq 0 \qquad (3)$$

→ The exact steady-state ($\partial u/\partial t \to 0$)

solution is given by:

$$\boxed{u(y) = U \cdot \frac{y}{h}} \qquad (4)$$

Numerical Solution : Explicit Scheme

$$\boxed{\frac{u_j^{n+1} - u_j^n}{\Delta t} = \nu \, \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta y^2}} \qquad (5)$$

∘ Consistency & Accuracy:

Expand the truncation error TE

about ε_j^n

→ Use known expansions ...

$$(6) \quad \frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{\partial u_j^n}{\partial t} + \frac{\Delta t}{2}\frac{\partial^2 u_j^n}{\partial t^2} + \frac{\Delta t^2}{6}\frac{\partial^3 u_j^n}{\partial t^3} + \mathcal{O}(\Delta t^3)$$

$$(7) \quad \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta y^2} = \frac{\partial^2 u_j^n}{\partial y^2} + \frac{\Delta y^2}{4!}\frac{\partial^4 u_j^n}{\partial y^4} + \mathcal{O}(\Delta y^4)$$

→ (6), (7) in (5) ...

$$\varepsilon_j^n = \cancel{\frac{\partial u_j^n}{\partial t}} + \frac{\Delta t}{2}\frac{\partial^2 u_j^n}{\partial t^2} + \frac{\Delta t^2}{6}\frac{\partial^3 u_j^n}{\partial t^3} + \mathcal{O}(\Delta t^3)$$
$$- \delta\left(\cancel{\frac{\partial^2 u_j^n}{\partial y^2}} + \frac{\Delta y^2}{4!}\frac{\partial^4 u_j^n}{\partial y^4} + \mathcal{O}(\Delta y^4)\right)$$

$$\varepsilon_j^n = \mathcal{O}(\Delta t, \Delta y^2)$$

⟹ The scheme (5) is consistent and 1st order accurate in time and 2nd order accurate in space.

- <u>Stability:</u>

Complex Fourier mode: $\boxed{u_j^n = g^n e^{ij\beta}}$ (8)

→ Equation (5) in update form ...

$$\boxed{u_j^{n+1} = u_j^n + \frac{\nu \Delta t}{\Delta y^2}\left(u_{j+1}^n - 2u_j^n + u_{j-1}^n\right)} \quad (9)$$

and define $\boxed{\sigma = \frac{\nu \Delta t}{\Delta y^2}}$ to start the

V. Neumann analysis ...

$$g^{n+1} e^{ij\beta} = g^n e^{ij}$$

$$+ \sigma\left(g^n e^{i(j+1)\beta} - 2g^n e^{ij\beta} + g^n e^{i(j-1)\beta}\right)$$

Divide by $g^n e^{ij\beta}$

$$g = 1 + \sigma\left(e^{i\beta} - 2 + e^{i(-\beta)}\right)$$

$$= 1 + \sigma\left(\cos\beta + \cancel{i\sin\beta} - 2 + \cos(-\beta) + \cancel{i\sin(-\beta)}\right)$$

$$= 1 + 2\sigma(\cos\beta - 1)$$

$$= 1 - 2\sigma(1 - \cos\beta) \qquad \text{"real"}$$

$$\|g\|^2 \leq 1$$

$$[1-2\sigma(1-\cos\beta)]^2 \le 1$$

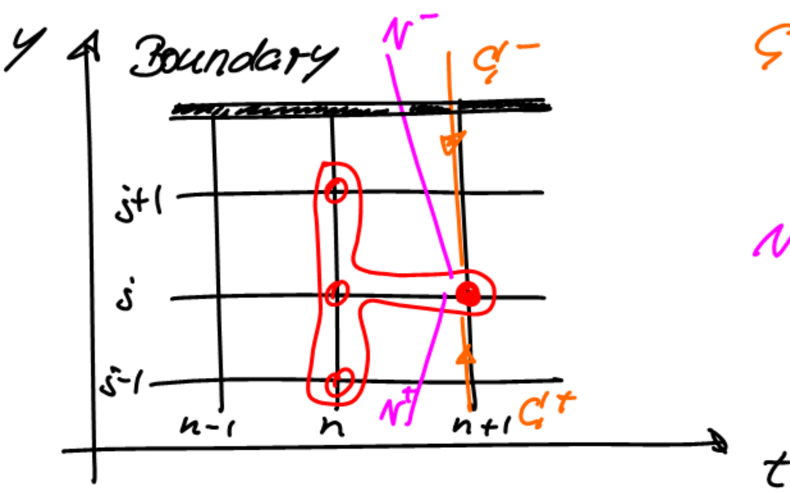
$$\cancel{1} - \underbrace{\cancel{4\sigma(1-\cos\beta)}}_{1} + \cancel{4}\sigma^{\cancel{2}}(1-\cos\beta)^{\cancel{2}} \le \cancel{1}$$

$$\sigma\underbrace{(1-\cos\beta)}_{\le 2} \le 1$$

$$\sigma \le \frac{1}{2} \quad \Longrightarrow \quad \boxed{\Delta t \le \frac{\Delta y^2}{2\nu}} \qquad (10)$$

→ Equation (10) describes a quite strong restriction on the time step $\Delta t \sim \Delta y^2$.
This can be computationally expensive!

→ Computational Molecule



$C \hat{=}$ Mathematical Characteristics w/ infinite slope

$N \hat{=}$ Numerical Characteristics

From (10) ...

$$\frac{\Delta y}{\Delta t} = \frac{2\nu}{\Delta y} = \mathcal{O}\left(\frac{1}{\Delta y}\right) \longrightarrow \infty \text{ for } \Delta y \to 0$$

- We know that a scheme is stable (for certain), if the numerical characteristics include the mathematical characteristics.
- What it actually means is that numerical characteristics have to include the region of dependence of the governing PDE.
- This can be achieved in the above example if the boundary is not too far away. Note though that the numerical characteristics do have a slope of $O(1/\Delta y) \rightarrow \infty$ that approaches the mathematical ones.

Numerical Solution: Implicit Scheme [Laasonen, 1949]

$$\boxed{\frac{u_j^{n+1} - u_j^{n}}{\Delta t} = \nu \, \frac{u_{j+1}^{n+1} - 2 u_j^{n+1} + u_{j-1}^{n+1}}{\Delta y^2}} \qquad (11)$$

→ We will see that the implicit scheme in (11) is unconditionally stable and therefore does <u>not</u> impose a large restriction on the time step Δt as in (10).

- <u>Consistency & Accuracy:</u>

Expand the truncation error TE about ε_j^{n+1}

⟹ Adjust indices and signs in (6), (7) to obtain ...

$$\varepsilon_j^{n+1} = \cancel{\frac{\partial u_j^{n+1}}{\partial t}} - \frac{\Delta t}{2}\frac{\partial^2 u_j^{n+1}}{\partial t^2} + \frac{\Delta t^2}{6}\frac{\partial^3 u_j^{n+1}}{\partial t^3} + \mathcal{O}(\Delta t^3)$$
$$- \nu\left(\cancel{\frac{\partial^2 u_j^{n+1}}{\partial y^2}} + \frac{\Delta y^2}{4!}\frac{\partial^4 u_j^{n+1}}{\partial y^4} + \mathcal{O}(\Delta y^4)\right)$$

$$\varepsilon_j^{n+1} = \mathcal{O}(\Delta t, \Delta y^2)$$

The scheme (11) is consistent and 1st order accurate in time and 2nd order accurate in space.

- Stability:

Equation (11) in update form ...

$$\boxed{u_j^{n+1} = u_j^n + r\left(u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}\right)} \qquad (12)$$

Use complex Fourier mode $u_j^n = g^n e^{ij\beta}$

$$g^{n+1} e^{ij\beta} = g^n e^{ij\beta} + r\left(g^{n+1} e^{i(j+1)\beta} - 2g^{n+1} e^{ij\beta} + g^{n+1} e^{i(j-1)\beta}\right)$$

Divide by $g^n e^{ij\beta}$

$$g = 1 + rg\left(e^{i\beta} - 2 + e^{i(-\beta)}\right)$$

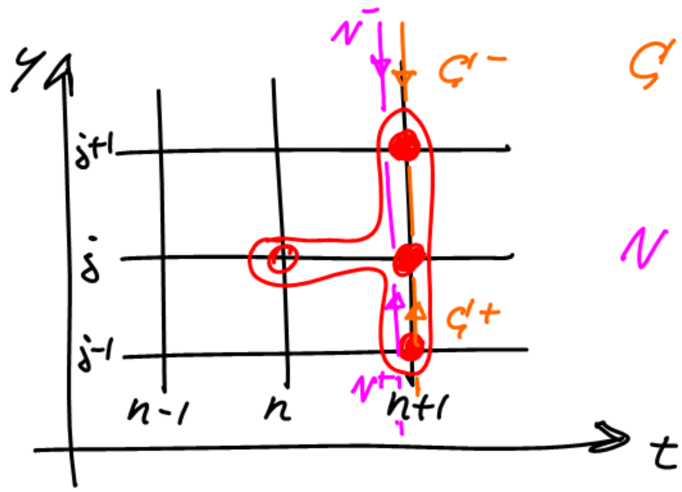
$$g = 1 + rg\left(\cos\beta + \cancel{i\sin\beta} - 2 + \cos(-\beta) + \cancel{i\sin(-\beta)}\right)$$

$$g = 1 - 2rg(1 - \cos\beta)$$

$$\Longrightarrow \boxed{g = \frac{1}{1 + 2r(1 - \cos\beta)}} \qquad (13)$$

It is apparent that $\|g\| \le 1$. Hence the implicit scheme (11) is unconditionally stable.

→ Computational Molecule



$C \hat{=}$ Mathematical Characteristics

$N \hat{=}$ Numerical Characteristics

Numerical Solution:

Combined Explicit-/Implicit Scheme

- One can construct a mixed scheme from equations (5) and (11) as

$$\boxed{\frac{u_j^{n+1} - u_j^{n}}{\Delta t} = (1-\Theta)\cdot\nu\,\frac{u_{j+1}^{n} - 2u_j^{n} + u_{j-1}^{n}}{\Delta y^2} + \Theta\cdot\nu\,\frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{\Delta y^2}} \qquad (14)$$

where $0 \le \Theta \le 1$ is a weighting parameter.

- The simple explicit scheme corresponds to $\Theta = 0$.

- The simple implicit scheme corresponds to $\Theta = 1$.

- In general, the combined method (14) is 1st order accurate in time and 2nd order accurate in space.

- However, there are some special cases:

a.) $\theta = \frac{1}{2} \Longrightarrow \boxed{\varepsilon_j^{n+\frac{1}{2}} = \mathcal{O}(\Delta t^2, \Delta y^2)}$

"Crank-Nicolson" Method (Semi-Implicit Method)

b.) $\theta = \frac{1}{2} - \frac{\Delta y^2}{12\nu\Delta t} \Longrightarrow \boxed{\varepsilon_j^{n} = \mathcal{O}(\Delta t^2, \Delta y^4)}$

c.) $\theta = \frac{1}{2} - \frac{\Delta y^2}{12\nu\Delta t}$ and $\frac{\Delta y^2}{\nu\Delta t} = \sqrt{20}$

$$\Longrightarrow \boxed{\varepsilon_j^{n} = \mathcal{O}(\Delta t^2, \Delta y^6)}$$

- The main benefit of the combined schemes lies in their 2nd order accuracy in time.

- Additional spatial accuracy in b.) and c.)

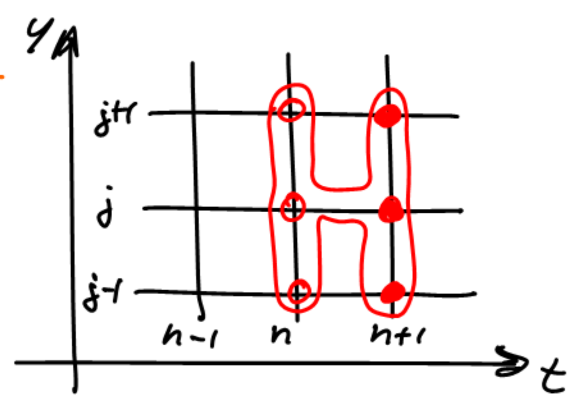
comes at the expense of a more restricted stability criterion.

- It can be shown that the combined schemes are unconditionally stable for $\boxed{\frac{1}{2} \leq \theta \leq 1}$ when (14) is mostly implicit.

  However, only the "Crank-Nicolson" scheme w/ $\theta = \frac{1}{2}$ retains 2nd order accuracy in time.

- For $\boxed{0 \leq \theta \leq \frac{1}{2}}$, the combined scheme (14) is stable for $0 \leq \sigma \leq \frac{1}{2-4\theta}$ which means that $\Delta t \sim \Delta y^2$ for stability. Note that the stability criterion for the explicit scheme (10) is recovered as $\sigma \leq \frac{1}{2}$ for $\theta = 0$!

- Computational Molecule



Numerical Implementation of "Implicit Schemes"

- The trouble with implicit schemes is that a computational molecule has more than one unknown. This is also true for mixed explicit-/implicit schemes such as (14).

- How to solve the system?

Example: Implicit scheme (11)

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \nu \frac{u_{j+1}^{n+1} - 2u_j^n + u_{j-1}^{n+1}}{\Delta y^2}$$

Rearrange as ...

$$\boxed{\frac{\nu}{\Delta y^2} u_{j-1}^{n+1} - \left(\frac{1}{\Delta t} + \frac{2\nu}{\Delta y^2}\right) u_j^{n+1} + \frac{\nu}{\Delta y^2} u_{j+1}^{n+1} = -\frac{1}{\Delta t} u_j^n} \tag{11a}$$

L.H.S. $\hat{=}$ Unknowns at new time step $n+1$

R.H.S. $\hat{=}$ Known quantities from previous time step n.

- Equation (11a) can be written in the general form

$$\boxed{p_j\, u_{j-1}^{n+1} + q_j\, u_j^{n+1} + r_j\, u_{j+1}^{n+1} = s_j} \quad (15)$$

- Equation (15) is valid for <u>all</u> implicit-like schemes. We can also write it in matrix form as:

$$\boxed{\begin{bmatrix} q_1 & r_1 & & & & & \\ p_2 & q_2 & r_2 & & & & \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ & & p_j & q_j & r_j & & \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ & & & & p_{jx-1} & q_{jx-1} & r_{jx-1} \\ & & & & & p_{jx} & q_{jx} \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_j \\ \vdots \\ x_{jx-1} \\ x_{jx} \end{bmatrix} = \begin{bmatrix} s_1 \\ s_2 \\ \vdots \\ s_j \\ \vdots \\ s_{jx-1} \\ s_{jx} \end{bmatrix}} \quad (16)$$

where $u_j^{n+1} = x_j$.

- The matrix in equation (16) is <u>tridiagonal</u>.

It can be solved with the well known "Thomas Algorithm". The Thomas algorithm (or double sweep method) is a special case of the Gauss elimination algorithm.

- In the direct sweep, the lower diagonal with elements p_j is eliminated to obtain an upper triangular system. Let us start @ $j=1$ and normalize the diagonal term (for $q_1 \neq 0$) as

$$\boxed{x_1 + \hat{r}_1 x_2 = \hat{s}_1} \quad ; \quad \hat{r}_1 = \frac{r_1}{q_1} \; ; \; \hat{s}_1 = \frac{s_1}{q_1} \qquad (17)$$

- Now we write (in a general sense) the $(i-1)^{st}$ and $(i)^{th}$ equation as

$$\left.\begin{aligned} x_{j-1} + \hat{r}_{j-1} x_j &= \hat{s}_{j-1} \quad \Big| * (-p_j) \\ p_j x_{j-1} + q_j x_j + r_j x_{j+1} &= s_j \end{aligned}\right\} +$$

$$0 \quad (q_j - p_j \hat{r}_{j-1}) x_j + r_j x_{j+1} = s_j - p_j \hat{s}_{j-1}$$

Or, if $q_j - p_j \hat{r}_{j-1} \neq 0$

$$\boxed{x_j + \hat{r}_j \, x_{j+1} = \hat{s}_j} \qquad j = 1, \dots, jx \qquad (18)$$

$$\hat{r}_j = \frac{r_j}{q_j - p_j \, \hat{r}_{j-1}} \quad ; \quad \hat{s}_j = \frac{s_j - p_j \, \hat{s}_{j-1}}{q_j - p_j \, \hat{r}_{j-1}}$$

- Note that equation (18) is a recurrence formula. Also be aware that (18) is not strictly valid for $j=1$ and $j=jx$. However, the associated x_1 and x_{jx} are oftentimes given through Dirichlet Boundary Conditions.
- Altenatively, the boundaries can be accounted for by setting

$$\boxed{\begin{array}{l} p_1 = 0 \quad ; \quad \hat{r}_1 = 0 \, ; \quad \hat{s}_0 = 0 \\ r_{jx} = 0 \end{array}} \qquad (19)$$

- At the end of the direct sweep, the system (16) has been transformed to an upper triangular matrix with two diagonals

$$
\begin{bmatrix}
1 & \hat{r}_1 & & & & \\
 & 1 & \hat{r}_2 & & & \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
 & & & 1 & \hat{r}_j & \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
 & & & & 1 & \hat{r}_{jx-1} \\
 & & & & & 1
\end{bmatrix}
\cdot
\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_j \\ \vdots \\ x_{jx-1} \\ x_{jx} \end{bmatrix}
=
\begin{bmatrix} \hat{s}_1 \\ \hat{s}_2 \\ \vdots \\ \hat{s}_j \\ \vdots \\ \hat{s}_{jx-1} \\ \hat{s}_{jx} \end{bmatrix}
\tag{20}
$$

- During the inverse sweep, the upper diagonal with entries $\hat{r}_j$ will be eliminated starting from the bottom as

$$x_{jx} = \hat{s}_{jx}$$

$$x_{jx-1} = \hat{s}_{jx-1} - \hat{r}_{jx-1}\, x_{jx}$$

$$\vdots$$

$$\boxed{x_j = \hat{s}_j - \hat{r}_j \cdot x_{j+1}} \qquad j = jx,\, jx-1,\, \cdots,\, 1 \tag{21}$$

- Equation (21) thus defines the solution x_j at the current marching step.

Remark:

The Thomas Algorithm is stable and insensitive to round-off errors, if the tridiagonal matrix is diagonally dominant!

$$\boxed{|q_j| \geq |p_j| + |r_j|} \qquad (22)$$