VII - Solution of partial differential equations

1 - Introduction

1.1 - Types of PDE's

Simplest case: Quasilinear PDEs

$$A \frac{\partial^2 \phi}{\partial x_1^2} + B \frac{\partial^2 \phi}{\partial x_1 \partial x_2} + C \frac{\partial^2 \phi}{\partial x_2^2} = f\left(x_1, x_2, \phi, \frac{\partial \phi}{\partial x_1}, \frac{\partial \phi}{\partial x_2}\right)$$

(A, B, C const.)

(*) Elliptic PDE's : $B^2 - 4AC < 0$

Example: $$\frac{\partial^2 U(x,y)}{\partial x^2} + \frac{\partial^2 U(x,y)}{\partial y^2} = f(x,y)$$

(Poisson equation)

(*) Parabolic PDE's : $B^2 - 4AC = 0$

Example: $$\frac{\partial U}{\partial t} = D \frac{\partial^2 U}{\partial x^2}$$

(Diffusion equation)

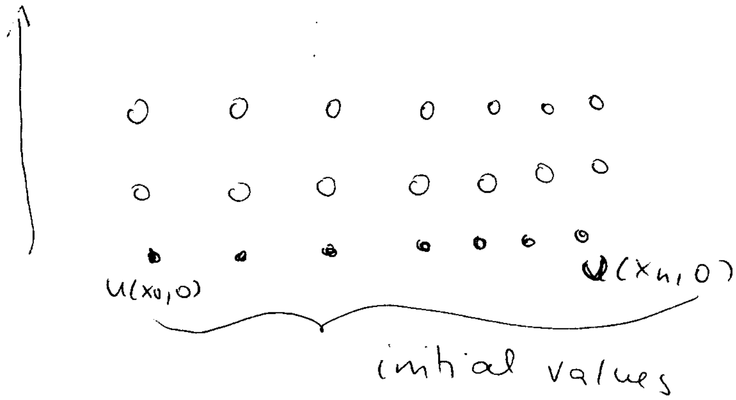
(*) Hiperbolic PDE's : $B^2 - 4AC < 0$

Example: $$\frac{\partial^2 U}{\partial t^2} = v^2 \frac{\partial^2 U}{\partial x^2}$$

(wave equation)

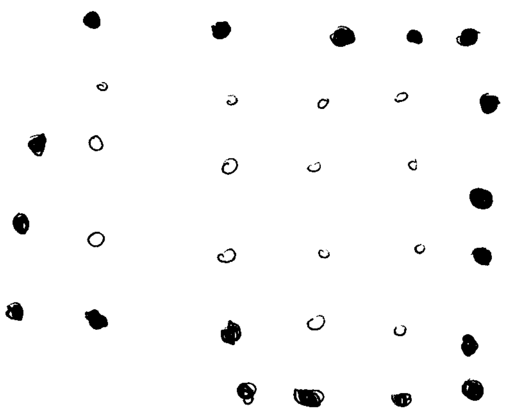
1.2 - Initial value problem (time evolution probl.)

$U(x,0)$ given and we wish to compute $U(x,t)$ (propagate forward in time)



1.3 - Boundary value problem (static solution probl.)

$U(x,y)$ is specified around the edge of a grid and we wish to find $u(x,y)$ everywhere

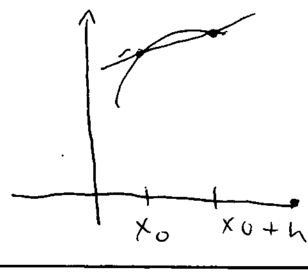


1.4 - Numerical differentiation

1.4.1 - One-dimensional case

1D : The derivative of a function at $x = x_0$ is

$$f'(x) = \lim_{h \to 0} \frac{f(x_0+h) - f(x_0)}{h}$$



Foward difference formula (of order $O(h)$)

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

On the other hand,

$$f'(x) \simeq \frac{f(x) - f(x-h)}{h} \quad \text{(Backward difference formula).}$$

(*) Please note: both formulae can be directly obtained from the Taylor expansions

$$f(x+h) = f(x) + f'(x)h + \frac{f^{(2)}(\cancel{x})h^2}{2!} + \dots \qquad (*)$$

$$\Rightarrow f'(x) = \frac{f(x+h) - f(x)}{h} - \underbrace{\frac{f^{(2)}(\cancel{x})h}{2!} + \dots}_{\text{error: } O\left(\frac{h}{2}\right)}$$

$$f(x-h) = f(x) - f'(x)h + \frac{f^{(2)}(x)h^2}{2} - \dots \qquad (**)$$

$$\Rightarrow f'(x) = \frac{f(x) - f(x-h)}{h} - \underbrace{\frac{f^{(2)}h}{2} + \dots}_{\text{error: } O\left(\frac{h}{2}\right)}$$

Problems: loss of significant digits for small h (one is subtracting nearly equal quantities)

Central difference formula (of $O(h^2)$)

$$(*) - (**) \Rightarrow \quad f(x+h) - f(x-h) = 2f'(x)h + \underbrace{\frac{O(h^3)}{3!}}_{\text{error}}$$

$$\Rightarrow f'(x) = \frac{f(x+h) - f(x-h)}{2h} + O\left(\frac{h^2}{6}\right)$$

more accurate than the previous ones!

(*) Please note: In principle one can derive approximations for derivatives with higher accuracy using either Taylor polynomials in a larger number of points, or Lagrange polynomials of higher order (alternatively, the forward and the central difference formulae can be obtained by differentiating $P_1(x)$ and $P_2(x)$)

1.4.2 - Partial differentiation

$$\frac{\partial(u(x,y))}{\partial x} = \frac{u(x+\Delta x, y) - u(x,y)}{\Delta x} \quad \text{(forward difference)}$$

or

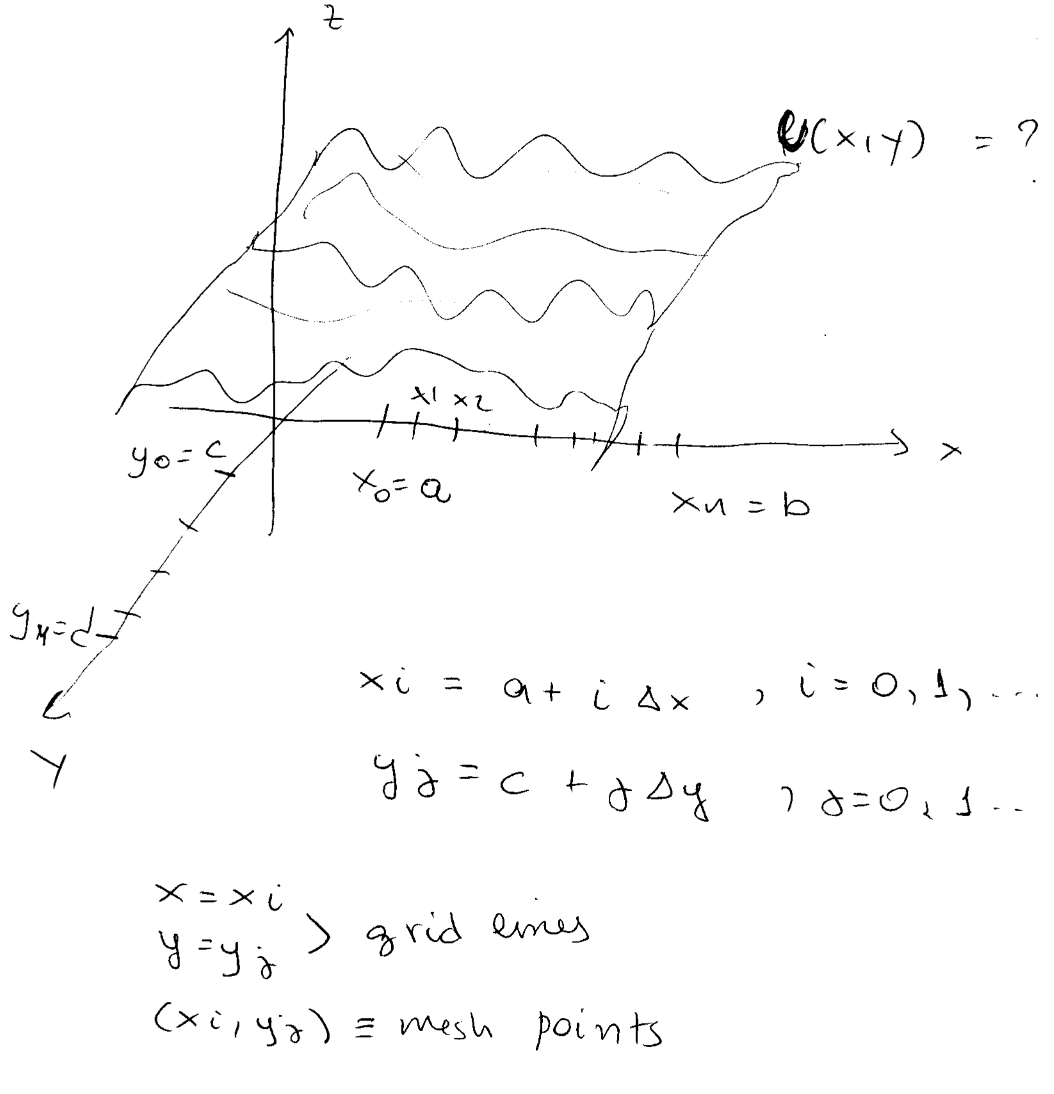
$$\frac{\partial(u(x,y))}{\partial x} = \frac{u(x,y) - u(x-\Delta x, y)}{\Delta x} \quad \text{(backward difference)}$$

$$\frac{\partial u(x,y)}{\partial x} = \frac{u(x+\Delta x, y) - u(x-\Delta x, y)}{2\Delta x} \quad \text{(central difference)}$$

2 - Boundary Value Problems (in elliptic PDE's)

$$\frac{\partial^2 u}{\partial x^2}(x,y) + \frac{\partial^2 u(x,y)}{\partial y^2} = f(x,y) \quad , \quad a<x<b$$
$$c<y<d$$

Boundary condition: $u(x,y) = g(x,y)$ for $(x,y) \in \underbrace{S}_{\text{boundary}}$



$x_i = a + i\Delta x \quad , \; i = 0, 1, \ldots, n$

$y_j = c + j\Delta y \quad , \; j = 0, 1 \ldots$

$\left.\begin{array}{l} x = x_i \\ y = y_j \end{array}\right\}$ grid lines

$(x_i, y_j) \equiv$ mesh points

Centered difference formulae (second derivatives)

$$\frac{\partial^2 u(x_i,y_j)}{\partial x^2} \simeq \frac{u(x_{i+1},y_j) - 2u(x_i,y_j) + u(x_{i-1},y_j)}{(\Delta x)^2}$$

(Check: consider the taylor expansions of $u(x, y_j)$ around x_i, $x_{i+1} = x+\Delta x$ and $x_{i-1} = x-\Delta x$)

$$\frac{\partial^2 u}{\partial y^2}(x_i, y_j) = \frac{u(x_i, y_{j+1}) - 2u(x_i, y_j) + u(x_i, y_{j-1})}{(\Delta y)^2}$$

Hence :

$$\frac{u(x_{i+1}, y_j) - 2u(x_i, y_j) + u(x_{i-1}, y_j)}{(\Delta x)^2} +$$

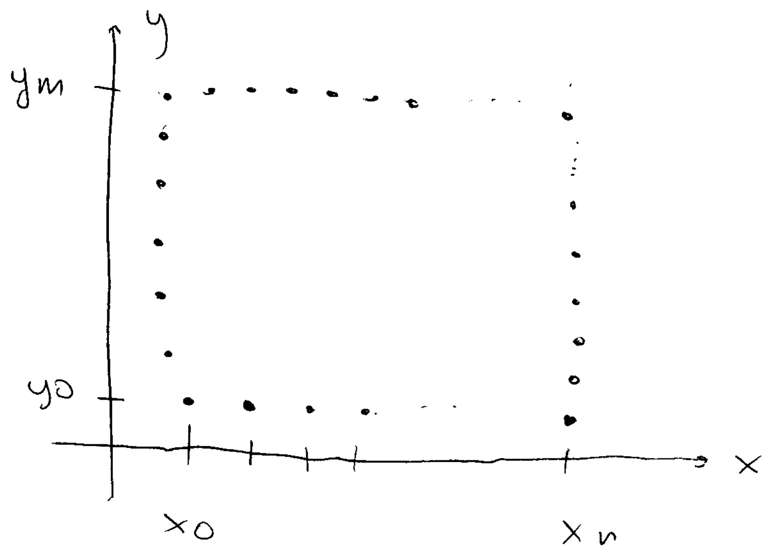
$$+ \frac{u(x_i, y_{j+1}) - 2u(x_i, y_j) + u(x_i, y_{j-1})}{(\Delta y)^2} = f(x_i, y_j)$$

for $i = 1, 2, \dots, n-1$ and $j = 1, 2, m-1$

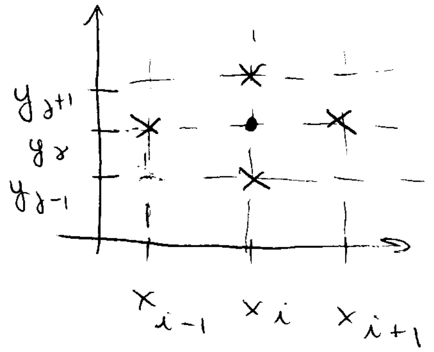
Boundary conditions :

$u(x_0, y_j) = g(x_0, y_j)$ and $u(x_n, y_j) = g(x_n, y_j)$
$(j = 0, 1, \dots, m)$

$u(x_i, y_0) = g(x_i, y_0)$ and $u(x_i, y_m) = g(x_i, y_m)$
$(i = 1, 2, \dots, n-1)$.



This involves approximations in a "star shaped" region in the grid centered at (x_γ, y_γ)



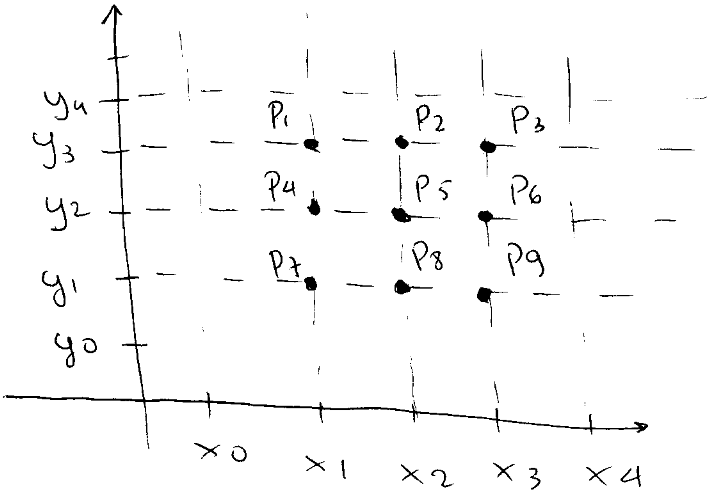
Redefining

$P_l = (x_i, y_\gamma)$, $w_l = u(i, \gamma)$

with $l = i + (m-1-\gamma)(n-1)$ for $i = 1, 2, \dots, n-1$

$\gamma = 1, 2, \dots, m-1$

(interior grid points)



Example : Determine the system of four equations in the four unknowns w_1, w_2, w_3, w_4 for computing approximations for

$$\frac{\partial^2 u(x,y)}{\partial x^2} + \frac{\partial^2 u(x,y)}{\partial y^2} = 0 \quad \text{for} \quad \begin{array}{l} 0 \le x \le 3 \\ 0 \le y \le 3 \end{array}$$

with the boundary conditions

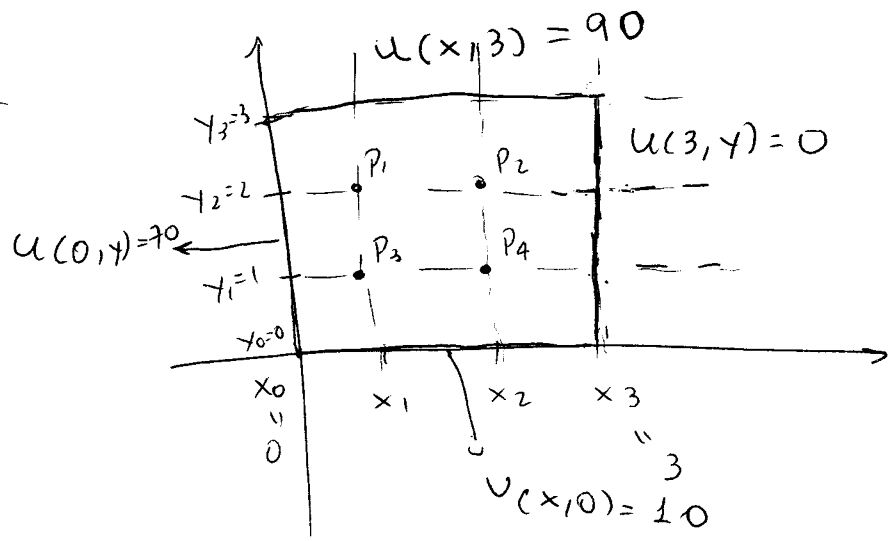
$u(x,0) = 10$ and $u(x,3) = 90$ for $0 < x < 3$

$u(0,y) = 70$ and $u(3,y) = 0$ for $0 < y < 3$

$$\Delta x = \frac{3-0}{3} = 1$$

$$\Delta y = 1$$

MESH



Laplace equation:

$$-4u(x_i, y_j) + u(x_{i+1}, y_j) + u(x_{i-1}, y_j) + u(x_i, y_{j+1}) + u(x_i, y_{j-1}) = 0$$

- $P_1 = (x_1, y_2)$; $w_1 = u(x_1, y_2)$

$$-4u(x_1, y_2) + u(x_2, y_2) + u(x_0, y_2) + u(x_1, y_3) + u(x_1, y_1) =$$

$$-4w_1 + w_2 + 70 + 90 + w_3 = 0$$

- $P_2 = (x_2, y_2)$, $w_2 = u(x_2, y_2)$

$$-4w_2 + \overbrace{u(x_3, y_2)}^{=0} + \overbrace{u(x_1, y_2)}^{w_1} + \overbrace{u(x_2, y_3)}^{=90} + w_4 = 0$$

- $P_3 = (x_1, y_1) \qquad w_3 = u(x_1, y_1)$

$$-4w_3 + \underbrace{u(x_2,y_1)}_{w_4} + \underbrace{u(x_0,y_1)}_{70} + \underbrace{u(x_1,y_2)}_{w_1} + \underbrace{u(x_1,y_0)}_{=10} = 0$$

- $P_4 : (x_2, y_1)$:

$$-4w_4 + \underbrace{u(x_3,y_1)}_{=0} + \underbrace{u(x_1,y_1)}_{w_3} + \underbrace{u(x_2,y_2)}_{w_2} + \overbrace{u(x_2,y_0)}^{10} = 0$$

$$\begin{aligned}
-4w_1 &+ w_2 + w_3 + 0 = -160 \\
w_1 &- 4w_2 \quad + w_4 = -90 \\
w_1 &\quad 0 \quad -4w_3 \quad w_4 = -80 \\
0 &\quad w_2 \quad w_3 \quad -4w_4 = -10
\end{aligned}$$

Matrix of the system.

$$A = \begin{pmatrix} -4 & 1 & 1 & 0 \\ 1 & -4 & 0 & 1 \\ 1 & 0 & -4 & 1 \\ 0 & 1 & 1 & -4 \end{pmatrix}$$

"Band-diagonal matrix" (can be solved by a generalization of the Crout algorithm)

→ Can also be solved by standard methods (Gaussian elimination, etc.)

3 - Diffusive initial value problems

Diffusion equation:

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(D \frac{\partial u}{\partial x} \right)$$

Speific case: D const.

$$\frac{\partial U}{\partial t} = D \frac{\partial^2 U}{\partial x^2}$$

Initial condition : $U(x,0) = f(x)$, $0 \leq x \leq \ell$

Boundary condition: $u(0,t) = u(\ell,t) = 0$

(we are putting the system in a "box" of length ℓ)

Steps in x : $\Delta x = \frac{\ell}{m}$ → size of "box". m → integer number

Steps in t : $\Delta t = \frac{t_{MAX}}{n}$ → maximum time. n → # of timesteps (integer)

$x_i = i * \Delta x \quad i = 0, 1, \dots, m$

$t_j = j * \Delta t \quad j = 0, 1, \dots, n$

We take $\frac{\partial^2 U(x_i, t_j)}{\partial x^2} \simeq \frac{U(x_i + \Delta x, t_j) - 2U(x_i, t_j) + U(x_i - \Delta x, t_j)}{(\Delta x)^2}$

Temporal derivatives:

i) Forward - difference method ("explicit" method)

$$\frac{\partial u}{\partial t}(x_i, t_j) = \frac{u(x_i, t_j + \Delta t) - u(x_i, t_j)}{\Delta t}$$

$$\frac{u(x_i, t_\gamma + \Delta t) - u(x_i, t_\gamma)}{\Delta t} = D\left[\frac{u(x_i + \Delta x, t_\gamma) - 2u(x_i, t_\gamma) + u(x_i - \Delta x, t_\gamma)}{(\Delta x)^2}\right]$$

$$u(x_i, t_\gamma + \Delta t) - u(x_i, t_\gamma) = \frac{D\Delta t}{(\Delta x)^2}\left[u(x_i + \Delta x, t_\gamma) - 2u(x_i, t_\gamma) + u(x_i - \Delta x, t_\gamma)\right]$$

$$u(x_i, t_\gamma + \Delta t) - u(x_i, t_\gamma) = \frac{D\Delta t}{(\Delta x)^2} u(x_i + \Delta x, t_\gamma) - \frac{2u(x_i, t_\gamma) D\Delta t}{(\Delta x)^2} +$$

$$+ \frac{D\Delta t}{(\Delta x)^2} u(x_i - \Delta x, t_\gamma)$$

$$u(x_i, \underbrace{t_\gamma + \Delta t}_{t_{\gamma+1}}) = \frac{D\Delta t}{(\Delta x)^2} u(\underbrace{x_i + \Delta x}_{x_{i+1}}, t_\gamma) + \left[1 - \frac{2D\Delta t}{(\Delta x)^2}\right] u(x_i, t_\gamma)$$

$$+ \frac{D\Delta t}{(\Delta x)^2} u(\underbrace{x_i - \Delta x}_{x_{i-1}}, t_\gamma)$$

($\gamma = 0, 1, \ldots, n$ (one can start from $\gamma = 0$ and find all $u(x,t)$)

The RHS can be written as:

$A \times \vec{\omega}$

$$A = \begin{bmatrix} \left[1 - \frac{D\Delta t}{(\Delta x)^2}\right] & \frac{D\Delta t}{(\Delta x)^2} & 0 & \cdots & 0 \\ \frac{D\Delta t}{(\Delta x)^2} & \ddots & \ddots & & 0 \\ 0 & \ddots & \ddots & \ddots & \\ \vdots & & & & \\ 0 & \cdots & & & 0 \end{bmatrix} \qquad \vec{\omega} = \begin{bmatrix} u(x_0, t_\gamma) \\ \vdots \\ u(x_n, t_\gamma) \end{bmatrix}$$

↓

tridiagonal matrix

ii) Backward difference method ("implicit method")

$$\frac{\partial u(x_i,t_j)}{\partial t} \simeq \frac{u(x_i,t_j)-u(x_i,\overbrace{t_{j-1}}^{=t_j-\Delta t})}{\Delta t}$$

Diffusion equation:

$$\frac{u(x_i,t_j)-u(x_i,t_j-\Delta t)}{\Delta t} = \frac{D}{(\Delta x)^2}\Big[u(x_i+\Delta x,t_j)-2u(x_i,t_j)+$$

$$+u(x_i-\Delta x,t_j)\Big]$$

Rearranging,

$$-\frac{D(\Delta t)}{(\Delta x)^2}u(x_i+\Delta x,t_j)+\left[1+\frac{2D(\Delta t)}{(\Delta x)^2}\right]u(x_i,t_j)-\frac{D(\Delta t)}{(\Delta x^2)}$$

$$u(x_i-\Delta x,t_j)\Big] = u(x_i,t_j-\Delta t)\Big]$$

- calling $a = \frac{-D(\Delta t)}{(\Delta x)^2}$; $b = 1+\frac{2D(\Delta t)}{(\Delta x)^2}$

$$u(x_i+\Delta x,t_j) = w_{i+1,j}$$
$$u(x_i,t_j) = w_{i,j}$$
$$u(x_i-\Delta x,t_j) = w_{i-1,j}$$
$$u(x_i,t_j-\Delta t) = w_{i,j-1}$$

We have

$$\boxed{a\,w_{i+1,j}+b\,w_{i,j}+a\cdot w_{i-1,j} = w_{i,j-1} \quad \text{for } j=1,\dots,m;\ i=1,\dots,n-1}$$

This yields the tridiagonal system

$$\begin{pmatrix} 1+\frac{2D(\Delta t)}{(\Delta x)^2} & -\frac{D(\Delta t)}{(\Delta x)^2} & 0 & \cdots & 0 \\ -\frac{D(\Delta t)}{(\Delta x)^2} & \ddots & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & 1+\frac{2D(\Delta t)}{(\Delta x)^2} \\ 0 & \cdots & 0 & -\frac{D(\Delta t)}{(\Delta x)^2} & \end{pmatrix} \begin{bmatrix} w_{1,j} \\ w_{2,j} \\ \vdots \\ w_{m-1,j} \end{bmatrix} = \begin{bmatrix} w_{1,j-1} \\ w_{2,j-1} \\ \vdots \\ w_{m-1,j-1} \end{bmatrix}$$

which has to be solved at each timestep

(+) Note that the matrix is strictly diagonally dominant so one expects this scheme to be

iii) Crank-Nicolson ("semi-implicit") method

we average (a) the Forward difference method at the j-th step at t

$$\frac{w_{i,j+1}-w_{ij}}{\Delta t} - \frac{D(w_{i+1,j}-2w_{i,j}+w_{i-1,j})}{(\Delta x)^2} = 0$$

and

(b) The Backward-difference method at the $(j+1)$st step in t

$$\frac{w_{i,j+1}-w_{i,j}}{\Delta t} - \frac{D}{(\Delta x)^2}\left[w_{i+1,j+1} - 2w_{i,j+1} + w_{i-1,j+1}\right] = 0$$

$$\frac{(a)+(b)}{2} \Rightarrow \frac{w_{i,j+1}-w_{ij}}{\Delta t} - \frac{D}{2(\Delta x)^2}\left[w_{i+1,j} - 2w_{ij} + w_{i-1,j} + \right.$$

$$w_{i+1,j+1} - 2w_{i,j+1} + w_{i-1,j+1}\Big] = 0$$

Multiplying by Δt and rearranging,

$$-\frac{D\Delta t}{2(\Delta x)^2} w_{i-1,j+1} + \left[1 + \frac{D\Delta t}{(\Delta x)^2}\right] w_{i,j+1} - \frac{D\Delta t}{2(\Delta x)^2} w_{i+1,j+1} =$$

$$= \frac{D\Delta t}{2(\Delta x)^2} w_{i+1,j} + \left[1 - \frac{D\Delta t}{(\Delta x)^2}\right] w_{ij} + \frac{D\Delta t}{2(\Delta x)^2} w_{i-1,j}$$

$\therefore$ One ends up with $A\,\vec{\omega}^{(j+1)} = B\,\vec{\omega}^{(j)}$ $\quad j = 0, 1, 2 \ldots$

$$\begin{bmatrix} 1 + \frac{\Delta t}{(\Delta x)^2} & -\frac{D\Delta t}{2(\Delta x)^2} & 0 & \cdots & 0 \\ -\frac{D\Delta t}{2(\Delta x)^2} & \ddots & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & -\frac{D\Delta t}{2(\Delta x)^2} \\ 0 & \cdots & 0 & -\frac{D\Delta t}{2(\Delta x)^2} & 1 + \frac{\Delta t}{(\Delta x)^2} \end{bmatrix} \begin{bmatrix} \omega_{1,j+1} \\ \omega_{2,j+1} \\ \vdots \\ \vdots \\ \omega_{n-1,j+1} \end{bmatrix} =$$

$$= \begin{bmatrix} 1 - \frac{D\Delta t}{(\Delta x)^2} & \frac{D\Delta t}{2(\Delta x)^2} & 0 & \cdots & 0 \\ \frac{D\Delta t}{2(\Delta x)^2} & \ddots & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \frac{D\Delta t}{2(\Delta x)^2} \\ 0 & \cdots & 0 & \frac{D\Delta t}{2(\Delta x)^2} & 1 - \frac{D\Delta t}{(\Delta x)^2} \end{bmatrix} \begin{bmatrix} \omega_{1,j} \\ \omega_{2,j} \\ \vdots \\ \vdots \\ \omega_{n-1,j} \end{bmatrix}$$

A is strictly diagonally dominant $\therefore$ the scheme is stable!