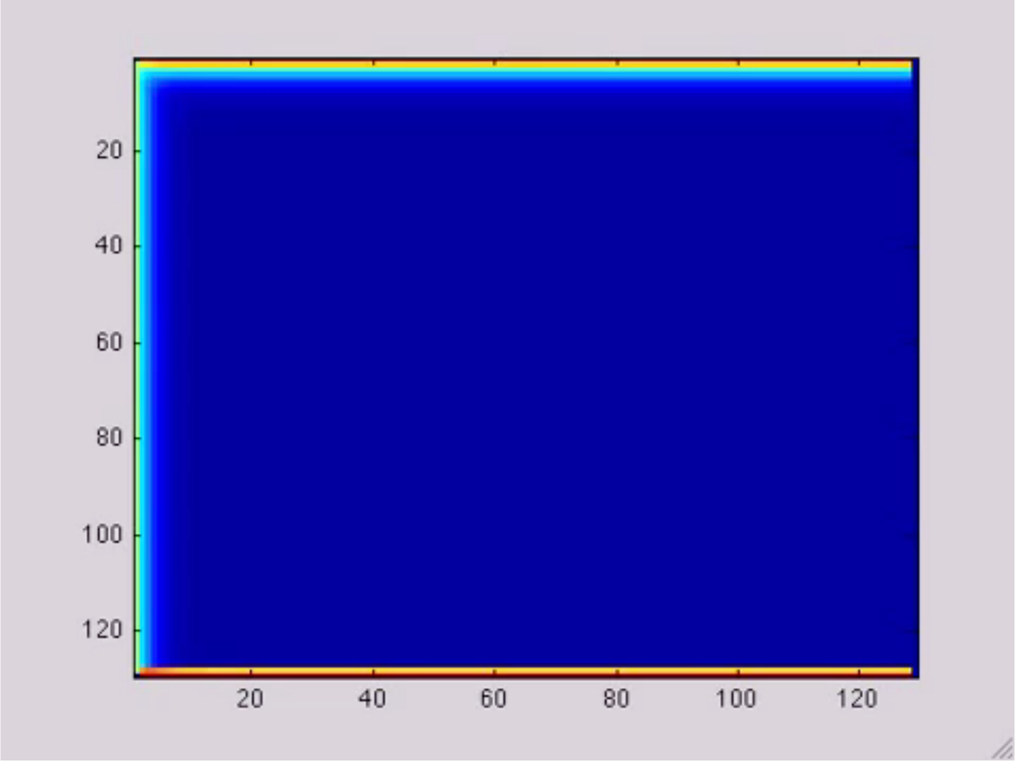
Numerical Methods for Partial Differential Equations

Lecture 4: Parabolic PDE

Parabolic PDE

- Parabolic PDE: initial value problem. Boundary conditions must be specified at all times.
- In physics, they typically describe *dissipative* processes (e.g. viscosity, conduction, resistivity, etc..).
- Examples: Heat equation $\frac{\partial T}{\partial t} = \kappa \nabla^2 T$



- Example: Schrodinger Equation

$$i\hbar \frac{\partial}{\partial t}\Psi(\mathbf{r},t) = \left[\frac{-\hbar^2}{2\mu}\nabla^2 + V(\mathbf{r},t)\right]\Psi(\mathbf{r},t)$$

Parabolic PDE in 1D

Explicit and Implicit Finite Difference Methods

Parabolic PDE

- We consider the prototype diffusion equation

$$\frac{\partial \varphi}{\partial t} = \nabla \cdot (D \nabla \varphi) + S$$

where D = diffusion coefficient, S = source term.

- This is also known as the *Heat Equation*.

- Note that $\varphi=\varphi(x,y,z,t)$ is now functions of *four* independent variables.

- Given the field $\varphi(x,y,z,0)$ for t=0 we seek solution for t>0 given some boundary conditions (e.g. heat flux specified on the surface boundary)

Diffusion Equation in 1D

- For 1D problem with constant diffusion D, we have: $$\frac{\partial \varphi}{\partial t} = D\frac{\partial^2 \varphi}{\partial x^2} + S(x,t)$$
- Where $\varphi=\varphi(x,t)$ is a function of space and time while
  - x is the space variable, $0 \le x \le L$;
  - t is the time variable, $t \ge 0$.
- To solve the PDE we must first specify an initial condition f(x) so that $\varphi(x,0) = f(x)$
- And a boundary condition: $\varphi(0,t) = g_0(t)\,, \qquad \varphi(L,t) = g_L(t)\,,$

Exact Solution

- For the heat equation subject to the following conditions

$$\frac{\partial \varphi}{\partial t} = D\frac{\partial^2 \varphi}{\partial x^2}, \qquad \begin{cases} \varphi(x,0) = f(x) & \text{(IC)} \\ \varphi(0,t) = \varphi(L,t) = 0 & \text{(BC)} \end{cases}$$

an exact solution in terms of Fourier series can be found:

$$\varphi(x,t) = \sum_{k=1}^{\infty} A_k \sin\left(\frac{k\pi x}{L}\right) e^{-\frac{k^2\pi^2 Dt}{L^2}} \quad \text{where} \quad A_k = \frac{2}{L}\int_0^L f(x)\sin\left(\frac{k\pi x}{L}\right) dx$$

- Note that high-order harmonics (k large) are damped faster than lower order ones.

Numerical Discretization

- For 1D problem with constant diffusion D,

$$\frac{\partial \varphi}{\partial t} = D\frac{\partial^2 \varphi}{\partial x^2} + S(x,t)$$

- Discretization is performed in both space *and* time.
- Spatial derivatives: finite differences on a uniform lattice of $N+1$ points with uniform spacing Δx.
- Time derivative by a simple first-order method:

$$\frac{\varphi_i^{n+1} - \varphi_i^n}{\Delta t} = D\frac{\varphi_{i+1}^n - 2\varphi_i^n + \varphi_{i-1}^n}{\Delta x^2} + S_i^n$$

- `i = ` spatial index, `n = ` time index

Diffusion Equation in 1D

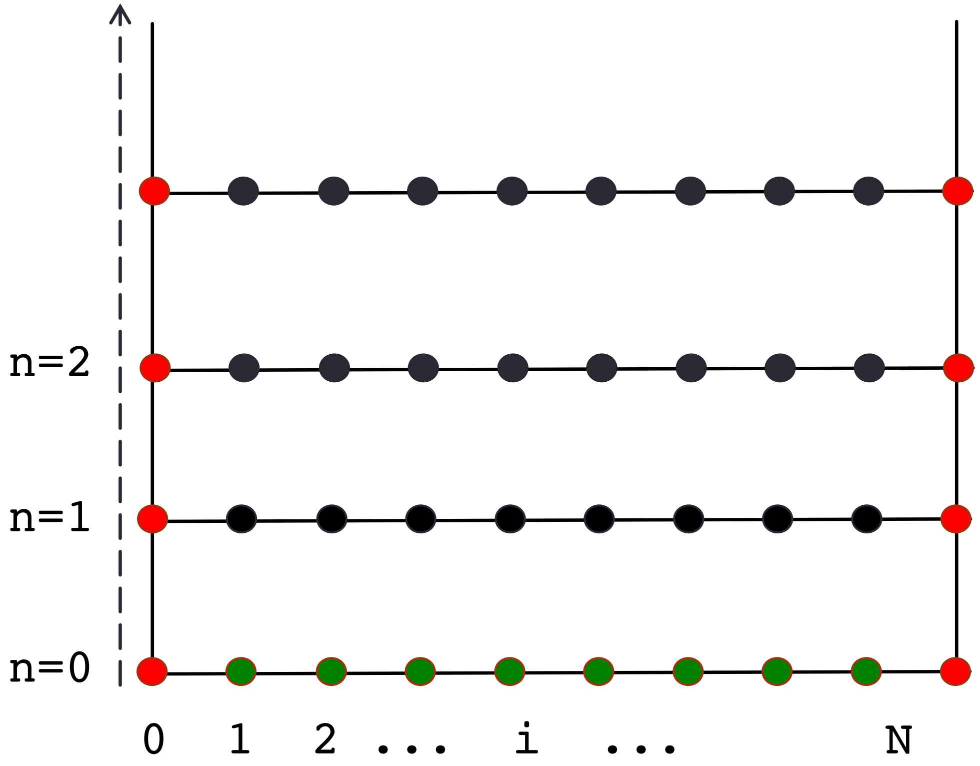
- At $t=0$ the *initial condition* must be provided:

$$\varphi_i^0, \qquad i = 1, ..., N-1$$

- *Boundary values* are provided at the boundaries of the domain for all t ≥ 0:

$$\varphi_0^n, \; \varphi_N^n$$

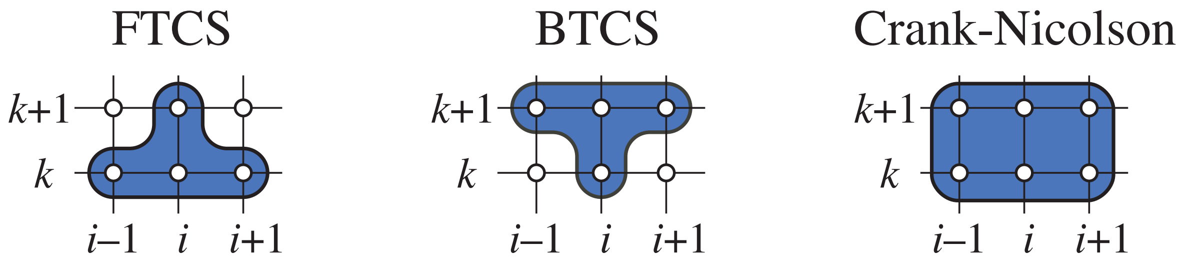
- *Solution values* are evolved starting from the initial condition inside the computation domain for all t > 0



Boundary Conditions (B.C.)

- Boundary conditions require information to be specified at all times at the boundary of the computational domain.

- This is necessary because the finite difference approximation require neighbor points:



- [Dirichlet]() b.c.: specify the value of the solution on the boundary region.
- [Neumann]() b.c.: specify the value of the derivative of the function on the boundary region.

The FTCS scheme

- The previous expression can be used to find φ^{n+1} as a function of the solution values at time t^n:

$$\varphi_i^{n+1} = \varphi_i^n + \frac{D\Delta t}{\Delta x^2}\left(\varphi_{i+1}^n - 2\varphi_i^n + \varphi_{i-1}^n\right) + \Delta t S_i$$

- This is an explicit scheme, called "FTCS" (Forward in Time, Centered in Space)
- The dimensionless number $C=D\Delta t/\Delta x^2$ is called the Courant (or CFL) number and plays an important role for stability.
- The previous equation can then be written as

$$\varphi_i^{n+1} = \varphi_i^n + C\left(\varphi_{i+1}^n - 2\varphi_i^n + \varphi_{i-1}^n\right) + \Delta t S_i$$

Stability of FTCS scheme

- The FTCS is *conditionally stable* since, it can be shown (see von Neumann stability) that

$$C \leq \frac{1}{2} \quad \Longleftrightarrow \quad \Delta t \leq \frac{\Delta x^2}{2D}$$

- A finite difference scheme is stable if the errors made at one time step of the calculation do not cause the errors to increase as the computations are continued.

Von Neumann Stability Analysis

The von Neumann method is based on the decomposition of the errors into Fourier series. To illustrate the procedure, consider the one-dimensional heat equation

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

defined on the spatial interval L, which can be discretized[5] as

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

where

$$r = \frac{\alpha\,\Delta t}{\Delta x^2}$$

and the solution u_j^n of the discrete equation approximates the analytical solution $u(x,t)$ of the PDE on the grid.

Von Neumann Stability Analysis

Define the round-off error ϵ_j^n as

$$\epsilon_j^n = N_j^n - u_j^n$$

where u_j^n is the solution of the discretized equation (1) that would be computed in the absence of round-off error, and N_j^n is the numerical solution obtained in finite precision arithmetic. Since the exact solution u_j^n must satisfy the discretized equation exactly, the error ϵ_j^n must also satisfy the discretized equation.[6] Thus

$$(2) \qquad \epsilon_j^{n+1} = \epsilon_j^n + r\left(\epsilon_{j+1}^n - 2\epsilon_j^n + \epsilon_{j-1}^n\right)$$

is a recurrence relation for the error. Equations (1) and (2) show that both the error and the numerical solution have the same growth or decay behavior with respect to time. For linear differential equations with periodic boundary condition, the spatial variation of error may be expanded in a finite Fourier series, in the interval L, as

$$(3) \qquad \epsilon(x) = \sum_{m=1}^{M} A_m e^{ik_m x}$$

Von Neumann Stability Analysis

where the wavenumber $k_m = \dfrac{\pi m}{L}$ with $m = 1, 2, \ldots, M$ and $M = L/\Delta x$. The time dependence of the error is included by assuming that the amplitude of error A_m is a function of time. Since the error tends to grow or decay exponentially with time, it is reasonable to assume that the amplitude varies exponentially with time; hence

$$(4) \qquad \epsilon(x,t) = \sum_{m=1}^{M} e^{at} e^{ik_m x}$$

where a is a constant.

Since the difference equation for error is linear (the behavior of each term of the series is the same as series itself), it is enough to consider the growth of error of a typical term:

$$(5) \qquad \epsilon_m(x,t) = e^{at} e^{ik_m x}$$

The stability characteristics can be studied using just this form for the error with no loss in generality. To find out how error varies in steps of time, substitute equation (5) into equation (2), after noting that

$$\begin{aligned}
\epsilon_j^n &= e^{at} e^{ik_m x} \\
\epsilon_j^{n+1} &= e^{a(t+\Delta t)} e^{ik_m x} \\
\epsilon_{j+1}^n &= e^{at} e^{ik_m (x+\Delta x)} \\
\epsilon_{j-1}^n &= e^{at} e^{ik_m (x-\Delta x)},
\end{aligned}$$

Von Neumann Stability Analysis

$$(6) \qquad e^{a\Delta t} = 1 + \frac{\alpha \Delta t}{\Delta x^2}\left(e^{ik_m\Delta x} + e^{-ik_m\Delta x} - 2\right).$$

Using the identities

$$\cos(k_m\Delta x) = \frac{e^{ik_m\Delta x} + e^{-ik_m\Delta x}}{2} \qquad \text{and} \qquad \sin^2\frac{k_m\Delta x}{2} = \frac{1-\cos(k_m\Delta x)}{2}$$

equation (6) may be written as

$$(7) \qquad e^{a\Delta t} = 1 - \frac{4\alpha\Delta t}{\Delta x^2}\sin^2(k_m\Delta x/2)$$

Define the amplification factor

$$G \equiv \frac{\epsilon_j^{n+1}}{\epsilon_j^n}$$

The necessary and sufficient condition for the error to remain bounded is that $|G| \leq 1$. However,

$$(8) \qquad G = \frac{e^{a(t+\Delta t)}e^{ik_m x}}{e^{at}e^{ik_m x}} = e^{a\Delta t}$$

Von Neumann Stability Analysis

Thus, from equations (7) and (8), the condition for stability is given by

$$(9) \qquad \left|1 - \frac{4\alpha\Delta t}{\Delta x^2}\sin^2(k_m\Delta x/2)\right| \leq 1$$

Note that the term $\frac{4\alpha\Delta t}{\Delta x^2}\sin^2(k_m\Delta x/2)$ is always positive. Thus, to satisfy Equation (9):

$$(10) \qquad \frac{4\alpha\Delta t}{\Delta x^2}\sin^2(k_m\Delta x/2) \leq 2$$

For the above condition to hold at all $\sin^2(k_m\Delta x/2)$, we have

$$(11) \qquad \frac{\alpha\Delta t}{\Delta x^2} \leq \frac{1}{2}$$

Equation (11) gives the stability requirement for the FTCS scheme as applied to one-dimensional heat equation. It says that for a given Δx, the allowed value of Δt must be small enough to satisfy equation (10).

Implicit Schemes: BTCS

- If we replace the right hand side with the solution at the new time level we obtain

$$\frac{\varphi_i^{n+1} - \varphi_i^n}{\Delta t} = \frac{\varphi_{i+1}^{n+1} - 2\varphi_i^{n+1} + \varphi_{i-1}^{n+1}}{h^2} + S_i^{n+1}$$

- This scheme is Backward in Time, Centered in Space (BTCS)
- Remember: the source term S does not depend on φ, but only on x and t.
- Repeating von-Neumann stability we'd find

$$G = e^{a\Delta t} = \frac{1}{1 + 4\alpha\frac{\Delta t}{\Delta x^2}\sin^2(k_m \Delta x/2)} \leq 1$$

- The method is *unconditionally stable* for all Δt > 0 !!

- This does not, of course, tell anything about its *accuracy*.

Implicit Scheme: Tridiagonal Matrix

- The previous equations can be written in matrix notation as a linear system in the unknowns φ^{n+1}:

$$\begin{pmatrix} a_1^0 & a_1^+ & 0 & 0 & 0 & 0 & 0 \\ a_2^- & a_2^0 & a_2^+ & 0 & 0 & 0 & 0 \\ 0 & a_3^- & a_3^0 & a_3^+ & 0 & 0 & 0 \\ 0 & 0 & \ddots & \ddots & \ddots & 0 & 0 \\ 0 & 0 & 0 & 0 & a_{N-1}^- & a_{N-1}^0 & a_{N-1}^+ \\ 0 & 0 & 0 & 0 & 0 & a_N^- & a_N^0 \end{pmatrix} \begin{pmatrix} \varphi_1^{n+1} \\ \varphi_2^{n+1} \\ \vdots \\ \varphi_{N-1}^{n+1} \\ \varphi_N^{n+1} \end{pmatrix} = \begin{pmatrix} b_1^n \\ b_2^n \\ \vdots \\ b_{N-1}^n \\ b_N^n \end{pmatrix}$$

- This system has tridiagonal form and can be efficiently inverted in (order) N operations (rather than N^2) by using a recurrence relation rather than inverting the full matrix.

Inversion of a Tridiagonal Matrix

- Written in components, `i = 1, ..., N-1`: $a_i^- \varphi_{i-1}^{n+1} + a_i^0 \varphi_i^{n+1} + a_i^+ \varphi_{i+1}^{n+1} = b_i$

where $a_i^\pm = -C\,, \quad a_i^0 = 1 + 2C\,, \quad b_i = \varphi_i^n + \Delta t S_i^{n+1}$

$$\varphi_{i+1}^{n+1} = \alpha_i \varphi_i^{n+1} + \beta_i$$

- To solve the system, assume that the solution satisfies as one-term forward recursion relation:
- Substituting in the original equation we obtain

$$a_i^- \varphi_{i-1}^{n+1} + a_i^0 \varphi_i^{n+1} + a_i^+ (\alpha_i \varphi_i^{n+1} + \beta_i) = b_i$$

$$\Longrightarrow \quad \varphi_i^{n+1} = \gamma_i \left[a_i^- \varphi_{i-1}^{n+1} + a_i^+ \beta_i - b_i\right] \quad \text{with} \quad \gamma_i = -\frac{1}{a_i^0 + a_i^+ \alpha_i}$$

Inversion of a Tridiagonal Matrix

- Upon comparing the previous expression with the recurrence relation we obtain

$$\alpha_i = \gamma_{i+1} a^{-}_{i+1}$$
$$\beta_i = \gamma_{i+1}(a^{+}_{i+1}\beta_{i+1} - b_{i+1})$$

- The previous expression is first used in a *backward sweep* to obtain α_i and β_i for $i=N-2, \ldots, 0$. The starting value are $\alpha_{N-1} = 0$ and $\beta_{N-1} = \varphi_N$. This guarantees the boundary condition at the last lattice point.
- Then perform a *forward sweep* to determine the solution φ_i using the recurrence relation for $i=1, \ldots, N-1$.
- This determines the solution in only two sweeps and involve of order N arithmetic operations.

The Crank-Nicholson Scheme

- With little effort, 2nd order accuracy in time can be achieved by replacing the backward Euler with an average between the current level and the new level (trapezoidal rule):

$$\varphi_i^{n+1} = \varphi_i^n + C\left[\frac{(\varphi_{i-1}^n - 2\varphi_i^n + \varphi_{i+1}^n) + (\varphi_{i-1}^{n+1} - 2\varphi_i^{n+1} + \varphi_{i+1}^{n+1})}{2}\right]$$

- This system can again be inverted using the tri-diagonal solver written before.

General θ-form

- FTCS, BTCS and CN can be cast in the following

$$\varphi_i^{n+1} = \varphi_i^n + C\left[(1-\theta)(\delta^2\varphi^n)_i + \theta(\delta^2\varphi^{n+1})_i\right]$$

where $(\delta^2\varphi)_i = (\varphi_{i+1} - 2\varphi_i + \varphi_{i-1})$ is the 2nd order discrete operator, $0 \leq \theta \leq 1$ so that:

  - $\theta = 0$ → FTCS; $\theta = 1$ → BTCS; $\theta = 1/2$ → Crank Nicholson

- The general form of the tridiagonal matrix is therefore

$$a_i^- = a_i^+ = -C\theta\,, \quad a_i^0 = 1 + 2C\theta\,,$$

$$b_i = \varphi_i^n + C(1-\theta)\left(\varphi_{i+1}^n - 2\varphi_i^n + \varphi_{i-1}^n\right) + \Delta t^n \frac{S_i^n + S_i^{n+1}}{2}$$

Exercise #1

- Let's solve the diffusion equation with D = 1 and S = 0 using at t=0 the simple Gaussian profile

$$\varphi(x,0) = \exp(-x^2/a^2) \quad \text{for } x \in [-1,1]$$

with *a* = ¼. Integration is carried for 0 ≤ t ≤ 1 using Nx = 100 points.

- The PDE has analytical solution

$$\varphi(x,t) = \frac{1}{\sqrt{1+4Dt/a^2}} \exp\left[-\frac{(x/a)^2}{1+4Dt/a^2}\right]$$

- Boundary conditions at x = ±1 can be specified using the exact solution.

1. *Try integrating the PDE using FTCS, BCTS and Crank-Nicholson (CN) by using different values of the CFL number.*
2. *For implicit schemes increase C by ten times. Compare the relative error.*
3. *Which scheme perform best ?*

Exercise #2

- Solve the diffusion equation with $D = 1$ and $S = 0$ inside the unit interval $0 \leq x \leq 1$ for $0 \leq t \leq 1$ using $Nx = 100$ points

  - Initial condition: $\varphi(x,0) = 0$;
  - Boundary condition: $\varphi(0,t) = 0$, $\varphi(1,t) = 5$.

- This situation correspond to a physical rod where the two extremities are kept at constant temperature.

- What is the final solution ? Is this a steady state solution ?

Exercise #3

- Solve the heat equation in the unit interval $0 \le x \le 1$ with I.C. given by

$$\varphi(x,0) = \sin(\pi x) + \frac{1}{10}\sin(10\pi x)$$

- This problem has exact solution

$$\varphi(x,t) = e^{-\pi^2 t}\sin(\pi x) + \frac{e^{-\pi^2 100 t}}{10}\sin(10\pi x)$$

which shows that high frequency are damped faster. Integrate until $t = 0.01$

Parabolic PDE in 2D

Explicit and Implicit ADI Methods

Two-Dimensional Diffusion Equation

- Assuming constant diffusion coefficients, the 2D heat equation reads

$$\frac{\partial\varphi}{\partial t} = D_x \frac{\partial^2\varphi}{\partial x^2} + D_y \frac{\partial^2\varphi}{\partial y^2}$$

- The solution now depends on 3 variables: $\varphi \equiv \varphi(x, y, t)$
- Generalizing our 1D results, we now must prescribe an initial condition:

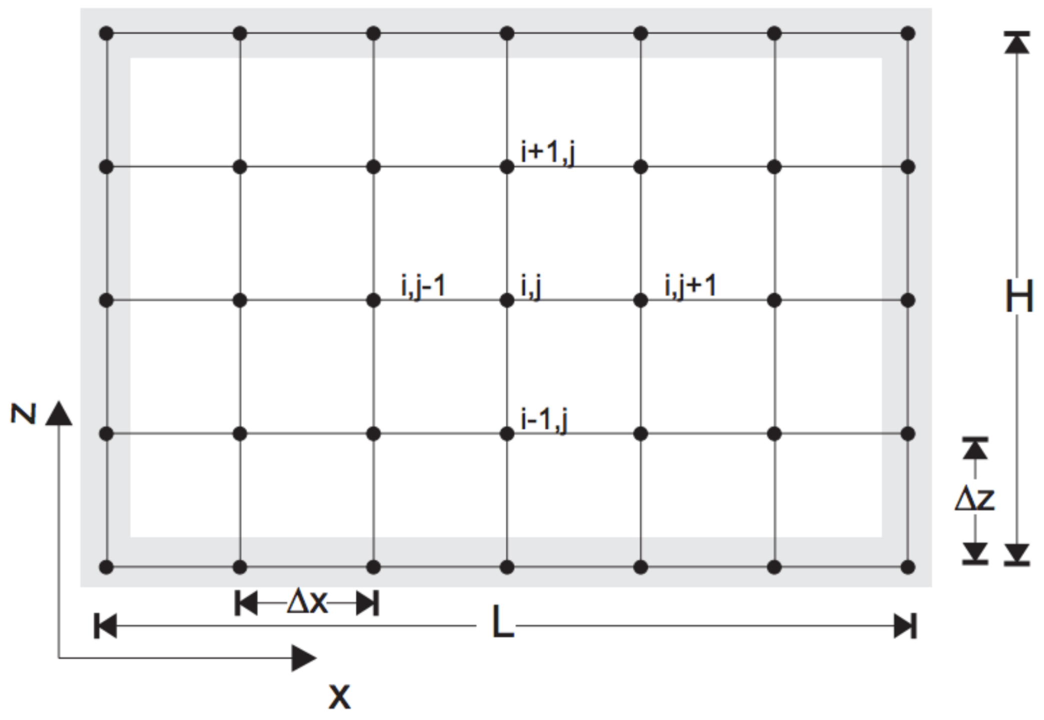
$$\varphi(x, y, 0) = f(x, y) \qquad (\text{for} \quad \text{t} = 0)$$

- And boundary conditions:

$$\begin{cases} \varphi(x_L, y, t) & = & f_L(y, t) \\ \varphi(x_R, y, t) & = & f_R(y, t) \\ \varphi(x, y_L, t) & = & f_B(x, t) \\ \varphi(x, y_R, t) & = & f_T(x, t) \end{cases}$$

Discretization in 2D

- We will assume a 2D spatial grid, with indices *i,j*:



$$\Rightarrow \quad \varphi(x_i, y_j, t^n) \equiv \varphi_{ij}^n \quad \Leftarrow$$

FTCS in 2D

- The FTCS scheme in 1D can be readily extended to the 2D case:

$$\frac{\phi_{ij}^{n+1} - \phi_{ij}^{n}}{\Delta t} = \delta_x^2 \phi_{ij}^n + \delta_y^2 \phi_{ij}^n$$

- Where the meaning of the difference operators on the rhs should now be clear.
- This is again an explicit scheme and rearranging terms yields

$$\phi_{ij}^{n+1} = \phi_{ij}^n + C_x(\varphi_{i+1,j}^n - 2\varphi_{i,j}^n + \varphi_{i-1,j}^n) + C_y(\varphi_{i,j+1}^n - 2\varphi_{i,j}^n + \varphi_{i,j-1}^n)$$

- where

$$C_x = D_x \frac{\Delta t}{\Delta x^2}, \quad C_y = D_y \frac{\Delta t}{\Delta y^2}$$

Stability of the 2D FTCS scheme

- Using von-Neumann analysis it is possible to show that the 2D scheme is stable under the restriction

$$C_x + C_y \leq \frac{1}{2} \quad \Rightarrow \quad \Delta t \leq \frac{1}{2} \frac{1}{\frac{D_x}{\Delta x^2} + \frac{D_y}{\Delta y^2}}$$

- In order to ensure stability of the FTCS, one has to impose a restriction that is essentially twice as strong as the analogous restriction in 1D.
- This scheme is not very computationally efficient.

Alternate Direction Implicit (ADI) Method

- Direct extension of the CN method in 2D poses serious problems since the resulting matrix is *banded tri-diagonal* rather than tri-diagonal. This makes the inversion costly.

- A different approach is given by ADI methods: split the finite difference equations into two: one with the *x*-derivative taken implicitly and the next with the *y*-derivative taken implicitly,

$$
\begin{aligned}
\frac{\phi_{ij}^{*} - \phi_{ij}^{n}}{\Delta t/2} &= \delta_x^2 \phi_{ij}^{*} + \delta_y^2 \phi_{ij}^{n} \\
\frac{\phi_{i}^{n+1} - \phi_{ij}^{*}}{\Delta t/2} &= \delta_x^2 \phi_{ij}^{*} + \delta_y^2 \phi_{ij}^{n+1}
\end{aligned}
$$

- ADI is unconditionally stable and 2nd order accurate in space and time.

Implementation of ADI

- Apply boundary conditions on φ^n;
- Obtain intermediate solution (x implicit, y explicit):

$$\varphi^*_{ij} = \varphi^n_{ij} + \frac{C_x}{2}(\varphi^*_{i+1,j} - 2\varphi^*_{i,j} + \varphi^*_{i-1,j}) + \frac{C_y}{2}(\varphi^n_{i,j+1} - 2\varphi^n_{i,j} + \varphi^n_{i,j-1})$$

- Invert implicit terms using tridiagonal solver with

$$a^0_i = 1 + C_x\,, \quad a^-_i = a^+_i = -\frac{C_x}{2}\,, \quad b_i = \varphi^n_i + \frac{C_y}{2}\Delta^2_y \varphi^n_{ij}$$

- Apply boundary conditions on φ^*;
- Obtain final solution (x explicit, y implicit):

$$\varphi^{n+1}_{ij} = \varphi^*_{ij} + \frac{C_x}{2}(\varphi^*_{i+1,j} - 2\varphi^*_{i,j} + \varphi^*_{i-1,j}) + \frac{C_y}{2}(\varphi^{n+1}_{i,j+1} - 2\varphi^{n+1}_{i,j} + \varphi^{n+1}_{i,j-1})$$

- Invert implicit terms using tridiagonal solver with

$$a^0_j = 1 + C_y\,, \quad a^-_j = a^+_j = -\frac{C_x}{2}\,, \quad b_j = \varphi^*_{ij} + \frac{C_x}{2}\Delta^2_x \varphi^*_{ij}$$

Excercise # 1

- Solve the diffusion equation with Dx = Dy = 1 on the square domain -1 < x,y < 1 with initial condition:

$$\varphi(x, y, t) = \exp\left[-\frac{x^2 + y^2}{a^2}\right]$$

- This is a Gaussian profile, use $a = ¼$.
- Integration is carried for 0 ≤ t ≤ 1 using NX,NY = 128,128 points.
- The PDE has analytical solution

$$\varphi(x, y, t) = \frac{1}{1 + 4Dt/a^2} \exp\left[-\frac{x^2 + y^2}{a^2 + 4Dt}\right]$$

- Boundary conditions at x = ±1 can be specified using the exact solution.