Module 02: Numerical Methods

Unit 06: Partial Differential Equation: IBVP

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Learning Objectives

- To discretize the spatial and temporal derivatives of single-valued multi-dimensional functions using finite difference approximations.

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- To discretize the spatial and temporal derivatives of single-valued multi-dimensional functions using finite difference approximations.
- To derive the algebraic form using discretized PDE, IC and BCs.

General Equation

A form of differential equation with a general variable ϕ:

$$\frac{\partial(\Lambda_\phi \phi)}{\partial t} + \nabla.(\Upsilon_\phi \phi \mathbf{u}) = \nabla.(\mathbf{\Gamma}_\phi.\nabla\phi) + F_{\phi_o} + S_\phi \tag{1}$$

where

ϕ = general variable

Λ_ϕ, Υ_ϕ = problem dependent parameters

$\mathbf{\Gamma}_\phi$ = tensor

F_{ϕ_o} = other forces

S_ϕ = source/sink term

Problem Definition

Governing equation

A two-dimensional (in space) IBVP can be written as,

$$\Omega : \quad \Lambda_\phi \frac{\partial \phi}{\partial t} = \Gamma_x \frac{\partial^2 \phi}{\partial x^2} + \Gamma_y \frac{\partial^2 \phi}{\partial y^2} + S_\phi(x, y)$$

Problem Definition

subject to

Initial Condition

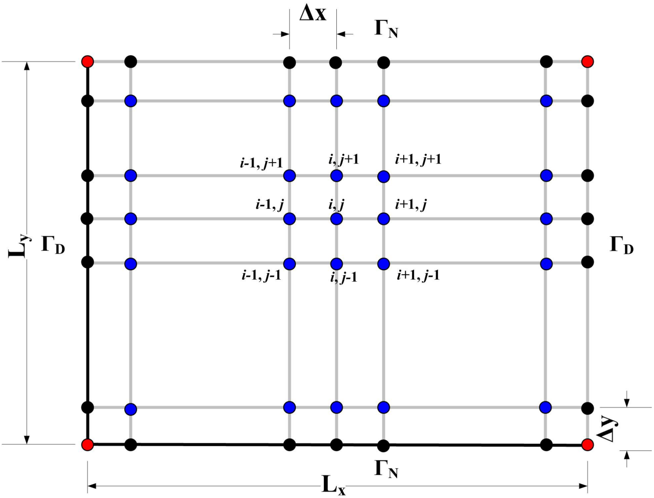
$$\phi(x, y, 0) = \phi_0(x, y)$$

and

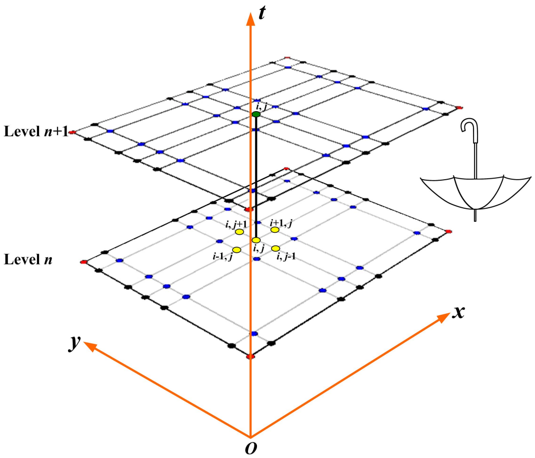
Boundary Condition

$$\begin{aligned}
\Gamma_D^1 : &\quad \phi(0, y, t) = \phi_1 \\
\Gamma_D^2 : &\quad \phi(L_x, y, t) = \phi_2 \\
\Gamma_N^3 : &\quad \left.\frac{\partial \phi}{\partial y}\right|_{(x,0,t)} = 0 \\
\Gamma_N^4 : &\quad \left.\frac{\partial \phi}{\partial y}\right|_{(x,L_y,t)} = 0
\end{aligned}$$

Domain Discretization (Space)



Space-Time Discretization
Explicit Scheme



Explicit Scheme

Governing Equation

$$\Lambda_\phi \frac{\partial \phi}{\partial t}\bigg|_{i,j}^{n} = \Gamma_x \frac{\partial^2 \phi}{\partial x^2}\bigg|_{i,j}^{n} + \Gamma_y \frac{\partial^2 \phi}{\partial y^2}\bigg|_{i,j}^{n} + S_\phi(x,y)\bigg|_{i,j}^{n}$$

Explicit Scheme

Governing Equation

$$\Lambda_\phi \frac{\partial \phi}{\partial t}\Big|_{i,j}^{n} = \Gamma_x \frac{\partial^2 \phi}{\partial x^2}\Big|_{i,j}^{n} + \Gamma_y \frac{\partial^2 \phi}{\partial y^2}\Big|_{i,j}^{n} + S_\phi(x,y)\Big|_{i,j}^{n}$$

Time Discretization

$$\frac{\partial \phi}{\partial t}\Big|_{i,j}^{n} = \frac{\phi_{i,j}^{n+1} - \phi_{i,j}^{n}}{\Delta t} + \mathcal{O}(\Delta t)$$

Explicit Scheme

Governing Equation

$$\Lambda_\phi \frac{\partial \phi}{\partial t}\bigg|_{i,j}^{n} = \Gamma_x \frac{\partial^2 \phi}{\partial x^2}\bigg|_{i,j}^{n} + \Gamma_y \frac{\partial^2 \phi}{\partial y^2}\bigg|_{i,j}^{n} + S_\phi(x,y)\bigg|_{i,j}^{n}$$

Time Discretization

$$\frac{\partial \phi}{\partial t}\bigg|_{i,j}^{n} = \frac{\phi_{i,j}^{n+1} - \phi_{i,j}^{n}}{\Delta t} + \mathcal{O}(\Delta t)$$

In *Explicit scheme*, space derivatives are discretized at the present time level (n).

Explicit Scheme

Space Discretization

$$\left.\frac{\partial^2 \phi}{\partial x^2}\right|_{i,j}^{n} = \frac{\phi_{i-1,j}^{n} - 2\phi_{i,j}^{n} + \phi_{i+1,j}^{n}}{\Delta x^2} + \mathcal{O}(\Delta x^2)$$

Explicit Scheme

Space Discretization

$$\left.\frac{\partial^2 \phi}{\partial x^2}\right|_{i,j}^{n} = \frac{\phi_{i-1,j}^n - 2\phi_{i,j}^n + \phi_{i+1,j}^n}{\Delta x^2} + \mathcal{O}(\Delta x^2)$$

$$\left.\frac{\partial^2 \phi}{\partial y^2}\right|_{i,j}^{n} = \frac{\phi_{i,j-1}^n - 2\phi_{i,j}^n + \phi_{i,j+1}^n}{\Delta y^2} + \mathcal{O}(\Delta y^2)$$

Explicit Scheme

Space Discretization

$$\left.\frac{\partial^2 \phi}{\partial x^2}\right|_{i,j}^{n} = \frac{\phi_{i-1,j}^{n} - 2\phi_{i,j}^{n} + \phi_{i+1,j}^{n}}{\Delta x^2} + \mathcal{O}(\Delta x^2)$$

$$\left.\frac{\partial^2 \phi}{\partial y^2}\right|_{i,j}^{n} = \frac{\phi_{i,j-1}^{n} - 2\phi_{i,j}^{n} + \phi_{i,j+1}^{n}}{\Delta y^2} + \mathcal{O}(\Delta y^2)$$

The corresponding difference equation can be written as,

$$\Lambda_\phi \frac{\phi_{i,j}^{n+1} - \phi_{i,j}^{n}}{\Delta t} = \Gamma_x \frac{\phi_{i-1,j}^{n} - 2\phi_{i,j}^{n} + \phi_{i+1,j}^{n}}{\Delta x^2} + \Gamma_y \frac{\phi_{i,j-1}^{n} - 2\phi_{i,j}^{n} + \phi_{i,j+1}^{n}}{\Delta y^2} + S_\phi\Big|_{i,j}^{n} + \mathcal{O}(\Delta x^2, \Delta y^2, \Delta t)$$

Compact Form

In simplified form, this can be written as

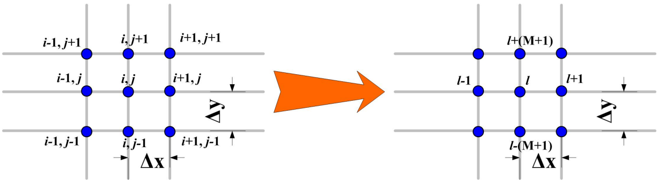
$$\phi_{i,j}^{n+1} = \alpha_y \phi_{i,j-1}^{n} + \alpha_x \phi_{i-1,j}^{n} + [1 - 2(\alpha_x + \alpha_y)]\, \phi_{i,j}^{n} + \alpha_x \phi_{i+1,j}^{n} + \alpha_y \phi_{i,j+1}^{n} + \frac{\Delta t}{\Lambda_\phi} S_\phi \Big|_{i,j}^{n}$$

with $\alpha_x = \frac{\Gamma_x \Delta t}{\Lambda_\phi \Delta x^2}$ and $\alpha_y = \frac{\Gamma_y \Delta t}{\Lambda_\phi \Delta y^2}$.

Single Index Notation

Single index l can be written as,

$$l = i + j \times (M + 1)$$



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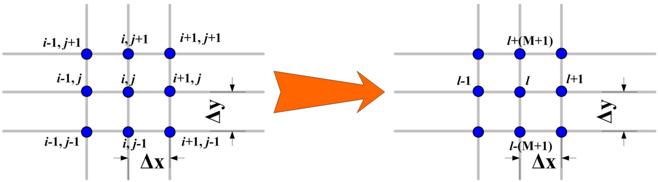

With single index notation, the equation can be written as,

$$\phi_l^{n+1} = \alpha_y \phi_{l-(M+1)}^n + \alpha_x \phi_{l-1}^n + \left[1 - 2(\alpha_x + \alpha_y)\right] \phi_l^n$$
$$+ \alpha_x \phi_{l+1}^n + \alpha_y \phi_{l+(M+1)}^n + \frac{\Delta t}{\Lambda_\phi} S_\phi \Big|_{i,j}^n$$

Standard Steps

Explicit Scheme: Time-stepping Algorithm

Data: Λ_ϕ, Γ_x, Γ_y, S_ϕ, Δx, Δy, Δt, ϕ^n at time-step n

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Data: Λ_ϕ, Γ_x, Γ_y, S_ϕ, Δx, Δy, Δt, ϕ^n at time-step n
Result: Updated ϕ^{n+1} at time-step $n+1$

Standard Steps

Explicit Scheme: Time-stepping Algorithm

Data: Λ_ϕ, Γ_x, Γ_y, S_ϕ, Δx, Δy, Δt, ϕ^n at time-step n
Result: Updated ϕ^{n+1} at time-step $n+1$
while *t <end time* **do**

For interior points: $\phi_{i,j}^{n+1} = \alpha_y \phi_{l-(M+1)}^n + \alpha_x \phi_{l-1}^n + \left[1 - 2(\alpha_x + \alpha_y)\right] \phi_l^n + \alpha_x \phi_{l+1}^n + \alpha_y \phi_{l+(M+1)}^n + \frac{\Delta t}{\Lambda_\phi} S_\phi \Big|_{i,j}^n$

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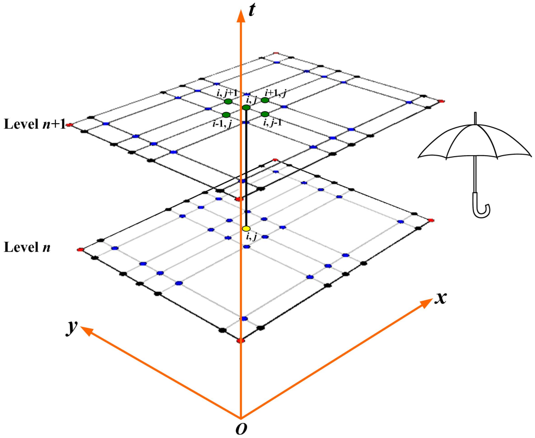
For boundary points: Use Boundary Conditions

$n \leftarrow n + 1$

end

Implicit Scheme



Implicit Scheme

Governing Equation

$$\Lambda_\phi \frac{\partial \phi}{\partial t}\bigg|_{i,j}^{n+1} = \Gamma_x \frac{\partial^2 \phi}{\partial x^2}\bigg|_{i,j}^{n+1} + \Gamma_y \frac{\partial^2 \phi}{\partial y^2}\bigg|_{i,j}^{n+1} + S_\phi(x,y)\bigg|_{i,j}^{n+1}$$

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Time Discretization

$$\frac{\partial \phi}{\partial t}\bigg|_{i,j}^{n+1} = \frac{\phi_{i,j}^{n+1} - \phi_{i,j}^{n}}{\Delta t} + \mathcal{O}(\Delta t)$$

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In *Implicit scheme*, space derivatives are discretized at the future time level $(n+1)$.

Implicit Scheme

Space Discretization

$$\left.\frac{\partial^2\phi}{\partial x^2}\right|_{i,j}^{n+1} = \frac{\phi_{i-1,j}^{n+1} - 2\phi_{i,j}^{n+1} + \phi_{i+1,j}^{n+1}}{\Delta x^2} + \mathcal{O}(\Delta x^2)$$

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The corresponding difference equation can be written as,

$$\Lambda_\phi \frac{\phi_{i,j}^{n+1} - \phi_{i,j}^{n}}{\Delta t} = \Gamma_x \frac{\phi_{i-1,j}^{n+1} - 2\phi_{i,j}^{n+1} + \phi_{i+1,j}^{n+1}}{\Delta x^2} + \Gamma_y \frac{\phi_{i,j-1}^{n+1} - 2\phi_{i,j}^{n+1} + \phi_{i,j+1}^{n+1}}{\Delta y^2} + \left.S_\phi\right|_{i,j}^{n+1} + \mathcal{O}(\Delta x^2, \Delta y^2, \Delta t)$$

Compact Form

In simplified form, this can be written as

$$\alpha_y \phi_{i,j-1}^{n+1} + \alpha_x \phi_{i-1,j}^{n+1} - \left[1 + 2(\alpha_x + \alpha_y)\right] \phi_{i,j}^{n+1}$$
$$+\alpha_x \phi_{i+1,j}^{n+1} + \alpha_y \phi_{i,j+1}^{n+1} = -\phi_{i,j}^{n} - \frac{\Delta t}{\Lambda_\phi} S_\phi\Big|_{i,j}^{n+1}$$

with $\alpha_x = \frac{\Gamma_x \Delta t}{\Lambda_\phi \Delta x^2}$ and $\alpha_y = \frac{\Gamma_y \Delta t}{\Lambda_\phi \Delta y^2}$.

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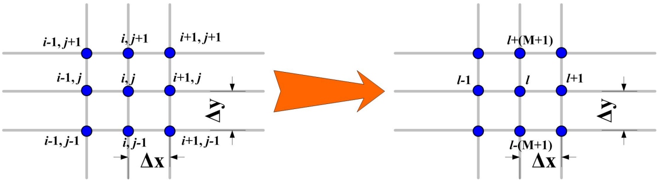

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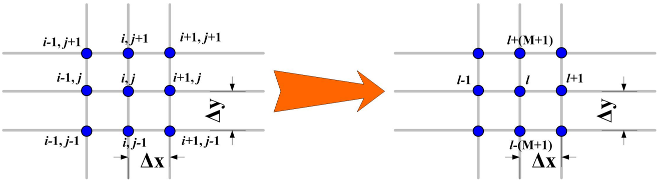

With single index notation, the equation can be written as,

$$\alpha_y \phi_{l-(M+1)}^{n+1} + \alpha_x \phi_{l-1}^{n+1} - \left[1 + 2(\alpha_x + \alpha_y)\right] \phi_l^{n+1}$$
$$+\alpha_x \phi_{l+1}^{n+1} + \alpha_y \phi_{l+(M+1)}^{n+1} = -\phi_l^n - \frac{\Delta t}{\Lambda_\phi} S_\phi \Big|_{i,j}^{n+1}$$

Standard Steps

Implicit Scheme: Time-stepping Algorithm

Data: Λ_ϕ, Γ_x, Γ_y, S_ϕ, Δx, Δy, Δt, ϕ^n at time-step n

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Data: Λ_ϕ, Γ_x, Γ_y, S_ϕ, Δx, Δy, Δt, ϕ^n at time-step n
Result: Updated ϕ^{n+1} at time-step $n+1$

Standard Steps

Implicit Scheme: Time-stepping Algorithm

Data: Λ_ϕ, Γ_x, Γ_y, S_ϕ, Δx, Δy, Δt, ϕ^n at time-step n
Result: Updated ϕ^{n+1} at time-step $n+1$
while $t <$ *end time* **do**
  For interior and boundary points: Solve governing equation and boundary conditions in discretized form.
  $n \leftarrow n+1$
end

θ-scheme

Governing Equation

Explicit Step

$$\Lambda_\phi \frac{\partial \phi}{\partial t}\bigg|_{i,j}^{n} = \Gamma_x \frac{\partial^2 \phi}{\partial x^2}\bigg|_{i,j}^{n} + \Gamma_y \frac{\partial^2 \phi}{\partial y^2}\bigg|_{i,j}^{n} + S_\phi(x,y)\bigg|_{i,j}^{n}$$

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Governing Equation

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$$\Lambda_\phi \frac{\partial \phi}{\partial t}\Big|_{i,j}^{n} = \Gamma_x \frac{\partial^2 \phi}{\partial x^2}\Big|_{i,j}^{n} + \Gamma_y \frac{\partial^2 \phi}{\partial y^2}\Big|_{i,j}^{n} + S_\phi(x,y)\Big|_{i,j}^{n}$$

Implicit Step

$$\Lambda_\phi \frac{\partial \phi}{\partial t}\Big|_{i,j}^{n+1} = \Gamma_x \frac{\partial^2 \phi}{\partial x^2}\Big|_{i,j}^{n+1} + \Gamma_y \frac{\partial^2 \phi}{\partial y^2}\Big|_{i,j}^{n+1} + S_\phi(x,y)\Big|_{i,j}^{n+1}$$

θ-scheme

Finite Difference Scheme

Explicit Step

$$\Lambda_\phi \frac{\phi_{i,j}^{n+\theta} - \phi_{i,j}^{n}}{\theta \Delta t} = \Gamma_x \frac{\phi_{i-1,j}^{n} - 2\phi_{i,j}^{n} + \phi_{i+1,j}^{n}}{\Delta x^2} + \Gamma_y \frac{\phi_{i,j-1}^{n} - 2\phi_{i,j}^{n} + \phi_{i,j+1}^{n}}{\Delta y^2} + S_\phi\Big|_{i,j}^{n} + \mathcal{O}(\Delta x^2, \Delta y^2, \theta \Delta t)$$

θ-scheme
Finite Difference Scheme

Explicit Step

$$\Lambda_\phi \frac{\phi_{i,j}^{n+\theta} - \phi_{i,j}^{n}}{\theta \Delta t} = \Gamma_x \frac{\phi_{i-1,j}^{n} - 2\phi_{i,j}^{n} + \phi_{i+1,j}^{n}}{\Delta x^2} + \Gamma_y \frac{\phi_{i,j-1}^{n} - 2\phi_{i,j}^{n} + \phi_{i,j+1}^{n}}{\Delta y^2} + S_\phi\Big|_{i,j}^{n} + \mathcal{O}(\Delta x^2, \Delta y^2, \theta\Delta t)$$

Implicit Step

$$\Lambda_\phi \frac{\phi_{i,j}^{n+1} - \phi_{i,j}^{n+\theta}}{(1-\theta) \Delta t} = \Gamma_x \frac{\phi_{i-1,j}^{n+1} - 2\phi_{i,j}^{n+1} + \phi_{i+1,j}^{n+1}}{\Delta x^2} + \Gamma_y \frac{\phi_{i,j-1}^{n+1} - 2\phi_{i,j}^{n+1} + \phi_{i,j+1}^{n+1}}{\Delta y^2} + S_\phi\Big|_{i,j}^{n+1} + \mathcal{O}(\Delta x^2, \Delta y^2, (1-\theta)\Delta t)$$

θ-scheme

Finite Difference Scheme

By combining explicit and implicit discretizations,

$$\Lambda_\phi \frac{\phi_{i,j}^{n+1} - \phi_{i,j}^{n}}{\Delta t} =$$

$$\Gamma_x \left[\theta \frac{\phi_{i-1,j}^{n} - 2\phi_{i,j}^{n} + \phi_{i+1,j}^{n}}{\Delta x^2} + (1-\theta) \frac{\phi_{i-1,j}^{n+1} - 2{\phi^{n+1}}_{i,j} + \phi_{i+1,j}^{n+1}}{\Delta x^2} \right]$$

$$+\Gamma_y \left[\theta \frac{\phi_{i,j-1}^{n} - 2\phi_{i,j}^{n} + \phi_{i,j+1}^{n}}{\Delta y^2} + (1-\theta) \frac{\phi_{i,j-1}^{n+1} - 2\phi_{i,j}^{n+1} + \phi_{i,j+1}^{n+1}}{\Delta y^2} \right]$$

$$+ \left[\theta S_\phi \Big|_{i,j}^{n} + (1-\theta) S_\phi \Big|_{i,j}^{n+1} \right] + \mathcal{O}(\Delta x^2, \Delta y^2, ?)$$

Truncation Error of θ-scheme

Time Discretization

Explicit Step

$$\phi_{i,j}^{n} = \phi_{i,j}^{n+\theta} - \theta\Delta t \frac{\partial \phi}{\partial t}\Big|_{i,j}^{n+\theta} + \frac{(\theta\Delta t)^2}{2!}\frac{\partial^2 \phi}{\partial t^2}\Big|_{i,j}^{n+\theta} - \frac{(\theta\Delta t)^3}{3!}\frac{\partial^3 \phi}{\partial t^3}\Big|_{i,j}^{n+\theta} + \cdots$$

Truncation Error of θ-scheme

Time Discretization

Explicit Step

$$\phi_{i,j}^{n} = \phi_{i,j}^{n+\theta} - \theta\Delta t \frac{\partial \phi}{\partial t}\Big|_{i,j}^{n+\theta} + \frac{(\theta\Delta t)^2}{2!}\frac{\partial^2 \phi}{\partial t^2}\Big|_{i,j}^{n+\theta} - \frac{(\theta\Delta t)^3}{3!}\frac{\partial^3 \phi}{\partial t^3}\Big|_{i,j}^{n+\theta} + \cdots$$

Implicit Step

$$\phi_{i,j}^{n+1} = \phi_{i,j}^{n+\theta} + (1-\theta)\Delta t \frac{\partial \phi}{\partial t}\Big|_{i,j}^{n+\theta} + \frac{(1-\theta)^2\Delta t^2}{2!}\frac{\partial^2 \phi}{\partial t^2}\Big|_{i,j}^{n+\theta} + \frac{(1-\theta)^3\Delta t^3}{3!}\frac{\partial^3 \phi}{\partial t^3}\Big|_{i,j}^{n+\theta} + \cdots$$

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Implicit Step

$$\phi_{i,j}^{n+1} = \phi_{i,j}^{n+\theta} + (1-\theta)\Delta t \frac{\partial \phi}{\partial t}\Big|_{i,j}^{n+\theta} + \frac{(1-\theta)^2\Delta t^2}{2!}\frac{\partial^2 \phi}{\partial t^2}\Big|_{i,j}^{n+\theta} + \frac{(1-\theta)^3\Delta t^3}{3!}\frac{\partial^3 \phi}{\partial t^3}\Big|_{i,j}^{n+\theta} + \cdots$$

Combined Step

$$\frac{\phi_{i,j}^{n+1} - \phi_{i,j}^{n}}{\Delta t} = \frac{\partial \phi}{\partial t}\Big|_{i,j}^{n+\theta} + \frac{[(1-\theta)^2 - \theta^2]\Delta t}{2!}\frac{\partial^2 \phi}{\partial t^2}\Big|_{i,j}^{n+\theta} + \frac{[(1-\theta)^3 + \theta^3]\Delta t^2}{3!}\frac{\partial^3 \phi}{\partial t^3}\Big|_{i,j}^{n+\theta} + \cdots$$

Crank-Nicolson Method

If $\theta = 0.5$

Crank-Nicolson Method

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$$\frac{[(1-\theta)^2-\theta^2]\Delta t}{2!}\frac{\partial^2\phi}{\partial t^2}\bigg|_{i,j}^{n+\theta} = 0$$

The truncation error of the scheme is $\mathcal{O}(\Delta x^2, \Delta y^2, \Delta t^2)$.

Crank-Nicolson Method

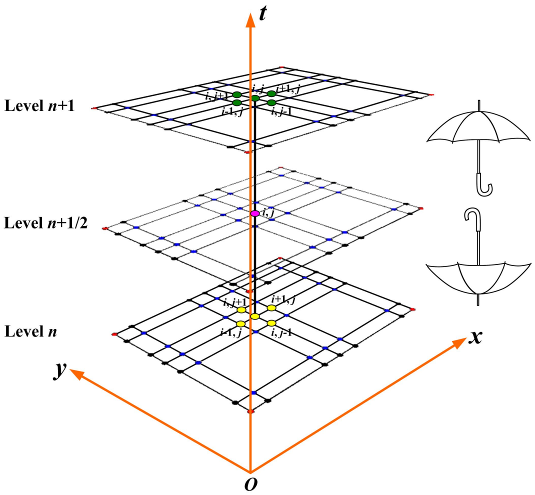
If $\theta = 0.5$

$$\frac{[(1-\theta)^2-\theta^2]\Delta t}{2!}\frac{\partial^2\phi}{\partial t^2}\bigg|_{i,j}^{n+\theta} = 0$$

The truncation error of the scheme is $\mathcal{O}(\Delta x^2, \Delta y^2, \Delta t^2)$.

The scheme is known as *Crank-Nicolson* method.

Crank-Nicolson Method



Thank You