Implicit/Explicit scheme for 2D advection diffusion problem

Mech587 Project #2

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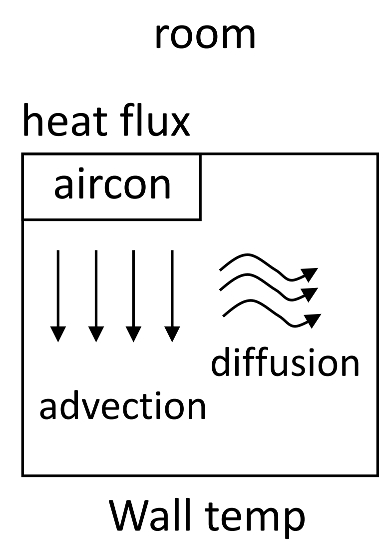
2D advection-diffusion: Definition

- Problem description:
  - The current value of the function is know.
  - The function follows certain condition on the boundary.
  - The evolution of the function is governed by the governing equation.
  - We want to predict the solution in the future
- Governing equation

$$\underbrace{\frac{\partial \phi}{\partial t}}_{\text{Evolution}} + \underbrace{u\frac{\partial \phi}{\partial x} + v\frac{\partial \phi}{\partial y}}_{\substack{\text{advection} \\ \text{Wave-like solution}}} = \underbrace{\alpha\left(\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2}\right)}_{\substack{\text{Diffusion} \\ \text{Damping/smear}}} \text{ in } (0, \mathrm{T}) \times \Omega$$



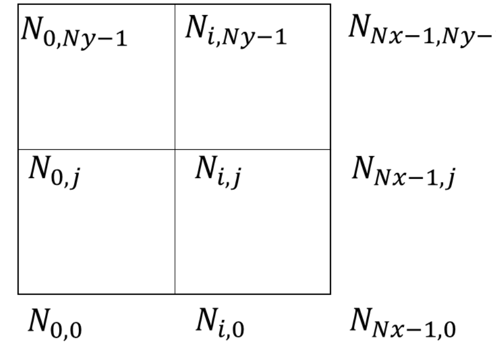
- Initial condition (IC)

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

- Boundary condition (BC)
  - Dirichlet (function value is given): $\phi = \phi_0$
  - Neumann (flux is given, e.g., heat flux): $\dfrac{\partial \phi}{\partial n} = g$

(n denote the normal direction to the boundary)

Discretization



- Governing equation is satisfied at every point (i, j)
- Discretization of the governing equation at each point gives us a algebra equation. Putting all of them together, we have a linear system.

$$\left(\frac{\partial \phi}{\partial t} + u\frac{\partial \phi}{\partial x} + v\frac{\partial \phi}{\partial y} = \alpha\left(\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2}\right)\right)_{i,j} \Rightarrow a\phi_{i,j} + b\phi_{i,j-1} + \cdots = 0$$

$\Downarrow$ All together

$$\begin{aligned} a\phi_{1,1} + b\phi_{1,0} + \cdots &= 0 \\ a\phi_{1,2} + b\phi_{1,1} + \cdots &= 0 \\ &\vdots \\ a\phi_{Nx-2,Ny-2} + b\phi_{Nx-2,Ny-3} + \cdots &= 0 \end{aligned}$$

$(Nx - 2 \times Ny - 2)$ interior points
$(Nx - 2 \times Ny - 2)$ algebra equations
$(Nx - 2 \times Ny - 2)$ unknowns
Can be solved!

$$\Longrightarrow \boldsymbol{A\phi} = \boldsymbol{b}$$

$\boldsymbol{b}$ come from BC or source term

- We can treat the terms one by one
- Spatial discretization
  - How the spatial derivatives are evaluated with given mesh?

Diffusion: $\left(\alpha\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\phi\right)_{i,j}$ Advection: $\left(\left(u\frac{\partial}{\partial x} + v\frac{\partial}{\partial y}\right)\phi\right)_{i,j}$

- Temporal discretization
  - At which moment am I approximating the evolution?

Explicit Euler: $\frac{\partial \phi}{\partial t} = f(\phi^n)$ Implicit Euler: $\frac{\partial \phi}{\partial t} = f(\phi^{n+1})$

Spatial discretization

- Example: diffusion with central difference

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

$\Downarrow$ All together

$$\boldsymbol{D\phi}$$

- $\boldsymbol{\phi}$ is the vector of unknown
- $\boldsymbol{D}$ is a matrix decided by:
  - PDE operator: diffusion operator $\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)$
  - Discretization scheme: central difference
- $\boldsymbol{D}$ has nothing to do with which variable you are discretizing
- $\boldsymbol{D\phi}$ is a vector which gives the approximated $\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\phi$ value on each grid point.
  - If ϕ is known, you can directly calculate the value. Formation of the matrix is not needed (Similar to calculate the residual in Project 1)
- Boundary value needs to be considered separately because governing equation don’t apply to the boundary nodes

PDE:

$$\frac{\partial\phi}{\partial t}=-u\frac{\partial\phi}{\partial x}-v\frac{\partial\phi}{\partial y}+\alpha\left(\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}\right)$$

Spatial discretization: $\Downarrow$

Semi discrete form:

$$\frac{\partial\boldsymbol{\phi}}{\partial t}=-\boldsymbol{A\phi}+\boldsymbol{D\phi}$$

Upwind discretization for advection term

- Advection term:

$$\left(u\frac{\partial}{\partial x}\phi\right)_i$$

- First order upwind
  - When $u > 0$, information propagates from left to right
  - We use ϕ_{i-1} and ϕ_i to approximate the derivative (backward)

$$\left(\frac{\partial}{\partial x}\phi\right)_i = \frac{\phi_i - \phi_{i-1}}{\Delta x}$$

  - When $u < 0$, information propagates from right to left
  - We use ϕ_{i+1} and ϕ_i to approximate the derivative (forward)

$$\left(\frac{\partial}{\partial x}\phi\right)_i = \frac{\phi_{i+1} - \phi_i}{\Delta x}$$

  - Define $u^+ = 0.5(u + |u|)$, we have $u^+ = u$ for $u > 0$ and $u^+ = 0$ for $u \leq 0$
  - Define $u^- = 0.5(u - |u|)$, we have $u^- = u$ for $u < 0$ and $u^- = 0$ for $u \geq 0$

$$\left(u\frac{\partial}{\partial x}\phi\right)_i = u^+\left(\frac{\phi_i - \phi_{i-1}}{\Delta x}\right) + u^-\left(\frac{\phi_{i+1} - \phi_i}{\Delta x}\right)$$

- Second order upwind

$$\left(u\frac{\partial}{\partial x}\phi\right)_i = u^+\left(\frac{3\phi_i - 4\phi_{i-1} + \phi_{i-2}}{2\Delta x}\right) + u^-\left(\frac{-3\phi_i + 4\phi_{i+1} - \phi_{i+2}}{2\Delta x}\right)$$

- $\left(u\frac{\partial}{\partial x}\phi\right)_i = \boldsymbol{A}\phi$. Upwind is not symmetry. $\boldsymbol{A}^{-1}$ may be hard to calculate

Temporal discretization

- Consider problem $$\frac{\partial \phi}{\partial t} = f(\phi)$$
- Explicit schemes evaluated the derivative at previous time steps:
  - Forward Euler: $$\frac{\partial \phi}{\partial t} = f(\phi^n) \Rightarrow \frac{\boldsymbol{I}}{\Delta t}(\boldsymbol{\phi}^{n+1} - \boldsymbol{\phi}^n) = \boldsymbol{M}\boldsymbol{\phi}^n$$
  $$\boldsymbol{\phi}^{n+1} = (\boldsymbol{I} + \boldsymbol{M}\Delta t)\boldsymbol{\phi}^n$$
  - Adams-Bashforth: $$\frac{\partial \phi}{\partial t} = 1.5 f(\phi^n) - 0.5 f(\phi^{n-1})$$

    Two-step method

    You can start with FE
  $$\frac{\boldsymbol{I}}{\Delta t}(\boldsymbol{\phi}^{n+1} - \boldsymbol{\phi}^n) = 1.5\boldsymbol{M}\boldsymbol{\phi}^n - 0.5\boldsymbol{M}\boldsymbol{\phi}^{\boldsymbol{n-1}}$$
  $$\boldsymbol{\phi}^{n+1} = \boldsymbol{\phi}^n + 1.5\boldsymbol{M}\Delta t\boldsymbol{\phi}^n - 0.5\boldsymbol{M}\Delta t\boldsymbol{\phi}^{n-1}$$
  - No inverse of matrix
- Implicit schemes evaluated the derivative at previous time steps:
  - Backward Euler: $$\frac{\partial \phi}{\partial t} = f(\phi^{n+1}) \Rightarrow \frac{\boldsymbol{I}}{\Delta t}(\boldsymbol{\phi}^{n+1} - \boldsymbol{\phi}^n) = \boldsymbol{M}\boldsymbol{\phi}^{n+1}$$
  $$\boldsymbol{\phi}^{n+1} = (\boldsymbol{I} - \boldsymbol{M}\Delta t)^{-1}\boldsymbol{\phi}^n$$
  - Need to calculate inverse of matrix

- For $\boldsymbol{M}$ which is easy to be inversed, we want to used implicit scheme.
- For $\boldsymbol{M}$ which is hard to be inversed, we want to used explicit scheme.

Implicit/Explicit scheme

- Consider the problem:

$$\frac{\partial \phi}{\partial t} = -\left(u\frac{\partial}{\partial x} + v\frac{\partial}{\partial y}\right)\phi + \alpha\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\phi$$

- The semi-discrete form:

$$\frac{\partial \boldsymbol{\phi}}{\partial t} = -\boldsymbol{A}\boldsymbol{\phi} + \boldsymbol{D}\boldsymbol{\phi}$$

  - With central difference, $\boldsymbol{D}$ is easy to be inverted
  - With upwind, $\boldsymbol{A}$ is hard to be inverted

- Explicit for $\boldsymbol{A}\boldsymbol{\phi}$ (AB2), Implicit for $\boldsymbol{D}\boldsymbol{\phi}$ (Trapezoidal)

$$\frac{\boldsymbol{I}}{\Delta t}(\boldsymbol{\phi}^{n+1} - \boldsymbol{\phi}^n) = -(1.5\boldsymbol{A}\boldsymbol{\phi}^n - 0.5\boldsymbol{A}\boldsymbol{\phi}^{n-1}) + \boldsymbol{D}(0.5\boldsymbol{\phi}^n + 0.5\boldsymbol{\phi}^{n+1})$$

Explicit scheme, forward calculation. Don't need to form matrix

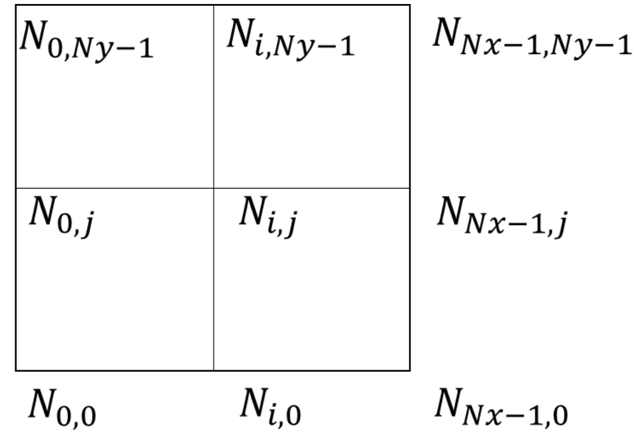
- You need to use Newton-Raphson method to calculate $\delta\boldsymbol{\phi}$

- **Use as much existing code as you can!**

Neumann boundary condition

- Suppose we have Neumann boundary condition on the bottom boundary:

$$\frac{\partial \phi}{\partial n} = \frac{\partial \phi}{\partial y}(y = 0) = h$$



- With first order one-side difference at $N_{i,0}$

$$\frac{\phi_{i,1} - \phi_{i,0}}{\Delta y} = h$$

- The boundary condition needs to be satisfied after updating:

$$\frac{\phi_{i,1}^{k+1} - \phi_{i,0}^{k+1}}{\Delta y} = h \qquad \frac{(\phi_{i,1}^{k} + \delta\phi_{i,1}^{k}) - (\phi_{i,0}^{k} + \delta\phi_{i,0}^{k})}{\Delta y} = h$$

- Finally we have the discrete form of the Neumann boundary condition:

$$\frac{1}{\Delta y}\delta\phi_{i,1}^{k} - \frac{1}{\Delta y}\delta\phi_{i,0}^{k} = h - \frac{\phi_{i,1}^{k} - \phi_{i,0}^{k}}{\Delta y}$$