Lecture 18: Time stepping

Logistics: - Australia 3/30 to 4/26

$\Rightarrow$ next week is last in person

after either zoom or pre-recorded ?

reshedule office hours or Piazza

- HW 6 due (9/17) ?

- HW 7 will be posted

Last time: - Diffusion

$Pe \to 0$

$$\frac{\partial c}{\partial t} - \nabla \cdot [D_m \nabla c] = 0$$

$$\boxed{\frac{\partial c}{\partial t} - D \frac{\partial^2 c}{\partial x^2} = 0}$$

- Bolzmann variable : $\eta = \dfrac{x}{\sqrt{4Dt}}$

$\Rightarrow$ similarity solution

PDE $\to$ ODE

- analytic solution

$$\boxed{c(x,t) = c_0 \,\mathrm{erf}\left(\frac{x}{\sqrt{4Dt}}\right)}$$

Today: - Numerical solution of transient problems $\Rightarrow$ time stepping

Transient Diffusion → Numerical solution

Transient PDE

$$\phi \frac{\partial c}{\partial t} - \underbrace{\nabla \cdot [\phi D_m \nabla c]}_{\underline{\underline{L}}\,\underline{c} = -\underline{\underline{D}} * \underline{\underline{Kd}} * \underline{\underline{G}} * \underline{c}} = f_s \qquad \underline{\underline{Kd}} = \phi D_m \underline{\underline{I}}$$

⇒ just need to discretize time derivative

Simple finite difference: $\frac{\partial c}{\partial t} \approx \frac{\underline{c}^{n+1} - \underline{c}^{n}}{\Delta t}$

$\Delta t = t^{n+1} - t^{n}$

substitute into PDE:

$$\underline{\underline{\Phi}} \frac{\underline{c}^{n+1} - \underline{c}^{n}}{\Delta t} + \underline{\underline{L}}\, c = f_s$$

$$\underline{\underline{\Phi}} = \text{spdiags}(\underline{\phi}, 0, Nx, Nx)$$

$$\underline{\underline{\Phi}} (\underline{c}^{n+1} - \underline{c}^{n}) + \Delta t\, \underline{\underline{L}}\, \underline{c}^{?} = \Delta t\, f_s$$

what time level ?

Theta method

Need to decide time level of $\underline{\underline{L}}\,\underline{c}$

choose: $\underline{c}^{\theta} = \theta\underline{c}^{n} + (1-\theta)\underline{c}^{n+1}$ $\quad 0 \leq \theta \leq 1$

substitute

$$\underline{\underline{\Phi}}(\underline{c}^{n+1} - \underline{c}^{n}) + \Delta t\,\underline{\underline{L}}(\theta\underline{c}^{n} + (1-\theta)\underline{c}^{n+1}) = \Delta t\,\underline{f_s}$$

$\underline{c}^{n}$ is known but $\underline{c}^{n+1}$ needs to be calculated

collect unknown $\underline{c}^{n+1}$ on l.h.s.

$$\underline{\underline{\Phi}}\,\underline{c}^{n+1} + \Delta t(1-\theta)\underline{\underline{L}}\,\underline{c}^{n+1} = \underline{\underline{\Phi}}\,\underline{c}^{n} - \Delta t\,\theta\,\underline{\underline{L}}\,\underline{c}^{n} + \Delta t\,\underline{f_s}$$

pull out $\underline{c}^{n+1}$ and $\underline{c}^{n}$

$$\underbrace{[\underline{\underline{\Phi}} + \Delta t(1-\theta)\underline{\underline{L}}]}_{\underline{\underline{IM}}}\,\underline{c}^{n+1} = \underbrace{[\underline{\underline{\Phi}} - \Delta t\,\theta\,\underline{\underline{L}}]}_{\underline{\underline{EX}}}\,\underline{c}^{n} + \Delta t\,\underline{f_s}$$

Linear system for single time step:

$$\boxed{\underline{\underline{IM}}\,\underline{c}^{n+1} = \underline{\underline{Ex}}\,\underline{c}^{n} + \Delta t\,\underline{f_s}}$$

Implicit matrix: $\underline{\underline{IM}} = \underline{\underline{\Phi}} + \Delta t(1-\theta)\underline{\underline{L}}$ $\quad \underline{\underline{L}} = -\underline{\underline{D}} * \underline{\underline{Kd}} * \underline{\underline{G}}$

$$\underline{\underline{EX}} = \underline{\underline{\Phi}} - \Delta t\,\theta\,\underline{\underline{L}}$$

Note: In general, we need to solve linear system at every time step

Properties of Theta Method

$\theta = 1$: Forward Euler Method

$\underline{\underline{IM}} = \underline{\underline{\Phi}}$ is diagonal

$\Rightarrow \quad \underline{c}^{n+1} = \underline{\underline{\Phi}}^{-1} \left(\underline{\underline{Ex}}\, \underline{c}^{n} + \Delta t\, f_s \right)$

- explicit method
- only requires matrix vector multiply (cheap)
- conditionally stable $\quad \Delta t \leq \dfrac{\Delta x^2}{2 D_m}$
- first-order accurate

$\theta = 0$: Backward Euler Method

$\underline{\underline{EX}} = \underline{\underline{\Phi}}$ diagonal

$\underline{\underline{IM}}$ not diagonal

$\underline{\underline{IM}}\, \underline{c}^{n+1} = \underline{\underline{Ex}}\, \underline{c}^{n} + \Delta t\, f_s$ implicit

- solve linear system $\rightarrow$ solve_lbvp.m

  $\Rightarrow$ expensive
- unconditionally stable
- first-order accurate

$\theta = \frac{1}{2}$: Crank-Nicholson Method

- $\underline{\underline{IM}}\, \underline{c}^{n+1} = \underline{\underline{EX}}\, \underline{c}^{n} + \Delta t\, f_s$

  → implicit method → solve linear system

- $c^{\theta} = \frac{1}{2} \underline{c}^{n} + \frac{1}{2} \underline{c}^{n+1} = \frac{\underline{c}^{n} + \underline{c}^{n+1}}{2}$ average

⇒ central difference in time

  ⇒ second order accurate

- unconditionally stable

  but has an oscillation limit

Amplification matrix

$\Delta t \qquad \underline{f}_D = -\underline{\underline{L}}\, \underline{c}_p$

$$\underline{\underline{IM}}\, \underline{c}^{n+1} = \underline{\underline{Ex}}\, \underline{c}^{n} + \Delta t\, \underline{f}_s + \underline{f}_N + \underline{f}_D$$

In absence of r.h.s terms, i.e. no sink/source ($\underline{f}_s = 0$) and homogeneous BC's ($\underline{f}_N = \underline{f}_D = 0$)

$$\underline{\underline{IM}}\, \underline{c}^{n+1} = \underline{\underline{EX}}\, \underline{c}^{n}$$

$$\underbrace{\underline{\underline{IM}}^{-1}\, \underline{\underline{IM}}\, \underline{c}^{n+1}}_{\underline{\underline{I}}\, \underline{c}^{n+1}} = \underline{\underline{IM}}^{-1}\, \underline{\underline{EX}}\, \underline{c}^{n}$$

$$\underline{c}^{n+1} = \underbrace{\underline{\underline{IM}}^{-1}\, \underline{\underline{EX}}}_{\underline{\underline{A}}}\, \underline{c}^{n}$$

$\underline{\underline{A}}$ = amplification matrix

$$\underline{c}^{n+1} = \underline{\underline{A}}\,\underline{c}^{n} = \underline{\underline{A}}(\underline{\underline{A}}\,\underline{c}^{n-1}) = \underline{\underline{A}}^{2}\,\underline{c}^{n-1} = \underline{\underline{A}}^{3}\,\underline{c}^{n-2} = \ldots = \underline{\underline{A}}^{n}\,\underline{c}^{0}$$

where $\underline{c}^{0}$ = initial condition

To evolve the solution we just keep multiplying by $\underline{\underline{A}}$

Evaluate matrix exponential $\underline{\underline{A}}^{n}$ using the spectral decomposition: $\underline{\underline{A}} = \underline{\underline{Q}}\,\underline{\underline{\Lambda}}\,\underline{\underline{Q}}^{-1}$

where $\underline{\underline{Q}}$ is square matrix of eigenvectors (columns)

$\underline{\underline{\Lambda}}$ is diagonal matrix of eigenvalues

$$\underline{\underline{A}}^{2} = \underline{\underline{A}}\,\underline{\underline{A}} = \underline{\underline{Q}}\,\underline{\underline{\Lambda}}\,\underbrace{\underline{\underline{Q}}^{-1}\,\underline{\underline{Q}}}_{\underline{\underline{I}}}\,\underline{\underline{\Lambda}}\,\underline{\underline{Q}}^{-1} = \underline{\underline{Q}}\,\underline{\underline{\Lambda}}^{2}\,\underline{\underline{Q}}^{-1}$$

in general: $\underline{\underline{A}}^{n} = \underline{\underline{Q}}\,\underline{\underline{\Lambda}}^{n}\,\underline{\underline{Q}}^{-1}$

The solution decays, i.e., method is stable, if

$$\max |\lambda_n| \leq 1$$