Lecture 1 - Mathematical Preliminaries

Gradient (grad/∇): $\nabla u = \langle \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}, \frac{\partial u}{\partial z} \rangle$ /vector/ $[m^{-1}]$
Directional derivative: $D_{\vec{v}} u = \nabla u \cdot \vec{v} = |\nabla u|\,|\vec{v}| \cos\theta = |\nabla u| \cos\theta$ /scalar/
∇u - direction of maximum rate of growth
Divergence (div/$\nabla \cdot$): $\nabla \cdot \vec{u} = \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z}$ /scalar/

<u>Def.</u> F - flux density; Φ - flux of F across S
$\Phi = \iint_S \vec{F} \cdot d\vec{S} = \iint_S (\vec{F} \cdot \vec{n})\, dS$

total amount — outward flux across S
Global conservation law: $\frac{\partial Q}{\partial t} = -\Phi + R$ — rate of creation/destruction in Ω

Divergence Theorem: $\iint_S \vec{F} \cdot d\vec{S} = \iiint_\Omega (\nabla \cdot \vec{F})\, dV$

Fourier's Law: $\vec{q} = -k \nabla T$ /heat flux density/
Heat Flow: $\Phi = \iint_S \vec{q} \cdot d\vec{S} = -\iint_S k \nabla T \cdot d\vec{S}$
Gauss's Law: $Q = \varepsilon_0 \iint_S \vec{E} \cdot d\vec{S}$ /net charge/

$\rho(x,y,z,t)$ - density; $f(x,y,z,t)$ - local rate of creation/destruction
$Q(t) = \iiint_\Omega \rho\, dV \qquad R(t) = \iiint_\Omega f\, dV$

$$\frac{dQ}{dt} = -\Phi + R \Rightarrow \frac{d}{dt} \iiint_\Omega \rho\, dV = -\iint_S \vec{J} \cdot d\vec{S} + \iiint_\Omega f\, dV$$
$$= -\iiint_\Omega (\nabla \cdot \vec{J})\, dV + \iiint_\Omega f\, dV$$

local conservation law: $\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{J} = f$
diffusion: $\vec{J} = -k \nabla \rho$
diffusion PDE: $\frac{\partial \rho}{\partial t} - \nabla \cdot (k \nabla \rho) = f$
ad/convection: $\vec{J} = \rho \vec{v}$
advection PDE: $\frac{\partial \rho}{\partial t} + \vec{v} \cdot \nabla \rho = f$

steady-state: $\frac{\partial \rho}{\partial t} = 0 \Rightarrow$ Poisson's equation: $-\nabla \cdot (k \nabla \rho) = f \Rightarrow -\Delta \rho = \frac{f}{k}$
Laplace operator ($\Delta = \nabla \cdot \nabla$): $\Delta \rho = \frac{\partial^2 \rho}{\partial x^2} + \frac{\partial^2 \rho}{\partial y^2} + \frac{\partial^2 \rho}{\partial z^2}$

Lecture 2 - Classification & Theoretical Analysis

second-order PDE: $F\left(x, y, u, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}, \frac{\partial^2 u}{\partial x^2}, \frac{\partial^2 u}{\partial x \partial y}, \frac{\partial^2 u}{\partial y^2}\right) = 0$

$$a_{11} \frac{\partial^2 u}{\partial x^2} + 2 a_{12} \frac{\partial^2 u}{\partial x \partial y} + a_{22} \frac{\partial^2 u}{\partial y^2} + F_1\left(x, y, u, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}\right) = 0$$

$$\left[\frac{\partial}{\partial x} \ \frac{\partial}{\partial y}\right] \begin{pmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \end{pmatrix} \begin{bmatrix} \frac{\partial u}{\partial x} \\ \frac{\partial u}{\partial y} \end{bmatrix} + F = 0 \Rightarrow \nabla . A \nabla u + F = 0$$

A - symmetric $\Rightarrow A = Q \Lambda Q^T \Rightarrow \nabla . Q \Lambda Q^T \nabla u + F = 0 \Rightarrow \tilde{\nabla} . \Lambda \tilde{\nabla} u + F = 0$

Λ - diagonal matrix of eigenvalues of A

$\tilde{\nabla}$ - gradient with respect to new variables ξ, η

$$\lambda_1 \frac{\partial^2 u}{\partial \xi^2} + \lambda_2 \frac{\partial^2 u}{\partial \eta^2} + F\left(\xi, \eta, u, \frac{\partial u}{\partial \xi}, \frac{\partial u}{\partial \eta}\right) = 0$$

$$\frac{\partial u}{\partial \xi} = \frac{\partial u}{\partial x} \frac{\partial x}{\partial \xi} + \frac{\partial u}{\partial y} \frac{\partial y}{\partial \xi} = \frac{\partial u}{\partial x} q_{11} + \frac{\partial u}{\partial y} q_{12}$$

1) elliptic: λ_1, λ_2 - nonzero, same sign ($a_{12}^2 - a_{11} a_{22} < 0$)

ex: $\frac{\partial^2 u}{\partial \xi^2} + \frac{\partial^2 u}{\partial \eta^2} + F\left(\xi, \eta, u, \frac{\partial u}{\partial \xi}, \frac{\partial u}{\partial \eta}\right) = 0$

2) hyperbolic: λ_1, λ_2 - nonzero, different signs ($a_{12}^2 - a_{11} a_{22} > 0$)

ex.: $\frac{\partial^2 u}{\partial \xi^2} - \frac{\partial^2 u}{\partial \eta^2} + F\left(\xi, \eta, u, \frac{\partial}{\partial \xi}, \frac{\partial u}{\partial \eta}\right) = 0$

3) parabolic: λ_1, λ_2 - one is zero ($a_{12}^2 - a_{11} a_{22} = 0$)

ex.: $\frac{\partial^2 u}{\partial \xi^2} + F\left(\xi, \eta, u, \frac{\partial}{\partial \xi}, \frac{\partial u}{\partial \eta}\right) = 0$

Poisson's: $-\nabla . (k \nabla u) = -k \nabla . \nabla u - (\nabla k) . (\nabla u) = f$

$$-k \frac{\partial^2 u}{\partial x^2} - k \frac{\partial^2 u}{\partial y^2} - \frac{\partial k}{\partial x} \frac{\partial u}{\partial x} - \frac{\partial k}{\partial y} \frac{\partial u}{\partial y} = f \rightarrow \text{elliptic}$$

Wave equation: $\frac{1}{c^2} \frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} = \frac{1}{c^2} \frac{\partial^2 u}{\partial t^2} - \Delta u = f \rightarrow$ hyperbolic

Advection: $\frac{\partial u}{\partial t} + \vec{v} . \nabla u = f \rightarrow$ hyperbolic

Diffusion: $\frac{\partial u}{\partial t} - D \frac{\partial^2 u}{\partial x^2} = \frac{\partial u}{\partial t} - \nabla . k \nabla u = f \rightarrow$ parabolic $\left(0 \times \frac{\partial^2 u}{\partial t^2}\right)$

Boundary Conditions

1) Dirichlet: $u(\vec{x}) = g_0(\vec{x})$, $\vec{x} \in \partial\Omega$

2) Neumann: $k(\vec{x}) D_{\vec{n}} u(\vec{x}) = g_1(\vec{x})$, $\vec{x} \in \partial\Omega$ $\qquad D_{\vec{n}} = \frac{\partial u}{\partial \vec{n}}$

3) Robin (mixed): $k(\vec{x}) D_{\vec{n}} u(\vec{x}) + \sigma u(\vec{x}) = g_2(\vec{x})$, $\vec{x} \in \partial\Omega$

4) (diffusion) initial condition: $u(\vec{x}, t) = u_0(\vec{x})$ at $t=0$

$\boxed{\text{Def}}$ $u(\vec{x})$, $\vec{x} \in \mathbb{R}^2$, maximum at $\vec{x}_0 \in \Omega \subset \mathbb{R}^2$

if $\exists \delta > 0$ s.t. $u(\vec{x}_0) \geq u(\vec{x})$, $\forall \vec{x}$, $\|x - x_0\| < \delta$

$\boxed{\text{Def.}}$ Hessian matrix of $u(\vec{x})$ at $\vec{x}_0 \in \mathbb{R}^2$

$$H(\vec{x}_0) = \begin{bmatrix} \frac{\partial^2 u}{\partial x^2}(\vec{x}_0) & \frac{\partial^2 u}{\partial x \partial y}(\vec{x}_0) \\ \frac{\partial^2 u}{\partial y \partial x}(\vec{x}_0) & \frac{\partial^2 u}{\partial y^2}(\vec{x}_0) \end{bmatrix}$$

condition: $u(\vec{x}) \in C^2(\Omega)$, $u(\vec{x})$ has maximum at $\vec{x}_0 \Rightarrow \nabla u(\vec{x}_0) = 0$

$\boxed{\text{Th}}$ $u(\vec{x}) \in C^2(\Omega)$, $\Omega \subset \mathbb{R}^2$ has maximum at $\vec{x}_0$

$\Rightarrow \exists \delta > 0$ s.t. $\forall \vec{x}$, $\|\vec{x} - \vec{x}_0\| < \delta$, Hessian matrix of $u(\vec{x})$ at $\vec{x}_0$ is negative semi-definite

i.e. $(\vec{x} - \vec{x}_0)^T H(\vec{x}_0)(\vec{x} - \vec{x}_0) \leq 0$ for $\forall \vec{x}$, $\|\vec{x} - \vec{x}_0\| < \delta$

$H(\vec{x}_0)$ is negative semi-definite $\Rightarrow -\Delta u(\vec{x}_0) \geq 0$

$\boxed{\text{Collary}}$ $u(\vec{x})$ has maximum at $\vec{x}_0 \Rightarrow \nabla u(\vec{x}_0) = 0$, $-\Delta u(\vec{x}_0) \geq 0$

$u(\vec{x})$ has minimum at $\vec{x}_0 \Rightarrow \nabla u(\vec{x}_0) = 0$, $-\Delta u(\vec{x}_0) \leq 0$

$\boxed{\text{Def}}$ 1) harmonic on Ω, $-\Delta u = 0$ for $\vec{x} \in \Omega$

2) subharmonic on Ω, $-\Delta u \leq 0$ for $\vec{x} \in \Omega$

3) superharmonic on Ω, $-\Delta u \geq 0$ for $\vec{x} \in \Omega$

$\boxed{\text{Th}}$ Maximal Principle

$u \in C^2(\Omega) \cap C^1(\bar{\Omega})$ is subharmonic on Ω

$\Rightarrow$ 1) maximum at $\partial\Omega \Rightarrow \max_{\vec{x} \in \bar{\Omega}} u = \max_{\vec{x} \in \partial\Omega} u$ (weak)

2) Ω-connected + $\exists \vec{x}_0 \in \Omega$, $u(\vec{x}_0) = \max_{\vec{x} \in \bar{\Omega}} \Rightarrow u(\vec{x}) = u(\vec{x}_0)$ on $\bar{\Omega}$ (strong)

$\boxed{\text{Th}}$ Minimal Principle

minimum for superharmonic functions

Th $-\Delta u = 0$ on Ω, homogeneous Dirichlet BC $u(\vec{x}) = 0$, $\vec{x} \in \partial\Omega$

$\Rightarrow$ only trivial solution $u(\vec{x}) = 0$ on Ω

Th
$$\left.\begin{array}{l} -\Delta u = f(\vec{x}),\ \vec{x} \in \Omega \\ u = g(\vec{x}),\ \vec{x} \in \partial\Omega \end{array}\right\} \begin{array}{l} \exists \text{ at most } 1 \text{ solution } u(\vec{x}) \\ \text{Dirichlet BC} \end{array}$$

Th
$$\left.\begin{array}{l} -\Delta u = f(\vec{x}),\ \vec{x} \in \Omega \\ \sigma u + D_{\vec{n}} u = g(\vec{x}),\ \vec{x} \in \partial\Omega,\ \sigma > 0 \end{array}\right\} \begin{array}{l} \exists \text{ at most } 1 \text{ solution } u(\vec{x}) \\ \text{Robin (mixed) BC} \end{array}$$

uniqueness

Th
$$\left.\begin{array}{l} -\nabla \cdot k \nabla u = f(\vec{x}),\ \vec{x} \in \Omega \\ -k D_{\vec{n}} u = g(\vec{x}),\ \vec{x} \in \partial\Omega \text{ (Neumann BC)} \end{array}\right\} \begin{array}{l} \text{if } u(\vec{x}) \text{ is solution, then} \\ u(\vec{x}) + c \text{ is solution} \end{array}$$

compatibility: $\int_{\partial\Omega} g \, ds = \iint_{\Omega} f \, dA$ non-uniqueness

Th
$$\left.\begin{array}{l} -\Delta u \geq 0,\ x \in \Omega \\ u = 0,\ x \in \partial\Omega \end{array}\right\} u(\vec{x}) \geq 0,\ \vec{x} \in \Omega$$

Th
$$\left.\begin{array}{l} -\Delta u_1 = f,\ \vec{x} \in \Omega \\ u_1 = g_1,\ \vec{x} \in \partial\Omega \\ -\Delta u_2 = f,\ \vec{x} \in \Omega \\ u_2 = g_2,\ \vec{x} \in \partial\Omega \end{array}\right\} |u_1(\vec{x}) - u_2(\vec{x})| \leq \max_{\vec{x} \in \partial\Omega} |g_1(\vec{x}) - g_2(\vec{x})|,\ \forall \vec{x} \in \Omega$$

Lecture 3 - 1D Finite Difference Method

$-\Delta u = -\frac{\partial^2 u}{\partial x^2} = f, \ x \in (0,1)$ (Poisson)
$u(0)=0, \ u(1)=0$ (Dirichlet BC)

grid - finite set of points on segment $\Omega = [a,b]$ (Ω_N)
$a = x_0 < x_1 < x_2 < \dots < x_{N-1} < x_N = b$
x_i - node of grid Ω_N
f_i - grid value of $f(x)$ at point $x_i \in \Omega_N$
$x_i, \ i=1,\dots,N-1 \to$ inner points/nodes
$i=0, N \to$ boundary points/nodes

$\Omega_h, \ f_i = f(x_i), \ u_i = u(x_i)$
$-u_i'' = f_i, \quad i=1,2,\dots,N-1$
$u_0 = 0, \ u_N = 0$

Taylor series of $u(x)$ around x_i:

$$u(x) = u(x_i) + u'(x_i)(x-x_i) + \frac{u''(x_i)}{2}(x-x_i)^2 + \frac{u'''(x_i)}{6}(x-x_i)^3 + \dots$$

$$= u_i + u_i'(x-x_i) + \frac{u_i''}{2}(x-x_i)^2 + \frac{u_i'''}{6}(x-x_i)^3 + \dots$$

$$u_{i+1} = u_i + u_i'(x_{i+1}-x_i) + \frac{u_i''}{2}(x_{i+1}-x_i)^2 + \frac{u_i'''}{6}(x_{i+1}-x_i)^3 + \dots$$
$$u_{i-1} = u_i + u_i'(x_{i-1}-x_i) + \frac{u_i''}{2}(x_{i-1}-x_i)^2 + \frac{u_i'''}{6}(x_{i-1}-x_i)^3 + \dots$$

$$-\frac{u_i''}{2} = \frac{-u_{i+1}+u_i}{(x_{i+1}-x_i)^2} + u_i'\frac{1}{x_{i+1}-x_i} + \frac{u_i'''}{6}(x_{i+1}-x_i) + \dots$$
$+$
$$-\frac{u_i''}{2} = \frac{-u_{i-1}+u_i}{(x_{i-1}-x_i)^2} + u_i'\frac{1}{x_{i-1}-x_i} + \frac{u_i'''}{6}(x_{i-1}-x_i) + \dots$$

$$-u_i'' = \frac{-u_{i+1}+u_i}{(x_{i+1}-x_i)^2} + \frac{-u_{i-1}+u_i}{(x_{i-1}-x_i)^2} + u_i'\left(\frac{1}{x_{i+1}-x_i} + \frac{1}{x_{i-1}-x_i}\right) + \frac{u_i'''}{6}(x_{i+1}-x_i+x_{i-1}-x_i)$$

Uniform grid: $x_{i+1}-x_i = h, \ i=0,\dots,N$

$$-u_i'' = \frac{-u_{i+1}+u_i}{h^2} + \frac{-u_{i-1}+u_i}{h^2} + u_i'\frac{1}{h} - u_i'\frac{1}{h} + \frac{u_i'''}{6}h - \frac{u_i'''}{6}h + \dots$$

$$\Rightarrow -u_i'' = \frac{-u_{i+1}+2u_i-u_{i-1}}{h^2} + \frac{u_i^{(4)}}{12}h^2$$

$$-u_i'' = \frac{-u_{i+1}+2u_i-u_{i-1}}{h^2} + \underbrace{O(h^2)}$$

order of approximation

local approximation error

left finite-difference derivative: $D_x^- u_i = \frac{u_i - u_{i-1}}{h}$

right finite-difference derivative: $D_x^+ u_i = \frac{u_{i+1} - u_i}{h}$

central finite-difference derivative: $D_x^c u_i = \frac{u_{i+1} - u_{i-1}}{2h}$

$$D_{xx}^{(2)} u_i = \frac{D_x^+ u_i - D_x^- u_i}{h}$$

$u_0 = f_0$ left BC

$-\frac{1}{h^2}(u_0 - 2u_1 + u_2) = f_1 \Rightarrow -\frac{1}{h^2}(-2u_1 + u_2) = f_1 + \frac{1}{h^2} f_0$

$-\frac{1}{h^2}(u_1 - 2u_2 + u_3) = f_2$

$\dots$

$-\frac{1}{h^2}(u_{N-2} - 2u_{N-1} + u_N) = f_{N-1} \Rightarrow -\frac{1}{h^2}(u_{N-2} - 2u_{N-1}) = f_{N-1} + \frac{1}{h^2} f_1$

$u_N = f_1$ right BC

$$-\frac{1}{h^2}\begin{bmatrix} -2 & 1 & 0 & 0 & \dots & 0 \\ 1 & -2 & 1 & 0 & \dots & 0 \\ 0 & 1 & -2 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & 1 & -2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_{N-1} \end{bmatrix} = \begin{bmatrix} f_1 + \frac{f_0}{h^2} \\ f_2 \\ \vdots \\ f_{N-1} + \frac{f_1}{h^2} \end{bmatrix}$$

$A\vec{u} = \vec{f}$, $\vec{u} = A^{-1}\vec{f} \in \mathbb{R}^{N-1}$, FDM approximation of grid-values of the solution

$$L = \frac{1}{h^2}\begin{bmatrix} 2 & -1 & 0 & 0 & \dots & 0 \\ -1 & 2 & -1 & 0 & \dots & 0 \\ \vdots & & & & & \vdots \\ 0 & 0 & 0 & \dots & -1 & 2 \end{bmatrix}$$

Def. Matrix $A \in \mathbb{R}^{n\times n}$ is positive if $\vec{u}^T A \vec{u} \geq 0$

positive definite if $\vec{u}^T A \vec{u} > 0$, $\forall \vec{u} \in \mathbb{R}^n$, $\vec{u} \neq 0$

Def. Matrix $A \in \mathbb{R}^{n\times n}$ is symmetric if $A^T = A$

Th L is symmetric definite positive.

Proof

$u^T L u = \frac{1}{h^2}(2u_1^2 - u_1u_2 - u_1u_2 + 2u_2^2 - u_2u_3 + \dots - u_{N-1}u_{N-2} + 2u_{N-1}^2)$

$= \frac{1}{h^2}(u_1^2 + u_1^2 - 2u_1u_2 + u_2^2 + u_2^2 - 2u_2u_3 + u_3^2 + \dots + u_{N-2}^2 - 2u_{N-2}u_{N-1} + u_{N-1}^2 + u_{N-1}^2)$

$= \frac{1}{h^2}\left(u_1^2 + \sum_{i=1}^{N-2}(u_i - u_{i+1})^2 + u_{N-1}^2\right) > 0, \quad \vec{u} \neq 0$

Collaries:

1) eigendecomposition, $\mathcal{L} = Q \Lambda Q^T$, where $Q^T Q = I$
2) $\forall \lambda$ (eigenvalue of $\mathcal{L}$) - distinct, real, positive
3) $\mathcal{L}$ - invertible
4) $\exists$ unique solution to $\mathcal{L}\vec{u} = \vec{f}$

$\mathcal{L}\vec{v_i} = \lambda_i \vec{v_i}$

$N-1$ eigenvalues of $\mathcal{L} \in \mathbb{R}^{(N-1)\times(N-1)}$:

$$\lambda_i = \frac{4}{h^2} \sin^2\left(\frac{\pi i}{2N}\right), \quad i = 1, 2, \dots, N-1$$

$$[\vec{v_i}]_j = \sin\left(\frac{\pi i j}{N}\right), \quad i, j = 1, 2, \dots, N-1$$

$-v_i'' = \lambda_i v_i, \quad v_i(0) = v_i(D) = 0$

$\tilde{\lambda}_i = \left(\frac{\pi i}{D}\right)^2, \quad v_i(x) = \sin\left(\frac{\pi i x}{D}\right), \quad i = 1, 2, \dots$

$[\vec{v_i}]_j = v_i(x_j)$

$$\lim_{h \to 0} \frac{4}{h^2} \sin^2\left(\frac{\pi i h}{2D}\right) = \left(\frac{\pi i}{D}\right)^2, \quad i = 1, 2, \dots, N-1$$

$\lambda_1 = \frac{4}{h^2} \sin^2\left(\frac{\pi}{2N}\right)$

$\tilde{\lambda}_1 = \left(\frac{\pi}{D}\right)^2$

Lecture 4 - 1D Finite Difference Method

k - constant coefficient

$-k \Delta u = f$

$k > 0,\ -ku'' = f,\ x \in (0,1)$

$$-ku_i'' = k\,\frac{-u_{i-1} + 2u_i - u_{i+1}}{h^2} + O(h^2)$$

k - non-constant coefficient

$-\nabla \cdot (k \nabla u) = f$

$-(k(x)u')' = f,\ x \in (0,1)$

$$(ku')_i' = \frac{1}{h}\left(a_{i+1}\frac{u_{i+1} - u_i}{h} - a_i \frac{u_i - u_{i-1}}{h}\right) + O(h^2)$$

$$\frac{u_{i+1} - u_i}{h} = u_i' + \frac{h}{2}u_i'' + \frac{h^2}{6}u_i''' + O(h^3)$$

$$\frac{u_i - u_{i-1}}{h} = u_i' - \frac{h}{2}u_i'' + \frac{h^2}{6}u_i''' + O(h^3)$$

$$\Rightarrow (ku')_i' = \frac{a_{i+1} - a_i}{h}u_i' + \frac{a_{i+1} + a_i}{h}u_i'' + \frac{h(a_{i+1} - a_i)}{6}u_i''' + O(h^2)$$

$$(ku')_i' = k_i u_i'' + k_i' u_i'$$

$$\frac{1}{h}\left(a_{i+1}\frac{u_{i+1} - u_i}{h} - a_i\frac{u_i - u_{i-1}}{h}\right) - (ku')_i' = \frac{a_{i+1} - a_i}{h}u_i' + \frac{a_{i+1} + a_i}{2}u_i'' + \frac{h(a_{i+1} - a_i)}{6}u_i''' + O(h^2) - k_i u_i'' - k_i' u_i'$$

$$= \left(\frac{a_{i+1} - a_i}{h} - k_i'\right)u_i' + \left(\frac{a_{i+1} + a_i}{2} - k_i\right)u_i'' + \frac{h(a_{i+1} - a_i)}{6}u_i''' + O(h^2)$$

$$\text{error} = O(h^2) \quad \text{if} \begin{cases} \dfrac{a_{i+1} - a_i}{h} = k_i' + O(h^2) \\ \dfrac{a_{i+1} + a_i}{2} = k_i' + O(h^2) \end{cases}$$

$$\Rightarrow \frac{1}{h}\left(a_{i+1}\frac{u_{i+1} - u_i}{h} - a_i\frac{u_i - u_{i-1}}{h}\right) - (ku')_i' = O(h^2)$$

$a_i = \dfrac{k(x_i) + k(x_{i-1})}{2}$ arithmetic mean of values

$a_i = k(x_i - 0.5h)$ values between x_i and x_{i-1}

$a_i = \sqrt{k(x_i)\,k(x_{i-1})}$ geometric mean of values

$a_i = k(x_i) \rightarrow$ first-order approximation

Arithmetic mean:

$$-(ku')'_i = -\frac{1}{h}\left(\frac{k_{i+1}+k_i}{2}\,\frac{u_{i+1}-u_i}{h} - \frac{k_i+k_{i-1}}{2}\,\frac{u_i-u_{i-1}}{h}\right) + O(h^2)$$

$$= \frac{1}{h^2}\left(-\frac{k_i+k_{i-1}}{2}u_{i-1} + \frac{k_{i+1}+2k_i+k_{i-1}}{2}u_i - \frac{k_{i+1}+k_i}{2}u_{i+1}\right) + O(h^2)$$

$$= \frac{1}{h^2}\left(-a_i u_{i-1} + (a_i+a_{i+1})u_i - a_{i+1}u_{i+1}\right) + O(h^2)$$

Approximation of boundary conditions

Dirichlet BC: $u_N = \mu_2$

$$\frac{1}{h^2}\left(-a_{N-1}u_{N-2} + (a_{N-1}+a_N)u_{N-1} - a_N u_N\right) = f_{N-1}$$

$$\frac{1}{h^2}\left(-a_{N-1}u_{N-2} + (a_{N-1}+a_N)u_{N-1}\right) = f_{N-1} + \frac{a_N}{h^2}\mu_2$$

Robin BC: $-k(0)u_0' + \beta u_0 = \mu_1$

$$u_0' = \frac{u_1-u_0}{h} + O(h) \qquad \left(\beta + \frac{k_0}{h}\right)u_0 - \frac{k_0}{h}u_1 = \mu_1$$

$$\frac{1}{h^2}\left(-a_1u_0 + (a_1+a_2)u_1 - a_2u_2\right) = f_1$$

$$x_{-1} = x_0 - h \qquad u_0' = \frac{u_1-u_{-1}}{2h} + O(h^2) \qquad -k_0\frac{1}{2h}(u_1-u_{-1}) + \beta u_0 = \mu_1$$

$$\frac{1}{h^2}\left(-a_0u_{-1} + (a_0+a_1)u_0 - a_1u_1\right) = f_0 \qquad \frac{1}{h^2}\left(-a_1u_0 + (a_1+a_2)u_1 - a_2u_2\right) = f_1$$

$$u_{-1} = -\left(\frac{2h}{k_0}\right)\beta u_0 + u_1 + \left(\frac{2h}{k_0}\right)\mu_1$$

$$\frac{1}{h^2}\left(\left(\frac{2h\beta}{k_0}a_0 + a_0 + a_1\right)u_0 - (a_0+a_1)u_1\right) = f_0 + \frac{2a_0\mu_1}{hk_0}$$

Global error of the numerical solution

$u_i = u(x_i)$ – exact solution, $\tilde{u}_i$ – numerical solution at x_i

RMSE, $\varepsilon = \sqrt{\frac{1}{N-1}\sum_{i=1}^{N-1}|u_i-\tilde{u}_i|^2}$

$u(x), v(x)$ – functions on $[a,b]$ and $u(a)=v(a)$, $u(b)=v(b)$

$$\|u-v\|_2 = \sqrt{\int_a^b |u(x)-v(x)|^2\,dx} \approx \sqrt{\sum_{i=1}^{N-1}|u_i-v_i|^2\,\frac{b-a}{N-1}}$$

$\vec{u}, \vec{v}$ – vectors in $\mathbb{R}^{N-1}$

$$\|\vec{u}-\vec{v}\|_2 = \sqrt{\sum_{i=1}^{N-1}|u_i-v_i|^2}$$

$$RMSE(\vec{u},\vec{v}) = \|\vec{u}-\vec{v}\|_{2,h} = \frac{1}{\sqrt{N-1}}\|\vec{u}-\vec{v}\|_2 \approx \frac{1}{\sqrt{b-a}}\|u-v\|_2$$

$$-u'' = \frac{1}{h^2}(-u_{i-1} + 2u_i - u_{i+1}) + p_i h^2$$

Dirichlet BC:
$$\left|\begin{array}{l} -\frac{1}{h^2}(2u_1 - u_2) = f_1 + u_0 h^{-2} + p_1 h^2 \\ -\frac{1}{h^2}(-u_1 + 2u_2 - u_3) = f_2 + p_2 h^2 \\ \vdots \\ -\frac{1}{h^2}(-u_{N-2} + 2u_{N-1}) = f_{N-1} + u_N h^{-2} + p_{N-1} h^2 \end{array}\right.$$

Numerical problem:
$$\left|\begin{array}{l} -\frac{1}{h^2}(2\tilde{u}_1 - \tilde{u}_2) = f_1 + u_0 h^{-2} \\ -\frac{1}{h^2}(-\tilde{u}_1 + 2\tilde{u}_2 - \tilde{u}_3) = f_2 \\ \vdots \\ -\frac{1}{h^2}(-\tilde{u}_{N-2} + 2\tilde{u}_{N-1}) = f_{N-1} + u_N h^{-2} \end{array}\right.$$

$$\begin{bmatrix} p_1 h^2 \\ p_2 h^2 \\ \dots \\ p_{N-1} h^2 \end{bmatrix} = h^2 \begin{bmatrix} p_1 \\ p_2 \\ \dots \\ p_{N-1} \end{bmatrix} = h^2 \vec{p}, \quad \vec{u} = \begin{bmatrix} u_1 \\ u_2 \\ \dots \\ u_{N-1} \end{bmatrix}, \quad \vec{\tilde{u}} = \begin{bmatrix} \tilde{u}_1 \\ \tilde{u}_2 \\ \dots \\ \tilde{u}_{N-1} \end{bmatrix}, \quad \vec{f} = \begin{bmatrix} f_1 + u_0 h^{-2} \\ f_2 \\ \dots \\ f_{N-1} + u_N h^{-2} \end{bmatrix}$$

$$A \in \mathbb{R}^{(N-1)\times(N-1)}: \begin{cases} A\vec{u} = \vec{f} + h^2\vec{p} \\ A\vec{\tilde{u}} = \vec{f} \end{cases}$$

$$A\vec{e} = h^2\vec{p}, \quad \vec{e} = \vec{u} - \vec{\tilde{u}}, \quad \vec{e} \in \mathbb{R}^{N-1}$$

Th Global numerical solution error of Poisson equation $-u'' = f$ with Dirichlet BC for $O(h^2)$ finite-difference method is $\|\vec{e}\|_{2,h} = O(h^2)$

Proof

A - symmetric positive definite

$\Rightarrow A = Q\Lambda Q^T$, $A^{-1} = Q\Lambda^{-1}Q^T$ with $\lambda_{max}(A^{-1}) = \frac{1}{\lambda_{min}(A)}$, $\|A\|_2 = \sqrt{\lambda_{max}(A^TA)}$

$A\vec{e} = h^2\vec{p} \Rightarrow \vec{e} = h^2A^{-1}\vec{p}$

$$\|\vec{e}\|_2 = \|h^2A^{-1}\vec{p}\|_2 \le h^2\|A^{-1}\|_2\,\|\vec{p}\|_2 = h^2\sqrt{\lambda_{max}(A^{-T}A^{-1})}\,\|\vec{p}\|_2 = \frac{h^2}{\lambda_{min}(A)}\|\vec{p}\|_2$$
$$= h^2\frac{(x_N - x_0)^2 + O(h^2)}{\pi^2}\|\vec{p}\|_2$$

$$\|\vec{e}\|_{2,h} \le h^2\frac{(x_N - x_0)^2 + O(h^2)}{\pi^2}\|\vec{p}\|_{2,h} = O(h^2)$$

Dirichlet + Neumann BC

$-u'' = f,\ u(x_0)=0,\ u'(x_N)=0$

$O(h^2): -\frac{1}{h^2}(u_{i-1}-2u_i+u_{i+1}) = f_i,\ i=1,\dots,N$

$O(h): \frac{1}{h}(u_{N+1}-u_N)=0$

$\tilde{A} \in \mathbb{R}^{N\times N} = \frac{1}{h^2}\begin{bmatrix} 2 & -1 & 0 & \dots & 0 \\ -1 & 2 & -1 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & -1 \\ 0 & 0 & 0 & -\frac{1}{h} & \frac{1}{h} \end{bmatrix} \Rightarrow \tilde{A}\vec{u} = \vec{f} + h^2\vec{p} + h\vec{q},\ \vec{q} = [0,\dots,0,q_N]^T$

$\tilde{A}\vec{\tilde{u}} = \vec{f},\ \vec{e} = \vec{u} - \vec{\tilde{u}} \Rightarrow \tilde{A}\vec{e} = h^2\vec{p} + h\vec{q}$

Let $\vec{e} = \vec{e}_1 + \vec{e}_2$ s.t. $\tilde{A}\vec{e}_1 = h^2\vec{p}$ and $\tilde{A}\vec{e}_2 = h\vec{q} \Rightarrow \|e\|_2 = \|e_1+e_2\| \le \|e_1\|_2 + \|e_2\|_2$

Th: Global numerical solution error of the Poisson equation $-u''=f,\ u(x_0)=0,$ $-u'(x_N)=\mu$ obtained with $O(h^2)$ finite-difference discretization at $x_i,\ i=1,\dots,N-1$ and $O(h)$ discretization at x_N is $\|\vec{e}\|_{2,h} = O(h^2)$

$h_2 = \frac{h_1}{k}$

$O(h)$ discretization error: $\frac{\|\vec{e_{h_1}}\|_{2,h}}{\|\vec{e_{h_2}}\|_{2,h}} = \frac{O(h_1)}{O(h_2)} \approx k$

$O(h^2)$ discretization error: $\frac{\|\vec{e_{h_1}}\|_{2,h}}{\|\vec{e_{h_2}}\|_{2,h}} = \frac{O(h_1^2)}{O(h_2^2)} \approx k$

$h \to 0$, asymptotic

$-\varepsilon c'' + vc' = 0,\ c(0)=0,\ c(1)=1$

$c(x) = \frac{e^{\frac{vx}{\varepsilon}}-1}{e^{\frac{v}{\varepsilon}}-1},\ Pe = \frac{vL}{\varepsilon}$

$-\varepsilon c_i'' + vc_i' \approx \varepsilon\frac{-c_{i-1}+2c_i-c_{i+1}}{h^2} + v\frac{c_{i+1}-c_{i-1}}{2h} = \varepsilon\left(\frac{-c_{i-1}+2c_i-c_{i+1}}{h^2} + \frac{vh}{2\varepsilon}\frac{c_{i+1}-c_{i-1}}{h^2}\right) = 0$

$p_h = \frac{vh}{2\varepsilon} = \frac{h}{2L}Pe = \frac{1}{2N}Pe,\ (-1-p_h)c_{i-1} + 2c_i + (-1+p_h)c_{i+1} = 0,\ i=2,3,\dots,N-2$

left: $-\varepsilon c_1'' + vc_1' = 0,\ c_0 = 0 \Rightarrow \frac{\varepsilon}{h^2}((-1-p_h)c_0 + 2c_1 + (-1+p_h)c_2) = 0 \Rightarrow 2c_1 + (-1+p_h)c_2 = 0$

right: $-\varepsilon c_{N-1}'' + vc_{N-1}' = 0,\ c_N = 1 \Rightarrow \frac{\varepsilon}{h^2}((-1-p_h)c_{N-2} + 2c_{N-1} + (-1+p_h)) = 0 \Rightarrow (-1-p_h)c_{N-2} + 2c_{N-1} = 1-p_h$

$A\vec{c} = \vec{f},\ A = \begin{bmatrix} 2 & -1+p_h & 0 & 0 & \dots & 0 \\ -1-p_h & 2 & -1+p_h & 0 & \dots & 0 \\ \vdots & & & & & -1+p_h \\ 0 & 0 & 0 & 0 & -1-p_h & 2 \end{bmatrix}\quad \vec{f} = \begin{bmatrix} 0 \\ 0 \\ \dots \\ 1-p_h \end{bmatrix}$

Lecture 5 - 2D Finite Difference Method

$\Omega \in \mathbb{R}^2 = (a,b) \times (c,d)$, boundary $\partial\Omega$

$-\Delta u(x,y) = f(x,y),\ (x,y) \in \Omega, \quad \Delta u = \dfrac{\partial^2 u}{\partial x^2} + \dfrac{\partial^2 u}{\partial y^2}$

$u(x,y) = 0,\ (x,y) \in \partial\Omega$

$\Omega_h = \{(x_i, y_j) \mid x_i = a + i h_x,\ i = 0, 1, \dots, N_x;\ y_j = c + j h_y,\ j = 0, 1, \dots, N_y\}$

$h_x = \dfrac{b-a}{N_x},\quad h_y = \dfrac{d-c}{N_y},\quad u_{ij} = u(x_i, y_j) \quad f_{ij} = f(x_i, y_j)$

$-\dfrac{\partial^2 u_{i,j}}{\partial x^2} = \dfrac{-u_{i-1,j} + 2u_{i,j} - u_{i+1,j}}{h_x^2} + O(h_x^2)$

$-\dfrac{\partial^2 u_{i,j}}{\partial y^2} = \dfrac{-u_{i,j-1} + 2u_{i,j} - u_{i,j+1}}{h_y^2} + O(h_y^2)$

$\Delta u_{i,j} = \dfrac{-u_{i-1,j} + 2u_{i,j} - u_{i+1,j}}{h_x^2} + O(h_x^2) + \dfrac{-u_{i,j-1} + 2u_{i,j} - 2u_{i,j-1}}{h_y^2} + O(h_y^2)$

inner points: $\dfrac{-u_{i-1,j} + 2u_{i,j} - u_{i+1,j}}{h_x^2} + \dfrac{-u_{i,j-1} + 2u_{i,j} - u_{i,j+1}}{h_y^2} = f_{i,j}$, $i = 1, 2, \dots, N_x - 1$, $j = 1, 2, \dots, N_y - 1$

boundary points (Dirichlet: $u(x,y) = 0$, $(x,y) \in \partial\Omega$):

- lower (South): $i = 0, 1, \dots, N_x;\ j = 0$
- upper (North): $i = 0, 1, \dots, N_x;\ j = N_y$
- left (West): $i = 0;\ j = 0, 1, \dots, N_y$
- right (East): $i = N_x,\ j = 0, 1, \dots, N_y$

$\vec{u} \in \mathbb{R}^{(N_x - 1)(N_y - 1)}$

lexicographic order: $\vec{u} = [u_{1,1} \dots u_{N_x-1,1}\ u_{1,2} \dots u_{N_x-1,2} \dots u_{1,N_y-1} \dots u_{N_x-1,N_y-1}]^T$

$A \in \mathbb{R}^{(N-1)\times(N-1)}$ $\qquad D \in \mathbb{R}^{N_x (N-1)}$

$A = \dfrac{1}{h^2}\begin{bmatrix} 2 & -1 & 0 & 0 & \dots & 0 \\ -1 & 2 & -1 & 0 & \dots & 0 \\ \vdots & & & & & -1 \\ 0 & 0 & 0 & 0 & -1 & 2 \end{bmatrix} \qquad D = \dfrac{1}{h}\begin{bmatrix} 1 & 0 & 0 & 0 & \dots & 0 \\ -1 & 1 & 0 & 0 & \dots & 0 \\ \vdots & & & & & 1 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{bmatrix} \Bigg\} \Rightarrow A = D^T D$

$D_x \in \mathbb{R}^{N_x \times (N_x - 1)}$ $\qquad D_y \in \mathbb{R}^{N_y \times (N_y - 1)}$

$D_x = \dfrac{1}{h_x}\begin{bmatrix} 1 & 0 & 0 & 0 & \dots & 0 \\ -1 & 1 & 0 & 0 & \dots & 0 \\ \vdots & & & & & 1 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{bmatrix} \qquad D_y = \dfrac{1}{h_y}\begin{bmatrix} 1 & 0 & 0 & 0 & \dots & 0 \\ -1 & 1 & 0 & 0 & \dots & 0 \\ \vdots & & & & & 1 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{bmatrix}$

$A_{xx} = D_x^T D_x \in \mathbb{R}^{(N_x-1)\times(N_x-1)} \qquad A_{yy} = D_y^T D_y \in \mathbb{R}^{(N_y-1)\times(N_y-1)}$

$I_x = I_{N_x-1},\ I_y = I_{N_y-1} \Rightarrow A = I_y \otimes A_{xx} + A_{yy} \otimes I_x$

Kronecker product $\otimes$: $A \in \mathbb{R}^{2\times 3},\ B \in \mathbb{R}^{m\times n} \Rightarrow A\otimes B \in \mathbb{R}^{2m\times 3n}$

$$A\otimes B = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \end{bmatrix} \otimes B = \begin{bmatrix} a_{11}B & a_{12}B & a_{13}B \\ a_{21}B & a_{22}B & a_{23}B \end{bmatrix}$$

$\boxed{\text{Th}}$ 2D FD negative Laplacian matrix A (with Dirichlet BC) is symmetric.

Proof: $A^T = A$

$$\vec{v}^T A \vec{u} = (\vec{v}^T A \vec{u})^T = \vec{u}^T A^T \vec{v} = \vec{u}^T A \vec{v}, \quad \vec{u} = \vec{v} = 0,\ x\in\partial\Omega, \quad h_x = h_y = h$$

$$\vec{v}^T A \vec{u} = \sum_{j=1}^{N_y-1}\sum_{i=1}^{N_x-1} v_{i,j}\left(\frac{u_{i,j}-u_{i-1,j}}{h^2} - \frac{u_{i+1,j}-u_{i,j}}{h^2} + \frac{u_{i,j}-u_{i,j-1}}{h^2} - \frac{u_{i,j+1}-u_{i,j}}{h^2}\right)$$

fixed $j = 1, \dots, N_y - 1$: $\displaystyle\sum_{i=1}^{N_x-1} v_{i,j}\left(\frac{u_{i,j}-u_{i-1,j}}{h^2} - \frac{u_{i+1,j}-u_{i,j}}{h^2}\right) = \sum_{i=1}^{N_x} \frac{v_{i,j}-v_{i-1,j}}{h}\cdot\frac{u_{i,j}-u_{i-1,j}}{h}$

fixed $i = 1, \dots, N_x - 1$: $\displaystyle\sum_{j=1}^{N_y-1} v_{i,j}\left(\frac{u_{i,j}-u_{i,j-1}}{h^2} - \frac{u_{i,j+1}-u_{i,j}}{h^2}\right) = \sum_{j=1}^{N_y} \frac{v_{i,j}-v_{i,j-1}}{h}\cdot\frac{u_{i,j}-u_{i,j-1}}{h}$

$\Rightarrow \vec{v}^T A \vec{u} = \vec{u}^T A \vec{v}$

$\boxed{\text{Th}}$ The 2D FD negative Laplacian matrix A (with Dirichlet BC) is positive-definite.

Proof $\vec{u}^T A \vec{u} > 0,\ \vec{u} \neq 0$

$$\vec{u}^T A \vec{u} = \sum_{j=1}^{N_y-1}\sum_{i=1}^{N_x}\left(\frac{u_{i,j}-u_{i-1,j}}{h^2}\right)^2 + \sum_{j=1}^{N_y}\sum_{i=1}^{N_x-1}\left(\frac{u_{i,j}-u_{i,j-1}}{h^2}\right)^2 > 0$$

$$A\vec{v}_k = \lambda_k \vec{v}_k \Rightarrow \frac{1}{h^2}\left(-v_k(i-1,j) - v_k(i,j-1) + 4v_k(i,j) - v_k(i+1,j) - v_k(i,j+1)\right) = \lambda_k v_k(i,j)$$

$v_k(0,:) = v_k(N_x,:) = v_k(:,0) = v_k(i,N_y) = 0,\ \vec{v}_k \neq 0$

$v_{k_x,k_y}(i,j) = \sin\left(\frac{\pi i k_x}{N_x}\right)\sin\left(\frac{\pi j k_y}{N_y}\right)$

$\sin(\alpha\pm\beta) = \sin(\alpha)\cos(\beta) \pm \cos(\alpha)\sin(\beta),\quad 1-\cos(2\alpha) = 2\sin^2(\alpha)$

$$\lambda_{k_x,k_y} = \frac{4}{h^2}\left(\sin^2\left(\frac{\pi k_x}{2N_x}\right) + \sin^2\left(\frac{\pi k_y}{2N_y}\right)\right)$$

A-diagonally dominant $\Rightarrow |a_{nn}| \geq \sum_{m\neq n} |a_{nm}|$

inner-point row of A: $\left[\dots -\frac{1}{h^2} \dots -\frac{1}{h^2}\ \frac{4}{h^2}\ -\frac{1}{h^2} \dots -\frac{1}{h^2} \dots\right]$

Boundary point rows of A - strictly diagonally dominant $\Rightarrow |a_{nn}| > \sum_{m\neq n} |a_{nm}|$

boundary-point row of A: $\left[\dots -\frac{1}{h^2}\ \frac{4}{h^2}\ -\frac{1}{h^2} \dots -\frac{1}{h^2} \dots\right]$

Lecture 6 - 1D Finite Volume Method

1D: $w' + qu = f, \quad w = -ku'$

$\nabla \cdot \vec{j} + qu = 0, \quad \vec{j} = -k\nabla u$

$-(ku')' + qu = f, \quad x \in (a,b)$

$-k(a)u'(a) + \beta u(a) = \mu_1, \quad u(b) = \mu_2$

$[a_i, b_i], \quad i = 1, \dots, N-1, \quad \Omega = [a,b]$

$$\frac{1}{b_i - a_i}\int_{a_i}^{b_i}\left[-(ku')' + qu\right] dx = \frac{1}{b_i - a_i}\int_{a_i}^{b_i} f \, dx$$

$\{x_i, \ i = 0, \dots, N\}, \quad h_i = x_i - x_{i-1}, \quad i = 1, \dots, N$

$x_{i-1/2} = x_i - 0.5h_i, \quad x_{i+1/2} = x_i + 0.5h_{i+1}$

$w(x) = -k(x)u'(x), \quad u_i = u(x_i), \quad w_{i\pm 1/2} = w(x_{i\pm 1/2})$

$$\int_{x_{i-1/2}}^{x_{i+1/2}} w'(x)\,dx + \int_{x_{i-1/2}}^{x_{i+1/2}} q(x)u(x)\,dx = \int_{x_{i-1/2}}^{x_{i+1/2}} f(x)\,dx$$

Fundamental Theorem of Calculus on w':

$$w_{i+1/2} - w_{i-1/2} + \int_{x_{i-1/2}}^{x_{i+1/2}} q(x)u(x)\,dx = \int_{x_{i-1/2}}^{x_{i+1/2}} f(x)\,dx$$

$w_{i\pm 1/2} = -\left[ku'\right]_{i\pm 1/2} = -k_{i\pm 1/2}\, u'_{i\pm 1/2}$

$O(h^2)$ central-difference approximations for $u'_{i\pm 1/2}$:

$$u'_{i+1/2} = \frac{u_{i+1} - u_i}{h_{i+1}} - \frac{u'''_{i+1/2}}{24} h_{i+1}^2 + \dots, \qquad u'_{i-1/2} = \frac{u_i - u_{i-1}}{h_i} - \frac{u'''_{i-1/2}}{24} h_i^2 + \dots$$

$O(h^2)$ approximation for $w_{i\pm 1/2}$:

$$w_{i+1/2} = -k_{i+1/2}u'_{i+1/2} = -k_{i+1/2}\frac{u_{i+1} - u_i}{h_{i+1}} + O(h_{i+1}^2) \qquad w_{i-1/2} = -k_{i-1/2}u'_{i-1/2} = -k_{i-1/2}\frac{u_i - u_{i-1}}{h_i} + O(h_i^2)$$

$$\int_{x_{i-1/2}}^{x_{i+1/2}} q(x)u(x)\,dx \approx \frac{h_i + h_{i+1}}{2} q_i u_i, \quad \int_{x_{i-1/2}}^{x_{i+1/2}} f(x) \approx \frac{h_i + h_{i+1}}{2} f_i$$

$$-k_{i+1/2}\frac{u_{i+1} - u_i}{h_{i+1}} + k_{i-1/2}\frac{u_i - u_{i-1}}{h_i} + \frac{h_i + h_{i+1}}{2} q_i u_i \approx \frac{h_i + h_{i+1}}{2} f_i$$

$$w_{i+1/2} - w_{i-1/2} = -k_{i+1/2}\frac{u_{i+1}-u_i}{h_{i+1}} + k_{i-1/2}\frac{u_i-u_{i-1}}{h_i} + O(h_{i+1}^2) - O(h_i^2)$$

$$\frac{1}{x_{i+1/2}-x_{i-1/2}}\int_{x_{i-1/2}}^{x_{i+1/2}} w'(x)\,dx + \frac{1}{x_{i+1/2}-x_{i-1/2}}\int_{x_{i-1/2}}^{x_{i+1/2}} q(x)u(x)\,dx = \frac{1}{x_{i+1/2}-x_{i-1/2}}\int_{x_{i-1/2}}^{x_{i+1/2}} f(x)\,dx$$

$$\frac{2}{h_i+h_{i+1}}\int_{x_{i-1/2}}^{x_{i+1/2}} v(x)\,dx = \frac{2}{h_i+h_{i+1}}\int_{x_{i-1/2}}^{x_{i+1/2}} [v_i + v_i'(x-x_i)+\dots]\,dx = \frac{2}{h_i+h_{i+1}} v_i \int_{x_{i-1/2}}^{x_{i+1/2}} dx + \frac{2}{h_i+h_{i+1}} v_i' \int_{x_{i-1/2}}^{x_{i+1/2}} (x-x_i)\,dx + \dots$$

$$= v_i + \frac{v_i'}{4}(h_{i+1}-h_i) + O\left(\frac{h_{i+1}^3+h_i^3}{h_{i+1}+h_i}\right)$$

$$\Rightarrow \frac{2}{h_i+h_{i+1}}\int_{x_{i-1/2}}^{x_{i+1/2}} w'(x)\,dx = w_i' + \frac{w_i''}{4}(h_{i+1}-h_i) + O\left(\frac{h_{i+1}^3+h_i^3}{h_{i+1}+h_i}\right), \quad w' = -(ku')'$$

$$\Rightarrow \frac{2}{h_i+h_{i+1}}\int_{x_{i-1/2}}^{x_{i+1/2}} w'(x)\,dx = -(ku')'_i + \frac{w_i''}{4}(h_{i+1}-h_i) + O\left(\frac{h_{i+1}^3+h_i^3}{h_{i+1}+h_i}\right),$$ $O(h_{i+1}-h_i)$ FD approximation of $-(ku')'_i$

$k=1 \Rightarrow w' = -u''$

$$u_i'' = \frac{2}{h_i+h_{i+1}}\left(\frac{u_{i+1}-u_i}{h_{i+1}} - \frac{u_i-u_{i-1}}{h_i}\right) + \frac{u_i'''}{3}(h_{i+1}-h_i) + O\left(\frac{h_{i+1}^3+h_i^3}{h_{i+1}+h_i}\right)$$

$$\frac{2}{h_i+h_{i+1}}\int_{x_{i-1/2}}^{x_{i+1/2}} [-u''(x)]\,dx = -\frac{2}{h_i+h_{i+1}}\left(\frac{u_{i+1}-u_i}{h_{i+1}} - \frac{u_i-u_{i-1}}{h_i}\right) + O(h_{i+1}-h_i) + O\left(\frac{h_{i+1}^3+h_i^3}{h_{i+1}+h_i}\right)$$

$w' = -(ku')'$

$$(ku')'_i = \frac{2}{h_i+h_{i+1}}\left(k_{i+1/2}\frac{u_{i+1}-u_i}{h_{i+1}} - k_{i-1/2}\frac{u_i-u_{i-1}}{h_i}\right) + O(h_{i+1}-h_i) + O\left(\frac{h_{i+1}^3+h_i^3}{h_{i+1}+h_i}\right)$$

$$\Rightarrow \frac{2}{h_i+h_{i+1}}\int_{x_{i-1/2}}^{x_{i+1/2}} [-(ku')'(x)]\,dx = -\frac{2}{h_i+h_{i+1}}\left(k_{i+1/2}\frac{u_{i+1}-u_i}{h_{i+1}} - k_{i-1/2}\frac{u_i-u_{i-1}}{h_i}\right) + O(h_{i+1}-h_i) + O\left(\frac{h_{i+1}^3+h_i^3}{h_{i+1}+h_i}\right)$$

$$\frac{2}{h_i+h_{i+1}}\int_{x_{i-1/2}}^{x_{i+1/2}} q(x)u(x)\,dx = q_i u_i + O(h_{i+1}-h_i) + O\left(\frac{h_{i+1}^3+h_i^3}{h_{i+1}+h_i}\right)$$

$$\frac{2}{h_i+h_{i+1}}\int_{x_{i-1/2}}^{x_{i+1/2}} f(x)\,dx = f_i + O(h_{i+1}-h_i) + O\left(\frac{h_{i+1}^3+h_i^3}{h_{i+1}+h_i}\right)$$

$$-\frac{2}{h_i+h_{i+1}}\left(k_{i+1/2}\frac{u_{i+1}-u_i}{h_{i+1}} - k_{i-1/2}\frac{u_i-u_{i-1}}{h_i}\right) + q_i u_i = f_i + O(h_{i+1}-h_i) + O\left(\frac{h_{i+1}^3+h_i^3}{h_{i+1}+h_i}\right)$$

uniform grid: $h_{i+1} = h_i = h \Rightarrow O(h^2)$

very nonuniform ($h_{i+1} = h_i(1-O(h))$, $h = \max h_i$): $O(h_{i+1}-h_i) = O(h_i(1-O(h))-h_i) = O(h_i O(h)) = O(h^2)$

Dirichlet BC: $u_N = \mu_2$

Vertex $i = N-1$: $$-\frac{2}{h_{N-1}+h_N}\left(k_{N-1/2}\frac{u_N - u_{N-1}}{h_{N-1/2}} - k_{N-3/2}\frac{u_{N-1}+u_{N-2}}{h_{N-1}}\right) + q_{N-1}u_{N-1} = f_{N-1} + O(h_N - h_{N-1}) + O\left(\frac{h_N^3 + h_{N-1}^3}{h_N + h_{N-1}}\right)$$

Robin BC: $-k(0)u'(0) + \beta u(0) = \mu_1$ or $w_0 + \beta u_0 = \mu_1 \Rightarrow w_0 = \mu_1 - \beta u_0$

$$\frac{2}{h_1}(w_{1/2} - w_0) + \frac{2}{h_1}\int_{x_0}^{x_{1/2}} q(x)u(x)\,dx = \frac{2}{h_1}\int_{x_0}^{x_{1/2}} f(x)\,dx$$

$$\frac{2}{h_1}(w_{1/2} - w_0) = \frac{2}{h_1}\left(-k_{1/2}\frac{u_1 - u_0}{h_1} + O(h_1^2) - \mu_1 + \beta u_0\right) = \frac{2}{h_1}\left(-k_{1/2}\frac{u_1 - u_0}{h_1} - \mu_1 + \beta u_0\right) + O(h_1)$$

$$\frac{2}{h_1}\int_{x_0}^{x_{1/2}} q(x)u(x)\,dx = q_0u_0 + O(h_1), \quad \frac{2}{h_1}\int_{x_0}^{x_{1/2}} f(x)\,dx = f_0 + O(h_1)$$

$$\frac{2}{h_1}\left(-k_{1/2}\frac{u_1 - u_0}{h_1} - \mu_1 + \beta u_0\right) + q_0u_0 = f_0 + O(h_1)$$

Conservation Law of $-(ku')' = f - qu$:

Continuous: $w(b) - w(a) = \int_a^b [f(x) - q(x)u(x)]\,dx$, $w(x) = -k(x)u'(x)$

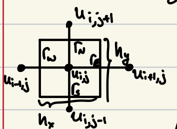
Discrete: $$-k_{i+1/2}\frac{u_{i+1}-u_i}{h_{i+1}} + k_{i-1/2}\frac{u_i - u_{i-1}}{h_i} + \frac{h_i + h_{i+1}}{2}q_iu_i = \frac{h_i + h_{i+1}}{2}f_i$$

$$-k_{N-1/2}\frac{u_N - u_{N-1}}{h_N} + k_{1/2}\frac{u_1 - u_0}{h_1} = \sum_{i=1}^{N-1}\frac{h_i + h_{i+1}}{2}(f_i - q_iu_i)$$

Lecture 7 - 2D Finite Volume Method

$\Omega \in \mathbb{R}^2,\quad -\nabla\cdot(k\nabla u) = f,\ (x,y)\in\Omega$

$-k\dfrac{\partial u}{\partial \vec{n}} = \alpha(u-u_0),\ (x,y)\in\partial\Omega$



$$\iint_{V_{ij}} \left[-\nabla\cdot(k\nabla u)\right] dv = \iint_{V_{ij}} f\, dV$$

$$\oint_{\Gamma_{ij}} (-k\nabla u\cdot\vec{n})\, d\Gamma = \iint_{V_{ij}} f\, dV$$

$$\oint_{\Gamma_{ij}} \left(-k\frac{\partial u}{\partial \vec{n}}\right) d\Gamma = \iint_{V_{ij}} f\, dV$$

$$\iint_{V_{ij}} f\, dV \approx f_{ij} h_x h_y$$

$$\oint_{\Gamma_{ij}} \left(-k\frac{\partial u}{\partial \vec{n}}\right) d\Gamma = \int_{\Gamma_W}\left(-k\left(-\frac{\partial u}{\partial x}\right)\right) dy + \int_{\Gamma_E}\left(-k\frac{\partial u}{\partial x}\right) dy + \int_{\Gamma_S}\left(-k\left(-\frac{\partial u}{\partial y}\right)\right) dx + \int_{\Gamma_N}\left(-k\frac{\partial u}{\partial y}\right) dx$$

$$\int_{\Gamma_W} k\frac{\partial u}{\partial x}\, dy \approx h_y k\frac{\partial u}{\partial x}\Big|_{(x_{i-1/2},y_j)} \approx h_y k_{i-1/2,j}\frac{u_{i,j}-u_{i-1,j}}{h_x}$$

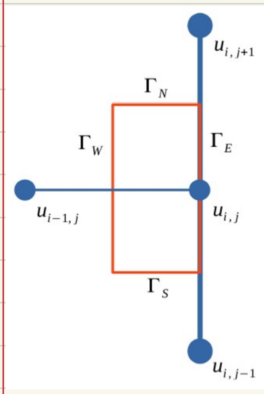
$$\int_{\Gamma_E}\left(-k\frac{\partial u}{\partial x}\right) dy \approx -h_y k\frac{\partial u}{\partial x}\Big|_{(x_{i+1/2},y_j)} \approx -h_y k_{i+1/2,j}\frac{u_{i+1,j}-u_{i,j}}{h_x}$$

$$\int_{\Gamma_S} k\frac{\partial u}{\partial y}\, dx \approx h_x k\frac{\partial u}{\partial y}\Big|_{(x_i,y_{j-1/2})} \approx h_x k_{i,j-1/2}\frac{u_{i,j}-u_{i,j-1}}{h_y}$$

$$\int_{\Gamma_N}\left(-k\frac{\partial u}{\partial y}\right) dx \approx -h_x k\frac{\partial u}{\partial y}\Big|_{(x_i,y_{j+1/2})} \approx -h_x k_{i,j+1/2}\frac{u_{i,j+1}-u_{i,j}}{h_y}$$

rearrange + divide by $h_x h_y$

$$f_{ij} = -\frac{k_{i-1/2,j}}{h_x^2}u_{i-1,j} - \frac{k_{i,j-1/2}}{h_y^2}u_{i,j-1} + \left(\frac{k_{i-1/2,j}}{h_x^2} + \frac{k_{i,j-1/2}}{h_y^2} + \frac{k_{i+1/2,j}}{h_x^2} + \frac{k_{i,j+1/2}}{h_y^2}\right)u_{i,j} - \frac{k_{i+1/2}}{h_x^2}u_{i+1,j} - \frac{k_{i,j+1/2}}{h_y^2}u_{i,j+1}$$



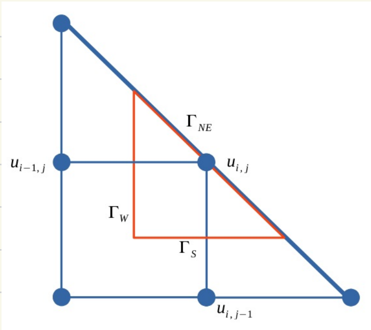
Neumann + Robin BC, Straight Boundary

$$\int_{\Gamma_E}\left(-k\frac{\partial u}{\partial x}\right) dy = \int_{\Gamma_E}\alpha(u-u_0)\, dy \approx h_y\alpha_{ij}(u_{ij}-u_0)$$

$\iint_{V_{ij}} f\, dV \approx \dfrac{h_x h_y}{2} f_{ij}$, Γ_S, Γ_N with coefficient $\dfrac{h_x}{2}$ instead of h_x

$$-\frac{2k_{i-1/2,j}}{h_x^2}u_{i-1,j} - \frac{k_{i,j-1/2}}{h_y^2}u_{i,j-1} + 2\left(\frac{k_{i-1/2,j}}{h_x^2} + \frac{k_{i,j-1/2}}{2h_y^2} + \frac{\alpha_{i,j}}{h_x} + \frac{k_{i,j+1/2}}{2h_y^2}\right)u_{i,j}$$

$$-\frac{k_{i,j+1/2}}{h_y^2}u_{i,j+1} = f_{ij} + \frac{2\alpha_{ij}}{h_x}u_0$$



Neumann + Robin BC, Skewed Boundary

$$\int_{\Gamma_{NE}} \left(-k\frac{\partial u}{\partial \vec{n}}\right) d\Gamma = \int_{\Gamma_{NE}} \alpha(u-u_0)\, d\Gamma \approx \sqrt{h_x^2+h_y^2}\, \alpha_{i,j}(u_{i,j}-u_0)$$

$$\iint_{V_{ij}} f\, dV \approx \frac{h_x h_y}{2} f_{ij}$$

$$-\frac{2k_{i-1/2,j}}{h_x^2}u_{i-1,j} - \frac{2k_{i,j-1/2}}{h_y^2}u_{i,j-1} + 2\left(\frac{k_{i-1/2,j}}{h_x^2}+\frac{k_{i,j-1/2}}{h_y^2}+\frac{\alpha_{i,j}\sqrt{h_x^2+h_y^2}}{h_x h_y}\right)u_{ij}$$
$$= f_{ij} + \frac{2\alpha_{ij}\sqrt{h_x^2+h_y^2}}{h_x h_y}u_0$$

$\vec{v}^T A\vec{u} = (\vec{v}^T A\vec{u})^T = \vec{u}^T A^T \vec{v} = \vec{u}^T A\vec{v}, \quad \vec{u},\vec{v} \in \mathbb{R}^{N-1}$

$$[A\vec{u}]_{ij} = k_{i-1/2,j}\frac{u_{i,j}-u_{i-1,j}}{h_x^2} - k_{i+1/2,j}\frac{u_{i+1,j}-u_{i,j}}{h_x^2} + k_{i,j-1/2}\frac{u_{i,j}-u_{i,j-1}}{h_y^2} - k_{i,j+1/2}\frac{u_{i,j+1}-u_{i,j}}{h_y^2}$$

Dirichlet BC: $u_{0,j} = u_{N_x,j} = 0, \ j = 1,\dots,N_y-1 \quad u_{i,0} = u_{i,N_y} = 0, \ i = 1,\dots,N_x-1$

fixed $j = 1,\dots,N_y-1$: $\displaystyle\sum_{i=1}^{N_x-1} v_{ij}\left[k_{i-1/2,j}\frac{u_{i,j}-u_{i-1,j}}{h_x^2} - k_{i+1/2,j}\frac{u_{i+1,j}-u_{i,j}}{h_x^2}\right] = \sum_{i=1}^{N_x}\frac{v_{i,j}-v_{i-1,j}}{h_x}k_{i-1/2,j}\frac{u_{i,j}-u_{i-1,j}}{h_x}$

fixed $i = 1,\dots,N_x-1$: $\displaystyle\sum_{j=1}^{N_y-1} v_{ij}\left[k_{i,j-1/2}\frac{u_{i,j}-u_{i,j-1}}{h_y^2} - k_{i,j+1/2}\frac{u_{i,j+1}-u_{i,j}}{h_y^2}\right] = \sum_{i=1}^{N_y}\frac{v_{i,j}-v_{i,j-1}}{h_y}k_{i,j-1/2}\frac{u_{i,j}-u_{i,j-1}}{h_y}$

$\Rightarrow \vec{v}^T A\vec{u} = \vec{u}^T A\vec{v}$

$k(x,y) > 0 \quad \displaystyle\vec{u}^T A\vec{u} = \sum_{j=1}^{N_y-1}\sum_{i=1}^{N_x} k_{i-1/2,j}\left(\frac{u_{i,j}-u_{i-1,j}}{h_x}\right)^2 + \sum_{j=1}^{N_y}\sum_{i=1}^{N_x-1} k_{i,j-1/2}\left(\frac{u_{i,j}-u_{i,j-1}}{h_y}\right)^2 > 0$

A - diagonally dominant if $|a_{nn}| \geq \sum_{m\neq n}|a_{nm}|$
A - Z-matrix if $a_{nm} \leq 0, \ m \neq n$
A - diagonally dominant Z-matrix
some rows -> strictly diagonally dominant, $|a_{nn}| > \sum_{m\neq n}|a_{nm}|$

Lecture 8 - Numerical Time Integration

Diffusion: $\frac{\partial u}{\partial t} - \nabla \cdot (k \nabla u) = f$

Wave: $\frac{1}{c^2} \frac{\partial^2 u}{\partial t^2} - \Delta u = f$

Unknown: $u(x,y,t)$, $u(x_i, y_j, t) = \vec{u}(t)$

$\vec{u}(t) \in \mathbb{R}^n$, $\vec{f}(t, \vec{u}) \in \mathbb{R}^n$

$$\frac{\partial \vec{u}}{\partial t} = \vec{f}(t, \vec{u}), \quad t \geq t_0, \quad \vec{u}(t_0) = \vec{u}_0$$

$$\frac{\partial}{\partial t} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \end{bmatrix} = \begin{bmatrix} f_1(t, u_1, u_2, \ldots) \\ f_2(t, u_1, u_2, \ldots) \\ \vdots \end{bmatrix}$$

$$\vec{u}' = -A\vec{u} + \vec{s}$$

$$\int_{t_0}^{t_0+h} \vec{u}' \, dt = \int_{t_0}^{t_0+h} \vec{f}(t, \vec{u}(t)) \, dt$$ (Fundamental Theorem of Calculus)

$$\vec{u}(t_0+h) - \vec{u}(t_0) = \int_{t_0}^{t_0+h} \vec{f}(t, \vec{u}(t)) \, dt$$

$$\vec{u}(t_0+h) = \vec{u}(t_0) + \int_{t_0}^{t_0+h} \vec{f}(t, \vec{u}(t)) \, dt$$

$$\int_{t_0}^{t_0+h} \vec{f}(t, \vec{u}(t)) \, dt \approx \sum_{k=1}^{K} w_k \vec{f}(t_k, \vec{u}(t_k)), \quad t_0 \leq t_k \leq t_0 + h$$

$$\left.\begin{aligned} &\int_{t_0}^{t_0+h} \vec{f}(t, \vec{u}(t)) \, dt \approx h \vec{f}(t_0, \vec{u}(t_0)) \\ &\vec{u}(t_0+h) \approx \vec{u}(t_0) + h\vec{f}(t_0, \vec{u}(t_0)) \\ &\vec{u}(t_k+h) \approx \vec{u}(t_k) + h\vec{f}(t_k, \vec{u}(t_k)), \quad k = 0, 1, \ldots \end{aligned}\right\} \text{Forward-Euler}$$

$$\left.\begin{aligned} &\int_{t_k}^{t_{k+1}} \vec{f}(t, \vec{u}(t)) \, dt \approx h \vec{f}(t_{k+1}, \vec{u}(t_{k+1})) \\ &\vec{u}(t_{k+1}) \approx \vec{u}(t_k) + h\vec{f}(t_{k+1}, \vec{u}(t_{k+1})), \quad k = 0, 1, \ldots \end{aligned}\right\} \text{Backward-Euler}$$

$$\left.\begin{aligned} &\int_{t_k}^{t_{k+1}} \vec{f}(t, \vec{u}(t)) \, dt \approx \frac{1}{2} h \left[\vec{f}(t_k, \vec{u}(t_k)) + \vec{f}(t_{k+1}, \vec{u}(t_{k+1}))\right] \\ &\vec{u}(t_{k+1}) \approx \vec{u}(t_k) + \frac{1}{2} h \left[\vec{f}(t_k, \vec{u}(t_k)) + \vec{f}(t_{k+1}, \vec{u}(t_{k+1}))\right], \quad k = 0, 1, \ldots \end{aligned}\right\} \text{Trapezoidal}$$

$$\int_{t_0}^{t_0+h} \vec{f}(t, \vec{u}(t)) \, dt \approx \sum_{i=1}^{k} w_i \vec{f}(t_k, \vec{u}(t_k)), \quad t_0 \leq t_k \leq t_0 + h$$

$t \in [t_0, t^*]$, $h = (t^* - t_0)/K$ time step, $\vec{u}_h(t_k)$ numerical approximation, $k = 0, 1, \ldots, K$

convergent: $\forall \vec{f}(t, \vec{u})$, $\forall t^* > t_0$, $\lim_{h \to 0^+} \max_k \| \vec{u}_h(t_k) - \vec{u}(t_k) \| = 0$

Th $\vec{u}(t)$ - continuously differentiable, $\vec{f}(t,\vec{u})$ - Lipschitz function

$\Rightarrow \exists \lambda > 0$ s.t. $\|\vec{f}(t,\vec{u}) - \vec{f}(t,\vec{v})\| \leq \lambda \|\vec{u}-\vec{v}\|,\ \forall \vec{u},\vec{v} \in \mathbb{R}^n$, Forward-Euler is convergent

Proof

$$\vec{e}_h(t_k) = \vec{u}_h(t_k) - \vec{u}(t_k)$$
$$\vec{u}(t_{k+1}) = \vec{u}(t_k) + h\vec{u}'(t_k) + O(h^2) = \vec{u}(t_k) + h\vec{f}(t_k, \vec{u}(t_k)) + O(h^2)$$
$$\vec{e}_h(t_{k+1}) = \vec{e}_h(t_k) + h\left[\vec{f}(t_k, \vec{u}(t_k) + \vec{e}_h(t_k)) - \vec{f}(t_k, \vec{u}(t_k))\right] + O(h^2)$$
$$\|\vec{e}_h(t_{k+1})\| \leq \|\vec{e}_h(t_k)\| + h\|\vec{f}(t_k, \vec{u}(t_k) + \vec{e}_h(t_k)) - \vec{f}(t_k, \vec{u}(t_k))\| + Ch^2$$
$$\|\vec{e}_h(t_{k+1})\| \leq (1+h\lambda)\|\vec{e}_h(t_k)\| + Ch^2,\quad k=0,1,\dots,n$$
$$\|\vec{e}_h(t_k)\| \leq \frac{C}{\lambda} h\left[(1+h\lambda)^k - 1\right] < \frac{C}{\lambda} h\left(e^{kh\lambda} - 1\right) \leq \frac{C}{\lambda}\left(e^{\lambda t^*} - 1\right)h$$
$$\lim_{h\to 0^+} \max_k \|\vec{e}_h(t_k)\| \leq \frac{C}{\lambda}\left(e^{\lambda t^*} - 1\right)\lim_{h\to 0^+} h = 0$$

$\vec{u}_h(t_1) - \vec{u}(t_1) = O(h^p)$, p-order of locality

Forward-Euler is locally $O(h^2)$: (explicit)

$$\vec{u}_h(t_1) - \vec{u}(t_1) = \vec{u}_h(t_0) + h\vec{f}(t_0, \vec{u}_h(t_0)) + O(h^2) - \vec{u}(t_0) + h\vec{f}(t_0, \vec{u}(t_0)) - O(h^2) = O(h^2)$$

Global error drops to $p-1$.

Backward-Euler: convergent, locally $O(h^2)$, globally $O(h)$ (implicit)

Trapezoidal: implicit, convergent, locally $O(h^3)$, globally $O(h^2)$

$$\|\vec{e}_h(t_k)\| \leq \frac{Ch^2}{\lambda} \exp\left(\frac{\lambda t^*}{1-\lambda h/2}\right),\quad k=0,1,\dots,K$$

FDM: $-\Delta u(\vec{x},t) \to A\vec{u}(t)$, $\vec{u}(t) \in \mathbb{R}^n$, $A \in \mathbb{R}^{n\times n}$, $\vec{u}' = -A\vec{u}$, $\vec{u}(0) = \vec{u}_0$

$\exists A = V\Lambda V^{-1} \Rightarrow \vec{u}(t) = V\vec{b}(t)$, $\vec{b}(t) = V^{-1}\vec{u}(t)$

$V\vec{b}' = -V\Lambda V^{-1}\vec{u}$, $\vec{u}_0 = V\vec{b}_0$, $\vec{b}' = -\Lambda\vec{b}$, $\vec{b}(0) = V^{-1}\vec{u}_0$

$b_j'(t) = -\lambda_j b_j(t),\ j=1,\dots,n;\quad b_j(t) = b_j(0)e^{-\lambda_j t},\ j=1,\dots,n$

$\vec{b}(t) = e^{-\Lambda t}\vec{b}(0) = e^{-\Lambda t}V^{-1}\vec{u}(0)$, $\vec{u}(t) = Ve^{-\Lambda t}V^{-1}\vec{u}(0)$

FDM: $-\Delta \to A$, $\lambda_j > 0$, $j=1,\dots,n$, $\vec{u}(t) = V\vec{b}(t)$

$$\vec{u}(t) = \sum_{j=1}^{n} b_j(t)\vec{v},\quad b_j(t) = b_j(0)e^{-\lambda_j t}$$

Stability

FDM/FVM: $\vec{u}' = -A\vec{u}, \ \vec{u}(t_0) = \vec{u}_0$

Forward-Euler:

$\vec{u}_h(t_k) = \vec{u}_h(t_{k-1}) - hA\,\vec{u}_h(t_{k-1}) = [I - hA]\,\vec{u}_h(t_{k-1}) = [I - hA]^k\,\vec{u}_0$

$A = V\Lambda V^{-1}, \quad \lambda_j, \ j = 1, \dots, n$

$\vec{u}(t_k) = V e^{\Lambda t_k} V^{-1} \vec{u}_0 = \sum_{j=1}^{n} b_j(0) e^{-\lambda_j t_k} \vec{v}_j$

$\vec{u}_h(t_k) = [I - hA]^k \vec{u}_0 = V[I - h\Lambda]^k V^{-1} \vec{u}_0 = \sum_{j=1}^{n} b_j(0)(1 - h\lambda_j)^k \vec{v}_j$

$\lambda_j > 0$, $e^{-\lambda_j t_k}$ decays with t_k, $|1 - h\lambda_j|^k$ growing with k if h is too large $\Rightarrow$ unstable

Conditional Stability: $|1 - h\lambda_j| < 1 \Rightarrow 0 < h < \frac{2}{\lambda_j}$, $j = 1, \dots, n$, $h = \Delta t \Rightarrow 0 < \Delta t < \frac{2}{\max_j \lambda_j}$

Backward-Euler:

$\vec{u}_h(t_k) = \vec{u}_h(t_{k-1}) - hA\,\vec{u}_h(t_k)$

$[I + hA]\,\vec{u}_h(t_k) = \vec{u}(t_{k-1})$

$\vec{u}_h(t_k) = [I + hA]^{-1}\,\vec{u}_{t_{k-1}} = [I + hA]^{-k}\,\vec{u}_0$

$\vec{u}_h(t_k) = [I + hA]^{-1}\,\vec{u}_0 = V[I + h\Lambda]^{-k} V^{-1} \vec{u}_0 = \sum_{j=1}^{n} b_j(0) \frac{1}{(1 + h\lambda_j)^k} \vec{v}_j$

$\lambda_j > 0 \Rightarrow$ stable for $\forall h > 0$

Trapezoidal:

$\vec{u}_h(t_k) = \vec{u}_h(t_{k-1}) - \frac{1}{2} hA\,[\vec{u}_h(t_{k-1}) + \vec{u}_h(t_k)]$

$[I + \frac{h}{2}A]\,\vec{u}_h(t_k) = [I - \frac{h}{2}A]\,\vec{u}(t_{k-1})$

$\vec{u}_h(t_k) = [I + \frac{h}{2}A]^{-1} [I - \frac{h}{2}A]\,\vec{u}_{t_{k-1}} = [I - \frac{h}{2}A]^k [I + \frac{h}{2}A]^{-k}\,\vec{u}_0$

$\vec{u}_h(t_k) = \sum_{j=1}^{n} b_j(0) \left(\frac{1 - \lambda_j h/2}{1 + \lambda_j h/2}\right)^k \vec{v}_j$

$\lambda_j > 0 \Rightarrow$ stable for $\forall h > 0$

$\frac{\partial u}{\partial t} - \Delta u = f, \quad (x, y) \in \Omega, \ 0 < t \le T$

$u(x, y, t) = g(x, y, t), \quad (x, y) \in \partial\Omega, \ 0 < t \le T$

$u(x, y, 0) = u_0(x, y), \quad (x, y) \in \Omega, \ t = 0$

$(x, y, t) \in \Omega \times (0, T]$

Forward-Euler:

$$\frac{\partial u(x,y,t)}{\partial t} = \Delta u(x,y,t) + f(x,y,t)$$

$$u(x,y,t_{k+1}) = u(x,y,t_k) + h[\Delta u(x,y,t_k) + f(x,y,t_k)]$$

$$u^{k+1}(x,y) = u^k(x,y) + h[\Delta u^k(x,y) + f^k(x,y)]$$

$k = 0, 1, \dots,\quad u(x,y,t_0) = u_0(x,y)$

BC: $u(x,y,t_k) = g(x,y,t_k)$, $(x,y) \in \partial\Omega$ must be enforced $\forall t_k$

Backward-Euler:

$$\frac{\partial u(x,y,t)}{\partial t} = \Delta u(x,y,t) + f(x,y,t)$$

$$u(x,y,t_{k+1}) = u(x,y,t_k) + h[\Delta u(x,y,t_{k+1}) + f(x,y,t_{k+1})]$$

$$u^{k+1}(x,y) - h\Delta u^{k+1}(x,y) = u^k(x,y) + hf^{k+1}(x,y)$$

$k = 0, 1, \dots,\quad u(x,y,t_0) = u_0(x,y)$

$(k+1)^{st}$ iteration:

$u^k(x,y)$, $f^{k+1}(x,y)$ – known for $(x,y) \in \Omega$

$u^{k+1}(x,y)$ – unknown

Space discretization: FDM/FVM

spacial grid, solution vector $\vec{u}^k \in \mathbb{R}^n$, $u(x_i, y_j, t_k)$

discretize $-\Delta \to A \in \mathbb{R}^{n \times n}$, Dirichlet BC to RHS $\vec{f}_k$

ex. Backward-Euler:

$$u^{k+1}(x,y) - h\Delta u^{k+1}(x,y) = u^k(x,y) + hf^{k+1}(x,y)$$

$$\vec{u}^{k+1} + hA\vec{u}^{k+1} = \vec{u}^k + h\vec{f}^{k+1}$$

$$[I + hA]\vec{u}^{k+1} = \vec{u}^k + h\vec{f}^{k+1}$$

$k = 0, 1, \dots,\quad \vec{u}^0 = \vec{u}_0$

find $\vec{u}^{k+1}$ → solve linear system

Lecture 9 - Numerical Solution of the Wave Equation

$$\frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} - \Delta u = f, \quad \vec{x} \in \Omega, \quad 0 < t \leq T$$

$$u(\vec{x}, t) = g(\vec{x}, t), \quad \vec{x} \in \partial\Omega, \quad 0 < t \leq T$$

$$u(\vec{x}, 0) = u_0(\vec{x}), \quad \vec{x} \in \Omega, \quad t = 0$$

$$\left.\frac{\partial u(\vec{x}, t)}{\partial t}\right|_{t=0} = v_0(\vec{x}), \quad \vec{x} \in \Omega, \quad t = 0$$

$$-\Delta u \to A\vec{u}, \quad \vec{u}(t) \in \mathbb{R}^n, \quad A \in \mathbb{R}^{n \times n}$$

$$\vec{u}'' = -c^2 A\vec{u}, \quad \vec{u}(0) = \vec{u}^0, \quad \vec{u}'(0) = \vec{w}^0$$

$$A = V\Lambda V^{-1} \Rightarrow \vec{u}(t) = V\vec{b}(t), \quad \vec{b}(t) = V^{-1}\vec{u}(t)$$

$$\vec{b}'' = -c^2\Lambda\vec{b}, \quad \vec{b}(0) = V^{-1}\vec{u}^0, \quad \vec{b}'(0) = V^{-1}\vec{w}^0$$

$$b_j''(t) = -c^2\lambda_j b_j(t), \quad j = 1, \dots, n$$

$$b_j(t) = a_j e^{ic\sqrt{\lambda_j}t} + d_j e^{-ic\sqrt{\lambda_j}t}$$

$$\vec{b}(t) = e^{ic\sqrt{\Lambda}t}\vec{a} + e^{-ic\sqrt{\Lambda}t}\vec{d}$$

$$\vec{b}(t) = \frac{1}{2}\left(e^{ic\sqrt{\Lambda}t} + e^{-ic\sqrt{\Lambda}t}\vec{d}\right)\vec{b}(0) + \frac{1}{2}\left(e^{ic\sqrt{\Lambda}t} - e^{-ic\sqrt{\Lambda}t}\right)\frac{1}{c}\sqrt{\Lambda}\,\vec{b}'(0)$$

$$\vec{u}'' = -c^2 A\vec{u}, \quad \vec{u}(0) = \vec{u}^0, \quad \vec{u}'(0) = \vec{w}^0$$

$$\vec{u}(t) = V\vec{b}(t), \quad \vec{u}(0) = \vec{u}^0, \quad \vec{u}'(0) = \vec{w}^0$$

$$\vec{u}(t) = V\left[\cos(c\sqrt{\Lambda}t)\vec{b}(0) + \sin(c\sqrt{\Lambda}t)\frac{1}{c\sqrt{\Lambda}}\vec{b}'(0) = \sum_{j=1}^{n}\left[b_j(0)\cos(ct\sqrt{\lambda_j}) + b_j'(0)\frac{1}{c\sqrt{\lambda_j}}\sin(ct\sqrt{\lambda_j})\right]\vec{v}_j\right.$$

$$\frac{\partial^2 u}{\partial t^2} = \frac{u^{k+1}(\vec{x}) - 2u^k(\vec{x}) + u^{k-1}(\vec{x})}{h_t^2} + O(h_t^2)$$

Explicit time-stepping: $\dfrac{u^{k+1}(\vec{x}) - 2u^k(\vec{x}) + u^{k-1}(\vec{x})}{c^2 h_t^2} = \Delta u^k(\vec{x}) + f^k(\vec{x})$

$$u^{k+1}(\vec{x}) = 2u^k(\vec{x}) - u^{k-1}(\vec{x}) + (ch_t)^2\Delta u^k(\vec{x}) + (ch_t)^2 f^k(\vec{x})$$

$$u(\vec{x}, 0) = u_0(\vec{x}), \quad \left.\frac{\partial u(\vec{x}, t)}{\partial t}\right|_{t=0} = v_0(\vec{x}), \quad \vec{x} \in \Omega$$

$$u^1(\vec{x}) = u^0(\vec{x}) + \left.\frac{\partial u(\vec{x}, t)}{\partial t}\right|_{t=0} h_t + \frac{1}{2}\left.\frac{\partial^2 u(\vec{x}, t)}{\partial t^2}\right|_{t=0} h_t^2 + O(h_t^3)$$

$$\frac{u^1(\vec{x}) - u^0(\vec{x})}{h_t} = \left.\frac{\partial u(\vec{x}, t)}{\partial t}\right|_{t=0} + O(h_t)$$

$$u^1(\vec{x}) = u^0(\vec{x}) + \left.\frac{\partial u(\vec{x}, t)}{\partial t}\right|_{t=0} h_t + \frac{1}{2}\left.\frac{\partial^2 u(\vec{x}, t)}{\partial t^2}\right|_{t=0} h_t^2 + O(h_t^3) = u_0(\vec{x}) + h_t v_0(\vec{x}) + \frac{(ch_t)^2}{2}\left[\Delta u_0(\vec{x}) + f^0(\vec{x})\right] + O(h_t^3)$$

$$\frac{1}{c^2}\left.\frac{\partial^2 u}{\partial t^2}\right|_{t=0} = \Delta u(\vec{x}, 0) + f(\vec{x}, 0)$$

$$u^0(\vec{x}) = u_0(\vec{x})$$
$$u^1(\vec{x}) = u_0(\vec{x}) + h_t v_0(\vec{x}) + \frac{(ch_t)^2}{2}\left[\Delta u_0(\vec{x}) + f^0(\vec{x})\right]$$
$$u^{k+1}(\vec{x}) = 2u^k(\vec{x}) - u^{k-1}(\vec{x}) + (ch_t)^2\left[\Delta u^k(\vec{x}) + f^k(\vec{x})\right]$$

$$-\Delta u^k(\vec{x}) \to A\vec{u}^k$$
$\vec{u}^0, \vec{w}^0$ - given
$$\vec{u}^1 = \vec{u}^0 + h_t\vec{w}_0 + \frac{(ch_t)^2}{2}\left[-A\vec{u}^0 + \vec{f}^0\right]$$
$$\vec{u}^{k+1} = 2\vec{u}^k - \vec{u}^{k-1} + (ch_t)^2\left[-A\vec{u}^k + \vec{f}^k\right]$$

$$\vec{u}^{k+1} = 2\vec{u}^k - \vec{u}^{k-1} - (ch_t)^2 A\vec{u}^k, \quad \vec{u}^k \in \mathbb{R}^n$$
$$A = V\Lambda V^{-1} \Rightarrow \vec{u}^k = V\vec{b}^k$$
$$\vec{b}^{k+1} = 2\vec{b}^k - \vec{b}^{k-1} - (ch_t)^2\Lambda\vec{b}^k, \quad \vec{b}^k \in \mathbb{R}^n$$
$$\vec{b}^{k+1} = 2b_j^k - b_j^{k-1} - (ch_t)^2\lambda_j b_j^k$$
$$b_j^k = (b_j)^k$$
$$b_j^2 - \left[2 - (ch_t)^2\lambda_j\right]b_j + 1 = 0$$
$$b_j = \frac{1}{2}\left[2 - (ch_t)^2\lambda_j \pm \sqrt{(2-(ch_t)^2\lambda_j)^2 - 4}\right.$$
$$(ch_t)^2\lambda_j = 4 \Rightarrow \frac{(ch_t)^2}{4}\lambda_j = 1$$

$$1D: \lambda_j = \frac{4}{h_x^2}\sin^2\left(\frac{\pi j}{2N}\right) \Rightarrow \left(\frac{ch_t}{h_x}\right)^2\sin^2\left(\frac{\pi j}{2N}\right) = 1 \quad \text{impossible}$$
$$\Rightarrow |b_j| \le 1 \Rightarrow \frac{(ch_t)^2}{4}\lambda_j \le 1$$

$$1D: \frac{(ch_t)^2}{4}\frac{4}{h_x^2}\sin^2\left(\frac{\pi j}{2N}\right) \le 1 \Rightarrow \frac{(ch_t)^2}{h_x^2} \le 1 \Rightarrow 0 \le \frac{ch_t}{h_x} \le 1$$

Lecture 10 - Nonlinear Problems

$\frac{\partial u}{\partial t} = f(u,t)$

Fisher's equation: $\frac{\partial u}{\partial t} = \Delta u + u(1-u)$

Newell-Whitehead-Segel equation: $\frac{\partial u}{\partial t} = \Delta u + u(1-u^2)$

Zeldovich equation: $\frac{\partial u}{\partial t} = \Delta u + u(1-u)(u-\alpha)$

$\vec{u}' = \vec{f}(\vec{u},t)$, $\vec{f}(\vec{u},t) \in \mathbb{R}^n$, $\vec{u} \in \mathbb{R}^n$

Fisher: $\vec{u}' = -A\vec{u} + \vec{u} \circ (1-\vec{u})$

NWS: $\vec{u}' = -A\vec{u} + \vec{u} \circ (1 - \vec{u} \circ \vec{u})$

Zeldovich: $\vec{u}' = -A\vec{u} + \vec{u} \circ (1-\vec{u}) \circ (\vec{u} - \alpha)$

$\vec{u} \circ \vec{v}$ - Hadamard (pointwise) product of two vectors

$\vec{u} \circ \vec{v} = \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{bmatrix} \circ \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix} = \begin{bmatrix} u_1 v_1 \\ u_2 v_2 \\ \vdots \\ u_n v_n \end{bmatrix}$ Scalar addition: $\vec{u} + \alpha = \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{bmatrix} + \begin{bmatrix} \alpha \\ \alpha \\ \vdots \\ \alpha \end{bmatrix} = \begin{bmatrix} u_1+\alpha \\ u_2+\alpha \\ \vdots \\ u_n+\alpha \end{bmatrix}$

FitzHugh-Nagumo equation:

$$\begin{cases} \frac{\partial u}{\partial t} = D_u \Delta u + \lambda u - u^3 - k - \sigma v \\ \tau \frac{\partial v}{\partial t} = D_v \Delta v + u - v \end{cases} \Rightarrow \begin{cases} \vec{u}' = -D_u A\vec{u} + \lambda\vec{u} - \vec{u}^3 - k - \sigma\vec{v} \\ \tau\vec{v}' = -D_v A\vec{v} + \vec{u} - \vec{v} \end{cases}$$

Forward-Euler: $\vec{u}' = \vec{f}(\vec{u},t) \Rightarrow \vec{u}^{k+1} = \vec{u}^k + h_t \vec{f}^k(\vec{u}^k)$

Fisher: $\vec{u}' = -A\vec{u} + \vec{u} - \vec{u}^2 \Rightarrow \vec{f}(\vec{u}) = -A\vec{u} + \vec{u} - \vec{u}^2 \Rightarrow \vec{u}^{k+1} = h_t\left[-A\vec{u}^k + \vec{u}^k - (\vec{u}^k)^2\right] + \vec{u}^k$

Backward Euler: $\vec{u}' = \vec{f}(\vec{u},t) \Rightarrow \vec{u}^{k+1} = \vec{u}^k + h_t \vec{f}^{k+1}(\vec{u}^{k+1})$

Fisher: $\vec{u}^{k+1} = \vec{u}^k + h_t\left[-A\vec{u}^{k+1} + \vec{u}^{k+1} - (\vec{u}^{k+1})^2\right]$

Picard's Method

$\vec{u} = h\vec{f}(\vec{u}) + \vec{v}$, $\vec{u}_0$ - initial guess, $\vec{u}_{i+1} = \vec{p}(\vec{u}_i)$

$\vec{p}(\vec{u}) = h\vec{f}(\vec{u}) + \vec{v}$

Convergence: $\lim_{i \to \infty} \vec{u}_i = \vec{\tilde{u}}$, $\vec{\tilde{u}} = h\vec{f}(\vec{\tilde{u}}) + \vec{v}$

$\|\vec{v} + h\vec{f}(\vec{u}_{i+1}) - \vec{u}_{i+1}\|$ (error)

Th Banach Fixed-Point

$h>0$, $\vec{u}_0 \in \mathbb{R}^n$, $\lambda \in (0,1)$, $\rho>0$

s.t. $\|\vec{f}(\vec{w})-\vec{f}(\vec{u})\| \le \frac{\lambda}{h}\|\vec{w}-\vec{u}\|$, $\vec{w},\vec{u} \in B_\rho(\vec{u}_0)$, $\|\cdot\|$ - vector norm, $B_\rho(\vec{u}_0) := \{\vec{u} \in \mathbb{R}^n \mid \|\vec{u}-\vec{u}_0\| \le \rho\}$

and $\vec{u}_1 \in B_{(1-\lambda)\rho}(\vec{u}_0)$

$\Rightarrow \vec{u}_{i+1} = h\vec{f}(\vec{u}_i)+\vec{v} \Rightarrow$
| $\vec{u}_i \in B_\rho(\vec{u}_0)$
| $\vec{\bar{u}}: \exists \lim_{i\to\infty} \vec{u}_i$, $\vec{\bar{u}} = h\vec{f}(\vec{\bar{u}})+\vec{v}$, $\vec{\bar{u}} \in B_\rho(\vec{u}_0)$
| no other point in $B_\rho(\vec{u}_0)$ is solution of $\vec{u} = h\vec{f}(\vec{u})+\vec{v}$

Picard for BE: $\vec{u}_{i+1}^{k+1} = h_t \vec{f}^{k+1}(\vec{u}_i^{k+1}) + \vec{u}^k$

$\|\vec{f}(\vec{u})-\vec{f}(\vec{w})\| \le \xi \|\vec{u}-\vec{w}\|$, $\forall \vec{u},\vec{w} \in B_\rho(\vec{u}_0)$, $\xi > 1 \Rightarrow \xi = \frac{\lambda}{h_t}$, $\lambda \in (0,1)$

Newton-Raphson Algorithm

$\vec{u} = h\vec{f}(\vec{u})+\vec{v}$, $\vec{u}_i$ - initial guess, $\vec{u} = \vec{u}_i + (\vec{u}-\vec{u}_i)$

$\vec{u}-\vec{u}_i \approx \vec{p}_i(\vec{u}_i) \Rightarrow \vec{u}_{i+1} = \vec{u}_i + \vec{p}_i(\vec{u}_i)$

$\vec{u} = h\vec{f}(\vec{u})+\vec{v} \Rightarrow \vec{u}-\vec{u}_i \approx \left[I - h\frac{\partial \vec{f}(\vec{u})}{\partial \vec{u}}\Big|_{\vec{u}=\vec{u}_i}\right]^{-1}\left[\vec{v}+h\vec{f}(\vec{u}_i)-\vec{u}_i\right]$

$\vec{p}_i(\vec{u}_i) = \left[I - hJ(\vec{u}_i)\right]^{-1}\{\vec{v}+h\vec{f}(\vec{u}_i)-\vec{u}_i\}$

$\vec{u} \in \mathbb{R}^n$, $\vec{f}(\vec{u}): \mathbb{R}^n \to \mathbb{R}^n$, Jacobian matrix $J \in \mathbb{R}^{n\times n}$

$J(\vec{u}_i) = \frac{\partial \vec{f}(\vec{u})}{\partial \vec{u}}\Big|_{\vec{u}=\vec{u}_i}$, $[J(\vec{u}_i)]_{qr} = \frac{\partial f_q(\vec{u})}{\partial u_r}\Big|_{\vec{u}=\vec{u}_i}$

Convergence: $\|\vec{\bar{u}}-\vec{u}_{i+1}\| \le c\|\vec{\bar{u}}-\vec{u}_i\|^2$, $J=0 \Rightarrow$ Picard, $J(\vec{u}_i) \approx J(\vec{u}_0) \Rightarrow$ Modified Newton-Raphson's

$\vec{f}(u) = -A\vec{u}+\vec{u}-\vec{u}^2$

$[J(\vec{u})]_{qr} = -a_{qr}+\delta_{qr}-2u_q\delta_{qr}$, δ_{qr} - Kronecker delta function

$J(\vec{u}_i^{k+1}) = -A+I-2\,\mathrm{diag}(\vec{u}_i^{k+1})$ $\hookrightarrow$ 1 if $q=r$ otherwise 0