AMATH 442 - Computational Methods for Partial Differential Equations

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PDEs
- → sound waves
- → heat distribution
- → fluids
- → quantum mechanics
- → electrodynamics
- ⋮

Exact closed form solution does not exist for many of these ...

↳ numerical methods

↳ approximate methods

→ Finite Difference (FD)

→ Finite Volume (FV)

→ Finite Element Method (FEM)

First and second order PDEs

$$A(x,y)\,\partial_{xx}u + B(x,y)\,\partial_{xy}u + C(x,y)\,\partial_{yy}u = W(u, \partial_x u, \partial_y u, x, y)$$

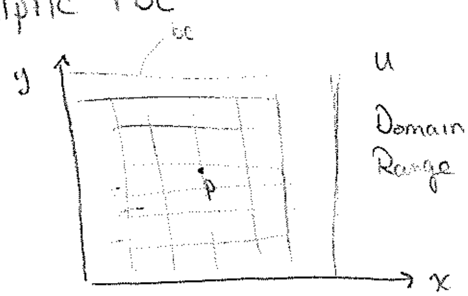
$$x,y \in \Omega$$

1/ Parabolic : $B^2 - 4AC = 0$

2/ Hyperbolic : $B^2 - 4AC > 0$

3/ Elliptic : $B^2 - 4AC < 0$

Elliptic PDE



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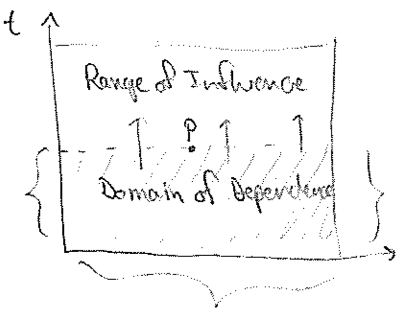
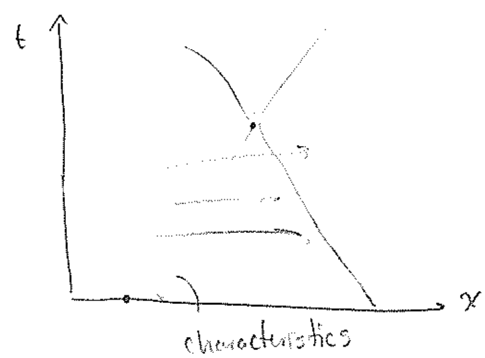
Domain of Dependence

Range of Influence

Parabolic PDE



Hyperbolic PDE

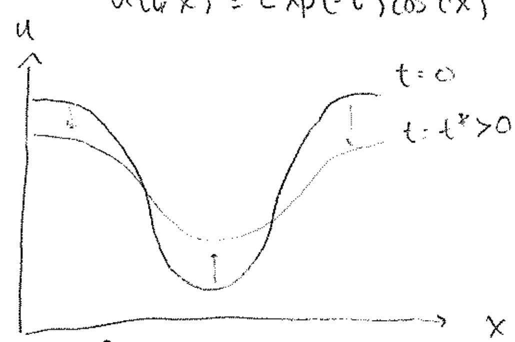


Parabolic PDE

Heat equation

$$\partial_t u - \partial_{xx} u = 0, \quad u = u(t, x)$$

$$u(t, x) = \exp(-t) \cos(x)$$



Decrease of amplitude = diffusion/dissipation

Hyperbolic PDE

Wave equation

$$\partial_{tt} u - a^2 \partial_{xx} u = 0$$

a = advection speed

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$L_1 = \partial_t - a\partial_x , \quad L_2 = \partial_t - a\partial_x$ [illegible]

$$L_1L_2 = (\partial_t - a\partial_x)(\partial_t - a\partial_x)$$
$$= \partial_{tt} + a\partial_{xt} - a\partial_{tx} - a^2\partial_{xx}$$
$$= \partial_{tt} - a^2\partial_{xx}$$

$L_1L_2u = 0$

$L_1u = 0 \quad L_2u = 0$

$L_1u = 0 \longrightarrow \partial_t u - a\partial_x u = 0$

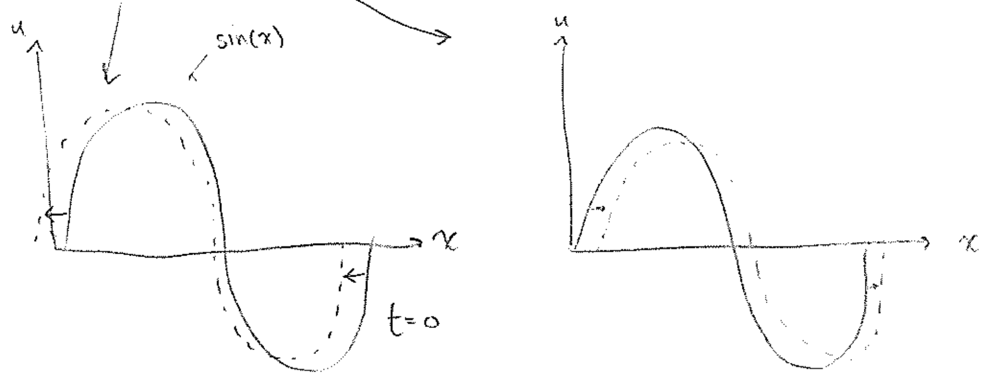
$\qquad u = f(x+at)$

$L_2u = 0 \longrightarrow \partial_t u + \partial_x u = 0$

$\qquad u = g(x-at)$

$$u = f(x+at) + g(x-at)$$

$a = 1$



$L_2u = 0$

First order hyperbolic PDE

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Elliptic PDE

Laplace equation

$$-\partial_{xx}u - \partial_{yy}u = 0$$

vector: $\vec{u} = (u_1, u_2)$

gradient: $\nabla u = (\partial_x u, \partial_y u)$

divergence: $\nabla \cdot \vec{u} = \partial_x u_1 + \partial_y u_2$

Laplacian: $\Delta u = \partial_{xx}u + \partial_{yy}u$

$u, \quad \nabla u = (\partial_x u, \partial_y u)$ $\qquad \Delta u = \nabla^2 u$

$\nabla \cdot \nabla u = \partial_{xx} u + \partial_{yy} u$

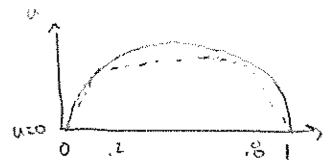
$-\Delta u = 0$ (Laplace)

$-\Delta u = f(x,y)$ (Poisson)

forcing

$-\nabla \cdot \nabla u = f$

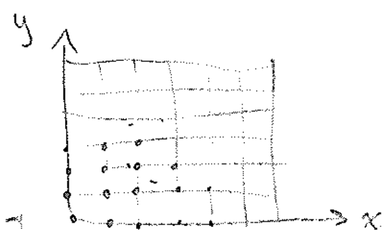
$-\nabla \cdot (a(x,y) \nabla u) = f$



$$a(x) = \begin{cases} 20, & x \in [0.2, 0.8] \\ 1, & \text{else} \end{cases}$$

$$\partial_t u + a\,\partial_x u = d\,\partial_{xx} u$$

Peclet no $\qquad Pe = \frac{aL}{b}$ → large - hyperbolic; → small - diffusion



squares

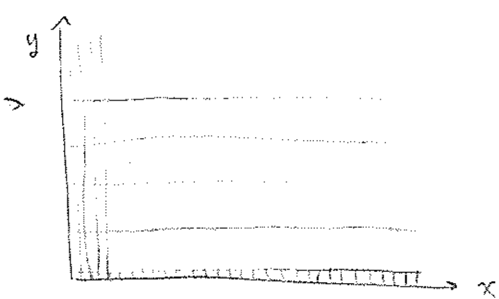
2D: triangles, rectangles quadrilaterals

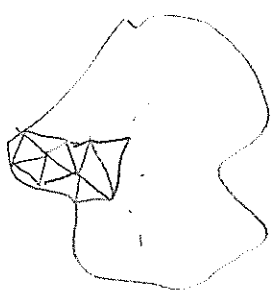
3D: tetrahedrons, pyramids, prisms, ...

Uniform grid

non-uniform

structured





unstructured grid

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	+	−
structured	computations can be very fast	"easy" domains
unstructured	general domains	more difficult to code, can be slow

	FD	FV	FEM
Uniform structured grids	✓	✓	✓
Non-uniform structured grids	✓	✓	✓
unstructured grids	×	✓	✓
advection dominated flows	✓	✓	×
diffusion dominated flows	✓	×	✓

Finite Difference Methods

Linear parabolic PDE

$$\partial_t u = \partial_x (b(x,t)\partial_x u) + c(x,t)\, u + d(x,t)$$

$$b>0,\ c,d \in \mathbb{R},\quad t>0$$

$$\left(\text{nonlinear pde} \quad \partial_t u = \partial_x (u \partial_x u) + u^2 \right)$$

$$x \in \Omega = [0,1]$$

① Boundary conditions: $\partial\Omega$

$$x=0: \quad \alpha_0(t)\, u + \alpha_1(t)\, \partial_x u = \alpha_2(t)$$

$$x=1: \quad \beta_0(t)\, u + \beta_1(t)\, \partial_x u = \beta_2(t)$$

$$\alpha_0 \geq 0,\ \alpha_1 \leq 0,\ \alpha_0 - \alpha_1 > 0$$

$$\beta_0 \geq 0,\ \beta_1 \geq 0,\ \beta_0 + \beta_1 > 0$$

② Initial Condition

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

Model problem: heat equation

$$\begin{cases} \partial_t u = \partial_{xx} u, & 0<x<1,\ t>0 \\ u(x,0) = u^0(x), & 0 \leq x \leq 1 \\ u(0,t) = u(1,t) = 0, & t>0 \end{cases}$$

Separation of variables

$$u(x,t) = f(x)g(t)$$

$$\partial_t u = \partial_{xx} u$$

$$\Leftrightarrow f(x)g'(t) = f''(x)g(t)$$

$$\Leftrightarrow \frac{g'(t)}{g(t)} = \frac{f''(x)}{f(x)} = \text{constant} = -K^2$$

① $g'(t) + K^2 g(t) = 0 \quad \Leftrightarrow \quad g(t) = c_1 e^{-K^2 t}$

② $f''(x) + K^2 f(x) = 0 \quad \Leftrightarrow \quad f(x) = c_2 \cos(Kx) + c_3 \sin(Kx)$

$$u(x,t) = \left(c_2 \cos(Kx) + c_3 \sin(Kx)\right)\exp(-K^2 t)$$

$$u(0,t) = u(1,t) = 0$$

$* \; u(0,t) = c_2 \exp(-K^2 t)$

$\longrightarrow c_2 = 0$

$* \; u(1,t) = c_3 \sin(K)\exp(-K^2 t) \longrightarrow \cancel{c_3 \neq 0}$

$\searrow K = m\pi, \quad m \in \mathbb{N} \setminus \{0\}$

To satisfy the bc's

$$u_m(x,t) = a_m \sin(m\pi x)\exp(-(m\pi)^2 t) \qquad m \in \mathbb{N}\setminus\{0\}$$

$$u(x,t) = \sum_{m=1}^{\infty} a_m \sin(m\pi x)\exp(-(m\pi)^2 t)$$

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$$u(x,0) = \sum_{m=1}^{\infty} a_m \sin(m\pi x) = u^{\circ}(x)$$

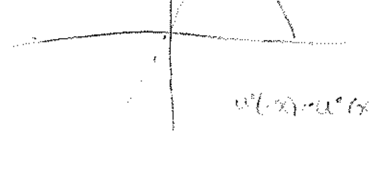
a_m are the coefficients of the Fourier sine series representation of $u^{\circ}(x)$

$u_0(x)$ defined $-\ell \le x \le \ell$

$$u_0(x) = \frac{1}{2}a_0 + \sum_{m=1}^{\infty}\left(b_m \cos\left(\frac{m\pi x}{\ell}\right) + a_m \sin\left(\frac{m\pi x}{\ell}\right)\right)$$

$$b_m = \frac{1}{\ell}\int_{-\ell}^{\ell} u_0(x)\cos\left(\frac{m\pi x}{\ell}\right)dx$$

$$a_m = \frac{1}{\ell}\int_{-\ell}^{\ell} u_0(x)\sin\left(\frac{m\pi x}{\ell}\right)dx$$



$$b_m = \frac{1}{l}\int_{-l}^{l} u_0(x)\cos\left(\frac{m\pi x}{l}\right)dx$$

$$= \int_{-1}^{0} u_0(x)\cos\left(\frac{m\pi x}{\cancel{l}}\right)dx + \int_{0}^{1} u_0(x)\cos\left(\frac{m\pi x}{\cancel{l}}\right)dx$$

$$= -\int_{-1}^{0} u_0(-z)\cos(m\pi(-z))dz + \int_{0}^{1} u_0(x)\cos(m\pi x)dx$$

$$= -\int_{0}^{1} u_0(z)\cos(m\pi z)dz + \quad " \quad = 0$$

$$a_m = \int_{-1}^{1} u_0(x)\sin(m\pi x)dx$$

$$= \int_{-1}^{0} u_0(x)\sin(m\pi x)dx + \int_{0}^{1} u_0(x)\sin(m\pi x)dx$$

$$= \int_{-1}^{0} u_0(-z)\sin(m\pi(-z))dz + \int_{0}^{1} u_0(x)\sin(m\pi x)dx$$

$$= 2\int_{0}^{1} u_0(x)\sin(m\pi x)dx$$

Finite Difference Methods

Step 1: Discretize the computational domain

J+1 discrete points

$x_0 = 0 \quad x_1 \quad x_2 \quad \cdots \quad x_{J-1} \quad 1 = x_J$

$$\Delta x_j = x_j - x_{j-1}$$
$$\Delta x_j = \Delta x \quad \forall j$$

$$x_j = \Delta x\, j \qquad j = 0, \ldots, J$$

Step 2: $t \in [0, T_F]$

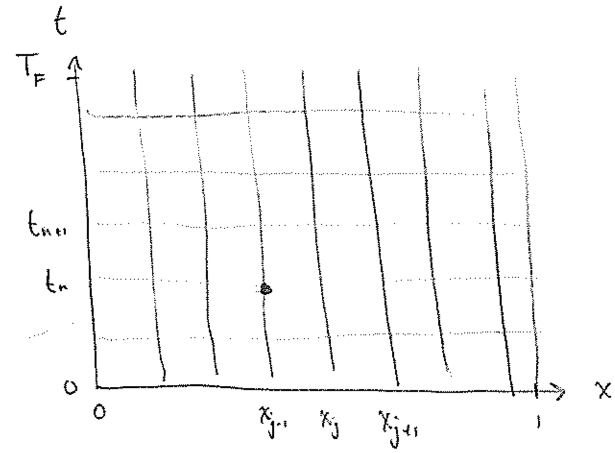
$0 = t_0 < t_1 < \cdots$

$\Delta t_n = t_n - t_{n-1}$

$\Delta t_n = \Delta t$

$t_n = n\Delta t \qquad n = 0, 1, 2, \ldots$

U_{j-1}^n



u exact solution
U numerical solution
U_s denotes U in $x = x_s$
U^n denotes U in $t = t^n$
U_s^n denotes ....

Main idea: replace derivatives by linear combinations of discrete function variables

$$\frac{\partial u}{\partial t}(x,t) = \lim_{\varepsilon \to 0} \frac{u(x,t+\varepsilon) - u(x,t)}{\varepsilon}$$

Motivation for

$$\frac{\partial u}{\partial t}(x_j,t_n) \approx \frac{u(x_j,t_n+\Delta t) - u(x_j,t_n)}{\Delta t}$$

$$\frac{\partial u}{\partial t}(x,t) = \lim_{\varepsilon \to 0} \frac{u(x,t) - u(x,t-\varepsilon)}{\varepsilon}$$

$$= \lim_{\varepsilon \to 0} \frac{u(x,t+\frac{1}{2}\varepsilon) - u(x,t-\frac{1}{2}\varepsilon)}{\varepsilon}$$

$$= \lim_{\varepsilon \to 0} \frac{u(x,t+\varepsilon) - u(x,t-\varepsilon)}{2\varepsilon}$$

<u>forward differences</u>

$$\frac{\partial u}{\partial t}(x_j,t_n) \approx \frac{u(x_j,t_n+\Delta t) - u(x_j,t_n)}{\Delta t}$$

$$\frac{\partial u}{\partial x}(x_j,t_n) \approx \frac{u(x_j+\Delta x,t_n) - u(x_j,t_n)}{\Delta x}$$

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Backward differences

$$\frac{\partial u}{\partial t}(x_j, t_n) \approx \frac{u(x_j, t_n) - u(x_j, t_n - \Delta t)}{\Delta t}$$

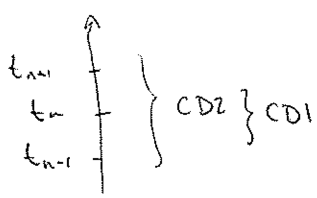
$\frac{\partial u}{\partial x}(x_j, t_n)$ similar

Central differences 1

$$\frac{\partial u}{\partial t}(x_j, t_n) \approx \frac{u(x_j, t_n + \frac{1}{2}\Delta t) - u(x_j, t_n - \frac{1}{2}\Delta t)}{\Delta t}$$

Central differences 2

$$\frac{\partial u}{\partial t}(x_j, t_n) \approx \frac{u(x_j, t_n + \Delta t) - u(x_j, t_n - \Delta t)}{2\Delta t}$$



$$\begin{aligned}
\frac{\partial^2 u}{\partial x^2}(x_j, t_n) &= \frac{\partial}{\partial x}\left(\frac{\partial u}{\partial x}\right)(x_j, t_n) \\
&\approx \frac{\partial}{\partial x}\left(\frac{u(x_j + \frac{1}{2}\Delta x, t_n) - u(x_j - \frac{1}{2}\Delta x, t_n)}{\Delta x}\right) \\
&= \frac{1}{\Delta x}\frac{\partial}{\partial x} u(x_j + \tfrac{1}{2}\Delta x, t_n) - \frac{1}{\Delta x}\frac{\partial}{\partial x} u(x_j - \tfrac{1}{2}\Delta x, t_n) \\
&\approx \frac{1}{\Delta x}\left(\frac{u(x_j + \Delta x, t_n) - u(x_j, t_n)}{\Delta x}\right) - \frac{1}{\Delta x}\left(\frac{u(x_j, t_n) - u(x_j - \Delta x, t_n)}{\Delta x}\right) \\
&= \frac{u(x_j + \Delta x, t_n) - 2u(x_j, t_n) + u(x_j - \Delta x, t_n)}{\Delta x^2} \qquad (ii)
\end{aligned}$$

(i) $$\frac{\partial u}{\partial t}(x_j, t_n) = \frac{u(x_j, t_n - \Delta t) - u(x_j, t_n)}{\Delta t}$$

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$$(**) \qquad \frac{U_j^{n+1} - U_j^n}{\Delta t} = \frac{U_{j+1}^n - 2U_j^n + U_{j-1}^n}{(\Delta x)^2}$$

$j = 1, 2, \ldots, J-1$

at $x = x_0$: $U_0^n = 0$ $\qquad U_j^0 = u_0(x_j)$

$x = x_J$: $U_J^n = 0$

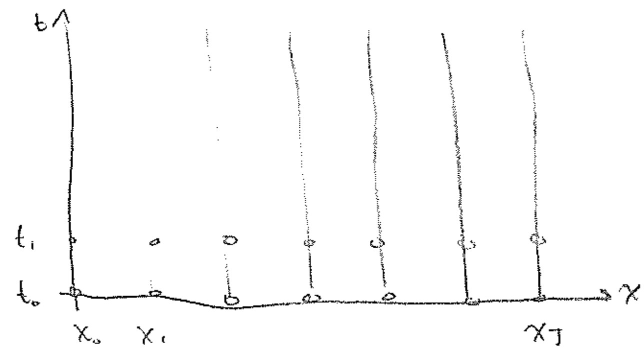
We can write (**)

$$U_j^{n+1} = U_j^n + \frac{\Delta t}{(\Delta x)^2}\left(U_{j+1}^n - 2U_j^n + U_{j-1}^n\right)$$

$$= U_j^n + \mu\left(U_{j+1}^n - 2U_j^n + U_{j-1}^n\right)$$

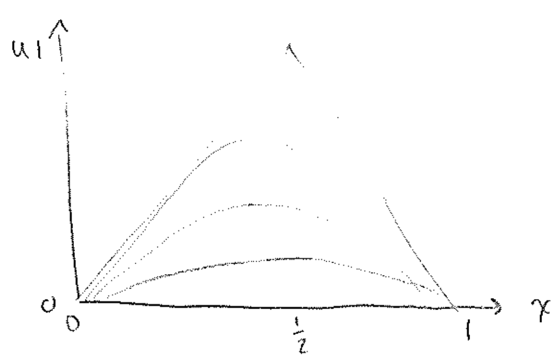
where

$$\mu = \frac{\Delta t}{(\Delta x)^2}.$$



time-stepping

$t \in [0, 100]$



- Stability
- Converges: $U \longrightarrow u$

Question: Does the numerical solution U converge to u (exact solution) and if so, under what conditions?

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Theorem: If the numerical scheme is <u>consistent</u> and <u>stable</u> U will converge to u.

<u>Truncation error</u>

$$\partial_t u - \partial_{xx} u = 0 \iff \frac{U_j^{n+1} - U_j^n}{\Delta t} - \frac{U_{j+1}^n - 2U_j^n + U_{j-1}^n}{(\Delta x)^2} = 0.$$

$$T(x,t) = \frac{u(x,t+\Delta t) - u(x,t)}{\Delta t} - \frac{u(x+\Delta x,t) - 2u(x,t) + u(x-\Delta x,t)}{(\Delta x)^2}$$

Bound for $T(x,t)$.

$\hookrightarrow$ Taylor series

- $u(x,t+\Delta t) = u(x,t) + \partial_t u \,\Delta t + \frac{1}{2}\partial_{tt} u (\Delta t)^2 + \frac{1}{6}\partial_{ttt} u (\Delta t)^3 + \cdots$

$$= u(x,t) + \partial_t u \,\Delta t + \frac{1}{2}\partial_{tt} u(x,q)(\Delta t)^2, \quad q \in (t, t+\Delta t)$$

- $u(x+\Delta x,t) = u(x,t) + \partial_x u \,\Delta x + \frac{1}{2}\partial_{xx} u (\Delta x)^2 + \frac{1}{6}\partial_{xxx} u (\Delta x)^3 + \frac{1}{24}\partial_{xxxx} u(\xi,t)(\Delta x)^4$

$\xi \in (x-\Delta x, x$

- $u(x-\Delta x,t) =$ " $-$ " $+$ " $-$ " $+$ "

$$T(x,t) = \left(\partial_t u + \frac{1}{2}\partial_{tt} u(x,q)\Delta t\right) - \left(\partial_{xx} u + \frac{1}{12}\partial_{xxxx} u(\xi,t)(\Delta x)^2\right)$$

$$= \underbrace{\left(\partial_t u - \partial_{xx} u\right)}_{0} + \left(\frac{1}{2}\partial_{tt} u \Delta t - \frac{1}{12}\partial_{xxxx} u (\Delta x)^2\right)$$

$$= \frac{1}{2}\partial_{tt} u \Delta t - \frac{1}{12}\partial_{xxxx} u (\Delta x)^2$$

$$|T(x,t)| = \left|\frac{1}{2}\partial_{tt} u \Delta t - \frac{1}{12}\partial_{xxxx} u (\Delta x)^2\right|$$

$$\leq \frac{1}{2}|\partial_{tt} u|\Delta t + \frac{1}{12}|\partial_{xxxx} u|(\Delta x)^2$$

$$= \frac{1}{2}\Delta t\left(|\partial_{tt} u| + \frac{1}{6\mu}|\partial_{xxxx} u|\right)$$

If u sufficiently smooth ~~then~~

$|\partial_{tt} u| \leq M_{tt}$ and $|\partial_{xxxx} u| \leq M_{xxxx}$

$$|T| \leq \frac{1}{2}\Delta t \left(M_{tt} + \frac{1}{6\mu} M_{xxxx}\right)$$

$\underline{|T| \to 0 \quad \text{as} \quad \Delta t \to 0}$ (μ is fixed)

Unconditionally Consistent

$|T| \sim \mathcal{O}(\Delta t)$

$\longrightarrow$ First order scheme in Δt

(if) $|T| \sim \mathcal{O}((\Delta t)^p)$

$\rightarrow$ the scheme has p^{th} order accuracy

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$$T(x_j, t_n) = \frac{U_j^{n+1} - U_j^n}{\Delta t} - \frac{U_{j+1}^n - 2U_j^n + U_{j-1}^n}{(\Delta x)^2}$$

<u>Convergence</u> ($U \to u$)

- Define the mesh st $\Delta t \to 0$, $\Delta x \to 0$ with $\mu = \Delta t/(\Delta x)^2$ fixed
- The scheme is convergent if for any point (x^*, t^*) in domain $(0,1) \times (0, T_F)$ we have

$$\left.\begin{array}{l} x_j \to x^* \\ t_j \to t^* \end{array}\right\} U_j^n \to u(x^*, t^*)$$

- We will prove convergence

(1) Define the error

$$e_j^n = U_j^n - u(x_j, t_n)$$

u satisfies $\partial_t u = \partial_{xx} u$

U satisfies $U_j^{n+1} = U_j^n + \mu\left(U_{j+1}^n - 2U_j^n + U_{j-1}^n\right)$ } (a)

(b) $\left\{ u(x_j, t_{n+1}) = u(x_j, t_n) + \mu\left(u(x_{j+1}, t_n) - 2u(x_j, t_n) + u(x_{j-1}, t_n)\right) + \Delta t \underbrace{T(x_j, t_n)}_{\text{truncation er.}} \right.$

(a) - (b) =

$$U_j^{n+1} - u(x_j, t_{n+1}) = \left(U_j^n - u(x_j, t_n)\right) + \mu\left(\left(U_{j+1}^n - u(x_{j+1}, t_n)\right) - 2\left(U_j^n - u(x_j, t_n)\right) + \cdots\right) - \Delta t T(x_j,$$

$$e_j^{n+1} = e_j^n + \mu\left(e_{j+1}^n - 2e_j^n + e_{j-1}^n\right) - \Delta t T_j^n$$

$$\Longleftrightarrow$$

$$e_j^{n+1} = (1 - 2\mu) e_j^n + \mu e_{j+1}^n + \mu e_{j-1}^n - \Delta t T_j^n$$

Observation: if $\mu < \frac{1}{2}$ then all coefficients of the terms e^n (?) (?) are positive and they add up to unity

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$$|e_j^{n+1}| \le |(1-2\mu)e_j^n| + |\mu e_{j+1}^n| + |\mu e_{j-1}^n| + |\Delta t\, T_j^n|$$

(assume $\mu \le \frac{1}{2}$) $\le (1-2\mu)|e_j^n| + \mu|e_{j+1}^n| + \mu|e_{j-1}^n| + \Delta t\,|T_j^n|$

$$\le (1-2\mu)\max_j |e_j^n| + \mu \max_j |e_j^n| + \mu \max_j |e_j^n| + \Delta t \max_j |T_j^n|$$

$$E^n := \max_{j=0,\dots,J} |e_j^n|, \quad \bar{T} = \max_{j,n} |T_j^n|$$

$$|e_j^{n+1}| \le (1-2\mu)E^n + \mu E^n + \mu E^n + \Delta t\,\bar{T}$$

$$E^{n+1} \le E^n + \Delta t\,\bar{T}$$

$$\left.\begin{array}{l} t=0: \quad U_j^0 = u(x_j, t_0) \rightarrow E^0 = 0 \\ t=t_1: \quad E^1 \le E^0 + \Delta t\,\bar{T} = \Delta t\,\bar{T} \\ t=t_2: \quad E^2 \le E^1 + \Delta t\,\bar{T} = 2\Delta t\,\bar{T} \\ t=t_3: \quad E^3 \le E^2 + \Delta t\,\bar{T} = 3\Delta t\,\bar{T} \end{array}\right\} \quad E^n \le n\bar{T}\Delta t$$

(proof by induction)

$$|T| \le \frac{1}{2}\Delta t\left(M_{tt} + \frac{1}{6\mu} M_{xxxx}\right) \quad \forall (x,t) \in (0,1)\times(0,T_F)$$

$$E^{n+1} \le (n+1)\frac{1}{2}\Delta t\left(M_{tt} + \frac{1}{6\mu}M_{xxxx}\right)\Delta t$$

$$\le \underbrace{\frac{1}{2}\Delta t\left(M_{tt} + \frac{1}{6\mu}(\cdot)\right)T_F}_{\text{just a number}}$$

$E^{n+1} \to 0$ as $\Delta t \to 0$
Convergence!

<u>Refinement path</u>: a sequence of pairs of mesh sizes Δx and Δt each of which tends to zero

Refinement path $= \left\{ ((\Delta x)_i, (\Delta t)_i), \quad i = 0,1,2,3,\dots \right.$

$$\mu = \frac{(\Delta t)^{(\cdot)}}{(\Delta x)^2} \quad \mu_i = \frac{(\Delta t)_i}{(\Delta x)_i} \qquad \left.\begin{array}{l}\Delta t \to 0 \\ \Delta x \to 0\end{array}\right\}$$

Theorem 2.1: If a refinement path satisfies $\mu_i \le \frac{1}{2}$ for all sufficiently large values of i and positive numbers n_i, j_i st

means Ix $\exists n_i j_i$ I think

$$n_i (\Delta t)_i \rightarrow t > 0$$

$$j_i (\Delta x)_i \rightarrow x \in [0,1]$$

<u>and</u> if $|\partial_{xxxx} u| \le M_{xxxx}$

then U_j^n converges to u (solution of $\partial_t u = \partial_{xx} u$) in $(x,t) \in (0,1)\times(0,T_F)$

consistency ✓
convergence ✓

$\sin^2 x = \frac{1}{2}(1-\cos 2x)$

Stability

- $u(x,t) = \sum_{m=-\infty}^{\infty} A_m \exp(-(m\pi)^2 t)\sin(m\pi x)$

$$a_m = 2\int_0^1 u_0(x)\sin(m\pi x)\,dx$$

- Suppose $U_j^n = \lambda^n \exp(ikx_j) = \lambda^n \exp(ikj\Delta x)$

$$U_j^{n+1} = \lambda^{n+1}\exp(ikj\Delta x) = \lambda U_j^n$$
$$U_{j+1}^n = \lambda^n \exp(ik(j+1)\Delta x) = \lambda^n \exp(ikj\Delta x)\exp(ik\Delta x) = U_j^n \exp(ik\Delta x)$$

$$U_{j-1}^n = U_j^n \exp(-ik\Delta x)$$
$$U_j^{n+1} = U_j^n + \mu\,(U_{j+1}^n - 2U_j^n + U_{j-1}^n)$$
$$\lambda \cancel{U_j^n} = \cancel{U_j^n} + \mu(\cancel{U_j^n}\exp(ik\Delta x) - 2\cancel{U_j^n} + \cancel{U_j^n}\exp(-ik\Delta x))$$
$$\lambda = 1 + \mu(\exp(ik\Delta x) - 2 + \exp(-ik\Delta x))$$
$$= 1 + \mu(\cos(k\Delta x) + \cancel{i\sin(k\Delta x)} - 2 + \cos(k\Delta x) - \cancel{i\sin(k\Delta x)})$$
$$= 1 + 2\mu(\cos(k\Delta x) - 1)$$
$$= 1 - 4\mu\sin^2(\tfrac{1}{2}k\Delta x)$$

$$\lambda(k) = 1 - 4\mu\sin^2(\tfrac{1}{2}k\Delta x) \quad \longleftarrow \text{amplification factor}$$

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$$U_j^n = \sum_{m=-\infty}^{\infty} A_m \exp(im\pi j\Delta x)[\lambda(im\pi)]^n$$

$(k=m\pi)$
$$u(x_j,t_n) = \sum_{m=-\infty}^{\infty} A_m \exp(im\pi j\Delta x)\underbrace{\exp(i(m\pi)^2 n\Delta t)}_{[\exp(i(m\pi)^2\Delta t)]^n}$$

- $\exp(-k^2\Delta t) = 1 - k^2\Delta t + \frac{1}{2}k^4(\Delta t)^2 + \cdots$
- $\lambda(k) = 1 - 4\mu\sin^2(\frac{1}{2}k\Delta x)$

$$= 1 - 2\mu(1-\cos(k\Delta x))$$
$$= 1 - 2\mu(1 - 1 + \tfrac{1}{2}(k\Delta x)^2 - \tfrac{1}{24}(k\Delta x)^4 + \cdots)$$
$$= 1 - \tfrac{\Delta t}{(\Delta x)^2}((k\Delta x)^2 - \tfrac{1}{12}(k\Delta x)^4 + \cdots)$$
$$= 1 - k^2\Delta t + \tfrac{1}{12}k^4(\Delta t)^2 + \cdots$$

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- For low frequencies (k small) the numerical expansion is a good approx. to the exact solution
- What about large k?
  - exact solutions: modes rapidly decay like $\exp(-k^2 t)$
  - numerical solution:

$$[\lambda(k)]^n, \quad \lambda = 1 - 4\mu \sin^2(\tfrac{1}{2}k\Delta x)$$

what happens if $|\lambda| > 1 \longrightarrow$ instability

For stability, we need $|\lambda| \le 1$.

$$|1 - 4\mu\sin^2(\tfrac{1}{2}k\Delta x)| \le 1$$

$$4\mu\underbrace{\sin^2(\tfrac{1}{2}k\Delta x)}_{\max 1} \le 2$$

$$4\mu \le 2 \longrightarrow \boxed{\mu \le \tfrac{1}{2}} \longrightarrow \Delta t \le \tfrac{1}{2}(\Delta x)^2$$

__Von Neumann Stability Condition__

For stability: $|\lambda(k)| \le 1 + K\Delta t$

$$(|\lambda(k)| \le 1)$$

__Convergence (2)__

- Convergence proof (1) $\longrightarrow$ u is smooth enough s.t. u_{xxxx} is bounded

__Conv #2__

$\rightarrow$ relax assumptions of proof 1 as follows:

- u is continuous
- $u_0(x)$ (initial condition) has absolutely convergent Fourier series

$$\hookrightarrow \sum_{l=1}^{\infty} |b_l| = S < \infty$$

Suppose $\mu \le \frac{1}{2}$

$$e_j^n = U_j^n - u_j^n$$

$$= \sum_{-\infty}^{\infty} A_m \exp(im\pi j\Delta x)\left\{[\lambda(im\pi)]^n - \exp(-m^2\pi^2 n\Delta t)\right\}$$

- Split infinite sum in 2 parts:

Given $\varepsilon > 0$ choose m_0 s.t.

$$\sum_{|m| > m_0} |A_m| \le \frac{1}{4}\varepsilon$$

· if $|\lambda_1| \le 1$ and $|\lambda_2| \le 1$ $\Big\}$ $|\lambda_1^n - \lambda_2^n| \le n\,|\lambda_1 - \lambda_2|$

$$|e_j^n| = \left|\sum_{|m|\le m_0} A_m \exp(im\pi j\Delta x)\left\{[\lambda(m\pi)]^n - \exp(-m^2\pi^2 n\Delta t)\right\}\right| + \frac{1}{2}\varepsilon$$

$$\le \sum_{|m|\le m_0} |A_m| \left|(\lambda(m\pi))^n - [\exp(-m^2\pi^2\Delta t)]^n\right| + \frac{1}{2}\varepsilon$$

$$\le \sum_{|m|\le m_0} |A_m|\, n\, |\lambda(m\pi) - \exp(-m^2\pi^2\Delta t)| + \frac{1}{2}\varepsilon$$

$$|\lambda(m\pi) - \exp(-m^2\pi^2\Delta t)| = \Big|\cancel{1} - (m\pi)^2\Delta t + \frac{1}{12}(m\pi)^4\Delta t(\Delta x)^2 + h.o.t.$$
$$\cancel{-1} + (m\pi)^2\Delta t - \frac{1}{2}(m\pi)^4(\Delta t)^2 + h.o.t.\Big|$$
$$\le C(\mu)(m^2\pi^2\Delta t)^2$$

$$|e_j^n| \le \sum_{|m|\le m_0} |A_m|\, n\, C(\mu)(m^2\pi^2\Delta t)^2 + \frac{1}{2}\varepsilon$$

$$= \sum_{|m|\le m_0} (|A_m| m^4)\underbrace{(n\Delta t)}_{\le T_F}\Delta t\, \pi^4 C(\mu) + \frac{1}{2}\varepsilon$$

$$\le T_F \pi^4 C(\mu)\Delta t \left\{\sum_{|m|\le m_0} |A_m| m^4\right\} + \frac{1}{2}\varepsilon$$

If we take Δt small enough

$$|e_j^n| \le \frac{1}{2}\varepsilon \quad \forall (x_j, t_n) \in [0,1]\times[0, T_F]$$

Finite difference method

Explicit
(forward difference in time)
$\mu \le \frac{1}{2} \rightarrow \Delta t \le \frac{1}{2}(\Delta x)^2$ severe restriction!!

Implicit
① backward difference in time
② Θ-method

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Explicit FD

→ truncation error

↳ consistency

→ convergence ($\mu \le \frac{1}{2}$)

→ stability → $\mu \le \frac{1}{2}$

$$\mu = \frac{\Delta t}{(\Delta x)^2}, \quad \underbrace{\Delta t \le \tfrac{1}{2}(\Delta x)^2}_{\text{severe restriction}}$$

Implicit FD

↳ less severe restriction

sometimes you can take Δt as big as you want

$$\partial_t u = \partial_{xx} u$$

Explicit

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \frac{U_{j+1}^n - 2U_j^n + U_{j-1}^n}{(\Delta x)^2} \quad \left(\text{rhs evaluated at } t^n\right)$$

Implicit

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \frac{U_{j+1}^{n+1} - 2U_j^{n+1} + U_{j-1}^{n+1}}{(\Delta x)^2} \quad \left(\text{rhs evaluated at } t^{n+1}\right)$$

Explicit $U^{n+1} = f(U^n)$

Implicit: $U_j^{n+1} = U_j^n + \mu\left(U_{j+1}^{n+1} - 2U_j^{n+1} + U_{j-1}^{n+1}\right)$

$$-\mu U_{j+1}^{n+1} + (1-2\mu)U_j^{n+1} - \mu U_{j-1}^{n+1} = U_j^n$$

$$\underbrace{f(U^{n+1}) = g(U^n)}_{\text{implicit equation for } U^{n+1}}$$

⟶ more difficult to solve

$u(0,t) = u(1,t) = 0$

$U_0^{n+1} = 0 \quad (j=0)$

$-\mu U_{j+1}^{n+1} + (1+2\mu)U_j^{n+1} - \mu U_{j-1}^{n+1} = U_j^n \quad (j = 1, 2, \ldots, J-1)$

$U_J^{n+1} = 0$

$$
\begin{array}{cc}
 & j \\
J & \begin{bmatrix} 1 & 0 & \cdots & & & 0 \\ -\mu & (1+2\mu) & -\mu & 0 & \cdots & 0 \\ & \ddots & & & & \\ & -\mu & (1+2\mu) & -\mu & & \\ & & \ddots & & & \\ & & & -\mu & (1+2\mu) & -\mu \\ 0 & \cdots & & & 0 & 1 \end{bmatrix}
\end{array}
\begin{bmatrix} U_0^{n+1} \\ U_1^{n+1} \\ \vdots \\ U_j^{n+1} \\ \vdots \\ U_{J-1}^{n+1} \\ U_J^{n+1} \end{bmatrix} = \begin{bmatrix} 0 \\ U_1^n \\ \\ U_j^n \\ \\ U_{J-1}^n \\ 0 \end{bmatrix}
$$

$A \in \mathbb{R}^{(J+1)\times(J+1)}$

$A(1,1) = 1$

$\left.\begin{array}{l} A(j,j-1) = -\mu \\ A(j,j) = 1+2\mu \\ A(j,j+1) = -\mu \end{array}\right\} \quad j = 1,2,\ldots,J$

$A(J+1, J+1) = 1$

$A(i,k) = 0$

$$A U^{n+1} = F$$

① Matlab: $U^{n+1} = A \backslash F;$

② Thomas Algorithm

③ Iterative Methods

General System

$$-a_j U_{j-1} + b_j U_j - c_j U_{j+1} = d_j \qquad j = 1, \ldots, J-1$$

$$U_0 = U_J = 0$$

required $a_j, b_j, c_j > 0$

$b_j > a_j + c_j$ — ensures that the matrix is diagonally dominant

$$AU^{n+1} = F \longrightarrow \tilde{A}U^{n+1} = \tilde{F} \quad (\tilde{A} \text{ upper triangular})$$

Stability

Fourier modes: $U_j^n = \lambda^n \exp(ikj\Delta x)$

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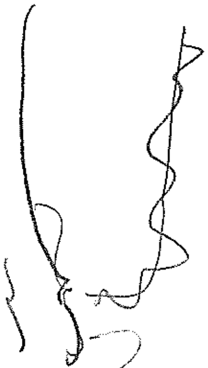

$$U_j^{n+1} = \lambda U_j^n$$
$$U_{j-1}^{n+1} = \lambda U_j^n \exp(-ik\Delta x)$$
$$U_{j+1}^{n+1} = \lambda U_j^n \exp(ik\Delta x)$$

$$\rightarrow -\mu U_{j-1}^{n+1} + (1+2\mu)U_j^{n+1} - \mu U_{j+1}^{n+1} = U_j^n$$
$$-\mu \lambda U_j^n \exp(-ik\Delta x) + (1+2\mu)U_j^n \lambda - \mu\lambda U_j^n \exp(ik\Delta x) = U_j^n$$
$$\lambda(-\mu\exp(-ik\Delta x) + (1+2\mu) - \mu\exp(ik\Delta x)) = 1$$
$$\lambda - 1 = \lambda\mu(\exp(-ik\Delta x) - 2 + \exp(ik\Delta x))$$
$$\lambda - 1 = \lambda\mu(\cos(k\Delta x) - 1)$$
$$\lambda - 1 = -4\lambda\mu \sin^2(\tfrac{1}{2}k\Delta x)$$
$$\lambda(1 + 4\mu\sin^2(\tfrac{1}{2}k\Delta x)) = 1$$
$$\lambda(k) = \frac{1}{1 + 4\mu\sin^2(\frac{1}{2}k\Delta x)} \quad \leftarrow \text{amplification factor}$$

For stability:

$$0 < \lambda \leq 1$$
$$\Leftrightarrow \quad 0 < \frac{1}{1 + 4\mu\sin^2(\frac{1}{2}k\Delta x)} \leq 1$$

True for <u>all</u> μ!

The implicit scheme is <u>unconditionally stable</u>

Explicit $$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \frac{U_{j-1}^n - 2U_j^n + U_{j+1}^n}{(\Delta x)^2} \qquad (A)$$

Implicit $$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \frac{U_{j-1}^{n+1} - 2U_j^{n+1} + U_{j+1}^{n+1}}{(\Delta x)^2} \qquad (B)$$

<u>Θ-method</u>

↳ weighted average of (A) and (B)

$$0 < \theta < 1$$
$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \theta B + (1-\theta)A$$
$$= \frac{\theta}{(\Delta x)^2}\left(U_{j-1}^{n+1} - 2U_j^{n+1} + U_{j+1}^{n+1}\right) + \frac{(1-\theta)}{(\Delta x)^2}\left(U_{j-1}^{n} - 2U_j^{n} + U_{j+1}^{n}\right)$$
$$\Leftrightarrow \quad U_j^{n+1} = U_j^n + \mu\theta\left(U_{j-1}^{n+1} - 2U_j^{n+1} + U_{j+1}^{n+1}\right) + \mu(1-\theta)\left(U_{j-1}^n - 2U_j^n + U_{j+1}^n\right)$$

$$-\mu\theta U_{j-1}^{n+1} + (1+2\mu\theta)U_j^{n+1} - \mu\theta U_{j+1}^{n+1}$$
$$= U_j^n + (1-\theta)\mu\left(U_{j+1}^n - 2U_j^n + U_{j-1}^n\right)$$

$\boxed{\theta\text{-method}}$

Observation 1

$\theta = 0 \rightarrow$ Explicit (forward difference in time)

$\theta = 1 \rightarrow$ Implicit

$0<\theta<1 \rightarrow$ somewhere between fully backward and fully forward in time (weighted average)

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Observation 2

$\theta = 0 \longrightarrow$ Explicit FD, $U^{n+1} = f(U^n)$

$0<\theta\le 1 \longrightarrow$ Implicit FD, $g(U^{n+1}) = h(U^n)$

$\partial_t u = \partial_{xx} u$

$\theta = 0 \longrightarrow \Delta t \le \frac{1}{2}(\Delta x)^2$

$\theta = 1 \longrightarrow \Delta t < \infty$

Stability. $\theta = 0$, $\mu \le \frac{1}{2}$

$\theta = 1 \rightarrow$ unconditionally stable

$0<\theta<1$?

$$U_j^n = \lambda^n \exp(ikj\Delta x)$$
$$-\mu\theta\lambda\exp(-ik\Delta x) + (1+2\mu\theta)\lambda - \mu\theta\lambda\exp(ik\Delta x)$$
$$= 1 + (1-\theta)\mu\exp(ik\Delta x) - 2\mu(1-\theta) + (1-\theta)\mu\exp(-ik\Delta x)$$
$$\Longrightarrow$$
$$\lambda - 1 = \mu\theta\lambda\left(\exp(ik\Delta x) - 2 + \exp(-ik\Delta x)\right) + (1-\theta)\mu\underbrace{\left(\exp(ik\Delta x) - 2 + \exp(-ik\Delta x)\right)}_{-4\sin^2(\frac{1}{2}k\Delta x)}$$
$$\Longrightarrow$$
$$\lambda - 1 = -4\mu\left(\lambda\theta + (1-\theta)\right)\sin^2\left(\tfrac{1}{2}k\Delta x\right)$$
$$\lambda\left(1 + 4\mu\theta\sin^2\left(\tfrac{1}{2}k\Delta x\right)\right) = 1 - 4\mu(1-\theta)\sin^2\left(\tfrac{1}{2}k\Delta x\right)$$
$$\lambda(k) = \frac{1 - 4\mu(1-\theta)\sin^2(\frac{1}{2}k\Delta x)}{1 + 4\mu\theta\sin^2(\frac{1}{2}k\Delta x)}$$

$\theta = 0 \rightarrow \lambda = 1 - 4\mu\sin^2(\frac{1}{2}k\Delta x)$

$\theta = 1 \rightarrow \lambda = (1 + 4\mu\sin^2(\frac{1}{2}k\Delta x))^{-1}$

$|\lambda| \le 1$ we know $\mu > 0$, $0 \le \theta \le 1 \rightarrow \lambda < 1$

We need to check that $\lambda \ge -1$

2015 09 30 (2)

$$1-4\mu(1-\theta)\sin^2(\quad) \geq -(1+4\mu\theta\sin^2(\quad))$$
$$\Leftrightarrow \quad 1-4\mu(1-2\theta)\sin^2(\quad) \geq -1$$
$$\Leftrightarrow \quad 4\mu(1-2\theta)\underbrace{\sin^2(\quad)}_{\leq 1} \leq 2$$
$$\Leftrightarrow \quad 4\mu(1-2\theta) \leq 2 \longrightarrow \mu(1-2\theta) \leq \tfrac{1}{2}$$

$\mu(1-2\theta) \leq \frac{1}{2}$ for stability of θ-method

- $\theta = 0 \rightarrow \mu \leq \frac{1}{2}$
- $\theta < \frac{1}{2} \rightarrow \mu(1-2\theta) \leq \frac{1}{2}$

} conditionally stable

- $\theta = 1 \rightarrow \forall\mu$
- $\theta \geq \frac{1}{2} \rightarrow \forall\mu$

} unconditionally stable

Accuracy

Truncation error θ-method

Taylor series expansion around $x_j, t_{n+\frac{1}{2}}$

$$u_j^{n+1} = \left[u + \tfrac{1}{2}\Delta t\,\partial_t u + \tfrac{1}{2}(\tfrac{1}{2}\Delta t)^2\partial_{tt}u + \tfrac{1}{6}(\tfrac{1}{2}\Delta t)^3\partial_{ttt}u + \cdots\right]_j^{n+1/2}$$

$$u_j^{n} = \left[u - \tfrac{1}{2}\Delta t\,\partial_t u + \tfrac{1}{2}(\tfrac{1}{2}\Delta t)^2\partial_{tt}u - \tfrac{1}{6}(\tfrac{1}{2}\Delta t)^2\partial_{ttt}u + \cdots\right]_j^{n+1/2}$$

$$u_j^{n+1} - u_j^{n} = \left[\Delta t\,\partial_t u + \tfrac{1}{24}(\Delta t)^3\partial_{ttt}u + \cdots\right]_j^{n+1/2}$$

$$u_{j+1}^{n+1} - 2u_j^{n+1} - u_{j-1}^{n+1} = \left[(\Delta x)^2\partial_{xx}u + \tfrac{1}{12}(\Delta x)^4\partial_{xxxx}u + \tfrac{2}{6!}(\Delta x)^6\partial_{xxxxxx}u + \cdots\right]_j^{n+1}$$

$\hookrightarrow$ Taylor around $(x_j, t_{n+1/2})$

$$= \left[(\Delta x)^2\partial_{xx}u + \tfrac{1}{12}(\Delta x)^4\partial_{xxxx}u + \tfrac{2}{6!}(\Delta x)^6\partial_{xxxxxx}u + \cdots\right]_j^{n+1/2} \leftarrow A$$

$$+\tfrac{1}{2}\Delta t\left[(\Delta x)^2\partial_{xxt}u + \tfrac{1}{12}(\Delta x)^4\partial_{xxxxt}u + \cdots\right]_j^{n+1/2} \leftarrow B$$

$$+\tfrac{1}{2}(\tfrac{1}{2}\Delta t)^2\left[(\Delta x)^2\partial_{xxtt}u + \cdots\right]_j^{n+1/2} \leftarrow C$$

$$u_{j+1}^{n} - 2u_j^{n} - u_{j-1}^{n} = A - \tfrac{1}{2}\Delta t\,B + \tfrac{1}{2}(\tfrac{1}{2}\Delta t)^2 C$$

$$T_j^{n+1/2} = \frac{u_j^{n+1} - u_j^n}{\Delta t} - \left(\frac{\theta}{(\Delta x)^2} \left(u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1} \right) + \frac{(1-\theta)}{(\Delta x)^2} \left(u_{j+1}^n - 2u_j^n + u_{j-1}^n \right) \right)$$

$$= \cancel{\left[\partial_t u - \partial_{xx} u \right]_j^{n+1/2}} + \left[\left(\tfrac{1}{2} - \theta \right) \Delta t \, \partial_{xxt} u - \tfrac{1}{12} (\Delta x)^2 \partial_{xxxx} u \right]_j^{n+1/2}$$

$$+ \left[\frac{1}{24} (\Delta t)^2 \partial_{ttt} u - \frac{1}{8} (\Delta t)^2 \partial_{xxtt} u \right]_j^{n+1/2}$$

$$+ \left[\frac{1}{12} \left(\tfrac{1}{2} - \theta \right) \Delta t (\Delta x)^2 \partial_{xxxxt} u - \frac{2}{6!} (\Delta x)^4 \partial_{xxxxxx} u \right]_j^{n+1/2} + \cdots$$

- Consistency: $|T| \to 0$ as $\Delta t, \Delta x \to 0$
- Accuracy: $T \sim \mathcal{O}(\Delta t)$, $\theta \neq \frac{1}{2}$
  $T \sim \mathcal{O}(\Delta t^2)$, $\theta = \frac{1}{2}$

$\boxed{\theta = \frac{1}{2}}$ $\quad T = \left[-\frac{1}{12} (\Delta x)^2 \partial_{xxxx} u - \frac{1}{12} (\Delta t)^2 \partial_{ttt} u \cdots \right]$

↳ Crank-Nicolson

Summary

$\theta = 0 \to$ · $T \sim \mathcal{O}(\Delta t), \mathcal{O}(\Delta x^2)$
· conditionally stable

$\theta = 1 \to$ · $T \sim \mathcal{O}(\Delta t), \mathcal{O}(\Delta x^2) \to \Delta t \sim \Delta x^2$ (accuracy)
· unconditional stability

$0 < \theta \leq 1, \theta \neq \frac{1}{2}$ too

$\theta = \frac{1}{2} \to$ · $T \sim \mathcal{O}(\Delta t^2), \mathcal{O}(\Delta x^2) \to \boxed{\Delta t \sim \Delta x}$
· unconditionally stable

we have done §2.1 §2.10

2015 10 02

Stability + Consistency = Convergence

We will prove convergence now Proof based on Max. Principle

- $\partial_t u = \partial_{xx} u$
  ↳ diffusion
  ↳ amplitude u decays in time

$\Rightarrow u(x,t)$ is bounded above and below by the extremes attained by i.c. and b.c.

Can we mimic this property with the θ-method?
↳ Yes, but only conditionally: μ has to satisfy $\mu(1-\theta) \leq \frac{1}{2}$

<Theorem 2.2 in book projected on board>

Proof of max principle:

- $(1+2\mu\theta)U_j^{n+1} = \theta\mu\left(U_{j-1}^{n+1} + U_{j+1}^{n+1}\right) + (1-\theta)\mu\left(U_{j-1}^{n} + U_{j+1}^{n}\right) + (1-2(1-\theta)\mu)U_j^n$

  if $\mu(1-\theta) \le 1/2$ all the coefs on RHS are positive and sum to $1+2\mu\theta$
- Assume U has max in interior point, and that max is $U^* = U_j^{n+1}$.

Define $\tilde{U}^* = \max\{U_{j-1}^{n+1}, U_{j+1}^{n+1}, U_{j-1}^{n}, U_j^n, U_{j+1}^n\}$

$$(1+2\mu\theta)U_j^{n+1} \le 2\theta\mu\tilde{U}^* + 2(1-\theta)\mu\tilde{U}^* + (1-2(1-\theta)\mu)\tilde{U}^*$$

$$\left.\begin{array}{l} U_j^{n+1} \le \tilde{U}^* \\ \text{But we assumed } U_j^{n+1} = U^* \ge \tilde{U}^* \end{array}\right\} U_j^{n+1} = \tilde{U}^*$$

still proof?

Part 2: Convergence

Error $e_j^n = U_j^n - u_j^n$

- Exact sol $(1+2\theta\mu)u_j^{n+1} = \theta\mu\left(u_{j-1}^{n+1} + u_{j+1}^{n+1}\right) + \theta\mu\left(u_{j-1}^{n} + u_{j+1}^{n}\right)$
  $+ (1-2(1-\theta)\mu)u_j^n + \Delta t\, T_j^{n+1/2}$
- Num. sol $(1+2\theta\mu)U_j^{n+1} = \theta\mu\left(U_{j-1}^{n+1} + U_{j+1}^{n+1}\right) + \theta\mu\left(U_{j-1}^{n} + U_{j+1}^{n}\right) + (1-2(1-\theta)\mu)U_j^n$.

Subtract:

$$(1+2\theta\mu)e_j^{n+1} = \theta\mu\left(e_{j-1}^{n+1} - e_{j+1}^{n+1}\right) + \theta\mu\left(e_{j-1}^{n} + e_{j+1}^{n}\right) + (1-2(1-\theta)\mu)e_j^n - \Delta t\, T_j^{n+1/2} \quad \leftarrow (*)$$

- for $j = 1, 2, \ldots, J-1$, $n = 0, 1, \ldots$
- b.c. $U_0^n = u_0^n$, $U_J^n = u_J^n$
- i.c. $U_j^0 = u_0(x)$

Define $E^n = \max_{0 \le j \le J} |e_j^n|$, $T^{n+1/2} = \max_{1 \le j \le J-1} |T_j^{n-1/2}|$

Bound for $|e_j^{n+1}|$: $|LHS| = |RHS|$

- use that all coefs are non-negative (as $\mu(1-\theta) \le 1/2$)
- use the triangle inequality

$(1+2\theta\mu)|e_j^{n+1}| \le$ $(*)$ with $|\cdot|$ on e terms and on $T_j^{n+1/2}$ (& total (1)

$(1+2\theta\mu)E^{n+1} \le 2\theta\mu E^{n+1} + E^n + \Delta t\, T^{n+1/2}$

$\Rightarrow E^{n+1} \le E^n + \Delta t\, T^{n+1/2}$

Since $E^0 = 0$,

$$E^{n+1} \le \Delta t \sum_{m=0}^{n-1} T^{m+1/2} \le n\Delta t \max_m T^{m+1/2}$$

We assumed that $|T| \to 0$ as $\Delta x, \Delta t \to 0$. So $E^n \to 0$ if $\Delta x, \Delta t \to 0$. $\therefore$ we have convergence!

2015 10 05

<see matlab code on learn>

Testing Implementation (§1.3 of pdf file)

$$\begin{cases} \partial_t u = \partial_{xx} u \\ u(0,t) = u(1,t) = 0 \\ u(0,x) = u_0(x) \end{cases}$$

- assume you implemented θ-method
- theory: θ-method is stable, consistent
  We expect $U \to u$ if $\Delta x, \Delta t$ small enough
- practice: there will be a bug in your code
  You need to find this bug

One way to make sure your code is correct is using manufactured solutions

Modify to problem of which you know the solution

I want $u = \sin(2\pi x)\cos(2\pi t)$ to be my exact solution

$$\begin{cases} \partial_t u - \partial_{xx} u = 4\pi^2 \cos(2\pi t)\sin(2\pi x) - 2\pi \sin(2\pi t)\sin(2\pi t) \\ u(0,t) = u(1,t) = 0 \\ u(x,0) = \sin(2\pi x) \end{cases}$$

Define $E = \max\{|e_j^n|, (x_j, t_n) \in [0,1] \times [0, T_f]\}$

Theory: $E \sim \mathcal{O}(\Delta x^p), \mathcal{O}(\Delta t^q)$

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Manufactured Solutions

Choose a "nice" function $u(x,t) = w(x,t)$

Modified problem
$$\begin{cases} \partial_t u - \partial_{xx} u = f(x,t) \\ u(0,t) = w(0,t) \\ u(1,t) = w(1,t) \\ u(x,0) = w(x,0) \end{cases}$$

$$f(x,t) = \partial_t w - \partial_{xx} w$$

Example

$w(x,t) = \sin(2\pi x)\cos(2\pi t)$

$f(x,t) = 4\pi^2 \cos(2\pi t)\sin(2\pi x) - 2\pi \sin(2\pi t)\cos(2\pi x)$

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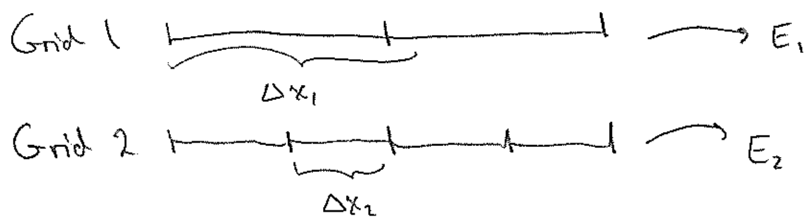
$u(0,t) = u(1,t) = 0$

$u(x,0) = \sin(2\pi x)$

$$E = \max\{|e_j^n|, \ (x_j, t_n) \in [0,1] \times [0, T_F]\}$$



⋮

Theory: $E \sim \mathcal{O}(\Delta x^{rate})$, μ is fixed, $\Delta t = \mu \Delta x^2$

$E = C \Delta x^{rate}$

$E_j = C \Delta x_j^{rate}$

$\dfrac{E_1}{E_2} = \left(\dfrac{\Delta x_1}{\Delta x_2}\right)^{rate}$ $\qquad$ $rate = \dfrac{\ln(E_1/E_2)}{\ln(\Delta x_1/\Delta x_2)}$

* Explicit $(\theta = 0)$

  if μ constant $E \sim \mathcal{O}(\Delta t) \sim \mathcal{O}(\Delta x^2)$

* Implicit $(\theta = 1)$
  - μ = constant $(\mu = \Delta t / \Delta x^2)$

    $E \sim \mathcal{O}(\Delta t) \sim \mathcal{O}(\Delta x^2)$
  - $\nu = \Delta t / \Delta x$ = constant

    $E \sim \mathcal{O}(\Delta t) \sim \mathcal{O}(\Delta x^1)$

* Crank Nicolson $(\theta = \frac{1}{2})$
  - μ constant $\longrightarrow$ $E \sim \mathcal{O}(\Delta t^2), \mathcal{O}(\Delta x^2)$
  - ν constant $\longrightarrow$ $E \sim \mathcal{O}(\Delta t^2), \mathcal{O}(\Delta x^2)$

$$\begin{cases} \partial_t u - \partial_{xx} u = 0 \\ u(0,t) = u(1,t) = 0 \\ u(x,0) = u_0(x) \end{cases}$$

$\Longrightarrow$ let's make it a <u>bit</u> more interesting

$$\begin{cases} \partial_t u = \partial_{xx} u \\ \partial_x u = \alpha(t) u + g(t) & \text{at } x = 0 \\ u = 0 & \text{at } x = 1 \\ u(x,0) = u_0(x) \end{cases}$$

Interior points

$$-\mu\theta U_{j-1}^{n+1} + (1+2\mu\theta)U_j^{n+1} - \mu\theta U_{j+1}^{n+1} = U_j^n + (1-\theta)\mu\left(U_{j+1}^n - 2U_j^n + U_{j-1}^n\right) \quad \Big\} (*)$$

$j = 1, 2, 3, \ldots, J-1$

Boundary points

$j = J \quad U_J^{n+1} = 0$

$j = 0$? $\quad t = t_n$

$$\frac{U_1^n - U_0^n}{\Delta x} = \alpha(t_n)U_0^n + g(t_n)$$

$$U_0^n = \frac{U_1^n - g^n \Delta x}{1 + \alpha^n \Delta x}$$

introduce $\beta^n = (1+\alpha^n \Delta x)^{-1} \Rightarrow \boxed{U_0^n = \beta^n U_1^n - \beta^n g^n \Delta x}$

Matrix Form $\qquad AU^{n+1} = F$

$$\begin{array}{c} \\ \\ \\ j \\ \\ \end{array}
\begin{bmatrix} 1 & -\beta^{n+1} & 0 & \cdots & & & 0 \\ & \ddots & \ddots & \ddots & & & \\ & & (-\mu\theta) & (1+2\mu\theta) & (-\mu\theta) & & \\ & & & \ddots & \ddots & \ddots & \\ 0 & \cdots & & & \cdots & 0 & 1 \end{bmatrix}
\begin{bmatrix} U_0^{n+1} \\ U_1^{n+1} \\ \vdots \\ U_j^{n+1} \\ \vdots \\ U_J^{n+1} \end{bmatrix}
=
\begin{bmatrix} \beta^{n+1} g^{n+1}\Delta x \\ \\ \\ (*) \\ \\ 0 \end{bmatrix}$$

Accuracy

Look only at $J=1$

$$-\mu\theta U_0^{n+1} + (1+2\mu\theta)U_1^{n+1} - \mu\theta U_2^{n+1} = U_1^n + (1-\theta)\mu\left(U_2^n - 2U_1^n + U_0^n\right)$$

But, $U_0^{n+1} = \beta^{n+1} U_1^{n+1} - \beta^{n+1} g^{n+1} \Delta x$

$$\underset{(A)}{[1+\theta\mu(2+\beta^{n+1})]U_1^{n+1}} = [1-(1-\theta)\mu(2-\beta^n)]U_1^n + \mu\theta U_2^{n+1} + (1-\theta)\mu U_2^n - \mu\Delta x\left(\theta\beta^{n+1}g^{n+1} + (1-\theta)\beta^n g^n\right) =: R(u^n, u^{n+1})$$

$$[1+\theta\mu)(2+\beta^{n+1})]u_1^{n+1} = R(u^n, u^{n+1}) + \Delta t\, T_1^{n+1/2} \quad (B)$$

$$e_j^n = U_j^n - u_j^n$$

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Subtract (B) from (A) to get equation for e_j^n

$$[1+\theta\mu(2-\beta^{n+1})]e_1^{n+1} = [1-(1-\theta)\mu(2-\beta^n)]e_1^n$$
$$-\mu\theta e_2^{n+1} - \mu(1-\theta)e_2^n - \Delta t T_1^{n+1/2}$$

We cannot use Fourier analysis!

$\rightarrow$ Use Max Principle

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$e_j^n = U_j^n - u_j^n$

Interior, $j>1$: (A) $(1+2\theta\mu)e_j^{n+1} = \theta\mu(e_{j-1}^{n+1}+e_{j+1}^{n+1}) + (1-\theta)\mu(e_{j-1}^n+e_{j+1}^n)$
$$+(1-2(1-\theta)\mu)e_j^n - \Delta t T_j^{n+1/2}$$

at $j=1$: (B) $(1+\theta\mu(2-\beta^{n+1}))e_1^{n+1} = \underline{(1-(1-\theta)\mu(2-\beta^n))}e_1^n$
$$\underline{+\mu\theta}e_2^{n+1} + \underline{(1-\theta)\mu}e_2^n - \Delta t T_1^{n+1/2}$$

Max. Principle: gives us a bound

$$E^n \le n\Delta t \max_n T^{n+1/2}$$

provided all the coefs of the RHS of (A) and (B) are positive and that the sum of all the coefs on RHS is smaller than or equal to those on the LHS

For (A): $\mu(1-\theta) \le \frac{1}{2}$ $\quad(\partial_x u = \alpha(t)u + g(t) \longrightarrow \alpha(t)\ge 0)$

For (B): we know $\beta^n = \frac{1}{1+\alpha^n\Delta x}$

If $\alpha^n \ge 0 \longrightarrow \beta^n \le 1$ and $\beta > 0$

First coef:

$$1-(1-\theta)\mu(2-\beta^n) = 1-2(1-\theta)\mu + (1-\theta)\beta\mu \ge 0 \text{ if } \mu(1-\theta)\le\tfrac{1}{2}$$

Sum: $1+\theta\mu(2-\beta^{n+1}) \ge 1-(1-\theta)\mu(2-\beta^n) + \theta\mu + (1-\theta)\mu$

$\iff$

$$\theta(1-\beta^{n+1}) \ge (1-\theta)(1-\beta^n)$$

but $0<\beta^n\le 1$ so this is always true

We can apply the Max Principle!

$$\Rightarrow E^n \le n\Delta t \max_m T^{m+1/2} \le T_F \max_m T^{m+1/2}$$

Question: What is $T^{m+1/2}$?

<u>Truncation Error</u> $T_j^{m+1/2}$, $j>1$ (known)

$j=1$ (consider just $\theta=0$)

- $T_1^{n+1/2} = \dfrac{u_1^{n+1}-u_1^n}{\Delta t} - \dfrac{u_2^n - 2u_1^n + u_0^n}{(\Delta x)^2}$

- boundary condition: $\dfrac{u_1^n - u_0^n}{\Delta x} - \alpha^n u_0^n - g^n \overset{\text{Taylor expansion } (x=0)}{=}$

$$\frac{1}{\Delta x}\left[\left(u_0^n + \Delta x u_x + \frac{1}{2}(\Delta x)^2 u_{xx} + \frac{1}{6}(\Delta x)^3 u_{xxx} + \cdots - u_0^n \right)\right]_0^n - \alpha^n u_0^n - g^n$$

$$= \underbrace{[u_x]_0^n - \alpha^n u_0^n - g_n}_{=0} + \left[\frac{1}{2}\Delta x u_{xx} + \frac{1}{6}(\Delta x)^2 u_{xxx} + \cdots\right]_0^n$$

Taylor expand $T_1^{n+1/2}$ around $x = \Delta x$

$$T_1^{n+1/2} = \frac{1}{\Delta t}\left[u_1^n + \Delta t u_t + \frac{1}{2}(\Delta t)^2 u_{tt} + \frac{1}{6}(\Delta t)^3 u_{ttt} + \cdots - u_1^n\right]_1^n$$

$$- \frac{1}{(\Delta x)^2}\Big[u_1^n + \Delta x u_x + \frac{1}{2}(\Delta x)^2 u_{xx} + \frac{1}{6}(\Delta x)^3 u_{xxx} + \frac{1}{24}(\Delta x)^4 u_{xxxx} + \cdots$$

$$- 2u_1^n + u_1^n - \Delta x u_x + \frac{1}{2}(\Delta x)^2 u_{xx} - \frac{1}{6}(\Delta x)^3 u_{xxx} + \frac{1}{24}(\Delta x)^4 u_{xxxx} + \cdots\Big]_1^n$$

$\vdots$

$$= \underbrace{\partial_t u - \partial_{xx} u}_{=0} + \left[\frac{1}{2}\Delta t u_{tt} - \frac{1}{12}(\Delta x)^2 u_{xxxx} + \cdots\right]_1^n$$

$$\left(T_1^{n+1/2} = \frac{u_1^{n+1} - u_1^n}{\Delta t} - \frac{u_2^n - 2u_1^n - u_0^n}{(\Delta x)^2} - \frac{\beta^n}{\Delta x}\left[\frac{u_1^n}{\Delta x} - \frac{u_0^n}{\beta^n \Delta x} - g^n\right] \right)$$

$$= \left[\frac{1}{2}\Delta t u_{tt} - \frac{1}{12}(\Delta x)^2 u_{xxxx} + \cdots\right]_1^n$$

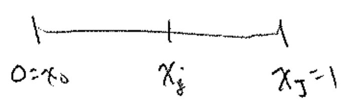
$$- \frac{\beta^n}{\Delta x}\left[\frac{1}{2}\Delta x u_{xx} + \frac{1}{6}(\Delta x)^2 u_{xxx} + \cdots\right]_0^n$$

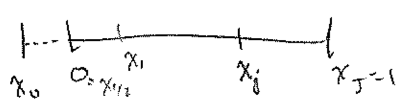
$$T_1^{n+1/2} \xrightarrow[\Delta x, \Delta t \to 0]{} -\frac{1}{2}u_{xx} \quad \text{oops!}$$

$$\partial_x u = \alpha(t) u + g(t), \quad x = 0$$

$$\frac{U_1^n - U_0^n}{\Delta x} = \alpha^n U_0^n + g^n$$

Alternative 1





$$\frac{U_1^n - U_0^n}{\Delta x} = \frac{1}{2}\alpha^n \left(U_0^n + U_1^n\right) + g^n$$

$$T^{n+1/2} \sim \Theta(\Delta x)!$$

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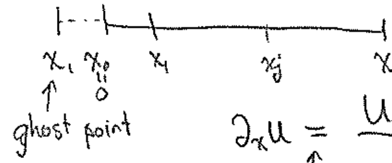
Alternative 2



$$\partial_x u = \frac{U_1^n - U_{-1}^n}{2\Delta x}$$
central differences

$$\frac{U_1^n - U_{-1}^n}{2\Delta x} = \alpha^n U_0^n + g^n \qquad T \sim \mathcal{O}(\Delta x)$$

Max Principle We need $\mu(1-\theta)(1+\alpha^n\Delta x) \le 1/2$

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$$\partial_t u = b(x,t)\,\partial_{xx} u, \quad b(x,t) > 0$$

$$\partial_t u\Big|_j^{n+1} \approx \frac{U_j^{n+1} - U_j^n}{\Delta t}$$

$$\partial_{xx} u\Big|_j^n \approx \frac{U_{j+1}^n - 2U_j^n + U_{j-1}^n}{(\Delta x)^2}$$

$$b(x,t)\Big|_j^n = b(x_j, t_n) = b_j^n$$

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \frac{b_j^n}{(\Delta x)^2}\left(U_{j+1}^n - 2U_j^n + U_{j-1}^n\right)$$

Truncation error

$$T(x,t) = \frac{1}{\Delta t}\left(u_j^n + \Delta t\, u_t + \tfrac{1}{2}(\Delta t)^2 u_{tt} + \cdots - u_j^n\right)$$
$$- \frac{b_j^n}{(\Delta x)^2}\Big(\cancel{u_j^n} + \cancel{\Delta x u_x} + \tfrac{1}{2}(\Delta x)^2 u_{xx} + \tfrac{1}{6}(\Delta x)^3 u_{xxx} + \tfrac{1}{24}(\Delta x)^4 u_{xxxx} + \cdots$$
$$- \cancel{2u_j^n} + \cancel{u_j^n} - \cancel{\Delta x u_x} + \tfrac{1}{2}(\Delta x)^2 u_{xx} - \tfrac{1}{6}(\Delta x)^3 u_{xxx} + \tfrac{1}{24}(\Delta x)^4 u_{xxxx} + \cdots$$

$$= \underbrace{(u_t - b(x,t)\,u_{xx})}_{=0} + \tfrac{1}{2}\Delta t\, u_{tt} - \tfrac{1}{12}(\Delta x)^2 u_{xxxx}\, b(x,t) + \cdots$$

$$T \longrightarrow 0 \quad \text{as } \Delta t, \Delta x \to 0$$

Stability

$$\mu b(x,t) \le \tfrac{1}{2}$$

because $U_j^{n+1} = U_j^n + \underline{b_j^n \mu}\left(U_{j+1}^n - 2U_j^n + U_{j-1}^n\right)$

so same analysis as before holds with $b\mu$ in place of μ

$$E^n \le \frac{1}{2}\Delta t\left(M_{tt} + \frac{1}{6\mu} B M_{xxxx}\right) T_F$$

$$B = \sup_{(x,t)\in[0,1]\times[0,T_F]} b(x,t)$$

$$\partial_t u = b(x,t)\,\partial_{xx}u + a(x,t)\,\partial_x u + c(x,t)\,u + d(x,t)$$

$$b(x,t) > 0$$

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \frac{b_j^n}{(\Delta t)^2}\left(U_{j+1}^n - 2U_j^n + U_{j-1}^n\right) + a_j^n\left(\frac{U_{j+1}^n - U_{j-1}^n}{2\Delta x}\right) + c_j^n U_j^n + d_j^n$$

Stability

Let $e_j^n = U_j^n - u_j^n$

$$e_j^{n+1} = \left(1 - 2\mu b_j^n + c_j^n \Delta t\right) e_j^n + \left(\mu b_j^n + \tfrac{1}{2}\nu a_j^n\right) e_{j+1}^n$$

$$+ \left(\mu b_j^n - \tfrac{1}{2}\nu a_j^n\right) e_{j-1}^n - \Delta t\, T_j^n$$

$$\mu = \frac{\Delta t}{(\Delta x)^2}, \quad \nu = \frac{\Delta t}{\Delta x}$$

For stability

(Max Principle)

all coef on RHS are non-negative and the sum no greater than unity

(i) $1 - 2\mu b_j^n + c_j^n \Delta t \ge 0 \iff \boxed{2\mu b_j^n - \Delta t c_j^n \le 1}$

(ii) $\mu b_j^n + \frac{1}{2}\nu a_j^n \ge 0 \iff -\frac{1}{2}\nu a_j^n \le \mu b_j^n$

(iii) $\mu b_j^n - \frac{1}{2}\nu a_j^n \ge 0 \iff \frac{1}{2}\nu a_j^n \le \mu b_j^n$

$\Big\}\ \frac{1}{2}\nu |a_j^n| \le \mu b_j^n$

(iv) $1 \cancel{- 2\mu b_j^n} + c_j^n \Delta t + \cancel{\mu b_j^n} \cancel{+ \frac{1}{2}\nu a_j^n} + \cancel{\mu b_j^n} \cancel{- \frac{1}{2}\nu a_j^n} \le 1 \iff c_j^n \le 0$

Summary:

$$\begin{cases} \frac{1}{2}\nu |a_j^n| \le \mu b_j^n \\ \Delta x \le 2b_j^n / |a_j^n| \\ c_j^n \le 0 \end{cases}$$

Practical applications: $b \ll a. \implies \Delta x$ very small

Central differences ✗

More efficient methods?

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$\hookrightarrow$ Implicit?
$\hookrightarrow$ what if you want explicit?

Assume $a \geq 0$

$$\frac{U_j^{n+1}-U_j^n}{\Delta t} = \frac{b_j}{(\Delta x)^2}\left(U_{j+1}^n - 2U_j + U_{j-1}^n\right) + \frac{a_j^n}{\Delta x}\left(U_{j+1}^n - U_j^n\right) + c_j^n U_j^n + d_j^n$$

$$e_j^{n+1} = (1-2\mu b_j^n - a_j^n \nu)e_j^n + (\mu b_j^n + \nu a_j^n)\, e_{j+1}^n + \mu b_j^n e_{j-1}^n - \Delta t\, T_j^n$$

(i) $1-2\mu b_j^n - a_j^n \nu \geq 0 \iff \boxed{2\mu b_j^n + \nu a_j^n \leq 1}$

(ii) $\mu b_j^n + \nu a_j^n \geq 0 \iff$ always true

(iii) $\mu b_j^n \geq 0 \iff$ always true

For stability: $\boxed{2\mu b_j^n + \nu a_j^n \leq 1}$

$$\partial_t u = \partial_x(p(x,t)\partial_x u) = p(x,t)\partial_{xx}u + \partial_x p \partial_x u$$

usually not a good idea to discretize this form

$\partial_t u = \partial_x F$

$$\partial_x F\Big|_j^n \approx \frac{F_{j+1/2}^n - F_{j-1/2}^n}{\Delta x}$$

Replace F by $p\partial_x u$

$$\partial_x(p\partial_x u)\Big|_j^n \approx \left([p\partial_x u]_{j+1/2}^n - [p\partial_x u]_{j-1/2}^n\right)/\Delta x$$

$$[p\partial_x u]_{j+1/2}^n \approx p_{j+1/2}^n\left(\frac{U_{j+1}^n - U_j^n}{\Delta x}\right)$$

$$[p\partial_x u]_{j-1/2}^n \approx p_{j-1/2}^n\left(\frac{U_j^n - U_{j-1}^n}{\Delta x}\right)$$

$$\frac{U_j^{n+1}-U_j^n}{\Delta t} = \frac{p_{j+1/2}^n(U_{j+1}^n - U_j^n) - p_{j-1/2}^n(U_j^n - U_{j-1}^n)}{(\Delta x)^2}$$

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2-D heat equation

$$\begin{cases} \partial_t u - \nabla^2 u = 0, & \vec{x} = (x,y) \in [0,1]\times[0,1], \quad t>0 \\ u(x,0) = u^0(x) \\ \text{boundary conditions} \end{cases}$$

u scalar

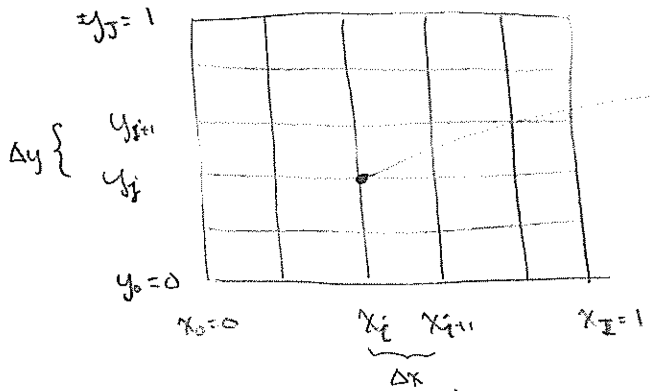
gradient: $\nabla u = \begin{bmatrix} \partial_x u \\ \partial_y u \end{bmatrix}$

$\vec{w} = (w_1, w_2)$

$\nabla \cdot \vec{w} = \partial_x w_1 + \partial_y w_2$

$$\nabla \cdot (\nabla u) = \partial_{xx} u + \partial_{yy} u = \nabla^2 u$$

$$\partial_t u - \nabla^2 u = \partial_t u - \partial_{xx} u - \partial_{yy} u = 0$$



$u(x_i, y_j, t_n) \approx U^n_{i,j}$

$$[\partial_t u]^n_{i,j} \xrightarrow[FD]{} \frac{U^{n+1}_{i,j} - U^n_{i,j}}{\Delta t}$$

$$[\partial_{xx} u]^n_{i,j} \longrightarrow \frac{U^n_{i+1,j} - 2U^n_{i,j} + U^n_{i-1,j}}{(\Delta x)^2}$$

$$[\partial_{yy} u]^n_{i,j} \longrightarrow \frac{U^n_{i,j+1} - 2U^n_{i,j} + U^n_{i,j-1}}{(\Delta y)^2}$$

$$\frac{U^{n+1}_{i,j} - U^n_{i,j}}{\Delta t} = \frac{U^n_{i+1,j} - 2U^n_{i,j} + U^n_{i-1,j}}{(\Delta x)^2} + \frac{U^n_{i,j+1} - 2U^n_{i,j} + U^n_{i,j-1}}{(\Delta y)^2}$$

$\frac{\Delta t}{(\Delta x)^2} \leq \frac{1}{2}$ (1-D) Stability

$\frac{\Delta t}{(\Delta x)^2} + \frac{\Delta t}{(\Delta y)^2} \leq \frac{1}{2}$ (2-D) Stability