AARMS Summer Course 2011

Introduction to Numerical Solution of Partial Differential Equations and Mesh Adaptation

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Overview: This course will be an introduction to the numerical solution of partial differential equations, particularly parabolic and elliptic equations. It will cover the finite difference method, the finite element method, concepts and analysis of consistency, stability, and convergence, the method of lines approach, programming skills, and basic concepts and principles of mesh adaptation. The objective is to provide students a background for treating more complicated problems arising in engineering and physics.

Prerequisites: Basic knowledge on partial differential equations. Knowledge in a programming language (such as Matlab, C, C++, or Fortran) is preferred but not required.

Texts: Lecture notes will be made available online. Reference books include
- Morton and Mayers, Numerical Solution of Partial Differential Equations (Cambridge, 2005)
- Johnson, Numerical Solution of Partial Differential Equations by the Finite Element Method (Dover, 2009)
- Huang and Russell, Adaptive Moving Mesh Methods (Springer, 2011). The first chapter of this book is available online at `http://www.springer.com/mathematics/numerical+and+computational+mathematics/book/978-1-4419-7915-5`

Grading: Grades will be based mainly on homework assignments and computer projects.

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Weizhang Huang
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References:

- Morton and Mayers: Numerical solution of partial differential equations (Cambridge 2005)
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Scientific Computing:

physical motivation
mathematical background
numerical analysis techniques
Computer knowledge

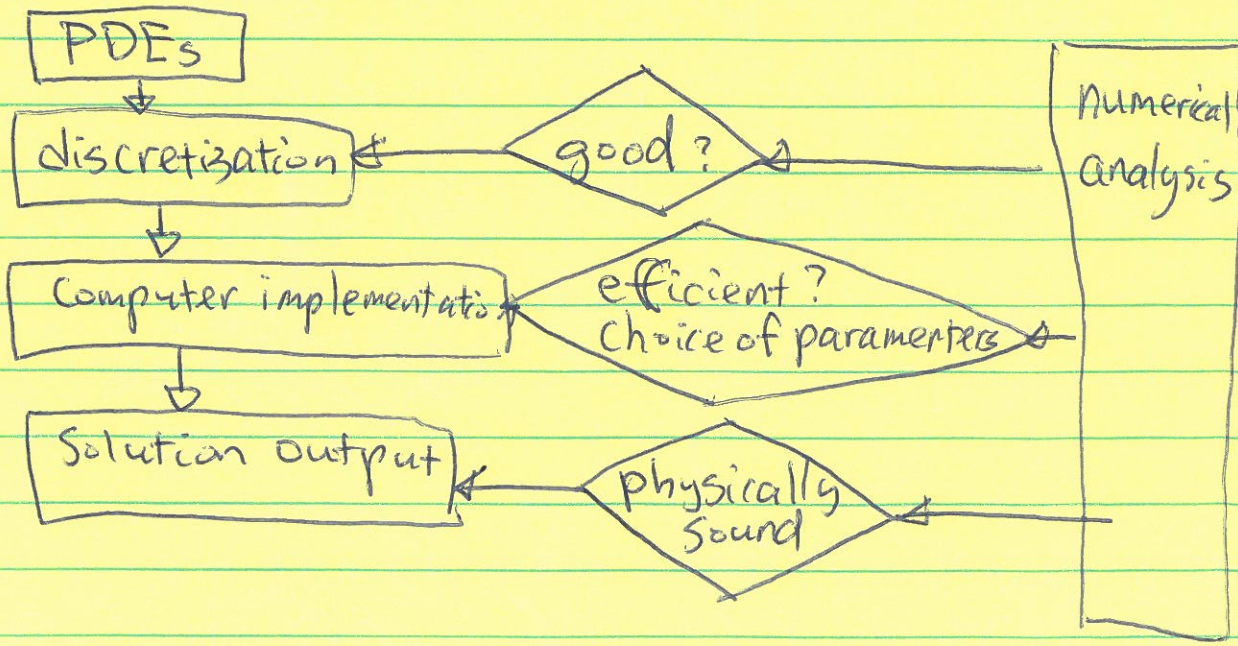
↓

find the numerical Solution of practical problems

↓

Show, illustrate and interpret your numerical solutions

Numerical PDEs.



<u>Consistency</u>: Numerical scheme ⟷ PDE

Does the numerical scheme approach close enough to the original, continuous PDE?

<u>Stability</u> Numerical scheme

Does the numerical solution stay bounded during the course of the solution of the discrete equations?

<u>Convergence</u> Numerical solution ⟷ exact solution of PDE

Does the solution of the numerical scheme approach close enough to the exact solution of the underlying PDE?

<u>Programming skills</u> is also a big factor in Numerical PDEs.

Lecture 1

Examples of PDEs

Independent variables

t — time

x, y, z — spatial coordinates

Three types of Second order PDEs:

- Parabolic PDEs

$$u_t = u_{xx} \qquad 1D$$

$$u_t = \frac{\partial}{\partial x}\left(a\frac{\partial u}{\partial x}\right) + b\frac{\partial u}{\partial x} + cu + f$$

$$a = a(x,t) \geq \alpha > 0 \qquad \alpha \text{ constant.}$$

IBVP (intial-boundary value problem)

PDE: $u_t = \frac{\partial}{\partial x}\left(a\frac{\partial u}{\partial x}\right) + b\frac{\partial u}{\partial x} + cu + f$ in $\Omega = (0,1)$, $0 < t < T$

BCs: $u(t,0) = g_0(t)$, $u(t,1) = g_1(t)$

IC: $u(0,x) = u^0(x)$

Multi-dimensions.

$$\nabla = \begin{bmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{bmatrix} \qquad \text{gradient operator}$$

Laplacian operator

$$\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \nabla \cdot \nabla = \nabla^2$$

$$u_t = \Delta u$$

$$\begin{cases} u_t = \nabla\cdot(a\nabla u) + \vec{b}\cdot\nabla u + cu + f \\ u|_{\partial\Omega} = g \\ u(0,x,y,z) = u^0(x,y,z) \end{cases}$$

- Elliptic PDEs

$$\begin{cases} u_{xx} = f \quad \text{in } (0,1) \\ u(0) = g_0 \\ u(1) = g_1 \end{cases} \qquad \text{(BVP)}$$

$$\Delta u = f \qquad \text{(poisson's eqn)}$$

$$\begin{cases} \nabla\cdot(a\nabla u) + \vec{b}\cdot\nabla u + cu = f \text{ in } \Omega \\ u|_{\partial\Omega} = g \end{cases}$$

Solution of elliptic PDE can often be viewed as the steady state solution of a corresponding parabolic PDE.

- Hyperbolic PDEs

$$u_t + a u_x = 0$$

$$u_{tt} = u_{xx}$$

$$u_{tt} = \Delta u$$

$$u_{tt} = \nabla\cdot(a\nabla u) + \vec{b}\nabla u + cu + f$$

Conservation laws (typerical with wave propagation problems with C soln. (discontinuous solutions))

More PDE examples

- Burgers' equation:

$$u_t + u u_x = \frac{1}{Re} u_{xx}$$

Re - Reynolds number

- Navier-Stokes equations (fluid dynamics) (incompressible fluid)

$$\begin{cases} u_t + u u_x + v u_y + w u_z = \frac{1}{Re} \Delta u - \frac{\partial p}{\partial x} + f_x \\ u_t + u v_x + v v_y + w v_z = \frac{1}{Re} \Delta v - \frac{\partial p}{\partial y} + f_y \\ w_t + u w_x + v w_y + w w_z = \frac{1}{Re} \Delta w - \frac{\partial p}{\partial z} + f_z \\ u_x + v_y + w_z = 0 \end{cases}$$

- Maxwell equations (Electromagnetism)

$$\begin{cases} \frac{\partial \vec{E}}{\partial t} = c \nabla \times \vec{B} - 4\pi \vec{J} \\ \frac{\partial \vec{B}}{\partial t} = - c \nabla \times \vec{E} \\ \nabla \cdot \vec{E} = 4\pi \rho \\ \nabla \cdot \vec{B} = 0 \end{cases}$$

- The Schrödinger equation (quantum mechanics)

$$i u_t = - \Delta u + V(x) u$$

- The Klein-Gordon equation (particle physics)

$$u_{tt} - c^2 \Delta u + m^2 u = - g u^3$$

sin(u) Sine-Gordon

- The KdV (Korteweg-de Vries) equation (shallow waves)

$$u_t + u_{xxx} + 6uu_x = 0$$

- Richard's equation

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left(D(\theta)\frac{\partial \theta}{\partial z}\right) - \frac{\partial K(\theta)}{\partial z}$$

θ: water content

$D(\theta) = \theta^3$: soil water diffusivity

$K(\theta) = 2.5\,\theta^3$: unsaturated hydraulic conductivity

- flame propagation:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} - f(u,v)$$

$$\frac{\partial v}{\partial t} = \frac{\partial^2 v}{\partial x^2} + f(u,v)$$

$$f(u,v) = 3.52 \times 10^6\, u\, e^{-\frac{4}{v}}$$

- Radiation diffusion

$$\frac{\partial E}{\partial t} = \varepsilon \frac{\partial}{\partial x}\left(D\frac{\partial E}{\partial x}\right) + \frac{\sigma_a}{\delta}\left(T^4 - E\right)$$

$$\frac{\partial T}{\partial t} = -\frac{\sigma_a}{\delta}\left(T^4 - E\right)$$

$$D = \frac{1}{3\sigma_a}, \quad \sigma_a = \frac{1}{T^3}$$

- FitzHugh-Nagumo equation (Biology)

$$\begin{cases} \dfrac{\partial u}{\partial t} = \varepsilon \dfrac{\partial^2 u}{\partial x^2} + \dfrac{1}{\delta}\left[u(1-u)(u-a) - w \right] \\ \dfrac{\partial w}{\partial t} = \beta (u - \gamma w) \end{cases}$$

⋮

⋮

$$\begin{cases} \dfrac{\partial u}{\partial t} = \dfrac{\partial^2 u}{\partial x^2} & \text{(parabolic)} \\ \dfrac{\partial^2 u}{\partial x^2} = f & \text{(elliptic)} \end{cases}$$

Lecture 2

Taylor's Theorem and finite Difference approximations of derivatives

- Taylor's Theorem
- big O notation for convergence
- finite difference (FD) approximations
- Order of convergence

▶ Taylor's Theorem

If $u \in C^n(a,b)$ and $u^{(n+1)}$ exists on (a,b), then for a given point x_0 and increment Δx satisfying $x_0 + \Delta x \in (a,b)$,

$$u(x_0+\Delta x) = u(x_0) + u'(x_0)\Delta x + \cdots + \frac{1}{n!}u^{(n)}(x_0)\Delta x^n + \frac{1}{(n+1)!}u^{(n+1)}(\xi)\Delta x^{n+1}$$

$$\equiv \sum_{k=0}^{n} \frac{1}{k!}u^{(k)}(x_0)\Delta x^k + \frac{1}{(n+1)!}u^{(n+1)}(\xi)\Delta x^{n+1}$$

where ξ is a point between $x_0+\Delta x$ and x_0.

Remark 1 Existence of ξ is known but its precise location or its expression is unknown.

Remark 2 $\frac{1}{(n+1)!}u^{(n+1)}(\xi)\Delta x^{n+1}$ is called the Lagrange remainder. The remainder can be expressed in an integral form.

Remark 3: $n=0$:

$$u(x_0+\Delta x) = u(x_0) + u'(\xi)\Delta x$$

or $u(b) - u(a) = (a-b)\, u'(\xi)$

or $$\frac{u(b)-u(a)}{b-a} = u'(\xi)$$

(Mean value Theorem).

Example 1

(a) $u(x) = \sin(x)$, $x_0 = 0$, $n=2$

(b) $u(x) = e^x$ $\quad x_0 = 0$, $n=3$

▶ Big O notation

Consider two functions

$$\begin{aligned} \alpha(x) &\to 0 \\ \beta(x) &\to 0 \end{aligned} \quad \text{as } x \to 0$$

we denote

$$\alpha(x) = O(\beta)$$

if there exists $c>0$ such that

$$\left|\frac{\alpha(x)}{\beta(x)}\right| \le c \quad \text{for all small } x. \ (\text{as } x\to 0)$$

We say

$$\alpha = o(\beta)$$

if

$$\left|\frac{\alpha(x)}{\beta(x)}\right| \to 0 \quad \text{as} \quad x \to 0.$$

Remark 1 if $\alpha = o(\beta)$, then $\alpha = O(\beta)$.
However, in this case, $\alpha = O(\beta)$ does not give a precise characterization.

Remark 2 Big O (and small o) notation can be used for sequences.

Ex 1 Taylor's expansion

$$u(x_0 + \Delta x) = \sum_{k=0}^{n} \frac{1}{n!} u^{(k)}(x_0)\,\Delta x^k + O(\Delta x^{n+1})$$

Ex 2

$$\sin(x) = O(x)$$

$$1 - \cos(x) = O(x^2) \qquad \text{as } x \to 0.$$

$$\frac{x}{1+x^2} = O(x)$$

Ex 3 As $n \to \infty$

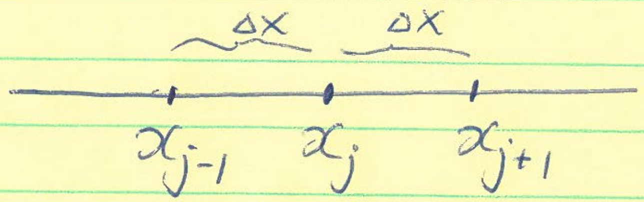
$$\sin\left(\frac{1}{n}\right) = o\left(\frac{1}{n}\right)$$

$$\frac{n}{1+n^3} = O\left(\frac{1}{n^2}\right).$$

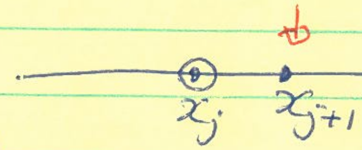
#

FD approximations of derivatives

- We want to use nodal values $u(x_j)$, $u(x_{j\pm1})$ to approximate derivatives $u'(x_j)$ and $u''(x_j)$



- forward FD:

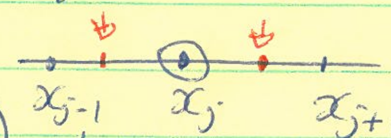


$$u'(x_j) \approx \frac{u(x_{j+1}) - u(x_j)}{\Delta x} \equiv \frac{1}{\Delta x}\Delta_+ u(x_j)$$

- backward FD

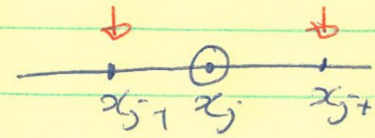
$$u'(x_j) \approx \frac{u(x_j) - u(x_{j-1})}{\Delta x} \equiv \frac{1}{\Delta x}\Delta_- u(x_j)$$

- central FD (half-point)



$$u'(x_j) \approx \frac{u(x_{j+\frac{1}{2}}) - u(x_{j-\frac{1}{2}})}{\Delta x} \equiv \frac{1}{\Delta x}\delta u(x_j)$$

- double-size central FD



$$u'(x_j) \approx \frac{u(x_{j+1}) - u(x_{j-1})}{2\Delta x} \equiv \frac{1}{\Delta x}\Delta_0 u(x_j)$$

- Use Taylor's expansion to show

$$\frac{1}{\Delta x}\Delta_+ u(x_j) = u'(x_j) + \frac{1}{2}u''(\xi)\Delta x$$

Thus, if $u''(\xi)$ is bounded, we have

$$\frac{1}{\Delta x}\Delta_+ u(x_j) = u'(x_j) + O(\Delta x)$$

(first order convergence in Δx)

Similarly,

$$\frac{1}{\Delta x}\Delta_- u(x_j) = u'(x_j) + O(\Delta x)$$

$$\frac{1}{\Delta x}\delta u(x_j) = u'(x_j) + O(\Delta x^2)$$

$$\frac{1}{\Delta x}\Delta_0 u(x_j) = u'(x_j) + O(\Delta x^2)$$

- Approximations for Second order derivative $u''(x_j)$:

$$\begin{aligned}
\frac{1}{\Delta x^2}\delta^2 u(x_j) &= \frac{1}{\Delta x^2}\Delta_+\Delta_- u(x_j) \\
&= \frac{1}{\Delta x^2}\Delta_-\Delta_+ u(x_j) \\
&= \frac{1}{\Delta x^2}\left(u(x_{j+1}) - 2u(x_j) + u(x_{j-1})\right) \\
&= u''(x_j) + O(\Delta x^2)
\end{aligned}$$

#

Lecture 3

FTCS Scheme for a model problem (I)

- model problem
- FTCS scheme
- local truncation error and Konsistency

Model problem

$$\begin{cases} u_t = u_{xx} & x \in (0,1) \quad t \in (0,T] \\ u(0,t) = 0, \ u(1,t) = 0 \\ u(x,0) = u^0(x) \end{cases}$$

Exact solution in Flourier series:

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

$$a_m = 2\int_0^1 u^0(x)\sin(m\pi x)\,dx \qquad m = 1, 2, \cdots$$

special case:

$$u^0(x) = \sin(\pi x)$$

$$u(x,t) = e^{-(\pi)^2 t}\sin(\pi x)$$

FD Discretization — FTCS scheme

partition of domain $(0,1)\times(0,T)$

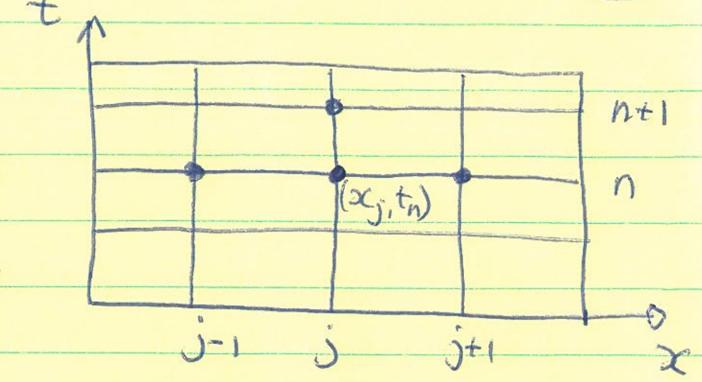
- For $(0,1)$: (in space)

$$x_0 = 0 < x_1 < \cdots < x_J = 1$$

$$x_j = j\Delta x, \quad j = 0, 1, \cdots, J$$

$$\Delta x = \frac{1}{J}$$

(J subintervals of equal length)



- For $(0,T)$: (in time)

$$t_0 = 0 < t_1 < \cdots < t_N \equiv T$$

$$t_n = n\Delta t, \quad n = 0, 1, \cdots, N$$

$$\Delta t = \frac{T}{N}$$

(N subintervals of equal length)

- We seek approximations to the solution at mesh points (x_j, t_n):

$$U_j^n \approx u(x_j, t_n) \qquad j = 0, 1, \cdots, J \quad n = 0, 1, \cdots, N$$

What are known:

$$U_j^n = 0 \qquad j = 0 \text{ or } j = J, \; n = 0, 1, \cdots, N \quad \text{(BCs)}$$

$$U_j^0 = u^0(x_j) \qquad j = 0, 1, \cdots, J \quad \text{(IC)}$$

What are unknown:

$$U_j^n \qquad j = 1, \cdots, J, \; n = 1, \cdots, N$$

(defined through PDE).

To develop the FD scheme, we recall that the PDE is defined at (x,t):

$$\frac{\partial u}{\partial t}(x,t) = \frac{\partial^2 u}{\partial x^2}(x,t)$$

Choose the "base" point as (x_j, t_n).

$$\frac{\partial u}{\partial t}(x_j,t_n) = \frac{\partial^2 u}{\partial x^2}(x_j,t_n)$$

↓ forward FD in time ↓ central FD in space

$$\frac{u(x_j,t_{n+1}) - u(x_j,t_n)}{\Delta t} \approx \frac{u(x_{j+1},t_n) - 2u(x_j,t_n) + u(x_{j-1},t_n)}{\Delta x^2}$$

FTCS Scheme (FT: forward in time
CS: central in space)

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta x^2}$$

$j = 1, \cdots, J-1$

$n = 0, 1, \cdots, N-1$

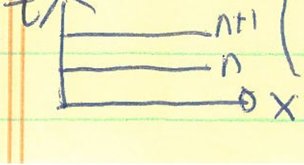
Computationally:

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

$j = 1, \cdots, J-1$

$n = 0, 1, \cdots, N-1$

The scheme is "matching style" in the sense that



$$\left(u_0^n, u_1^n, \cdots, u_J^n\right) \longrightarrow \left(u_0^{n+1}, u_1^{n+1}, \cdots, u_J^{n+1}\right)$$

▶ local truncation error and consistency

Q How close is the FTCS scheme to the PDE $u_t = u_{xx}$?

FTCS scheme: discrete equations about approximations u_j^n

PDE: continuous equation for function $u(x,t)$

Cannot perform direct comparison between FTCS scheme and PDE (apples and oranges?)

We may take a step furthere

Q: How close u_j^n and $u(x_j, t_n)$?

Define the error

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

Then

$$u_j^n = e_j^n + u(x_j, t_n)$$

Substituting this into FTCS scheme, we get the error equation

$$\frac{(e_j^{n+1} + u(x_j, t_{n+1})) - (e_j^n + u(x_j, t_n))}{\Delta t} = \frac{1}{\Delta x^2}\Big[(e_{j+1}^n + u(x_{j+1}, t_n)) - 2(e_j^n + u(x_j, t_n)) + (e_{j-1}^n + u(x_{j-1}, t_n))\Big]$$

$$\Rightarrow \frac{e_j^{n+1} - e_j^n}{\Delta t} = \frac{1}{\Delta x^2}\left(e_{j+1}^n - 2e_j^n + e_{j-1}^n\right) - \tau_j^n$$

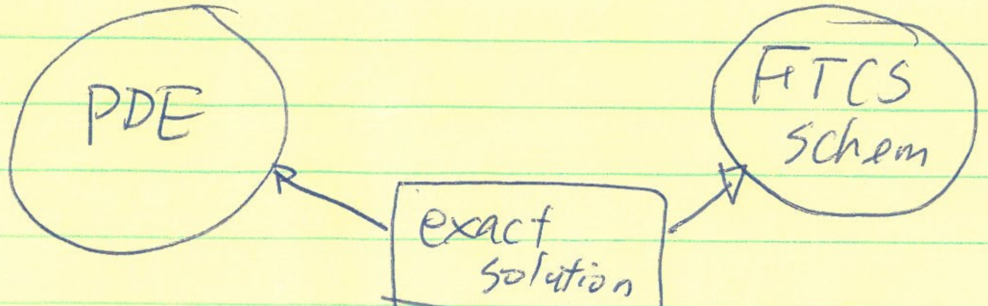
where

$$\tau_j^n = \frac{u(x_j, t_{n+1}) - u(x_j, t_n)}{\Delta t} - \frac{1}{\Delta x^2}\Big[u(x_{j+1}, t_n) - 2u(x_j, t_n) + u(x_{j-1}, t_n)\Big]$$

<u>Remark 1</u>. Quantity τ_j^n (called local truncation error) ~~can be considered~~ is the difference between the two sides of the FTCS scheme after u_j^n being replaced by $u(x_j, t_n)$.

<u>Remark 2</u> It measures how closely the exact solution $u(x,t)$ satisfies the FTCS scheme.

If τ_j^n were zero, both PDE and FTCS admit the same solution
$\Longrightarrow$ PDE and FTCS scheme the same



- τ_j^n is used to measure how closely the FTCS scheme approaches to the PDE as $\Delta t \to 0$, $\Delta x \to 0$.

<u>Definition</u> The FTCS scheme is ~~called~~ said to be consistent with the PDE if

$$\tau_j^n = O(\Delta t^q) + O(\Delta x^p)$$

as $\Delta t \to 0$, $\Delta x \to 0$

with $q \geq 1$ and $p \geq 1$.

<u>Remark 3</u> Consider the error over one time step. That is, we assume that $u_j^n = u(x_j, t_n)$ (or $e_j^n = 0$). We would like to see how big e_j^{n+1} is. From the error eqn, we have

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

i.e. $\Delta t \, \tau_j^n$ is the discretization error over one time step.

- Computation of the local truncation error: (Taylor's expansion)

$$\tau_j^n = \frac{\Delta t}{2} u_{tt}(x_j, \eta_n) - \frac{\Delta x^2}{12} u_{xxxx}(\xi_j, t_n)$$

$$= O(\Delta t) + O(\Delta x^2)$$

$$t_n < \eta_n < t_{n+1}, \quad x_{j-1} < \xi_j < x_{j+1}.$$

Lecture 4

FTCS scheme for a model problem (II)

- Convergence analysis (error estimation)
- Stability analysis $\begin{cases} L^\infty \text{ analysis} \\ \text{Fourier analysis} \end{cases}$

▶ Convergence analysis

Always starts with the error equation

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

Recall that

$$\tau_j^n = \frac{\Delta t}{2} u_{tt}(x_j, \eta_n) - \frac{\Delta x^2}{12} u_{xxxx}(\xi_j, t_n)$$

Let

$$M_{tt} = \max_{(x,t)} |u_{tt}(x,t)|$$

$$M_{xxxx} = \max_{(x,t)} |u_{xxxx}(x,t)|$$

$$|\tau_j^n| \le \frac{\Delta t}{2} M_{tt} + \frac{\Delta x^2}{12} M_{xxxx}$$

Define

$$\|e^n\|_\infty = \max_j |e_j^n|$$

From the error equation

$$e_j^{n+1} = \frac{\Delta t}{\Delta x^2} e_{j+1}^n + \left(1 - \frac{2\Delta t}{\Delta x^2}\right) e_j^n + \frac{\Delta t}{\Delta x^2} e_{j-1}^n - \Delta t\, \tau_j^n$$

$$|e_j^{n+1}| \leq \frac{\Delta t}{\Delta x^2}|e_{j+1}^n| + \left|1-\frac{2\Delta t}{\Delta x^2}\right||e_j^n| + \frac{\Delta t}{\Delta x^2}|e_{j+1}^n|$$

$$+ \Delta t\left(\frac{M_{tt}\Delta t}{2} + \frac{M_{xxxx}}{12}\Delta x^2\right)$$

$$\leq \left(\left|1-\frac{2\Delta t}{\Delta x^2}\right| + \frac{2\Delta t}{\Delta x^2}\right)\|e^n\|_\infty$$

$$+ \Delta t\left(\frac{M_{tt}}{2}\Delta t + \frac{M_{xxxx}}{12}\Delta x^2\right)$$

$$|e_j^{n+1}| \leq \left(\left|1-\frac{2\Delta t}{\Delta x^2}\right| + \frac{2\Delta t}{\Delta x^2}\right)\|e^n\|_\infty$$

$$+ \Delta t\left(\frac{M_{tt}}{2}\Delta t + \frac{M_{xxxx}}{12}\Delta x^2\right)$$

rhs is independent of j:

$$\|e^{n+1}\|_\infty \leq \left(\left|1-\frac{2\Delta t}{\Delta x^2}\right| + \frac{2\Delta t}{\Delta x^2}\right)\|e^n\|_\infty$$

$$+ \Delta t\left(\frac{M_{tt}}{2}\Delta t + \frac{M_{xxxx}}{12}\Delta x^2\right)$$

repeat the inequality:

$$\|e^n\|_\infty \leq \Big(\underbrace{\left|1-\frac{2\Delta t}{\Delta x^2}\right| + \frac{2\Delta t}{\Delta x^2}}_{\alpha}\Big)^n \|e^0\|_\infty$$

$$+ \left(\alpha^{n-1} + \cdots + 1\right)\Delta t\left(\frac{M_{tt}}{2}\Delta t + \frac{M_{xxxx}}{12}\Delta x^2\right)$$

$$= \begin{Bmatrix} \dfrac{\alpha^n - 1}{\alpha - 1}, & \alpha \neq 1 \\ n, & \alpha = 1 \end{Bmatrix} \cdot \Delta t(\ldots)$$

Thus, if $\alpha = 1$ or

$$\frac{2\Delta t}{\Delta x^2} \leq 1 \quad \text{or} \quad \boxed{\Delta t \leq \frac{1}{2}\Delta x^2},$$

we have

$$\|e^n\|_\infty \leq (n\Delta t)\left[\frac{M_{tt}}{2}\Delta t + \frac{M_{vxxx}}{12}\Delta x^2\right]$$

or

$$\boxed{\|e^n\|_\infty \leq T\left(\frac{M_{tt}}{2}\Delta t + \frac{M_{xxxx}}{12}\Delta x^2\right)}$$

$$\boxed{e_j^n = O(\Delta t) + O(\Delta x^2)} \quad \text{as } \Delta t \to 0,\ \Delta x \to 0.$$

FTCS: first order in time
second order in space.

Stability analysis.

We are concerned with the propagation of roundoff error in the computation using the FTCS scheme. Since roundoff error can occur at every step and in every operation, it is extremely difficult, if not impossible, to study the propagation of all roundoff errors.

For this reason, we consider a special but representive scenario:

We assume that roundoff error occurs when we calculate the initial solution. We want to see how the error evolves with FTCS scheme, provided that no more roundoff error is introduced in later computation.

Mathematically,

$$\begin{cases} u_j^{n+1} = u_j^n + \frac{\Delta t}{\Delta x^2}\left(u_{j+1}^n - 2u_j^n + u_{j-1}^n\right) & j = 1, \cdots J-1 \\ & n = 0, 1, \cdots N-1 \\ u_j^0 = u^0(x_j) & \end{cases} \quad (*)$$

$$\begin{cases} v_j^{n+1} = v_j^n + \frac{\Delta t}{\Delta x^2}\left(v_{j+1}^n - 2v_j^n + v_{j-1}^n\right) & j = 1, \cdots J-1 \\ & n = 0, 1 \cdots N-1 \\ v_j^0 = u^0(x_j) + \varepsilon_j & \end{cases}$$

ε_j initial roundoff error

error propagation can be characterized by $w_j^n = v_j^n - u_j^n$:

$$\begin{cases} w_j^{n+1} = w_j^n + \frac{\Delta t}{\Delta x^2}\left(w_{j+1}^n - 2w_j^n + w_{j-1}^n\right) & n = 0, 1, \cdots N-1 \\ w_j^0 = \varepsilon_j & \end{cases} \quad (**)$$

we would like to know if $|w_j^n| \leq C$ for all n, j as $\Delta t \to 0$, $\Delta x \to 0$.

<u>Remark</u> Since the equation (**) for w_j^n has the same form as (*) for u_j^n (homogeneous equation of FTCS scheme), for notational simplicity we simply consider the homogeneous equation

$$\begin{cases} u_j^{n+1} = u_j^n + \frac{\Delta t}{\Delta x^2}(u_{j+1}^n - 2u_j^n + u_{j-1}^n) \\ u_j^0 = u^0(x_j) \end{cases}$$

and check if

$$|u_j^n| \leq C \quad \text{for all } j, n \text{ as } \Delta t \to 0 \ \Delta x \to 0$$

for stability.

▶ <u>L^∞ stability analysis</u>

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

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

If $1 - \frac{2\Delta t}{\Delta x^2} \geq 0$ or

$$\boxed{\Delta t \leq \frac{1}{2}\Delta x^2} \text{ (CFL condition)}$$

Caurant-Friedrichs-Lewy

we have

$$\|u^{n+1}\|_\infty \leq \|u^n\|_\infty \leq \cdots \leq \|u^0\|_\infty$$

FTCS scheme is conditionally stable.

Fourier stability analysis

Recall: the exact solution of the IBVP is

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

We guess the finite difference solution has the form:

$$u_j^n = \sum_{m=1}^{J-1} b_m (\lambda_m)^n \sin(m\pi x_j)$$

where b_m, $m=1,\cdots,J-1$ determined by the initial solution, λ_m determined by the FD Equation.

By the superposition principle, we can consider each "Fourier mode" separately.

$$u_j^n = (\lambda)^n \sin(m\pi x_j) \qquad m=1,\cdots,J-1$$

where λ depends on m.

More generally, we can ~~first~~ consider a more general form:

$$u_j^n = (\lambda)^n e^{im\pi x_j} \qquad i^2 = -1$$

Substituting this into

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta x^2}$$

We get

$$\frac{\lambda - 1}{\Delta t} = \frac{1}{\Delta x^2}\left[e^{im\pi\Delta x} - 2 + e^{-im\pi\Delta x}\right]$$

$$\lambda = 1 - \frac{4\Delta t}{\Delta x^2}\sin^2\left(\tfrac{1}{2}m\pi\Delta x\right)$$

$|\lambda| \leq 1$ for all $m = 1, \cdots, J-1$

$\Longrightarrow$ $\Delta t \leq \frac{1}{2}\Delta x^2$ (CFL).

#

Lecture 5

The θ method for the model problem

- The θ method
- local truncation error
- Stability analysis
- Convergence analysis
- implicit vs. explicit

▶ The θ method

- Recall: FTCS scheme (explicit Euler)

$$\frac{\partial u}{\partial t}(x_j, t_n) = \frac{\partial^2 u}{\partial x^2}(x_j, t_n)$$

$$\Rightarrow \quad \frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta x^2}$$

- BTCS scheme (implicit Euler)

$$\frac{\partial u}{\partial t}(x_j, t_{n+1}) = \frac{\partial^2 u}{\partial x^2}(x_j, t_{n+1})$$

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{\Delta x^2}$$

(backward) (central)

- The θ method ($\theta \in [0,1]$)

$$\frac{\partial u}{\partial t}(x_j, t_{n+\theta}) = \frac{\partial^2 u}{\partial x^2}(x_j, t_{n+\theta})$$

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

($\theta = 0 \Rightarrow$ FTCS scheme
$\theta = 1 \Rightarrow$ BTCS scheme)

$\theta = \frac{1}{2}$: Crank-Nicolson Scheme

Local truncation error

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

$$\Rightarrow \quad u_j^n = e_j^n + u(x_j, t_n)$$

$$\Rightarrow \frac{e_j^{n+1} - e_j^n}{\Delta t} = (1-\theta)\frac{e_{j+1}^n - 2e_j^n + e_{j-1}^n}{\Delta x^2} + \theta \frac{e_{j+1}^{n+1} - 2e_j^{n+1} + e_{j-1}^{n+1}}{\Delta x^2} - \tau_j^n$$

(error eqn)

$$\tau_j^n = \frac{u(x_j, t_{n+1}) - u(x_j, t_n)}{\Delta t} - (1-\theta)\frac{u(x_{j+1}, t_n) - 2u(x_j, t_n) + u(x_{j-1})}{\Delta x^2} - \theta \frac{u(x_{j+1}, t_{n+1}) - 2u(x_j, t_{n+1}) + u(x_{j-1}, t_{n+1})}{\Delta x^2}$$

$$\frac{u(x_j, t_{n+1}) - u(x_j, t_n)}{\Delta t} = u_t(x_j, t_n) + \frac{u_{tt}(x_j, t_n)}{2!}\Delta t + \frac{u_{ttt}(x_j, \eta_n)}{3!}\Delta t^2$$

$$\frac{1}{\Delta x^2}\delta_x^2 u(x_j, t_n) = \frac{1}{12} u_{xxxx}(\xi_j, t_n)\Delta x^2 + u_{xx}(x_j, t_n)$$

$$\frac{1}{\Delta x^2}\delta_x^2 u(x_j, t_{n+1}) = u_{xx}(x_j, t_{n+1}) + \frac{\Delta x^2}{12} u_{xxxx}(\bar{\xi}_j, t_{n+1})$$

$$= u_{xx}(x_j, t_n) + u_{txx}(x_j, t_n)\Delta t + \frac{\Delta t^2}{2} u_{ttxx}(x_j, \bar{\eta}_n) + \frac{\Delta x^2}{12} u_{xxxx}(\bar{\xi}_j, t_{n+1})$$

$u_{txx} = u_{tt}$

$u_{ttxx} = u_{ttt}$

$$\tau_j^n = u_t(x_j, t_n) + \frac{\Delta t}{2} u_{tt}(x_j, t_n) + \frac{\Delta t^2}{3} u_{ttt}(x_j, \eta_n) - u_{xx}(x_j, t_n) - \frac{(1-\theta)}{12}\Delta x^2 u_{xxxx}(\xi_j, t_n) - \theta \Delta t\, u_{tt}(x_j, t_n) - \frac{\theta \Delta t^2}{2} u_{ttt}(x_j, \bar{\eta}_n) - \frac{\theta \Delta x^2}{12} u_{xxxx}(\bar{\xi}_j, t_{n+1})$$

$$= \left(\tfrac{1}{2} - \theta\right)\Delta t\, u_{tt}(x_j, t_n) + O(\Delta t^2) + O(\Delta x^2)$$

$$\tau_j^n = \begin{cases} O(\Delta t) + O(\Delta x^2) & \theta \neq \frac{1}{2} \\ O(\Delta t^2) + O(\Delta x^2) & \theta = \frac{1}{2} \end{cases}$$

Consistent with PDE!

▶ stability

- L^∞ stability analysis:

$$\|u^{n+1}\|_\infty \leq \|u^n\|_\infty \quad \text{when} \quad \Delta t \leq \frac{\Delta x^2}{2(1-\theta)}$$

CFL Condition

- Fourier stability analysis

$$u_j^n = (\lambda)^n e^{i m \pi x_j}$$

CFL condition

$$2(1-2\theta)\Delta t \le \Delta x^2 : \begin{cases} \text{on restriction on } \Delta t & \frac{1}{2} \le \theta \le 1 \\ \Delta t \le \dfrac{\Delta x^2}{2(1-2\theta)} & 0 \le \theta < \frac{1}{2} \end{cases}$$

$\frac{1}{2} \le \theta \le 1$: unconditionally stable
$0 \le \theta < \frac{1}{2}$: conditionally stable

Comparison:

L^∞: CFL: $2(1-\theta)\Delta t \le \Delta x^2$ stronger
Fourier CFL: $2(1-2\theta)\Delta t \le \Delta x^2$ weaker

▷ Convergence (in L^∞ norm)

$$\|e^n\|_\infty \to 0 \text{ as } n \to \infty$$

~~$\|e^n\| \le O(\Delta t$~~

$$\|e^n\|_\infty = \begin{cases} O(\Delta t) + O(\Delta x^2) & \theta \ne \frac{1}{2} \\ O(\Delta t^2) + O(\Delta x^2) & \theta = \frac{1}{2} \end{cases}$$

under condition

$$2(1-\theta)\Delta t \le \Delta x^2.$$

Implicit vs explicit

FTCS scheme ($\theta = 0$): explicit

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

$\theta > 0$: implicit

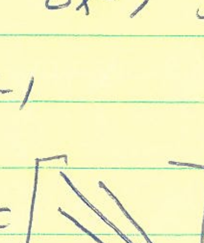
$$u_0^{n+1}, u_1^{n+1}, \cdots, u_{J-1}^{n+1}, u_J^{n+1}$$

must be solved simultaneously.

$$\begin{cases} -\frac{\theta \Delta t}{\Delta x^2} u_{j-1}^{n+1} + \left(1 + \frac{2\theta \Delta t}{\Delta x^2}\right) u_j^{n+1} - \frac{\theta \Delta t}{\Delta x^2} u_{j+1}^{n+1} \\ \qquad = u_j^n + \frac{\Delta t (1-\theta)}{\Delta x^2}\left(u_{j+1}^n - 2u_j^n + u_{j-1}^n\right) \\ \qquad\qquad j = 1, \cdots, J-1 \\ u_0^{n+1} = 0 \\ u_J^{n+1} = 0 \end{cases}$$

$$A\vec{u}^{\,n+1} = \vec{b}^{\,n}$$

$$\begin{cases} A_{j,j} = 1 + \frac{2\theta \Delta t}{\Delta x^2}, \quad A_{j,j-1} = -\frac{\theta \Delta t}{\Delta x^2}, \quad A_{j,j+1} = -\frac{\theta \Delta t}{\Delta x^2}, \\ b_j^n = \cdots \qquad j = 1, \cdots, J-1 \\ A_{0,0} = 1, \quad b_0^n = 0 \\ A_{J,J} = 1, \quad b_J^n = 0 \end{cases}$$

$A =$  tridiagonal