

Numerical Methods for Differential Equations

Chapter 5: Elliptic and Parabolic PDEs

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1. Brief overview of PDE problems

Classification Three basic types, four prototype equations

Elliptic $-\Delta u = f$ + BC *Poisson equation*

Parabolic $u_t = \Delta u$ + BC & IV *Diffusion equation*

Hyperbolic $u_{tt} = \Delta u$ + BC & IV *Wave equation*
 $u_t + a(u)u_x = 0$ + BC & IV *Advection equation*

We will consider these equations in 1D (one space dimension only)

$$-u'' = f; \quad u_t = u_{xx}; \quad u_{tt} = u_{xx}; \quad u_t + a(u)u_x = 0$$

Classification of PDEs

Classical approach Linear PDE with two independent variables

$$Au_{xx} + 2Bu_{xy} + Cu_{yy} + L(u_x, u_y, u, x, y) = 0$$

with L linear in u_x, u_y, u . Study

$$\delta := \det \begin{pmatrix} A & B \\ B & C \end{pmatrix} = AC - B^2$$

$\delta > 0$ *Elliptic*

$\delta = 0$ *Parabolic*

$\delta < 0$ *Hyperbolic*

Highest derivatives wrt t and x determines the PDE type

Let $F(\omega, x) = e^{i\omega x}$ and let u and its derivatives go to zero as $x \rightarrow \pm\infty$, and introduce the Fourier transform $\mathcal{F} : u \mapsto \hat{u}$ by

$$\hat{u}(\omega) = \mathcal{F}u = \langle F, u \rangle = \int_{-\infty}^{\infty} \bar{F}u \, dx = \int_{-\infty}^{\infty} e^{-i\omega x} u \, dx$$

Then

$$\mathcal{F}u_t = \langle F, u_t \rangle = d(\mathcal{F}u)/dt = d\hat{u}/dt$$

$$\mathcal{F}u_x = \langle F, u_x \rangle = -\langle F_x, u \rangle = -\langle i\omega F, u \rangle = i\omega \mathcal{F}u = i\omega \hat{u}$$

$$\mathcal{F}u_{xx} = \langle F, u_{xx} \rangle = \langle F_{xx}, u \rangle = -\langle \omega^2 F, u \rangle = -\omega^2 \mathcal{F}u = (i\omega)^2 \hat{u}$$

etc.

General classification. . .

Highest order terms (real coefficients)

$$\frac{\partial^p u}{\partial t^p} = \frac{\partial^q u}{\partial x^q}$$

Hyperbolic if $p + q$ is even, parabolic if $p + q$ is odd

$$u_t = u_x \quad \text{Hyperbolic}$$

$$u_t = u_{xx} \quad \text{Parabolic}$$

$$i u_t = u_{xx} \quad \text{Hyperbolic}$$

$$u_t = u_{xxx} \quad \text{Hyperbolic}$$

$$u_t = -u_{xxxx} \quad \text{Parabolic}$$

$$u_{tt} = u_{xx} \quad \text{Hyperbolic}$$

$$u_{tt} = -u_{xxxx} \quad \text{Hyperbolic}$$

General classification. . .

Mostly about the properties of the solutions:

Elliptic steady-state solutions, no time evolution

Parabolic energy dissipation, solutions gain regularity

Hyperbolic energy conservation, no regularity gain

Classification breaks down for nonlinear problems

PDE method types

FDM *Finite difference methods*

FEM *Finite element methods*

FVM *Finite volume methods*

BEM *Boundary element methods*

... *Spectral methods*

We will mostly study FDM to cover basic theory and some FEM

PDE methods for elliptic problems

Simple geometry FDM or Fourier methods

Complex geometry FEM

Special problems FVM or BEM

Very large, sparse systems, e.g. 10^6 — 10^{10} equations

Often combined with *iterative solvers* such as multigrid methods

PDE methods for parabolic problems

Simple geometry FDM or Fourier methods

Complex geometry FEM

Stiffness calls for A -stable implicit time-stepping methods

Need Newton-type solvers for large sparse systems, e.g. 10^6 — 10^9 equations. May be combined with multigrid methods

FDM, **FVM**. Sometimes FEM

Very challenging problems, with *conservation properties*, sometimes *shocks*, and sometimes *multiscale phenomena* such as turbulence

Solutions may be discontinuous, cf. “sonic booms”

Highly specialized methods are often needed

2. Elliptic problems with FDM

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

Laplace equation $\Delta u = 0$

with boundary conditions $u = u_0(x, y, z) \quad x, y, z \in \partial\Omega$

Poisson equation $-\Delta u = f$

with boundary conditions $u = u_0(x, y, z) \quad x, y, z \in \partial\Omega$

Other boundary conditions also of interest (Neumann)

- *Equilibrium problems*
 - Structural analysis (strength of materials)
 - Heat distribution
- *Potential problems*
 - Potential flow (inviscid, subsonic flow)
 - Electromagnetics (fields, radiation)
- *Eigenvalue problems*
 - Acoustics
 - Microphysics

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

Computational domain $\Omega = [0, 1] \times [0, 1]$ (unit square), Dirichlet conditions $u(x, y) = 0$ on boundary

Uniform grid $\{x_i, y_j\}_{i,j=1}^{N,M}$ with equidistant mesh widths $\Delta x = 1/(N + 1)$ and $\Delta y = 1/(M + 1)$

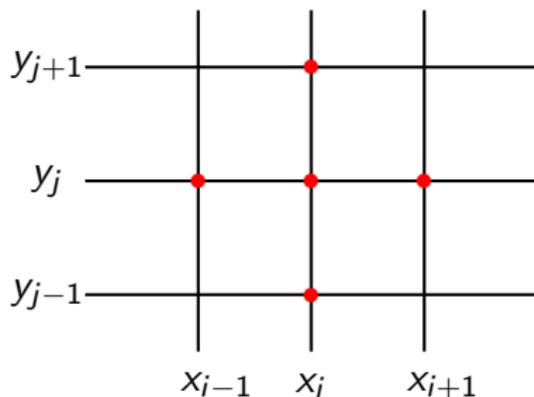
Discretization Finite differences with $u_{i,j} \approx u(x_i, y_j)$

$$\frac{u_{i-1,j} - 2u_{i,j} + u_{i+1,j}}{\Delta x^2} + \frac{u_{i,j-1} - 2u_{i,j} + u_{i,j+1}}{\Delta y^2} = f(x_i, y_j)$$

Equidistant mesh $\Delta x = \Delta y$

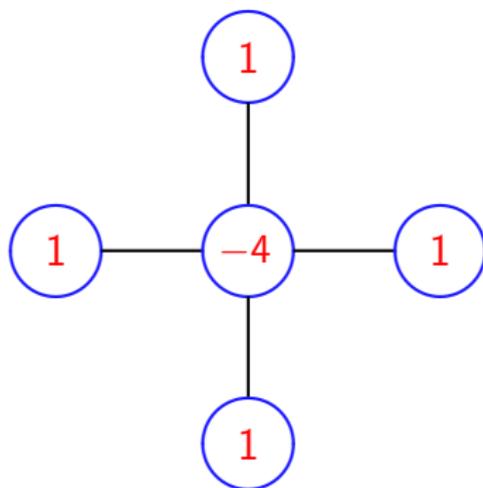
$$\frac{u_{i-1,j} + u_{i,j-1} - 4u_{i,j} + u_{i,j+1} + u_{i+1,j}}{\Delta x^2} = f(x_i, y_j)$$

Participating approximations and mesh points



Computational stencil for $\Delta x = \Delta y$

$$\frac{u_{i-1,j} + u_{i,j-1} - 4u_{i,j} + u_{i,j+1} + u_{i+1,j}}{\Delta x^2} = f(x_i, y_j)$$



“Five-point operator”

3. Elliptic problems with FEM

A general finite element method

Linear PDE	$Lu = f$	in domain Ω
Ansatz	$u = \sum c_i \varphi_i$	$\Rightarrow Lu = \sum c_i L\varphi_i$
Requirement	$\langle \varphi_i, Lu - f \rangle = 0$	gives coefficients $\{c_i\}$

FEM is a *least squares approximation*, fitting a linear combination of basis functions $\{\varphi_i\}$ to the solution using *orthogonality*

Simplest case Piecewise linear basis functions: 2nd-order cG(1)

Strong and weak forms

Strong form

$$-\Delta u = f \quad \text{in } \Omega; \quad u = 0 \quad \text{on } \partial\Omega$$

Take v with $v = 0$ on $\partial\Omega$

$$\int_{\Omega} -\Delta u v \, d\Omega = \int_{\Omega} f v \, d\Omega$$

Integrate by parts to get weak form

$$\int_{\Omega} \nabla u \cdot \nabla v = \int_{\Omega} f v$$

Note: \cdot means scalar product on \mathbb{R}^d here; ∇u is a vector

Recall integration by parts in 1D

$$\int_0^1 -u''v \, dx = [-u'v]_0^1 + \int_0^1 u'v' \, dx$$

or in terms of an inner product

$$-\langle u'', v \rangle = \langle u', v' \rangle$$

Generalization to 2D, 3D uses vector calculus

Weak form of $-\Delta u = f$

$$\Delta u = \operatorname{div}(\operatorname{grad} u)$$

Define inner product

$$\langle v, u \rangle = \int_{\Omega} vu \, d\Omega$$

and *bilinear form*

$$a(v, u) = - \int_{\Omega} v \Delta u \, d\Omega = \int_{\Omega} \nabla v \cdot \nabla u \, d\Omega = \int_{\Omega} \operatorname{grad} v \cdot \operatorname{grad} u \, d\Omega$$

to get the *weak form* of $-\Delta u = f$ as

$$a(v, u) = \langle v, f \rangle$$

Galerkin method (Finite Element Method)

1. *Basis functions* $\{\varphi_i\}$
2. *Approximate* $u = \sum c_j \varphi_j$
3. *Determine* c_j from $\sum c_j a(\varphi_i, \varphi_j) = \langle \varphi_i, f \rangle$

The c_j are determined by the *linear system*

$$Kc = F$$

The matrix K is called the *stiffness matrix*

Stiffness matrix elements $k_{ij} = a(\varphi_i, \varphi_j) = \int \nabla \varphi_i \cdot \nabla \varphi_j \, d\Omega$

Right-hand side $F_i = \langle \varphi_i, f \rangle = \int \varphi_i f \, d\Omega$

Dealing with the right-hand side

Typically $\int \varphi_i f \, d\Omega$ cannot be evaluated exactly so we approximate

$$f \approx \sum_j f_j \varphi_j$$

Then

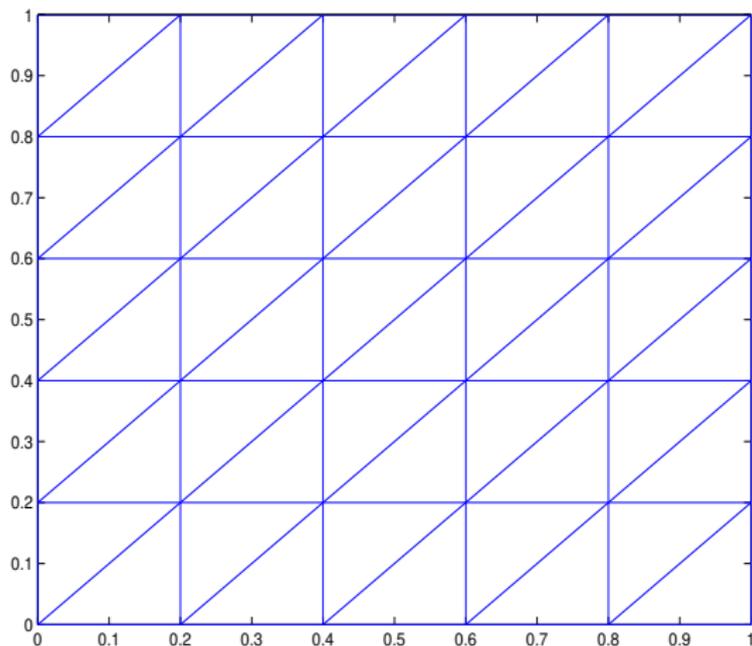
$$F_i \approx \langle \varphi_i, \sum_j f_j \varphi_j \rangle = \int \varphi_i \sum_j f_j \varphi_j \, d\Omega = \sum_j \langle \varphi_i, \varphi_j \rangle f_j$$

The matrix M is called the *mass matrix*, with matrix elements

$$m_{ij} = \langle \varphi_i, \varphi_j \rangle = \int \varphi_i \varphi_j \, d\Omega$$

Finite element equations, using $\bar{f} = \{f_j\}$, finally becomes $Kc = M\bar{f}$

Piecewise linear basis $\{\varphi_j\}$ require domain *triangulation*



The prototypical equation is the *diffusion equation*

$$u_t = \Delta u$$

Also nonlinear diffusion

$$u_t = \operatorname{div}(k(u) \operatorname{grad} u)$$

Boundary and initial conditions are needed

Solution methods are now built by *combining time-stepping* methods with *space discretization* of the spatial derivative operator

- *Diffusive processes*

Heat conduction

$$u_t = d \cdot u_{xx}$$

- *Chemical reactions*

Reaction–diffusion

$$u_t = d \cdot u_{xx} + f(u)$$

Convection–diffusion

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

- *Seismology*

Parabolic waves

$$u_t = uu_x + d \cdot u_{xx}$$

Irreversibility $u_t = -\Delta u$ is not well-posed!

Equation	$u_t = u_{xx}$
Initial values	$u(0, x) = g(x)$
Boundary values	$u(t, 0) = u(t, 1) = 0$

Separation of variables $u(t, x) := X(x)T(t) \Rightarrow$

$$u_t = X\dot{T}, \quad u_{xx} = X''T \quad \Rightarrow \quad \frac{\dot{T}}{T} = \frac{X''}{X} =: \lambda$$

$$T = Ce^{\lambda t} \quad X = A \sin \sqrt{-\lambda}x + B \cos \sqrt{-\lambda}x$$

Parabolic model problem...

Boundary values $X(0) = X(1) = 0 \Rightarrow \lambda_k = -(k\pi)^2$, therefore

$$X_k(x) = \sqrt{2} \sin k\pi x \quad T_k(t) = e^{-(k\pi)^2 t}$$

Fourier expansion of initial values $g(x) = \sum_1^\infty c_k \sqrt{2} \sin k\pi x \Rightarrow$

Solution can be assembled

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

5. Method of lines (MOL) discretization

In $u_t = u_{xx}$, discretize $\partial^2/\partial x^2$ by

$$u_{xx} \approx \frac{u_{i-1} - 2u_i + u_{i+1}}{\Delta x^2}$$

System of ODEs (semidiscretization) $\dot{u} = T_{\Delta x} u$ reads

$$\dot{u} = \frac{1}{\Delta x^2} \begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & & \ddots & & \\ & & & 1 & -2 \end{pmatrix} u$$

Full FDM discretization

Note $u_i(t) \approx u(t, x_i)$ along the *line* $x = x_i$ *in the* (t, x) *plane*

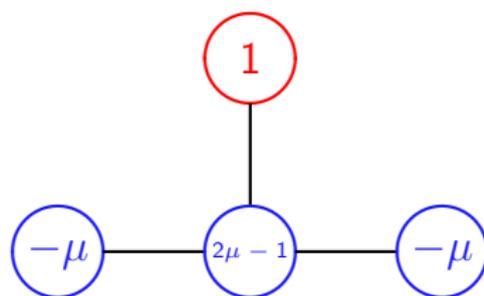
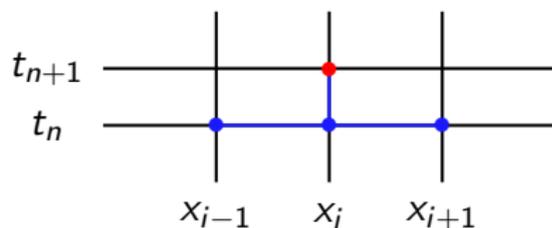
Using Explicit Euler time-stepping with $u_i^n \approx u(t_n, x_i)$ implies

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

With the *Courant number* $\mu = \Delta t / \Delta x^2$ we obtain recursion

$$u_i^{n+1} = u_i^n + \mu \cdot (u_{i-1}^n - 2u_i^n + u_{i+1}^n)$$

Explicit Euler time stepping. Participating grid points



Courant number $\mu = \Delta t / \Delta x^2$

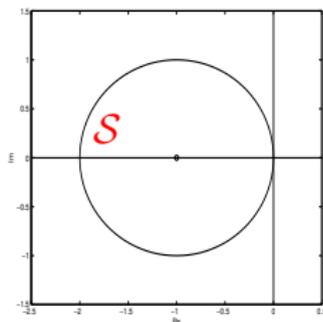
Explicit Euler with $\Delta x = 1/(N + 1)$ implies recursion

$$u_i^{n+1} = u_i^n + \Delta t \cdot T_{\Delta x} u_i^n$$

Recall $\lambda_k[T_{\Delta x}] = -4(N + 1)^2 \sin^2 \frac{k\pi}{2(N + 1)}$ for $k = 1 : N$

Stability requires $\Delta t \cdot \lambda_k \in \mathcal{S}$ for all eigenvalues

$$\Delta t \cdot \lambda_k \in \left[-\frac{4\Delta t}{\Delta x^2}, -\pi^2 \Delta t \right]$$



The CFL condition

For **explicit Euler** stability we need $4\Delta t/\Delta x^2 \leq 2$

CFL condition (Courant, Friedrichs, Lewy 1928)

$$\frac{\Delta t}{\Delta x^2} \leq \frac{1}{2}$$

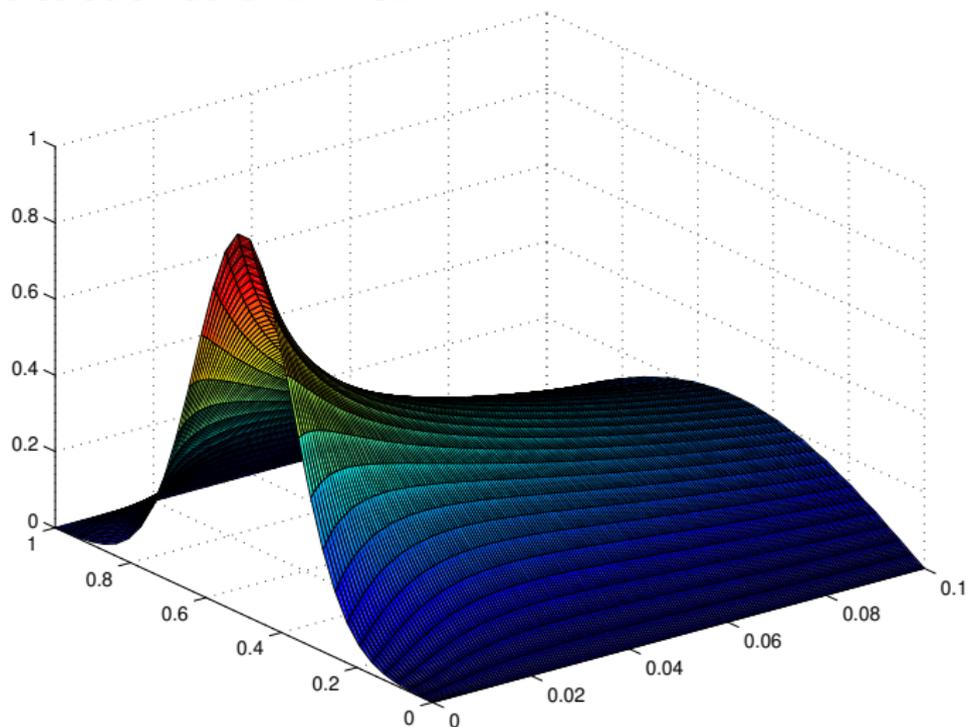


The CFL condition is a severe restriction on time step Δt

Stiffness The CFL condition can be avoided by using A-stable methods, e.g. Trapezoidal Rule or Implicit Euler

Experimental stability investigation

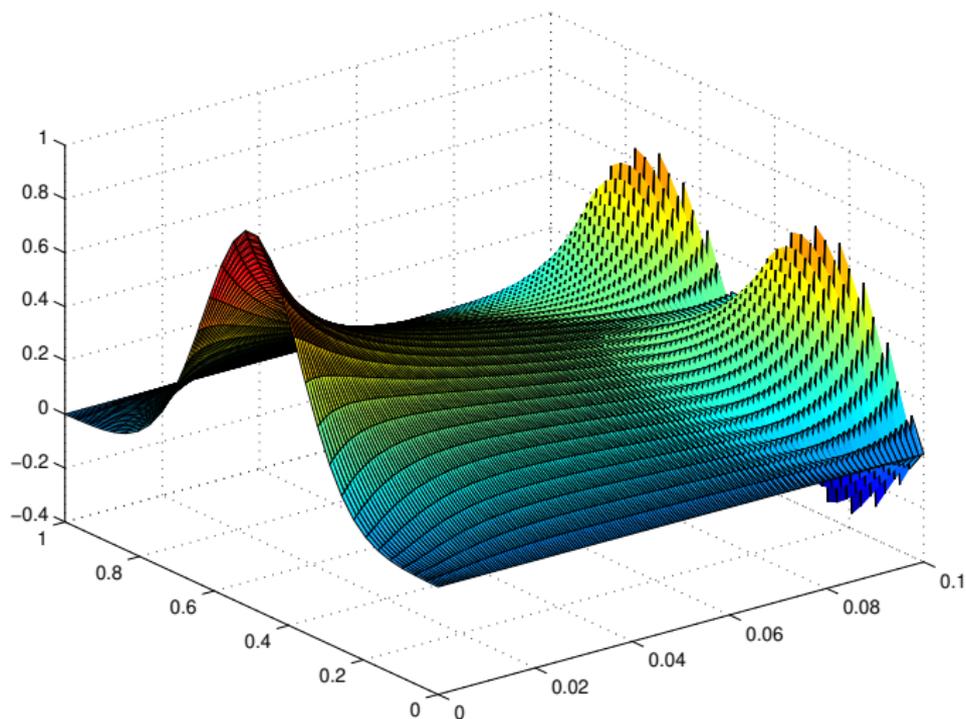
$N = 30$ internal pts in $[0, 1]$, $M = 187$ time steps on $[0, 0.1]$.
Stable solution at $\text{CFL} = .514$



Violating the CFL condition

Instability!

$N = 30$ internal pts in $[0, 1]$, $M = 184$ time steps on $[0, 0.1]$.
Unstable solution at $\text{CFL} = .522$



Crank–Nicolson method (1947)

Crank–Nicolson method \Leftrightarrow Trapezoidal Rule for PDEs

The Trapezoidal Rule is

- implicit \Rightarrow *more work/step*
- A–stable \Rightarrow *no restriction on Δt*
- Far more efficient

Theorem Crank–Nicolson is *unconditionally stable*

There is *no CFL condition* on the time-step Δt which is why the Crank–Nicolson method is preferable

Crank–Nicolson method...

$$u^{n+1} = u^n + \frac{\Delta t}{2} \left(T_{\Delta x} u^n + T_{\Delta x} u^{n+1} \right)$$

Courant number $\mu = \Delta t / \Delta x^2 \Rightarrow$ recursion

$$\left(I - \frac{\mu}{2} T \right) u^{n+1} = \left(I + \frac{\mu}{2} T \right) u^n$$

with Toeplitz matrix $T = \text{tridiag}(1 \quad -2 \quad 1)$

Tridiagonal structure \Rightarrow low complexity

Refactorize only if Courant number $\mu = \Delta t / \Delta x^2$ changes

MOL with explicit Euler for $u_t = u_{xx}$

Global error $e_i^n = u_i^n - u(t_n, x_i)$

Local error Insert exact solution to get

$$\frac{u(t_{n+1}, x_i) - u(t_n, x_i)}{\Delta t} = \frac{u(t_n, x_{i-1}) - 2u(t_n, x_i) + u(t_n, x_{i+1}))}{\Delta x^2} - l_i^n$$

Expand in Taylor series

$$-l_i^n = \frac{\Delta t}{2} u_{tt} + \frac{\Delta x^2}{12} u_{xxxx} + O(\Delta t^2, \Delta x^4)$$

The Lax Principle

Conclusion

<i>Consistency</i>	$l_i^n \rightarrow 0$	as $\Delta t, \Delta x \rightarrow 0$
<i>Stability</i>	CFL condition	$\Delta t / \Delta x^2 \leq 1/2$
<i>Convergence</i>	$e_i^n \rightarrow 0$	as $\Delta t, \Delta x \rightarrow 0$

Theorem (Lax Principle)

Consistency + Stability \Rightarrow Convergence

Note Choice of norm is very important

With local error

$$-l_i^n = \frac{\Delta t}{2} u_{tt} + \frac{\Delta x^2}{12} u_{xxxx} = O(\Delta t, \Delta x^2)$$

and stability in terms of CFL condition $\mu = \Delta t / \Delta x^2 \leq 1/2$ we have global error $e_i^n = O(\Delta t, \Delta x^2)$

For fixed μ we have $\Delta t \sim \Delta x^2$ and it follows that

Global error $e_i^n = O(\Delta t, \Delta x^2) = O(\Delta x^2) \Rightarrow$

Theorem *The order of convergence is $p = 2$*

$$A_\mu = \left(I - \frac{\mu}{2}T\right)^{-1} \left(I + \frac{\mu}{2}T\right) \quad \text{with the usual Toeplitz matrix } T$$

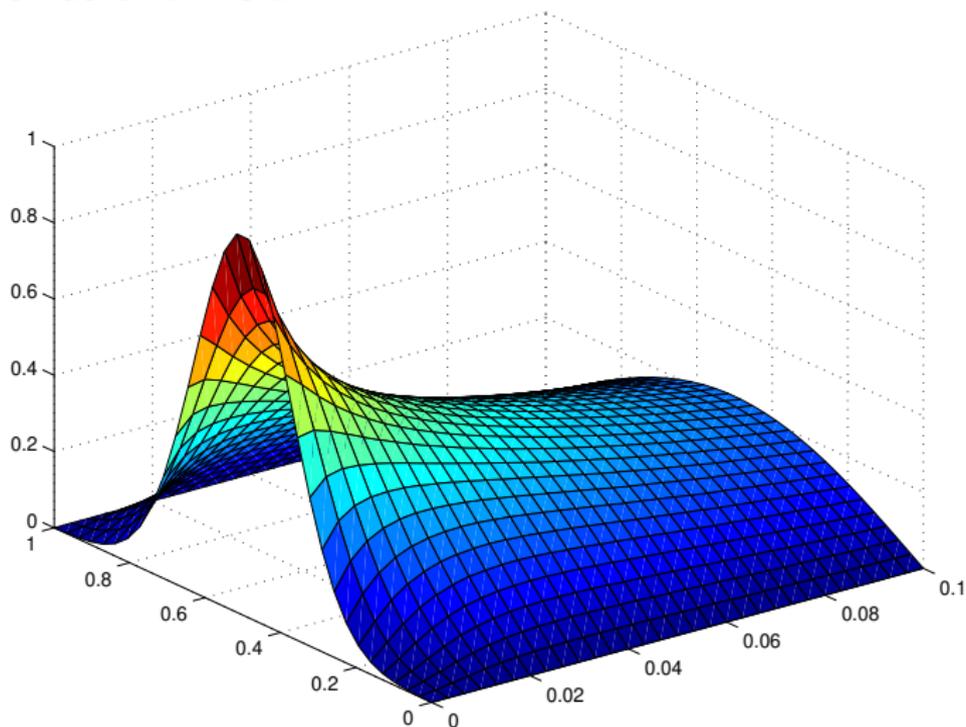
Theorem The eigenvalues are $\lambda[A_\mu] = \frac{1 + \frac{\mu}{2}\lambda[T]}{1 - \frac{\mu}{2}\lambda[T]}$

Note $\lambda[T] \in (-4, 0) \Rightarrow -1 < \lambda[A_\mu] < 1$. This implies that there is no CFL stability condition on the Courant ratio μ . The method is stable for all $\Delta t > 0$

Theorem Crank–Nicolson is *unconditionally stable* and convergent of order $p = 2$

Experimental stability investigation

$N = 30$ internal pts in $[0, 1]$, $M = 30$ time steps on $[0, 0.1]$ Stable solution at $CFL = 3.2$



Space operator with homogeneous Dirichlet conditions on $[0, 1]$

$$\mathcal{L}_\alpha u = u'' + \alpha u'$$

Convection dominated for Péclet numbers $|\alpha| \gg 1$, with boundary layer at $x = 1$ for $\alpha < 0$ and at $x = 0$ for $\alpha > 0$

\mathcal{L}_α is *not self-adjoint*, but it is *equi-elliptic* wrt Péclet number:

$$\lambda_k[\mathcal{L}_\alpha] = -(k\pi)^2 - \frac{\alpha^2}{4}$$
$$u^k(x) = e^{-\alpha x/2} \sin k\pi x$$

$\Rightarrow \mu_{[\mathcal{L}_\alpha]} \leq -(k\pi)^2$ for all α

$N \times N$ Toeplitz matrix $T_{\Delta x}$ with $\Delta x = 1/(N + 1)$

$$\mathcal{L}_\alpha = \frac{d^2}{dx^2} + \alpha \frac{d}{dx} \sim \frac{1}{\Delta x^2} \text{tridiag}(1 \ -2 \ 1) + \frac{\alpha}{2\Delta x} \text{tridiag}(-1 \ 0 \ 1) \\ =: T_{\Delta x}$$

While \mathcal{L}_α has negative real eigenvalues, the discrete eigenvalues

$$\lambda_k[T_{\Delta x}] = -\frac{2}{\Delta x^2} + \frac{2}{\Delta x^2} \sqrt{1 - \frac{\alpha^2 \Delta x^2}{4}} \cos \frac{k\pi}{N+1}, \quad k = 1 : N$$

are negative real only if *mesh Péclet number satisfies* $|\alpha \Delta x| < 2$

7. Parabolic problems with cG(1) FEM

Consider diffusion problem in strong form $u_t - u_{xx} = 0$ with Dirichlet boundary conditions

Multiply by test function v and integrate by parts

$$\int_0^1 v u_t \, dx + \int_0^1 v' u' \, dx = 0$$

In terms of inner product and energy norm:

Weak form $\langle v, u_t \rangle + a(v, u) = 0$ for all v with $v(0) = v(1) = 0$

Galerkin cG(1) FEM for parabolic equations

1. *Basis functions* $\{\varphi_i\}$
2. *Approximate* $u(t, x) = \sum c_j(t)\varphi_j(x)$
3. *Determine c_j from* $\langle \varphi_i, u_t \rangle + a(\varphi_i, u) = 0$

Note $\langle \varphi_i, u_t \rangle = \sum \dot{c}_j \langle \varphi_i, \varphi_j \rangle$ and $a(\varphi_i, u) = \sum c_j \langle \varphi'_i, \varphi'_j \rangle$

We get an initial value problem

$$M_{\Delta x} \dot{c} + K_{\Delta x} c = 0$$

for the determination of the coefficients $c_j(t)$ with $c(0)$ determined by the initial condition

Galerkin cG(1) FEM for parabolic equations

Simplest case Piecewise linear elements on equidistant grid

Stiffness matrix elements $k_{ij} = \langle \varphi'_i, \varphi'_j \rangle$

$$K_{\Delta x} = \frac{1}{\Delta x} \text{tridiag}(-1 \quad 2 \quad -1)$$

and mass matrix elements $m_{ij} = \langle \varphi_i, \varphi_j \rangle$

$$M_{\Delta x} = \frac{\Delta x}{6} \text{tridiag}(1 \quad 4 \quad 1)$$

Galerkin cG(1) FEM for parabolic equations. . .

Note that in the initial value problem

$$M_{\Delta x} \dot{c} + K_{\Delta x} c = 0$$

the matrix $M_{\Delta x}$ is tridiagonal \Rightarrow *no advantage from explicit time stepping methods*

Explicit Euler

$$M_{\Delta x}(c_{n+1} - c_n) = -\Delta t \cdot K_{\Delta x} c_n$$

requires the solution of a tridiagonal system on every step

Galerkin cG(1) FEM for parabolic equations. . .

As the system is *stiff*, use implicit A-stable method instead

$$M_{\Delta x}(c_{n+1} - c_n) = -\frac{\Delta t}{2} \cdot K_{\Delta x}(c_n + c_{n+1})$$

and solve tridiagonal system

$$(M_{\Delta x} + \frac{\Delta t}{2} K_{\Delta x})c_{n+1} = (M_{\Delta x} - \frac{\Delta t}{2} K_{\Delta x})c_n$$

on every step

Trapezoidal rule has *same cost, but better stability*

8. Well-posedness

Linear partial differential equation

$$u_t = \mathcal{L}u + f, \quad 0 \leq x \leq 1, \quad t \geq 0, \quad u(0, x) = h(x), \\ u(t, 0) = \phi_0(t), \quad u(t, 1) = \phi_1(t)$$

Suppose
$$\begin{cases} w_t = \mathcal{L}w + f, & w(0, x) = h(x) \\ v_t = \mathcal{L}v + f, & v(0, x) = h(x) + g(x) \end{cases}$$

Subtract to get *homogeneous Dirichlet problem*

$$u_t = \mathcal{L}u, \quad u(0, x) = g(x), \quad \phi_0(t) \equiv 0, \quad \phi_1(t) \equiv 0$$

Suppose time evolution $u(t, x) = \mathcal{E}(t)g(x)$

Definition The equation is *well-posed* if for every $t^* > 0$ there is a constant $0 < C(t^*) < \infty$ such that $\|\mathcal{E}(t)\| \leq C(t^*)$ for all $0 \leq t \leq t^*$

Definition A well-posed equation has a *solution* that

- depends continuously on the initial value (the “data”)
- is uniformly bounded in any compact interval

A small change in initial condition results in a small change in the solution

$u_t = u_{xx}$ is well posed

Fourier series expansion $g(x) = \sqrt{2} \sum_1^{\infty} c_k \sin k\pi x$ implies

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

$$\begin{aligned} \|\mathcal{E}(t)g\|_2^2 &= \int_0^1 |u(t, x)|^2 dx \\ &= 2 \sum_{k=1}^{\infty} \sum_{j=1}^{\infty} c_k c_j e^{-(k^2+j^2)\pi^2 t} \int_0^1 \sin k\pi x \sin j\pi x dx \\ &= \sum_{k=1}^{\infty} c_k^2 e^{-2(k\pi)^2 t} \leq \sum_{k=1}^{\infty} c_k^2 = \|g\|_2^2 \end{aligned}$$

Hence $\|\mathcal{E}(t)\|_2 \leq 1$ for every $t \geq 0$