

1. Introduction
2. Solution of first order partial differential equations
- 3. Solution of second order partial differential equation**
4. High performance methods

General form:

$$Lu := \sum_{i=1}^n \sum_{j=1}^n a_{ij}(x) \frac{\partial^2 u}{\partial x_i \partial x_j} + \sum_{i=1}^n b_i(x) \frac{\partial u}{\partial x_i} + c(x)u = f(x, u) \quad (9)$$

Ingredients:

- $a_{ij}, b_i, c : \mathbb{R}^n \rightarrow \mathbb{R}$ continuously differentiable
- wanted function u in n variables, thus $u = u(x_1, \dots, x_n)$
- homogeneous if $f = 0$, inhomogeneous otherwise

Example

1. For the three-dimensional Poisson equation $\Delta u = f$ holds

$$A(x) = I \in \mathbb{R}^{3 \times 3} \quad \text{as} \quad u_{x_1 x_1} + u_{x_2 x_2} + u_{x_3 x_3} = \sum_{i=1}^3 \frac{\partial^2 u}{\partial x_i^2}.$$

2. For the heat equation $u_t = \Delta u$ in 2D with $u = u(x_1, x_2, t)$ the operator reads

$$Lu = \frac{\partial^2 u}{\partial x_1^2} + \frac{\partial^2 u}{\partial x_2^2} - \frac{\partial u}{\partial t}$$

and the coefficients are

$$A = \text{diag}(1, 1, 0) \in \mathbb{R}^{3 \times 3}, \quad b = (0, 0, -1)^T.$$

3. For the 2D wave equation $u_{tt} = \Delta u$ holds

$$Lu = \frac{\partial^2 u}{\partial x_1^2} + \frac{\partial^2 u}{\partial x_2^2} - \frac{\partial^2 u}{\partial t^2} \quad \text{and thus} \quad A = \text{diag}(1, 1, -1).$$

3. Solution of second order partial differential equation

- 3.1 Characteristics of second order partial differential equations
- 3.2 Classification of linear second order partial differential equations
- 3.3 Canonical form of a linear second order PDE
- 3.4 Analytical solution of the Laplace equation
- 3.5 Analytical solution of the wave equation
- 3.6 Analytical solution of the heat equation
- 3.7 Difference methods for elliptic problems
- 3.8 Difference methods for parabolic problems
- 3.9 Difference methods for hyperbolic problems

Definition 3.1

For the PDE from (9) the second order term

$$L_0 u := \sum_{i=1}^n \sum_{j=1}^n a_{ij}(x) \frac{\partial^2 u}{\partial x_i \partial x_j}$$

is called the principal part of the operator Lu .

Remarks:

- the principal part decides about the main properties of the considered PDE
- the spectrum of the matrix $A(x)$ defines the type of the equation
- without limitation of generality we assume always $A(x) \in \mathbb{R}^{n \times n}$ to be symmetric, otherwise use $\frac{1}{2}(A(x) + A(x)^T)$

Definition 3.2

The quadratic polynomial

$$L_0(x, \xi) := \sum_{i=1}^n \sum_{j=1}^n a_{ij}(x) \xi_i \xi_j = \xi^T A(x) \xi$$

is called the principal symbol of a linear second order PDE.

Example

1. *For the Laplace equation $\Delta u = 0$ the principal symbol is*

$$L_0 = \xi_1^2 + \xi_2^2 + \xi_3^2 = \|\xi\|_2^2.$$

2. *For the heat equation $u_t = \Delta u$ the principal symbol is*

$$L_0 = \xi_2^2 + \xi_3^2.$$

3. *For the wave equation $u_{tt} = \Delta u$ the principal symbol is*

$$L_0 = \xi_1^2 + \xi_2^2 - \xi_3^2.$$

Definition 3.3

The characteristic equation of a given PDE is

$$L_0(x, \xi) = 0.$$

A solution ξ of the characteristic equation is called characteristic direction or characteristic of the principal symbol. A differentiable hypersurface in \mathbb{R}^n such that its normal vector $\xi \in \mathbb{R}^n$ points in a characteristic direction is called a characteristic surface (or characteristic curve if $n = 2$).

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Definition 3.4

Let $\lambda_1, \dots, \lambda_n$ be the eigenvalues of $A(x) \in \mathbb{R}^{n \times n}$ with respect to their multiplicities. At the point x the PDE is called

- (a) elliptic if all eigenvalues of $A(x)$ are positive or all eigenvalues of $A(x)$ are negative,
- (b) parabolic if one eigenvalue is zero and all others are positive or all others are negative,
- (c) hyperbolic if one eigenvalue is positive and all others are negative or one eigenvalue is negative and all others are positive.

The PDE is called elliptic, parabolic resp. hyperbolic if it is elliptic, parabolic resp. hyperbolic at every point of the domain Ω .

Example

1. For the n th-dimensional Laplace equation the matrix is $A = I_n$. Its eigenvalues are $\lambda_1 = \dots = \lambda_n = 1$ and the PDE is elliptic.
2. For the 2D heat equation $u_t = \Delta u$ with $u = u(x_1, x_2, t)$ the matrix is

$$A = \text{diag}(1, 1, 0) \in \mathbb{R}^{3 \times 3}$$

and the eigenvalues are $\lambda_1 = \lambda_2 = 1, \lambda_3 = 0$. Thereby the PDE is parabolic.

Example

3. For the 2D wave equation $u_{tt} = \Delta u$ the matrix is

$$A = \text{diag}(1, 1, -1)$$

and has the eigenvalues $\lambda_1 = \lambda_2 = 1, \lambda_3 = -1$. The PDE is hyperbolic.

4. Consider the PDE

$$3u_{xx} + 2u_{xy} + 2u_{xz} + 2u_{yy} + 2u_{zz} = f(x).$$

The matrix is

$$A(x) = A = \begin{pmatrix} 3 & 1 & 1 \\ 1 & 2 & 0 \\ 1 & 0 & 2 \end{pmatrix}.$$

A check of the main minors shows, that A is positive definite and thereby all eigenvalues are positive. Indeed they are $\lambda_1 = 4, \lambda_2 = 2, \lambda_3 = 1$. Thus the PDE is elliptic.

Remark 6

A special case is for $n = 2$. Using (x, y) instead of (x_1, x_2) we can write the PDE as

$$a_{11}u_{xx} + 2a_{12}u_{xy} + a_{22}u_{yy} + b_1u_x + b_2u_y + c = f.$$

Without using the eigenvalues directly we can classify the PDE with $a_{11} > 0$ as

- *elliptic if $\det(A) = a_{11}a_{22} - a_{12}^2 > 0$,*
- *parabolic if $\det(A) = a_{11}a_{22} - a_{12}^2 = 0$ and*
- *hyperbolic if $\det(A) = a_{11}a_{22} - a_{12}^2 < 0$.*

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Definition 3.5

A linear second order PDE is called of canonical form if it does not include mixed derivatives $\frac{\partial^2 u}{\partial x_i \partial x_j}$ with $i \neq j$ of the unknown function. Thus the PDE is of the form

$$Lu = \sum_{i=1}^n a_{ii}(x) \frac{\partial^2 u}{\partial^2 x_i} + \sum_{i=1}^n b_i(x) \frac{\partial u}{\partial x_i} + c(x)u(x) = f(x).$$

In the special case of just $n = 2$ coordinates we also call a form

$$Lu = \frac{\partial^2 u}{\partial x \partial y} + b_1(x, y)u_x + b_2(x, y)u_y + c(x, y) = f(x, y)$$

a canonical form.

Transformation into the canonical form

Symmetric but not diagonal

$$A \in \mathbb{R}^{n \times n}, \quad A^T = A$$

Diagonalization by eigenvalues and -vectors

$$C^T A C = \text{diag}(\lambda_1, \dots, \lambda_n)$$

New coordinates

$$\xi \in \mathbb{R}^n, \quad \xi = C^T x, \quad \nabla_x u = C \nabla_\xi u$$

Canonical form

$$\sum_{i=1}^n \lambda_i \frac{\partial^2 u}{\partial \xi_i^2} + \sum_{i=1}^n \tilde{b}_i \frac{\partial u}{\partial \xi_i} + cu = f$$

Example

Consider the PDE $u_{xx} + 2u_{xz} + u_{yy} + 2u_{yz} + 2u_{zz} = 0$. The matrix reads

$$A = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 2 \end{pmatrix}$$

and its eigenvalues and -vectors are $\lambda_1 = 0$, $\lambda_2 = 1$, $\lambda_3 = 3$,

$$v_1 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix}, \quad v_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}, \quad v_3 = \frac{1}{\sqrt{6}} \begin{pmatrix} 1 \\ 1 \\ 2 \end{pmatrix}.$$

The new coordinates are

$$\xi = \frac{1}{\sqrt{3}}(x + y - z), \quad \eta = \frac{1}{\sqrt{2}}(x - y), \quad \zeta = \frac{1}{2}(x + y + 2z)$$

and the transformed PDE reads

$$u_{\eta\eta} + 3u_{\zeta\zeta} = 0.$$

Consider the PDE

$$Lu = a_{11}u_{xx} + 2a_{12}u_{xy} + a_{22}u_{yy} + \text{lower order terms} = f.$$

Transformation by introducing functionally independent new coordinates

$$\xi = \xi(x, y), \quad \eta = \eta(x, y) \quad \text{with} \quad \det(J_{\xi, \eta}(x, y)) = \begin{vmatrix} \xi_x & \xi_y \\ \eta_x & \eta_y \end{vmatrix} \neq 0. \quad (10)$$

Theorem 3.6

The type of a PDE does not change under a nonsingular coordinate transformation from (10).

Constructing the coordinate system:

- compute the characteristics of the PDE using

$$a_{11}(x, y)w_x^2 + 2a_{12}(x, y)w_xw_y + a_{22}w_y^2 = 0$$

- the solutions of the quadratic equation

$$a_{11}(x, y)\mu^2 + 2a_{12}(x)\mu + a_{22}(x, y) = 0$$

are

$$\frac{w_x}{w_y} = \mu_{1,2} = \frac{-a_{12} \pm \sqrt{a_{12}^2 - a_{11}a_{22}}}{a_{11}}$$

Three cases:

- elliptic case, $a_{12}^2 - a_{11}a_{22} < 0$, both solutions μ_1 and μ_2 are not real
- parabolic case, $a_{12}^2 - a_{11}a_{22} = 0$, $\mu_1 = \mu_2 = -a_{12}(x, y)/a_{11}(x, y)$
- hyperbolic case, $a_{12}^2 - a_{11}a_{22} > 0$, two different real solutions

Hyperbolic case:

- the transformation is based on the solution of the homogeneous linear first order PDEs

$$w_x - \mu_{1,2}(x, y)w_y = 0$$

- solve the ODEs

$$\frac{dy}{dx} = -\mu_{1,2}(x, y) \quad (11)$$

- their solutions result in the new coordinates

$$\xi(x, y) = C_1, \quad \eta(x, y) = C_2$$

- in the new coordinates the PDE has the canonical form

$$u_{\xi\eta} + \text{lower order terms} = f$$

Transformation into the canonical form for $n = 2$

Parabolic case:

- solve the ODE

$$\frac{dy}{dx} = -\mu_{1,2}(x, y) = -a_{12}(x, y)/a_{11}(x, y)$$

- the new coordinates are

$$\xi = x, \quad \eta = \eta(x, y)$$

- the transformed PDE has the canonical form

$$u_{\xi\xi} + \text{lower order terms} = f$$

Elliptic case:

- both solutions are complex with $\mu_2 = \bar{\mu}_1$
- with $w(x, y) = c$ being the (complex-valued) solution of the ODE from (11) use

$$\begin{aligned}\xi(x, y) &= w(x, y) + \overline{w(x, y)} = 2 \operatorname{Re}(w(x, y)), \\ \eta(x, y) &= 2 \operatorname{Im}(w(x, y))\end{aligned}$$

- the transformed PDE has the canonical form

$$u_{\xi\xi} + u_{\eta\eta} + \text{lower order terms} = f.$$

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Definition 3.7

A function $u \in C^2(\Omega)$ is called harmonic if $\Delta u = 0$ on Ω .

Example

1. The function $u(x) = x_1 x_2 \cdot \dots \cdot x_n$ is harmonic on \mathbb{R}^n as also $\Delta u = 0$.
2. The function $u(x, y) = \ln(x^2 + y^2)$ is harmonic outside the origin.
3. The function $u(x, y, z) = (x^2 + y^2 + z^2)^{-1/2}$ is harmonic outside the origin.
4. The fundamental solution of the Laplace equation

$$E(x) = \begin{cases} -\frac{1}{2\pi} \ln \frac{1}{\|x\|} & \text{for } n = 2, \\ -\frac{1}{(n-2)w_n} \frac{1}{\|x\|^{n-2}} & \text{for } n \geq 3, \end{cases}$$

is harmonic in $\mathbb{R}^n \setminus \{0\}$. Therein w_n is the measure of the unit sphere in \mathbb{R}^n and $\Gamma(z)$ is the Gamma function, both defined as

$$w_n = \frac{2\pi^{n/2}}{\Gamma(n/2)}, \quad \Gamma(z) = \int_0^\infty t^{z-1} \exp(-t) dt.$$

The Laplace equation

The maximum principle:

- is of fundamental importance in the study of elliptic and parabolic PDEs
- Green's representation theorem and the mean value theorem are needed
- Green's theorem (a special case of Stokes' theorem) allows to express the integral over a plane surface by a curve integral
- the mean value theorem says that the value of u at the center equals the average of u over the sphere $S_R(x_0)$ and over the ball $B_R(x_0)$

Theorem 3.8 (Green's representation theorem)

Let u be harmonic on a domain $\Omega \subset \mathbb{R}^n$. For $x_0 \in \Omega$ holds

$$u(x_0) = \int_{\partial\Omega} \left(u(x) \frac{\partial E(x - x_0)}{\partial \vec{n}} - E(x - x_0) \frac{\partial u(x)}{\partial \vec{n}} \right) d\sigma$$

with $\vec{n} = \vec{n}(x)$ being the normal derivative at $\partial\Omega$ in the direction of the outside.

Theorem 3.9 (Mean value theorem)

Let

$$B_R(x_0) = \{x \in \mathbb{R}^n : \|x - x_0\| < R\}$$

be the n -dimensional ball with radius R and center x_0 as well as

$$S_R(x_0) = \{x \in \mathbb{R}^n : \|x - x_0\| = R\}$$

its boundary (S for sphere) and $\overline{B_R(x_0)} = B_R(x_0) \cup S_R(x_0)$ be the closure. If u is harmonic in $B_R(x_0)$ and continuous on $\overline{B_R(x_0)}$, then

$$u(x_0) = \frac{1}{\text{mes}(S_R)} \int_{S_R(x_0)} u(x) \, d\sigma$$

and

$$u(x_0) = \frac{1}{\text{mes}(B_R)} \int_{B_R(x_0)} u(x) \, dx.$$

Theorem 3.10 (Maximum principle)

Let u be harmonic in Ω and continuous on $\bar{\Omega} = \Omega \cup \partial\Omega$.

- (a) Then u attains its maximum and its minimum on the boundary of $\partial\Omega$.
- (b) If u is not constant, then u attains its maximum and its minimum only on the $\partial\Omega$.

Remark 7

Part (a) from Theorem 3.10 is called the weak maximum principle and part (b) is called the strong maximum principle.

Example

Let $\Omega = (-2, 2) \times (0, 2)$ and $u : \mathbb{R}^2 \rightarrow \mathbb{R}$ be the solution of the Cauchy-problem

$$\Delta u = 0 \quad \text{for } x \in \Omega,$$

$$u(x) = |x_1| + 2x_2 \quad \text{for } x \in \partial\Omega.$$

In order to compute $m_1 = \max_{x \in \bar{\Omega}} u(x)$ as well as $m_2 = \min_{x \in \bar{\Omega}} u(x)$ we apply the maximum principle and get

$$m_1 = \max_{x \in \partial\Omega} |x_1| + 2x_2 = 6$$

$$m_2 = \min_{x \in \partial\Omega} |x_1| + 2x_2 = 0.$$

Further, e. g. locations of the extrema are $\tilde{x} = (-2, 2)$ and $\bar{x} = (0, 0)$ with $u(\tilde{x}) = m_1$ and $u(\bar{x}) = m_2$.

Solution for the Laplace equation on a disc

Domain:

$$B_R = \{(x, y) \in \mathbb{R}^2 : x^2 + y^2 < R^2\}$$

Boundary value problem:

$$\begin{aligned}u_{xx}(x, y) + u_{yy}(x, y) &= 0 \quad \text{for } (x, y) \in B, \\u(x, y) &= g(x, y) \quad \text{for } (x, y) \in \partial B\end{aligned}$$

Work with polar coordinates:

$$x = r \cos(\varphi), \quad y = r \sin(\varphi)$$

Transformed problem:

$$\begin{aligned}\frac{\partial^2 u}{\partial r^2} + \frac{1}{r} \frac{\partial u}{\partial r} + \frac{1}{r^2} \frac{\partial^2 u}{\partial \varphi^2} &= 0 \quad \text{for } 0 \leq r < R, 0 \leq \varphi < 2\pi, \\u(R, \varphi) &= g(R \cos(\varphi), R \sin(\varphi)) \quad \text{for } 0 \leq \varphi < 2\pi.\end{aligned}$$

Solution for the Laplace equation on a disc

Factorial approach:

$$u(r, \varphi) = F(r) \cdot \Phi(\varphi)$$

Substituting this u in the PDE:

$$F''(r)\Phi(\varphi) + \frac{1}{r}F'(r)\Phi(\varphi) + \frac{1}{r^2}F(r)\Phi''(\varphi) = 0$$

Separation of variables

$$\frac{r^2 F''(r) + r F'(r)}{F(r)} = -\frac{\Phi''(\varphi)}{\Phi(\varphi)}$$

Both fractions have to be constant

$$\frac{r^2 F''(r) + r F'(r)}{F(r)} = -\frac{\Phi''(\varphi)}{\Phi(\varphi)} = \mu \quad \text{with} \quad \mu = n^2, \quad n = 0, 1, 2, \dots$$

Solution for the Laplace equation on a disc

The solutions of the PDE are

$$u_n(r, \varphi) = r^n (c_n \cos(n\varphi) + d_n \sin(n\varphi)), \quad n = 0, 1, 2, \dots$$

The general solution can be written as

$$u(r, \varphi) = \frac{c_0}{2} + \sum_{n=1}^{\infty} r^n (c_n \cos(n\varphi) + d_n \sin(n\varphi))$$

Theorem 3.11

Let $\tilde{g}(R, \varphi) = g(R \cos(\varphi), R \sin(\varphi))$ be continuous and 2π periodic. Then the coefficients to determine the solution are

$$c_n = \frac{1}{\pi R^n} \int_0^{2\pi} \tilde{g}(R, \varphi) \cos(n\varphi) \, d\varphi,$$

$$d_n = \frac{1}{\pi R^n} \int_0^{2\pi} \tilde{g}(R, \varphi) \sin(n\varphi) \, d\varphi.$$

Example

Consider with $\Omega = \{x \in \mathbb{R}^2 : \|x\|_2 < 2\}$ the boundary value problem

$$\Delta u = 0 \text{ in } \Omega,$$

$$u(x, y) = |y| \text{ on } \partial\Omega.$$

With $g(\varphi) = 2|\sin(\varphi)|$ we get $d_n = 0$ for all n as well as

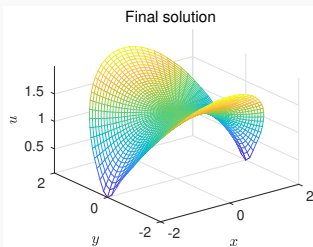
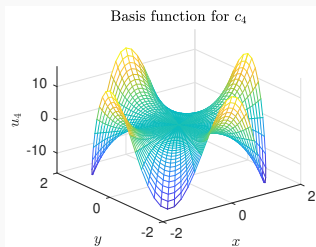
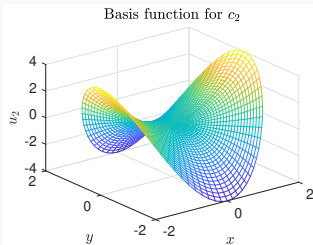
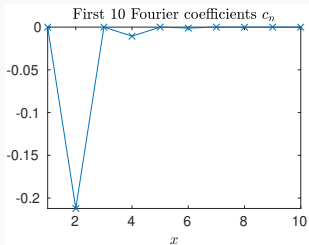
$$c_n = \begin{cases} -\frac{8}{\pi 2^n (n^2 - 1)} & \text{for even } n, \\ 0 & \text{for odd } n \end{cases}$$

and the solution is

$$u(r, \varphi) = \frac{4}{\pi} - \frac{8}{\pi} \left(\frac{r^2 \cos(2\varphi)}{2^2(2^2 - 1)} + \frac{r^4 \cos(4\varphi)}{2^4(4^2 - 1)} + \frac{r^6 \cos(6\varphi)}{2^6(6^2 - 1)} + \dots \right).$$

Solution for the Laplace equation on a disc

Example (Continuation)



Theorem 3.12 (Poisson's formula)

Consider the boundary value problem

$$\begin{aligned}\Delta u &= 0 && \text{on } B, \\ u &= g && \text{on } \partial B.\end{aligned}$$

Its solution has the form

$$u(r, \varphi) = \frac{1}{w_n R} \int_{\partial B} \frac{(R^2 - r^2)g(y)}{\|x - y\|^n} d\sigma_y$$

with w_n being the measure of the unit sphere in \mathbb{R}^n .

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The wave equation

General form of the PDE:

$$\frac{\partial^2 u}{\partial t^2} - \Delta u = 0 \quad \text{for } x = (x_1, \dots, x_n)^T \in \mathbb{R}^n, \quad t > 0$$

Initial conditions:

$$\begin{aligned} u(x, 0) &= \phi(x) \quad \text{for } x \in \mathbb{R}^n, \\ u_t(x, 0) &= \psi(x) \quad \text{for } x \in \mathbb{R}^n \end{aligned}$$

Problem in 1D:

$$\begin{aligned} \frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} &= 0 \quad \text{for } -\infty < x < \infty, \quad t > 0, \\ u(x, 0) &= \phi(x) \quad \text{for } -\infty < x < \infty, \\ u_t(x, 0) &= \psi(x) \quad \text{for } -\infty < x < \infty. \end{aligned}$$

Coordinate transformation ($x + t = C_1$ and $x - t = C_2$ are the characteristic curves of the PDE):

$$\xi = x + t, \quad \eta = x - t$$

Theorem 3.13 (d'Alembert's formula)

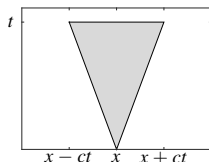
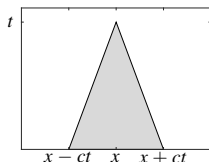
For the one-dimensional wave equation with initial conditions $\phi \in C^2(\mathbb{R})$ and $\psi \in C^1(\mathbb{R})$ the unique solution is

$$u(x, t) = \frac{\phi(x + t) + \phi(x - t)}{2} + \frac{1}{2} \int_{x-t}^{x+t} \psi(\tau) \, d\tau.$$

Remark 8

1. Dependency domain: the solution $u(x, t)$ at a position x and the time t depends on the initial data ϕ and ψ in the domain $[x - t, x + t]$.
2. Domain of influence: the initial data $\phi(x, 0)$ and $\psi(x, 0)$ at a position x affects the solution at the time t in the range $[x - t, x + t]$.

For $u_{tt} - c^2 u_{xx} = 0$ holds

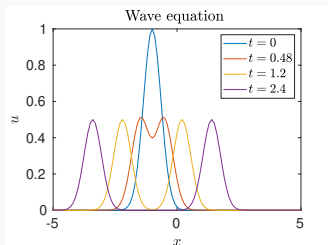
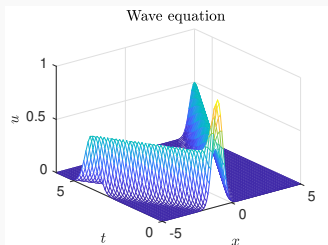


One-dimensional wave equation

Example

Consider the one dimensional wave equation for the initial condition $\phi(x) = \exp(-4(x + 1)^2)$ and $\psi(x) = 0$. Following d'Alembert's formula the solution is

$$u(x, t) = \frac{\exp(-4(x + t + 1)^2) + \exp(-4(x - t + 1)^2)}{2}.$$

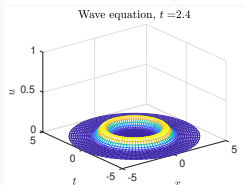
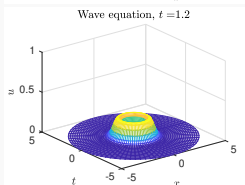
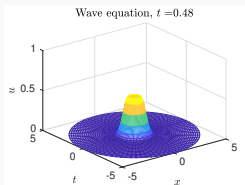
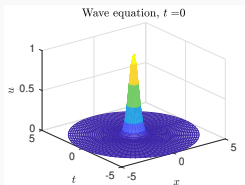


Two-dimensional wave equation

Example

The two dimensional wave equation on a disc for the initial data

$$u(x, 0) = \exp(-4(x^2 + y^2)).$$



Consider $u_{tt} = u_{xx}$ and the quantities

$$z = \begin{pmatrix} v \\ \varepsilon \end{pmatrix} = \begin{pmatrix} u_t \\ u_x \end{pmatrix}$$

Reformulation as a system of two first order PDEs

$$\begin{pmatrix} v_t \\ \varepsilon_t \end{pmatrix} + A \begin{pmatrix} v_x \\ \varepsilon_x \end{pmatrix} = 0 \quad \Rightarrow \quad A(x, t) = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$$

Encoupling the system with the new coordinates $w_1 = z_1 + z_2$, $w_2 = z_1 - z_2$ results in

$$\begin{pmatrix} w_1 \\ w_2 \end{pmatrix}_t + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \end{pmatrix}_x = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

Theorem 3.14 (Kirchhoff's formula)

The solution of the initial boundary value problem

$$\frac{\partial^2 u}{\partial t^2} - \Delta u = 0 \quad \text{for } x \in \Omega, \quad t > 0$$

$$u(x, 0) = 0, \quad u_t(x, 0) = p(x) \quad \text{for } x \in \Omega$$

for $\Omega \subset \mathbb{R}^3$ and a two times continuously differentiable function $p : \Omega \rightarrow \mathbb{R}$ is

$$u(x, t) = u_p(x, t) = \frac{1}{4\pi t} \iint_{S(x,t)} p(y) \, dy$$

with $S(x, t)$ the three-dimensional sphere with radius t and center x , thus $S(x, t) = \{y \in \mathbb{R}^3 : \|y - x\|_2 = t\}$.

Theorem 3.15

The solution of the initial boundary value problem

$$\begin{aligned}\frac{\partial^2 u}{\partial t^2} - \Delta u &= 0 \quad \text{for } x \in \Omega, \quad t > 0 \\ u(x, 0) &= u_0, \quad u_t(x, 0) = v_0(x) \quad \text{for } x \in \Omega\end{aligned}$$

for $\Omega \subset \mathbb{R}^2$ and $u_0, v_0 \in C^2(\Omega)$ is

$$u(x, t) = \frac{1}{2\pi} \iint_{B(x,t)} \frac{v_0(y)}{\sqrt{t^2 - \|y - x\|^2}} dy + \frac{\partial}{\partial t} \left(\iint_{B(x,t)} \frac{u_0(y)}{\sqrt{t^2 - \|y - x\|^2}} dy \right).$$

The initial boundary value problem in the one-dimensional case

Consider the problem

$$\begin{aligned}u_{tt} - u_{xx} &= 0, & 0 < x < 1, t > 0, \\u(0, t) = u(1, t) &= 0, & t \geq 0, \\u(x, 0) = \phi(x), u_t(x, 0) &= \psi(x), & 0 < x < 1.\end{aligned}$$

Factorial approach and Fourier series result in the following theorem.

Theorem 3.16

The solution reads

$$u(x, t) = \sum_{n=1}^{\infty} \sin(n\pi x) (a_n \cos(n\pi t) + b_n \sin(n\pi t)) \quad (12)$$

and the coefficients are

$$a_n = 2 \int_0^1 \phi(x) \sin(n\pi x) \, dx, \quad b_n = \frac{2}{n\pi} \int_0^1 \psi(x) \sin(n\pi x) \, dx$$

The initial boundary value problem in the one-dimensional case

Example

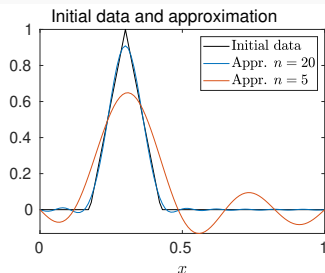
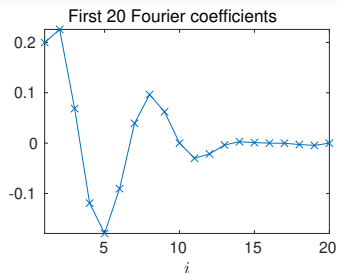
With $\Omega = (0, 1)$ consider the problem

$$u_{tt} - u_{xx} = 0 \quad \text{for } x \in \Omega, t > 0,$$

$$u(0, t) = u(1, t) = 0 \quad \text{for } t \geq 0,$$

$$u(x, 0) = \max(1 - 8|x - 0.3|, 0), \quad u_t(x, 0) = 0.$$

We compute the coefficients for Fourier's series and the final solution for any $t > 0$.



The initial boundary value problem in the one-dimensional case

Example

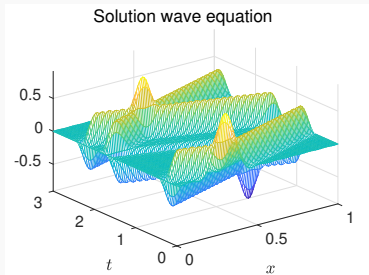
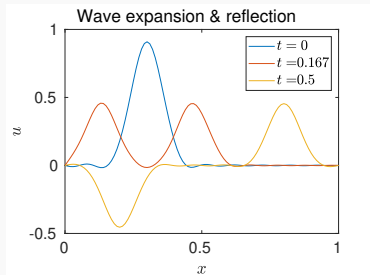
With $\Omega = (0, 1)$ consider the problem

$$u_{tt} - u_{xx} = 0 \quad \text{for } x \in \Omega, t > 0,$$

$$u(0, t) = u(1, t) = 0 \quad \text{for } t \geq 0,$$

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We compute the coefficients for Fourier's series and the final solution for any $t > 0$.



3. Solution of second order partial differential equation

- 3.1 Characteristics of second order partial differential equations
- 3.2 Classification of linear second order partial differential equations
- 3.3 Canonical form of a linear second order PDE
- 3.4 Analytical solution of the Laplace equation
- 3.5 Analytical solution of the wave equation
- 3.6 Analytical solution of the heat equation**
- 3.7 Difference methods for elliptic problems
- 3.8 Difference methods for parabolic problems
- 3.9 Difference methods for hyperbolic problems

Concentrated energy in one point

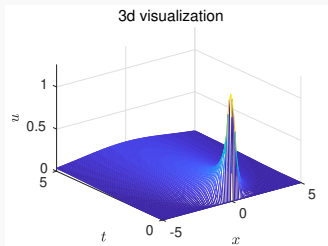
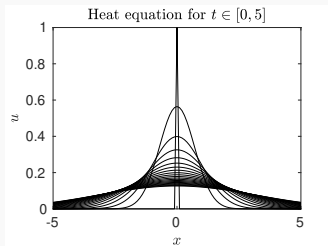
Theorem 3.17

The 1D initial value problem

$$u_t - u_{xx} = 0 \quad \text{for } x \in \mathbb{R}, t > 0,$$
$$u(x, 0) = \begin{cases} \infty & \text{for } x = 0 \\ 0 & \text{else} \end{cases} \quad \text{for } x \in \mathbb{R},$$

has the solution

$$u(x, t) = E(x, t) = \frac{1}{2\sqrt{\pi t}} \exp\left(-\frac{x^2}{4t}\right).$$



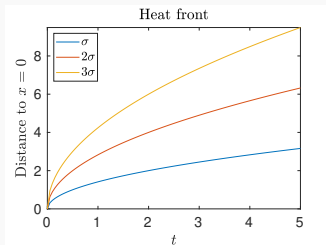
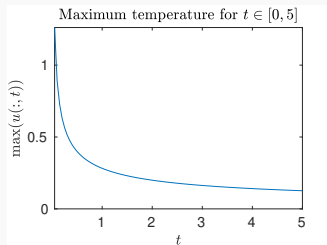
Theorem 3.17

The 1D initial value problem

$$u_t - u_{xx} = 0 \quad \text{for } x \in \mathbb{R}, t > 0,$$
$$u(x, 0) = \begin{cases} \infty & \text{for } x = 0 \\ 0 & \text{else} \end{cases} \quad \text{for } x \in \mathbb{R},$$

has the solution

$$u(x, t) = E(x, t) = \frac{1}{2\sqrt{\pi t}} \exp\left(-\frac{x^2}{4t}\right).$$



The initial value problem (Cauchy problem) for the heat equation

Theorem 3.18

Let ϕ be continuous and bounded in \mathbb{R}^n . Then the uniquely determined solution of the homogeneous heat equation is

$$u(x, t) = \frac{1}{(4\pi t)^{n/2}} \int_{\mathbb{R}^n} \phi(y) \exp\left(-\frac{\|y-x\|_2^2}{4t}\right) dy \quad (13)$$

with $x, y \in \mathbb{R}^n$ and $t > 0$.

Remark 9

Formula (13) can also be written as

$$u(x, t) = \int_{\mathbb{R}^n} \phi(y) E(y-x, t) dy.$$

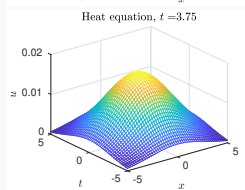
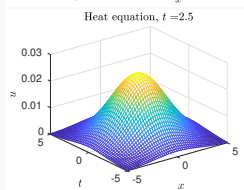
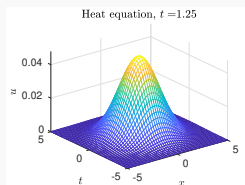
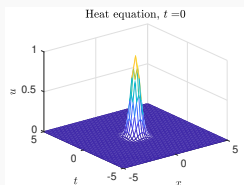
This means $u(x, t)$ is the convolution of the fundamental solution for $y-x$ and ϕ .

Homogeneous heat equation in the two-dimensional case

Example

Consider the two dimensional heat equation for the initial condition

$$\phi(x) = \exp(-4(x_1^2 + x_2^2)).$$



Theorem 3.19 (Maximum principle)

Let $T > 0$ and $u \in C^2(\Omega \times (0, T)) \cap C^0(\overline{\Omega} \times [0, T])$ be a smooth solution of the homogeneous heat equation

$$u_t(x, t) = u_{xx}(x, t) \quad \text{for } (x, t) \in \Omega \times (0, T)$$

then

$$\min_{(x,t) \in A} u(x, t) \leq \inf_{(x,t) \in B} u(x, t) \leq \sup_{(x,t) \in B} u(x, t) \leq \max_{(x,t) \in A} u(x, t)$$

with $A = \partial\Omega \times [0, T] \cup \Omega \times \{0\}$ and $B = \overline{\Omega} \times [0, T]$.

The initial-boundary value problem for the heat equation

Consider the one-dimensional initial-boundary value problem

$$u_t - u_{xx} = 0 \text{ for } x \in (0, 1), t > 0, \quad (14)$$

$$u(0, t) = u(1, t) = 0 \text{ for } t > 0, \quad (15)$$

$$u(x, 0) = \phi(x) \text{ for } x \in (0, 1) \quad (16)$$

Theorem 3.20

Let $\phi \in C^1([0, 1])$ and compatible condition $\phi(0) = \phi(1) = 0$.

Then the series

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

with the coefficients

$$c_n = 2 \int_0^1 \phi(x) \sin(n\pi x) dx$$

is the uniquely determined solution of (14), (15) and (16).

The initial-boundary value problem for the heat equation

Example

We consider the one-dimensional initial-boundary value heat equation with $\phi(x) = x \sin(\pi x)$. The formula for computing c_n is

$$c_n = 2 \int_0^1 x \sin(\pi x) \sin(n\pi x) dx.$$

The coefficients are

$$c_1 = \frac{1}{2}, \quad c_n = \begin{cases} -\frac{8n}{\pi^2(n^2-1)^2} & \text{for even } n, \\ 0 & \text{for odd } n \end{cases}$$

Using them the solution reads

$$u(x, t) = \frac{1}{2} \sin(\pi x) \exp(-\pi^2 t) - \sum_{i=1}^{\infty} \frac{16i}{(4i^2 - 1)^2 \pi^2} \sin(2i\pi x) \exp(-4i^2 \pi^2 t).$$

3. Solution of second order partial differential equation

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- 3.8 Difference methods for parabolic problems
- 3.9 Difference methods for hyperbolic problems

Idea/approach:

- extension of the 1D approach for boundary value problems with ODEs
- no time dependence, only the static case
- discretization of the bounded domain Ω by a grid with step size h
- approximation of the exact solution in the grid points $U_i \approx u(x^{(i)})$
- substitution of derivatives in the PDE by finite differences, e. g.

$$u_{xx} \approx \frac{1}{h^2} (u(x+h, y) - 2u(x, y) + u(x-h, y))$$

Result:

- large systems of linear equations for U_1, \dots, U_N with N the number of grid points
- quadratic systems $AU = b$, solution by iterative methods

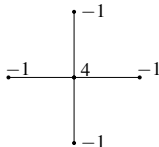
Difference methods for elliptic problems

Consider the 2D problem, thus $x \in \mathbb{R}^2$,

$$\begin{aligned} -\Delta u &= f(x) && \text{in } \Omega \\ u(x) &= g(x) && \text{on } \partial\Omega \end{aligned}$$

5-point stencil from Definition 1.7:

$$L_h^{(5)} = \frac{1}{h^2} \begin{bmatrix} & & & & \\ & & -1 & & \\ -1 & & 4 & & -1 \\ & & -1 & & \\ & & & & \end{bmatrix}$$



With $h_x = h_y = h$ this results in

$$-\Delta u = -u_{xx} - u_{yy} \approx \frac{-u(x-h, y) - u(x, y-h) + 4u(x, y) - u(x+h, y) - u(x, y+h)}{h^2}$$

Difference methods for elliptic problems

In practice:

- use $x \in \mathbb{R}^2$ instead of (x, y) in order to avoid conflicts in the numbering
- with m nodes in x_1 -direction and nodes in x_2 -direction we have $N = mn$ grid points

$$x_1, x_2, \dots, x_N \in \mathbb{R}^2$$

- their associated approximations to $u(x)$ are

$$U_i \approx u(x_i)$$

5-point stencil:

- grid point $x_{(j-1)m+i}$ has connections to the neighbours

$$x_{(j-2)m+i}, x_{jm+i}, x_{(j-1)m+i-1}, x_{(j-1)m+i+1}$$

- consequently a discretization of $-\Delta u$ with $h_x = h_y$ is

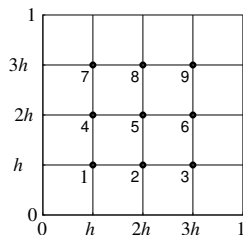
$$-\frac{U_{(j-2)m+i} + U_{jm+i} - 4U_{(j-1)m+i} + U_{(j-1)m+i-1} + U_{(j-1)m+i+1}}{h^2}$$

Example

Consider for $\Omega = (0, 1)^2$ the boundary value problem

$$-\Delta u = 7, \quad \text{in } \Omega, \quad u(x, y) = g(x, y), \quad \text{on } \partial\Omega.$$

For $m = 3$ and $h = 1/(m + 1)$ the grid is



Example

Consider for $\Omega = (0, 1)^2$ the boundary value problem

$$-\Delta u = 7, \quad \text{in } \Omega, \quad u(x, y) = g(x, y), \quad \text{on } \partial\Omega.$$

Next we derive the equations for the single points using the PDE $-\Delta u = 7$.

Point 1

$$\begin{aligned} \frac{1}{h^2} \left(- \underbrace{u(h, 0)}_{g(h, 0)} - \underbrace{u(0, h)}_{g(0, h)} + 4U_1 - U_2 - U_4 \right) &= 7 \\ \Rightarrow \frac{1}{h^2} (4U_1 - U_2 - U_4) &= 7 + \frac{1}{h^2} (g(h, 0) + g(0, h)). \end{aligned}$$

Example

Consider for $\Omega = (0, 1)^2$ the boundary value problem

$$-\Delta u = 7, \quad \text{in } \Omega, \quad u(x, y) = g(x, y), \quad \text{on } \partial\Omega.$$

Next we derive the equations for the single points using the PDE $-\Delta u = 7$.

Point 2

$$\begin{aligned} \frac{1}{h^2}(-U_1 - u(2h, 0) + 4U_2 - U_3 - U_5) &= 7 \\ \Rightarrow \frac{1}{h^2}(-U_1 + 4U_2 - U_3 - U_5) &= 7 + \frac{1}{h^2}g(2h, 0). \end{aligned}$$

Example

Consider for $\Omega = (0, 1)^2$ the boundary value problem

$$-\Delta u = 7, \quad \text{in } \Omega, \quad u(x, y) = g(x, y), \quad \text{on } \partial\Omega.$$

Next we derive the equations for the single points using the PDE $-\Delta u = 7$.

Point 5

$$\frac{1}{h^2}(-U_2 - U_4 + 4U_5 - U_6 - U_8) = 7.$$

Example

Consider for $\Omega = (0, 1)^2$ the boundary value problem

$$-\Delta u = 7, \quad \text{in } \Omega, \quad u(x, y) = g(x, y), \quad \text{on } \partial\Omega.$$

The system of linear equations is

$$A \begin{pmatrix} U_1 \\ U_2 \\ \vdots \\ U_9 \end{pmatrix} = \frac{1}{h^2} \begin{pmatrix} 7h^2 + g(0, h) + g(h, 0) \\ 7h^2 + g(2h, 0) \\ 7h^2 + g(3h, 0) + g(1, h) \\ 7h^2 + g(0, 2h) \\ 7h^2 \\ 7h^2 + g(1, 2h) \\ 7h^2 + g(0, 3h) + g(h, 1) \\ 7h^2 + g(2h, 1) \\ 7h^2 + g(3h, 1) + g(1, 3h) \end{pmatrix}.$$

Kronecker-product of $U \in \mathbb{R}^{m \times n}$ and $V \in \mathbb{R}^{p \times q}$:

$$U \otimes V = \begin{pmatrix} u_{11}V & \cdots & u_{1n}V \\ \vdots & \ddots & \vdots \\ u_{m1}V & \cdots & u_{mn}V \end{pmatrix} \in \mathbb{R}^{mp \times nq}$$

Representation of the discretization matrix:

$$A = \frac{1}{h^2} (I_m \otimes T_m + T_m \otimes I_m) \in \mathbb{R}^{m \times m},$$

with $T_m = \text{tridiag}(-1, 2, -1) \in \mathbb{R}^{m \times m}$, $I_m \in \mathbb{R}^{m \times m}$

Remark 10

1. *The system of linear equations comprises only equations for values at inner nodes.*
2. *The structure of the matrix A depends on the enumeration of the grid points.*
3. *The right-hand side of the system at grid points x_ℓ , which are not connected to the boundary, includes only the values of $f(x_\ell) = b_\ell$. Points close to the boundary, i.e. points which have a stencil that contains at least one boundary point, feature a contribution from the corresponding Dirichlet values to the right-hand side b of the system.*

Definition 3.21

A regular matrix $A \in \mathbb{R}^{n \times n}$ is called an M-matrix, if

$$A_{ij} \leq 0 \quad \text{for } i \neq j, \quad \sum_{j=1}^n A_{ij} \geq 0 \quad \text{for } i = 1, \dots, n,$$

and all entries of A^{-1} are nonnegative.

Difference to the analytical solutions:

- due to the construction of the difference approximation holds

$$D_h = L_h^{(5)} u(x) = Lu(x) + \mathcal{O}(h^2)$$

- with $u \in C^4(\Omega) \cap C(\bar{\Omega})$ the local error for D_h is controlled by the 4. derivatives of u

$$L_h^{(5)} u(x) = f(x) + E(x, h), \quad L_h^{(5)} U(x) = f(x), \quad \|E(x, h)\| \leq \frac{h^2}{12} \max_{x \in \Omega} (|u^{(4)}(x)|)$$

- consistency and stability result in

$$\|u_h - U\|_{\infty} \leq Ch^2,$$

- the constant C depends on the operator and the domain

Summary of the procedure:

1. discretize the domain with the step size h resp. different step sizes h_{x_1}, h_{x_2}, \dots
2. number the grid points $x^{(1)}, \dots, x^{(N)}$
3. derive a proper difference stencil for the PDE
4. set up equations for the unknown U_i
5. include boundary conditions in the equations
6. solve the system of linear equations

Example

Consider for $\Omega = (0, 1)^2$ the boundary value problem

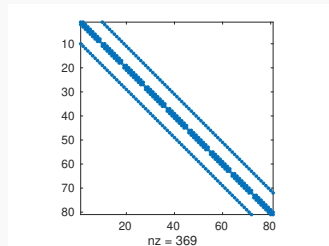
$$\begin{aligned} -\Delta u + au_{x_1} + bu_{x_2} + cu &= f \quad \text{in } \Omega, \\ u &= g \quad \text{on } \partial\Omega. \end{aligned}$$

Using $h_x = h_y = h$ the stencil reads

$$= \frac{1}{h^2} \begin{bmatrix} & -1 + \frac{h}{2}b_i & \\ -1 - \frac{h}{2}a_i & 4 + h^2c_i & -1 + \frac{h}{2}a_i \\ & -1 - \frac{h}{2}b_i & \end{bmatrix}.$$

Example (Continuation)

For $m = 9$ and $h = 0.1$ with $a = b = c = 0$ the structure of the matrix is

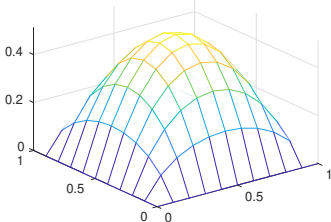


Only 369 of 6561 matrix elements are nonzero (5.6%). The system matrix is weakly diagonally dominant and irreducible. Therefore use iterative methods to solve the system of linear equations instead of the Gaussian elimination.

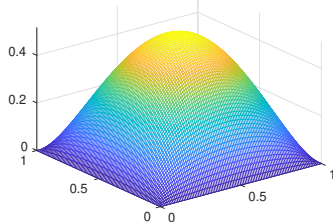
Example (Continuation)

Solution with $f(x) = 12$ and for a grid with $h = 0.1$ resp. $h = 0.01$.

Low resolution $h = 0.1$, $A \in \mathbb{R}^{81 \times 81}$



Fine resolution $h = 0.01$, $A \in \mathbb{R}^{9801 \times 9801}$



Example

Next we derive a difference stencil for the PDE

$$-u_{xx} - u_{xy} - u_{yy} + u_x + u_y + u = 0.$$

With $h_x = h_y = h$ the single parts of the stencil are

$$-\frac{1}{h^2} \begin{bmatrix} & 1 & \\ 1 & -2 & 1 \\ & 1 & \end{bmatrix} - \frac{1}{4h^2} \begin{bmatrix} -1 & 1 \\ & \\ 1 & -1 \end{bmatrix} + \frac{1}{2h} \begin{bmatrix} & & \\ -1 & & \\ & & 1 \end{bmatrix} + \frac{1}{2h} \begin{bmatrix} & 1 & \\ & & \\ & -1 & \end{bmatrix} + \begin{bmatrix} & & \\ & 1 & \\ & & \end{bmatrix}$$

Thus the stencil reads

$$\frac{1}{h^2} \begin{bmatrix} \frac{1}{4} & -1 + \frac{h}{2} & -\frac{1}{4} \\ -1 - \frac{h}{2} & 4 + h & -1 + \frac{h}{2} \\ -\frac{1}{4} & -1 - \frac{h}{2} & \frac{1}{4} \end{bmatrix}$$

Neumann boundary conditions:

$$\frac{\partial u}{\partial \vec{n}}(x) = \alpha \text{ for } x \in \partial\Omega$$

One-dimensional:

$$\frac{U_n - U_{n-1}}{h} = \alpha \quad \Leftrightarrow \quad U_n - U_{n-1} = h\alpha \quad \text{with } U_n \approx u(b)$$

Two-dimensional:

- extend the number of nodes for boundary point with Neumann conditions

$$\frac{U_{i(m+1)} - U_{i(m+1)-1}}{h} = w(ih) \quad \Leftrightarrow \quad U_{i(m+1)} - U_{i(m+1)-1} = hw(ih)$$

- or use the connection directly for the stencil as

$$u(b, ih) = U_{i(m+1)-1} + hw(ih), \quad i = 1, \dots, n$$

Definition 3.22

For a (possibly non-symmetric) matrix $A \in \mathbb{R}^{n \times n}$ we call $G_A = (V, E)$ the adjacency graph with the set of nodes $V = \{1, \dots, n\}$ and the set of edges

$$E = \{(i, j) \in V^2 : a_{ij} \neq 0\}.$$

Definition 3.23

A matrix A is called irreducible if every node i is connected to every node j by a chain of edges. In the case of a non-symmetric matrix of a chain of equally oriented edges in both directions.

Important also for:

- Perron-Frobenius theory of nonnegative matrices
- Graph theory
- via Perron-Frobenius indirectly for Page-rank, Markov chains, etc.

Theorem 3.24

Let $A \in \mathbb{R}^{n \times n}$ be irreducible, weakly diagonally dominant, thus

$$\sum_{j=1, j \neq i}^n |a_{ij}| \leq a_{ii}$$

and let for at least one j the inequality be strict $<$.

Then the Jacobean as well as the Gauss-Seidel iteration converge to the solution of the system of linear equations $Ax = b$ for each initial guess to the solution x^* .

Theorem 3.25

Let $A \in \mathbb{R}^{n \times n}$ be irreducible with

$$a_{ij} \leq 0 \quad \text{for } i \neq j, \quad \sum_{j=1}^n a_{ij} \geq 0 \quad \text{for } i = 1, \dots, n,$$

as well as $\sum_{j=1}^n a_{\ell j} > 0$ for at least one ℓ .

Then

1. A is inverse positive, that means $A^{-1} \geq 0$ holds component wise,
2. A is an M -matrix,
3. the Jacobean method to solve $AU = b$ converges,
4. A is inverse monotone, that means

$$Ax \leq Ay \quad \Rightarrow \quad x \leq y.$$

Theorem 3.26

Let the assumptions from Theorem 3.25 be fulfilled.

It holds:

1. If for the boundary value problem holds $L_h U \geq 0$ in Ω_h and $U \geq 0$ on $\partial\Omega_h$, then holds $U \geq 0$ on $\bar{\Omega}_h$.
2. For the Laplace operator $L = -\Delta = f$ on $\Omega = (0, 1)^2$ and a four times continuously differentiable solution u of the boundary value problem holds

$$\|U(x) - u(x)\|_{\bar{\Omega}_h} \leq Ch^2 \max(|u^{(4)}(x)|).$$

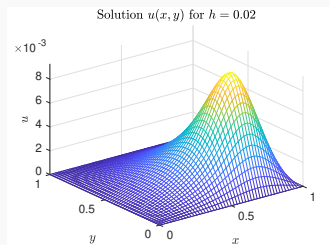
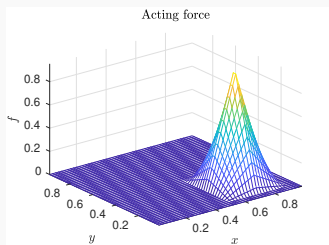
Example

Consider the boundary value problem

$$-\Delta u(x) = f(x) \quad \text{in } \Omega = (0, 1)^2, \quad u(x) = 0 \quad \text{on } \partial\Omega$$

with $f(x) = \max(0, 1 - 8|x_1 - 0.5|) \cdot \max(0, 1 - 8|x_2 - 0.5|)$.

The acting force and the solution are



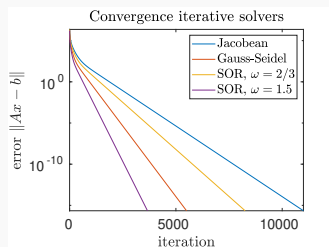
Example

Consider the boundary value problem

$$-\Delta u(x) = f(x) \quad \text{in } \Omega = (0, 1)^2, \quad u(x) = 0 \quad \text{on } \partial\Omega$$

with $f(x) = \max(0, 1 - 8|x_1 - 0.5|) \cdot \max(0, 1 - 8|x_2 - 0.5|)$.

Convergence speed for Jacobean, Gauss-Seidel and SOR with $w \in \{\frac{2}{3}, \frac{3}{2}\}$



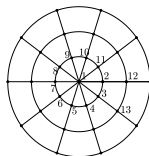
Keep in mind, that the cg-method converges much faster!

Grid for a circ:

- use a discretization for the rectangle $(0, R] \times [0, 2\pi)$ by m resp. n nodes with

$$r = (h, 2h, \dots, mh), \quad \varphi = (0, k, 2k, \dots, 2\pi - k)$$

- one additional grid point (1st) is the origin
- polar coordinates $x = r \cos \varphi$, $y = r \sin \varphi$ result in



E. g. the transformed Laplace operator reads:

$$\Delta u(x, y) = u_{rr} + \frac{1}{r}u_r + \frac{1}{r^2}u_{\varphi\varphi}$$

3. Solution of second order partial differential equation

- 3.1 Characteristics of second order partial differential equations
- 3.2 Classification of linear second order partial differential equations
- 3.3 Canonical form of a linear second order PDE
- 3.4 Analytical solution of the Laplace equation
- 3.5 Analytical solution of the wave equation
- 3.6 Analytical solution of the heat equation
- 3.7 Difference methods for elliptic problems
- 3.8 Difference methods for parabolic problems**
- 3.9 Difference methods for hyperbolic problems

Consider the 1D heat equation for an unknown function $u = u(x, t)$

$$u_t - u_{xx} = f(x, t) \quad \text{in } (0, 1) \times (0, T),$$

$$u(x, 0) = u_0(x) \quad \text{for } x \in [0, 1],$$

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

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

Given:

- right-hand side f , heat sources and sinks
- continuously (differentiable) functions u_0 , l and r as initial temperature for $t = 0$ and the temperatures at the boundaries $x = 0$ and $x = 1$

Discretization:

- domain $(0, 1) \times (0, T)$ is discretized by the grid

$$x_i = ih, \quad i = 0, \dots, N$$

$$t_j = jk, \quad j = 0, \dots, M$$

- compute approximations

$$U_i^j \approx u(x_i, t_j).$$

Semi-discretization:

- $u(x, 0)$ is given, successive calculation for later time layers

$$U_{1:N}^0 = u(x, 0) \rightarrow U_{1:N}^1 \approx u(x, k) \rightarrow \dots \rightarrow U_{1:N}^M \approx u(x, T)$$

- transition from time layer $U_{1:N}^j$ to time layer $U_{1:N}^{j+1}$ using single step methods
(Euler, Crank-Nicolson, etc.)

Discretization of the time derivative by two-point approximation in t -direction:

$$u_t(x_i, t_j) \approx \frac{U_i^{j+1} - U_i^j}{k}.$$

Discretization in x -direction:

- use the average over both involved time layers

$$u_{xx}(x_i, t_j) \approx (1 - \sigma) \frac{U_{i-1}^j - 2U_i^j + U_{i+1}^j}{h^2} + \sigma \frac{U_{i-1}^{j+1} - 2U_i^{j+1} + U_{i+1}^{j+1}}{h^2}$$

- $\sigma \in [0, 1]$ as a shift for an explicit ($\sigma = 0$) or an implicit ($\sigma > 0$) method

Initial and boundary conditions:

$$U_i^0 = u_0(x_i), \quad i = 0, \dots, N,$$

$$U_0^j = l(t_j), \quad U_N^j = r(t_j), \quad j = 0, \dots, M$$

Euler explicit for parabolic problems

Case $\sigma = 0$:

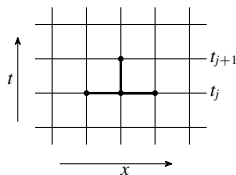
- Euler-method in time

$$U_i^{j+1} = U_i^j + \frac{k}{h^2}(U_{i-1}^j - 2U_i^j + U_{i+1}^j) + kf_i^j$$

with $\gamma = \frac{k}{h^2}$

- starting with $U_i^j, i = 0, \dots, N$, of the time layer j , the explicit scheme enables to compute approximations $U_i^{j+1}, i = 0, \dots, N$, for the new time layer $(j + 1)$

The stencil:



Associated matrix:

$$A = \begin{pmatrix} 1 - 2\gamma & \gamma & & & \\ \gamma & 1 - 2\gamma & \gamma & & \\ & & \ddots & \ddots & \ddots \\ & & & \ddots & \ddots \end{pmatrix}$$

Crank-Nicolson for parabolic problems

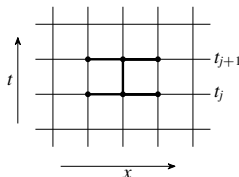
Case $\sigma = 0.5$:

- Crank-Nicolson-method in time

$$2(1 + \gamma)U_i^{j+1} - \gamma(U_{i-1}^{j+1} + U_{i+1}^{j+1}) = 2(1 - \gamma)U_i^j + \gamma(U_{i-1}^j + U_{i+1}^j) + 2kf(x_i, t_j + 0.5k)$$

- in each layer one has to solve a system of linear equations with a tridiagonal matrix to compute the new approximations U_i^{j+1} , $i = 0, \dots, N$

The stencil:



Case $\sigma = 0.5$:

- Crank-Nicolson-method in time

$$2(1 + \gamma)U_i^{j+1} - \gamma(U_{i-1}^{j+1} + U_{i+1}^{j+1}) = 2(1 - \gamma)U_i^j + \gamma(U_{i-1}^j + U_{i+1}^j) + 2kf(x_i, t_j + 0.5k)$$

- in each layer one has to solve a system of linear equations with a tridiagonal matrix to compute the new approximations U_i^{j+1} , $i = 0, \dots, N$

System of equations:

$$\begin{pmatrix} 2(1 + \gamma) & -\gamma & & & \\ -\gamma & \ddots & \ddots & & \\ & \ddots & \ddots & & \\ & & \ddots & -\gamma & \\ & & & -\gamma & 2(1 + \gamma) \end{pmatrix} U_{\cdot}^{j+1} = \begin{pmatrix} 2(1 - \gamma) & \gamma & & & \\ \gamma & \ddots & \ddots & & \\ & \ddots & \ddots & & \\ & & \ddots & -\gamma & \\ & & & -\gamma & 2(1 - \gamma) \end{pmatrix} U_{\cdot}^j + 2kf_{\cdot}^{j+\frac{1}{2}}$$

Euler implicit for parabolic problems

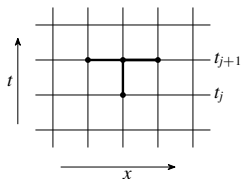
Case $\sigma = 1$:

- implicit Euler-method in time direction

$$(1 + 2\gamma)U_i^{j+1} - \gamma(U_{i-1}^{j+1} + U_{i+1}^{j+1}) = U_i^j + kf_i^{j+1}$$

- a system of linear equations has to be solved in each time layer, too

The stencil:



Euler implicit for parabolic problems

Case $\sigma = 1$:

- implicit Euler-method in time direction

$$(1 + 2\gamma)U_i^{j+1} - \gamma(U_{i-1}^{j+1} + U_{i+1}^{j+1}) = U_i^j + kf_i^{j+1}$$

- a system of linear equations has to be solved in each time layer, too

System of equations:

$$\begin{pmatrix} 1 + 2\gamma & -\gamma & & & \\ -\gamma & \ddots & \ddots & & \\ & \ddots & \ddots & & \\ & & & -\gamma & \\ & & & -\gamma & 1 + 2\gamma \end{pmatrix} U_i^{j+1} = U_i^j + kf_i^{j+1}$$

Difference methods for parabolic problems

Local truncation error/consistency:

$\mathcal{O}(h^2 + k)$ for Euler's methods, thus the orders are 2/1

$\mathcal{O}(h^2 + k^2)$ for Crank-Nicolson, thus the orders are 2/2

Theorem 3.27 (Stability)

For the solution of the discretized boundary value problem

$$\frac{U_i^{j+1} - U_i^j}{k} - D^{(2)}(\sigma U_i^{j+1} + (1 - \sigma)U_i^j) = f_i^j$$

holds

$$\max_{i,j} |U_i^j| \leq \max_{0 \leq x \leq 1} |u_0(x)| + k \sum_{j=0}^M \max_{i=1, \dots, N} |f_i^j|,$$

if

$$0 \leq \sigma \leq 1 \quad \text{and} \quad 1 - 2(1 - \sigma) \frac{k}{h^2} \geq 0.$$

Numerical stability:

- limiting of time step size k depending on step size in space direction h

$$(1 - \sigma) \frac{k}{h^2} \leq \frac{1}{2}$$

- Euler explicit ($\sigma = 0$):

$$k \leq \frac{h^2}{2},$$

- Crank-Nicolson ($\sigma = 0.5$):

$$k \leq h^2,$$

- Euler implicit ($\sigma = 1$):

No restriction!

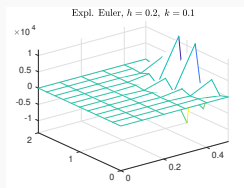
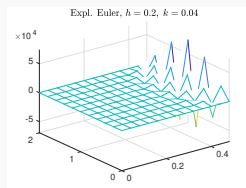
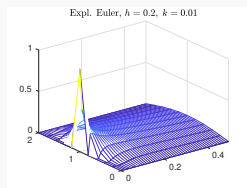
Example

Consider the parabolic initial boundary value problem

$$u_t = u_{xx} + 0.1 \sin(0.5\pi x) \quad \text{in } \Omega = (0, 2), \quad t > 0,$$
$$u(x, 0) = \max(1 - 5|1 - x|, 0), \quad u(0, t) = u(2, t) = 0.$$

Computation of a solution by explicit Euler, Crank-Nicolson and implicit Euler for various step sizes in time direction. With respect to stability we get

$$h = 0.2 \quad \Rightarrow \quad k_{Euler} \leq 0.02, \quad k_{CN} \leq 0.04.$$



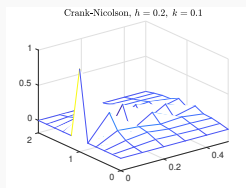
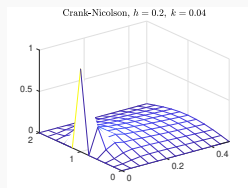
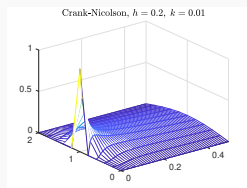
Example

Consider the parabolic initial boundary value problem

$$u_t = u_{xx} + 0.1 \sin(0.5\pi x) \quad \text{in } \Omega = (0, 2), \quad t > 0,$$
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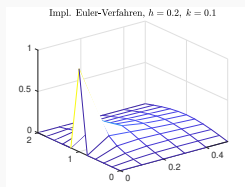
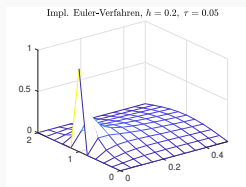
Example

Consider the parabolic initial boundary value problem

$$u_t = u_{xx} + 0.1 \sin(0.5\pi x) \quad \text{in } \Omega = (0, 2), \quad t > 0,$$
$$u(x, 0) = \max(1 - 5|1 - x|, 0), \quad u(0, t) = u(2, t) = 0.$$

Computation of a solution by explicit Euler, Crank-Nicolson and implicit Euler for various step sizes in time direction. With respect to stability we get

$$h = 0.2 \quad \Rightarrow \quad k_{Euler} \leq 0.02, \quad k_{CN} \leq 0.04.$$



Example

Consider the initial-boundary value problem

$$u_t = u_{xx}, \quad (x, y) \in \Omega = (0, 1),$$
$$u(x, 0) = \begin{cases} 1 & \text{for } x \in [0.3, 0.5] \\ 0 & \text{otherwise} \end{cases}, \quad u(0, t) = u(1, t) = 0.$$

Example

Numerical solution of 2D heat equation

$$u_t = 0.1\Delta u.$$

We use the implicit Euler method. This means

$$\frac{U(:, i+1) - U(:, i)}{k} = 0.1L_h^{(5)}U(:, i+1)$$

and thus

$$U(:, i+1) = (I_{n^2, n^2} - 0.1kA)^{-1}U(:, i), \quad i = 0, 1, 2, \dots$$

The system matrix is defined using

$$A = \frac{1}{h^2}(T \otimes I_{n,n} + I_{n,n} \otimes T) \quad \text{with} \quad T = \text{tridiag}(1, -2, 1) \in \mathbb{R}^{n \times n}.$$

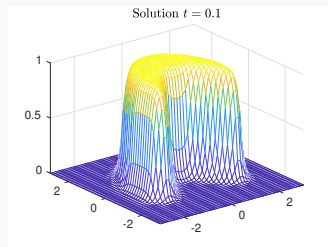
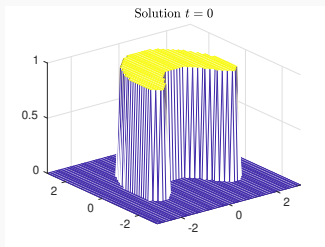
In MatLab use `kron(T, I_{n,n})` for $T \otimes I_{n,n}$.

Example

Numerical solution of 2D heat equation

$$u_t = 0.1\Delta u.$$

Some intermediary plots.

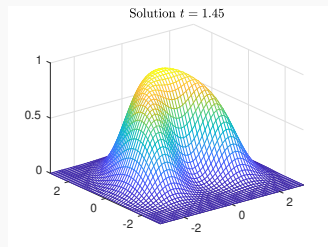
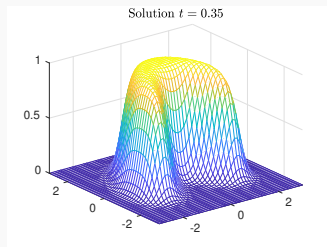


Example

Numerical solution of 2D heat equation

$$u_t = 0.1\Delta u.$$

Some intermediary plots.



3. Solution of second order partial differential equation

- 3.1 Characteristics of second order partial differential equations
- 3.2 Classification of linear second order partial differential equations
- 3.3 Canonical form of a linear second order PDE
- 3.4 Analytical solution of the Laplace equation
- 3.5 Analytical solution of the wave equation
- 3.6 Analytical solution of the heat equation
- 3.7 Difference methods for elliptic problems
- 3.8 Difference methods for parabolic problems
- 3.9 Difference methods for hyperbolic problems**

Standard 1D hyperbolic initial-boundary value problem:

$$\begin{aligned}u_{tt} &= c^2 u_{xx} && \text{in } [0, L] \times [0, \infty), \\u(x, 0) &= f(x), && u_t(x, 0) = g(x), \\u(0, t) &= h_1(t), && u(L, t) = h_2(t)\end{aligned}$$

Solution in $\mathbb{R} \times [0, \infty)$:

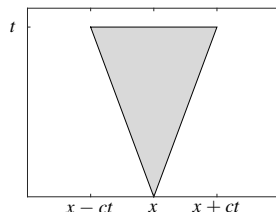
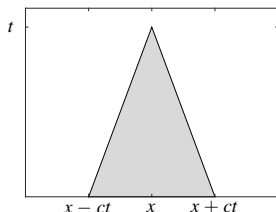
$$u(x, t) = \frac{f(x+ct) + f(x-ct)}{2} + \frac{1}{2c} \int_{x-ct}^{x+ct} g(s) \, ds$$

Dependency domain for (x, t) :

$$B(x, t) = \{(\xi, t - k) : k \geq 0, |x - \xi| \leq ck\}$$

Domain of influence:

$$E(x, t) = \{(\xi, t + k) : k \geq 0, |x - \xi| \leq ck\}$$



Discretization of u_{xx} in the current time layer (explicit scheme):

$$\frac{1}{k^2} (U_i^{j+1} - 2U_i^j + U_i^{j-1}) = \frac{c^2}{h^2} (U_{i+1}^j - 2U_i^j + U_{i-1}^j)$$

Explicit scheme

$$\begin{aligned} U_i^{j+1} &= 2U_i^j - U_i^{j-1} + \frac{c^2 k^2}{h^2} (U_{i+1}^j - 2U_i^j + U_{i-1}^j) \\ &= \rho^2 U_{i-1}^j + 2(1 - \rho^2) U_i^j + \rho^2 U_{i+1}^j - U_i^{j-1} \quad \text{with } \rho = \frac{ck}{h} \end{aligned}$$

The error behaves as:

$$\mathcal{O}(h^2 + k^2)$$

Initial conditions (displacement):

$$U_i^0 = f(x_i)$$

Initial speed (only order 1 in time):

$$\frac{U_i^1 - U_i^0}{k} = g(x_i) \quad \Rightarrow \quad U_i^1 = kg(x_i) + U_i^0$$

Instead use (order 2 in time):

$$\begin{aligned}u(x, t_1) &= u(x, t_0) + ku_t(x, t_0) + \frac{k^2}{2}u_{tt}(x, t_0) \\&= U_i^0 + kg(x_i) + \frac{c^2k^2}{2}u_{xx}(x_i, t_0) = U_i^0 + kg(x_i) + \frac{c^2k^2}{2}f''(x_i) \\&\Rightarrow U_i^1 = U_i^0 + kg(x_i) + \frac{c^2k^2}{2}f''(x_i)\end{aligned}$$

Boundary conditions:

$$U_0^j = h_1(t_j), \quad U_{L/h}^j = h_2(t_j)$$

General scheme (with $0 \leq \sigma \leq \frac{1}{2}$):

$$\begin{aligned}u_{xx} &\approx h^{-2} \sigma (U_{i-1}^{j+1} - 2U_i^{j+1} + U_{i+1}^{j+1}) && \text{layer } j + 1 \\ &+ h^{-2} (1 - 2\sigma) (U_{i-1}^j - 2U_i^j + U_{i+1}^j) && \text{layer } j \\ &+ h^{-2} \sigma (U_{i-1}^{j-1} - 2U_i^{j-1} + U_{i+1}^{j-1}) && \text{layer } j - 1\end{aligned}$$

Numerical stability:

- similar to parabolic problems the time step size is limited by the step size in space direction due to the dependence area
- for explicit Euler this is the so called CFL-condition (Courant-Friedrichs-Levy)

$$ck \leq h$$

- otherwise the approximations may diverge, although the solution is bounded

Example

Consider the initial-boundary value problem

$$u_{tt} = u_{xx}, \quad (x, y) \in \Omega = (0, 1),$$

$$u_t(x, 0) = 0, \quad u(0, t) = u(1, t) = 0.$$

Example (Oscillation of a square membrane without external influences)

Boundary value problem for $\Omega = (0, 1)^2$:

$$\begin{aligned}u_{tt}(x, y, t) &= \Delta u(x, y, t) = u_{xx}(x, y, t) + u_{yy}(x, y, t) && \text{for } (x, y) \in \Omega, \\u(x, y) &= 0 && \text{for } (x, y) \in \partial\Omega.\end{aligned}$$

Again the same approach as in 1D $u(x, y, t) = v(x, y)w(t)$ results in

$$\begin{aligned}u_{tt} &= vw''', & \Delta u &= w\Delta v \\w''v &= \Delta vw \\ \frac{\Delta v}{v} &= \frac{w''}{w} =: -\lambda.\end{aligned}$$

Example (Continuation)

First problem: computation of the eigenmodes in 2D

$$\begin{aligned}\Delta v &= -\lambda v && \text{in } \Omega, \\ v &= 0 && \text{on } \partial\Omega.\end{aligned}$$

Second problem: due to $w'' = -\lambda w$ the oscillation is

$$w(t) = a \cos(\sqrt{\lambda}t) + b \sin(\sqrt{\lambda}t).$$

λ with a small amount: low-frequency (fundamental) natural oscillations,

λ with a large amount; high-frequency natural oscillations.

Example (Continuation)

The eigenvalues for the analytical problem are

$$\lambda = -(k\pi)^2 - (\ell\pi)^2, \quad k, \ell = 1, 2, 3, \dots$$

and thus

$$(k, \ell) = (1, 1) \Rightarrow \lambda_1 = -2\pi^2, \text{ multiplicity } 1$$

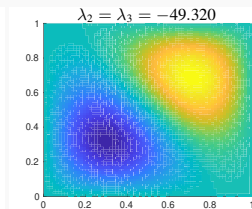
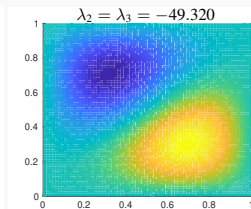
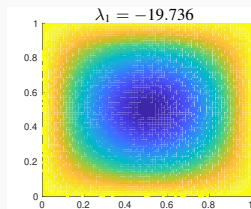
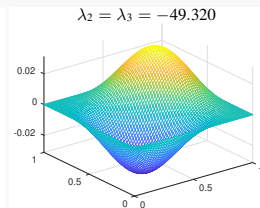
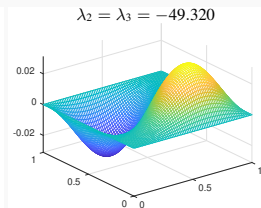
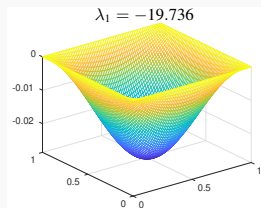
$$(k, \ell) = (1, 2) \Rightarrow \lambda_{2,3} = -5\pi^2, \text{ mult. } 2 \text{ as } (k, \ell) = (2, 1)$$

$$(k, \ell) = (2, 2) \Rightarrow \lambda_4 = -8\pi^2, \text{ mult. } 1$$

$$(k, \ell) = (1, 3) \Rightarrow \lambda_{5,6} = -10\pi^2, \text{ mult. } 2 \text{ as } (k, \ell) = (3, 1)$$

Example (Continuation)

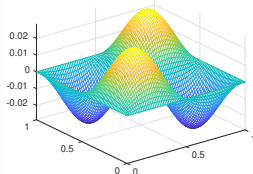
Numerical approximations for $n = 69$ (eigen value problem for $\mathbb{R}^{4761 \times 4761}$)



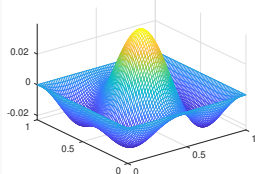
Example (Continuation)

Numerical approximations for $n = 69$ (eigen value problem for $\mathbb{R}^{4761 \times 4761}$)

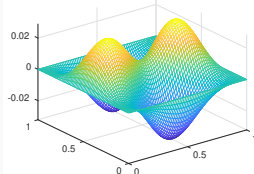
$$\lambda_4 = -78.904$$



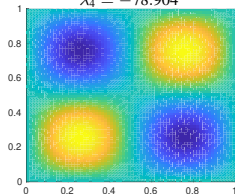
$$\lambda_5 = \lambda_6 = -98.560$$



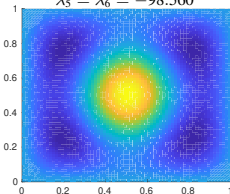
$$\lambda_5 = \lambda_6 = -98.560$$



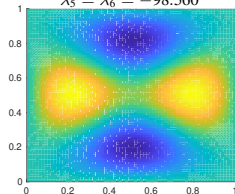
$$\lambda_4 = -78.904$$



$$\lambda_5 = \lambda_6 = -98.560$$



$$\lambda_5 = \lambda_6 = -98.560$$



Example (Continuation)

Computing the complete solution based on the eigenmodes. The single eigenmodes behave as

$$u_j(x, t) = (a_j \cos(\sqrt{\lambda_j t}) + b_j \sin(\sqrt{\lambda_j t})) V_{:,j}, \quad j = 1, 2, 3, \dots$$

The complete solution reads

$$u(x, t) = \sum_{j=0}^n (a_j \cos(\sqrt{\lambda_j t}) + b_j \sin(\sqrt{\lambda_j t})) V_{:,j}$$

with a number of $n \leq N$ eigenmodes. The coefficients a_j depend on the initial data and the coefficients b_j on the initial speed.

Procedure for an arbitrary initial displacement and without initial speed:

1. compute the eigenmodes $v_i \in \mathbb{R}^N$, store them in $V = (v_1, \dots, v_N)$
2. decompose the discretized initial displacement into the eigenmodes

$$U(:, 0) = Va$$

with coefficients $a \in \mathbb{R}^N$

3. due to $w''(t) = -\lambda w(t)$ the oscillation for mode λ_i is

$$w_i(t) = \alpha \cos(\sqrt{\lambda_i}t) + \beta \sin(\sqrt{\lambda_i}t)$$

and as $w'(x, 0) = 0$ and all v_1, \dots, v_N are linear independent it holds

$$\beta_1 = \dots = \beta_n = 0, \quad \alpha_i = a_i$$

4. the numerical solution is

$$U_i^j = \sum_{\ell=1}^n a_\ell \cos(\sqrt{\lambda_\ell}t_j) V_{\ell,j}$$

based on the first $n \leq N$ eigenmodes

Example

We solve the 2D wave equation $u_{tt} = \Delta u$ for $\Omega = (-1, 1)^2$ and with the initial condition

$$u(x, y, 0) = u_0(x, y) = \exp(-200(x^2 + y^2)),$$
$$u_t(x, y, 0) = 0$$

and on the boundary holds $u(x, y, t) = 0$ for all $t \geq 0$.

BUT: for $h = 0.02$ and thus $A \in \mathbb{R}^{9801 \times 9801}$ we have to use a large number of eigenmodes to get reasonable results. For $m = 600$ the results are

