Scientific Computing 1

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Contents

Start of lecture 1 (10.10.2023)

Introduction

- Tuesday 10:15 - 12:00
- Thursday: 08:25 - 10:00
- Orga infos and literature on ecampus

1 Partial differential equations

1.1 Laplace equation

Problem: How to model soap membrane spanned by a wire sling?
Notation:

- $\Omega \subset \mathbb{R}^2$ a bounded domain (open and connected set)
- $\Gamma = \partial\Omega$
- $g : \Gamma \to \mathbb{R}$ describing the wire sling
- $u : \Omega :\to \mathbb{R}$ describing the soap membrane

Question: Given Ω and g, how can we characterize the soap membrane?
u has minimal surface area.

$$\min_u \int_{u(\Omega)} 1 d\sigma = \int_\Omega \|\overrightarrow{u_x} \times \overrightarrow{u_y}\|_2 \, dxdy = \left\| \begin{pmatrix} 1 \\ 0 \\ u_x(x,y) \end{pmatrix} \times \begin{pmatrix} 0 \\ 1 \\ u_y(x,y) \end{pmatrix} \right\|_2 = \left\| \begin{pmatrix} -u_x(x,y) \\ u_y(x,y) \\ 1 \end{pmatrix} \right\|_2 = \sqrt{1 + u_x(x,y)^2 + u_y(x,y)^2}$$

Observation: $\sqrt{1+z} = 1 + z + O(z^2), z \to 0$.
$\implies$ Alternate minimization problem:

$$\min_u \underbrace{\frac{1}{2} \int_\Omega \left(u_x(x,y)^2 + u_y(x,y)^2\right) dxdy}_{F(u)} = \min_u F(u)$$

Assume: We have a minimizer $u \in C^2(\Omega) \cap C(\overline{\Omega})$ with $u|_\Gamma = g$
For $v \in C^1(\Omega) \cap C(\overline{\Omega})$ with $v|_\Gamma = 0$, we obtain

$$\begin{aligned}
0 &= \lim_{\epsilon \to 0} \frac{F(u+\epsilon) - F(u)}{\epsilon} && (1) \\
&= \lim_{\epsilon \to 0} \frac{1}{2\epsilon} \int_\Omega \left((u_x + \epsilon v_x)^2 + (u_y + \epsilon v_y)^2 - (u_x^2 + u_y^2)\right) dydx = (\star) && (2) \\
&= \lim_{\epsilon \to 0} \frac{1}{2\epsilon} \int_{\epsilon \to 0} \int_\Omega (2\epsilon u_x v_x + \epsilon^2 v_x^2 + 2\epsilon u_y + v_y + \epsilon^2 v_y^2) dxdy && (3) \\
&= \lim_{\epsilon \to 0} \frac{1}{2} \int_\Omega (2u_x v_x + \epsilon v^2 + 2u_y v_y + \epsilon v_y^2) dxdy && (4) \\
&= \int_\Omega (u_x v_x + u_y v_y) dxdy && (5) \\
&= \int_\Omega \langle \nabla u, \nabla v \rangle dxdy && (6)
\end{aligned}$$

Observation: A similar term as (1.1) also appears in the Gaus theorem, i.e.

$$\int_\Omega \operatorname{div}\overrightarrow{f}\,\overrightarrow{x} = \int_\Gamma \langle \overrightarrow{f}, \overrightarrow{n} \rangle d\sigma$$

where $\overrightarrow{n}$ is the outward pointing normal to Γ, and $f : \Omega \to \mathbb{R}^3$. If $f = \nabla(u)v$ we obtain

$$\begin{aligned}\int_\Omega \operatorname{div}(\nabla u) v dx + \int_\Omega \langle \nabla u, \nabla v \rangle dx \\ = \int_\Omega \operatorname{div} f dx \\ = \int_\Gamma \langle f, n \rangle d\sigma \\ = \int_\Gamma \frac{\partial u}{\partial n} \underbrace{v}_{=0} d\sigma = 0\end{aligned}$$

Summarizing, u needs to satisfy

$$\int_\Omega \underbrace{\operatorname{div}(\nabla u)}_{=\Delta u} v dx = 0$$

for all $v \in C^1(\Omega) \cap C(\overline{\Omega})$
By the fundamental lemma of calculus of variations, u must satisfy

$$\begin{cases} \Delta u(x) = 0 & x \in \Omega \\ u(x) = g(x) & x \in \Gamma \end{cases}$$

This equation is called the **Laplace equation** or a **potential equation**.

1.2 Heat equation

Problem: How to model temperature in a fixed volume over time?
Notation:

- $\Omega \subset \mathbb{R}^d$ a bounded domain, $d \in \mathbb{N}_+$
- $\Gamma = \partial\Omega$
- $u : \mathbb{R}_{>0} \times \Omega \to \mathbb{R}$
- $u(0, x) = u_0(x), x \in \Omega$
- $u(t, x) = g(t, x)$ $(t, x) \in \mathbb{R}_{>0} \times \Omega$.
- $f(t, x)$ heat source in Ω $(t, x) \in \mathbb{R}_{>0} \times \Omega$.

Question: Given Ω, u_0, f, g how can we characterize u?
First law of thermodynamics:
For any given $V \subset \Omega$ it must hold

$$\underbrace{\int_V \frac{\partial}{\partial} u(t,x) dx}_{\text{Change of temperature in } V} = \underbrace{- \int_{\partial V} \langle q(t,x), n \rangle d\sigma}_{heatflowthrough} V + \int_V f(t,x) dx$$

with the material law

$$q(t,x) = c(x\nabla u(t,x)), c(x) \geq c_0 > 0$$

$$\begin{aligned} \implies \int_{\partial V} \langle q(t,x), u\rangle d\sigma &= \int_V \operatorname{div}(q(t,x))dx \\ &= \int_V \operatorname{div}(c(x)\nabla u(t,x))dx \end{aligned}$$

$$\implies \int_v \frac{\partial}{\partial t} U(t,x) - \operatorname{div}_x((c(x)\nabla u(t,x)))dx = \int_V f(t,x)dx$$

By a variation of the fundamental lemma of calculus of variations we obtain the **heat equation**

$$\begin{cases} \frac{\partial}{\partial t} u(t,x) - \operatorname{div}(c(x)\nabla u(t,x)) = f(t,x) & (x, t \in \mathbb{R}_{>0} \times \Omega) \\ u(0,x) = u_0(x) & x \in \Omega \\ u(t,x) = g(t,x) & (t,x) \in \mathbb{R}_{>0} \times \Gamma \end{cases}$$

For $c(x) = 1$ and f, g time independent, the temperature will tend towards an equilibrium for $t \to \infty$. Then $\frac{\partial u}{\partial t} = 0$ and we obtain the poisson equation

$$\begin{cases} -\delta u(x) = f(x) & x \in \Omega \\ u(x) = g(x) & x \in \Gamma \end{cases}$$

1.3 Wave equation

Problem: How can we model waves in an ideal gas?
Notation:

- $\Omega \subset \mathbb{R}^d$ a bounded domain, $d \in \mathbb{N}_{>0}$
- $\Gamma = \partial\Omega$
- velocity $v : \mathbb{R}_{>0} \times \Omega \to \mathbb{R}^d$ of particles
- density $\rho = \rho_0 + \rho_1 : \mathbb{R}_{>0} \times \Omega \to \mathbb{R}$, ρ_0 is constant with $|\rho_1| << \rho_0$
- pressure $p : \mathbb{R}_{>0} \times \Omega \to \mathbb{R}$ of gas
- $p(0,x) = p_0(x), t = 0$
- $g(t,x)$ pressure at boundary Γ, at $t > 0$

Question: Given Ω, v, ρ, p_0, g can we characterize p?
1. Contiuity Equation: (mass conservation) in any $V \subset \mathbb{R}$.

$$\begin{aligned} \underbrace{\int_V \frac{\partial}{\partial t}\rho(t,x)dx}_{\text{Change of mass}} &= \underbrace{-\int_{\partial V} \rho(t,x)\langle v(t,x), n\rangle d\sigma}_{\text{flux through } \partial V} \\ &= \kappa - \rho_0 \int_{\partial V} \langle v(t,x), n\rangle d\sigma \\ &= -\rho_0 \int_V \operatorname{div}_x(v(t,x))dx \end{aligned}$$

As before $\implies$

$$\frac{\partial}{\partial t}\rho(t,x) \approx -\rho_0 \mathrm{div}_x(v(t,x))$$

2. Newton's law:

$$-\nabla_x p(t,x) = \rho(t,x)\frac{\partial}{\partial}v(t,x) \approx \rho_0 \frac{\partial}{\partial t}v(t,x)$$

3. Equation of state:

$$p(t,x) = c^2\rho(t,x)$$

Combining these 3 laws:

$$\begin{aligned}
\frac{\partial^2}{\partial t^2}p(t,x) &= c^2\frac{\partial^2}{\partial t^2}\rho(t,x) \\
&= -c^2\frac{\partial}{\partial t}\mathrm{div} : x(\rho_0 v(t,x)) = (\star) \\
&= -c^2\mathrm{div}_x(\rho_0\frac{\partial}{\partial t}v(t,x)) \\
&= c^2\mathrm{div}_x(\nabla p(t,x)) \\
&= c^2\Delta p(t,x)
\end{aligned}$$

This yields the **wave equation**

$$\begin{cases} \frac{\partial^2}{\partial t^2}p(t,x - \Delta p(t,x)) = 0 & (t, x \in \mathbb{R}_{>0} \times \Omega) \\ p(t,x) = g(t,x) & (t,x) \in \mathbb{R}_{>0} \times \Gamma \\ p(0,x) = p_0(x) & x \in \Omega \end{cases}$$

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Start of lecture 2 (12.10.2023)

1.4 Helmholz equation

Observation: Waves are quite often time-periodic, i.e.

$$p(t,x) = e^{\pm i\omega t}\hat{p}(x), \omega > 0$$

Substituting into the wave equation:

$$\begin{aligned}
0 &= -\omega^2 p(t,x) - c^2\Delta_x p(t,x) \\
&= e^{i\omega t}\left(-\omega^2\hat{p}(x) - c^2\Delta_x\hat{p}(x)\right)
\end{aligned}$$

$$\implies -\Delta_x\hat{p}(x) - \underbrace{\frac{\omega^2}{c^2}}_{=k^2}\hat{p}(x) = 0, x \in \Omega$$

If the boundary data are time periodic as well, $g(t,x) = e^{i\omega t}g(x)$, we obtain the **Helmholz equation:**

$$\begin{cases} -\Delta\hat{p}(x) - k^2\hat{p}(x) = 0 & x \in \Omega \\ \hat{p}(x) = \hat{g}(x) & x \in \Gamma \end{cases} \tag{7}$$

Advantage: We have gotten rid of the time-dimension.

1.5 Characterization of partial differential equations

Question: Can we find some structure in the partial differential equations above?
Observation: Given a sufficiently smooth function $u : \Omega \to \mathbb{R}$, all of the above PDE can be written in terms of a general partial differential operator

$$(Lu)(x) = -\sum_{i,j=1}^{d} a_{i,j}(x) \frac{\partial^2}{\partial x_i \partial x_k} u(x) + \sum_{i=1}^{d} b_i(x) \frac{\partial}{\partial x_i} u(x) + c(x) \cdot u(x) \tag{8}$$

where

$$A(x) = [a_{i,j}(x)]_{i,j}^{d} \in C(\overline{\Omega})^{d \times d}$$
$$b(x) = [b_i(x)]_{i=1}^{d} \in C(\overline{\Omega})^{d}$$
$$c(x) \in C(\overline{\Omega})$$

Observation: For $u \in C^2(\Omega)$ we have

$$\frac{\partial^2}{\partial x_i \partial x_j} u = \frac{\partial^2}{\partial x_j \partial x_i} u$$

$\implies$ w.l.o.g. we cab assume that $A(x)$ is symmetric. $\implies$ $A(x)$ has real eigenvalues.

definition 1.1. *We call $-\sum_{i,j=1}^{d} a_{i,j}(x) \frac{\partial^2}{\partial x_i \partial x_j} u(x)$ the* ***principle part*** *of the operator. Partial differential operators are called*

- ***elliptic in*** $x \in \Omega$ *if all eigenvalues of $A(x)$ are positive*
- ***parabolic in*** $x \in \Omega$ *if $d-1$ eigenvalues of A are positive, one eigenvalue vanishes and*

$$\mathit{rank}\begin{pmatrix} A(x) & b(x) \end{pmatrix} = d$$

- ***hyperbolic in*** $x \in \Omega$ *if $d-1$ eigenvalues of $A(x)$ are positive and one eigenvalue is negative.*

A partial differential operator is called elliptic, parabolic, hyperbolic if it is so for all $x \in \Omega$

example 1.2.
- *Laplace and Poisson equations are elliptic*
- *The heat equation is parabolic*
- *The wave equation is hyperbolic*
- *The Helmholz equation is elliptic*

These three classes have fundamentally different properties.

- Elliptic PDE are (mostly) similar to Laplace od Poisson equations. For $f \in C(\Omega), g \in C(\Omega)$, look for $u \in C^2(\Omega) \cap C(\overline{\Omega})$ s.t.

$$\begin{cases} \mathcal{L}u = f & \text{in } \Omega \\ u = g & \text{on } \partial\Omega \end{cases}$$

  These boundary conditions are called **Dirichlet** boundary conditions. They can be replaced by **Neumann boundary conditions** $\frac{\partial u}{\partial n} = g$ an others.

- Parabolic PDE: The coordinate direction from the vanishing eigenvalue is usually taken as time derivative, while the rest of the differential operator is elliptic, call it $\mathcal{L}$. Write

$$\frac{\partial}{\partial t} u + \mathcal{L}u = f$$

- Hyperbolic PDE: Take the coordinate direction with the negative eigenvalue as time. Write

$$\frac{\partial^2}{\partial t^2} u + \mathcal{L} u = f$$

Observation: We need to look at elliptic differential operators.
Question: When is it reasonable to look at solutions to PDE?

definition 1.3. *A problem is well-posed if there exists a solution, the solution is unique and it depends continuously on the data.*

Question: Are the PDE above well posed?

1.6 Maximum principle

Simplification: Consider a bounded domain $\Omega \subset \mathbb{R}^d$ and

$$(\mathcal{L}u)(x) = -\sum_{i,j=1}^{d} a_{i,j}(x) \frac{\partial^2}{\partial x_i \partial x_j} u(x) \tag{9}$$

which is elliptic.

theorem 1.4 (Maximum principle)**.** *Let $u \in C^2(\Omega) \cap C(\overline{\Omega})$ a solution to $\mathcal{L}(u) = f \leq 0$. Then u attains its maximum on the boundary, i.e.*

$$\max_{x \in \overline{\Omega}} u(x) = \max_{x \in \partial\Omega} u(x)$$

Proof. **Case 1:** $f < 0$ Assume there is $y \in \Omega$ with $u(y) = \max_{x \in \overline{\Omega}} > \max_{x \in \Gamma} u(x)$.
Observation: $A(x)$ is symmetric, $\mathcal{L}$ is elliptic.
$\implies$ $A(y)$ is symmetric and has positive, real eigenvalues.
$\implies$ there is $Q \in \mathbb{R}^{d \times d}$ such that

$$QA(y)Q^t$$

is diagonal and has positive entries.
Observation: Rotating the coordinate system on Ω by Q, i.e., setting $\zeta = Qx$ changes the differential operator to our advantage.

$$(\mathcal{L}\sqcap)(\zeta) \overset{\text{exercise}}{=} -\sum_{i,j=1}^{d} \left(QA(\zeta)Q^t\right)_{ij} \frac{\partial^2}{\partial \zeta_i \partial \zeta_j} u(\zeta)$$

$$\implies ()\mathcal{L}u)(y) = -\sum_{i,j=1}^{d} \underbrace{\left(QA(y)Q^t\right)_{ij} \frac{\partial^2}{\partial \zeta_i \partial \zeta_j}}_{=0 \text{ if } i \neq j} u(\zeta)$$

$$= -\sum_{i=1}^{d} \underbrace{(QA(y)Q^t)_{ii}}_{>0} \frac{\partial^2}{\partial \zeta_i^2} u(\zeta)$$

Observation: y is an extremal point of u

$$\implies \partial_{\zeta_i} u(y) = 0, \frac{\partial^2}{\partial \zeta_i^2} u(y) \leq 0$$

$f(y) = (\mathcal{L}u)(y) = -\sum_{i=1}^{d} \left(QA(y)Q^t\right)_{ii} \frac{\partial^2}{\partial \zeta_i^2} u(y) \geq 0$
Contradiction to $f < 0$.
Case: $f \leq 0$
Assumption: As before assume there is $y \in \Omega$, s.t. $u(y) = \max_{x \in \overline{\Omega}} > \max_{x \in \Gamma} u(x)$.

Observation: Setting

$$h(x) = \|x - y\|_2^2 = \sum_{i=1}^{d} |x_i - y_i|^2$$

and $\delta > 0$ small enough and set $w = \delta h$.
For δ small enough, w has its maximum in Ω.

$\square$

———————————————End of lecture 2 (12.10.2023)———————————————
———————————————Start of lecture 3 (17.10.2023)———————————————

Proof. (continued) **Case $f \leq 0$:**
Assumption: There exists

$$y \in \Omega \text{ s.t. } u(y) = \max_{x\in\Omega} u(x) > \max_{x\in\Gamma} u(x)$$

Observation:

$$h(x) = \|x - y\|_2^2 = \sum_{i=1}^{d} (x_i - y_i)^2$$

and u is convex.
For $\delta > 0$ small enough, set

$$w = u + \delta h$$

such that w still attains its maximum in Ω.
Observe:

$$\frac{\partial^2}{\partial x_i \partial x_j} h(x) = 2\delta_{ij}$$

$$\implies (\mathcal{L}w)(x) = \underbrace{\mathcal{L}\sqcap(x)}_{=f\leq 0} + \underbrace{\delta(\mathcal{L}h)(x)}_{=-\sum_{j=1}^{d} a_{i,j}(x)\frac{\partial^2}{\partial x_i \partial x_j}h(x)\frac{\partial^2}{\partial x_i \partial x_j}h(x)=\star} < 0$$

$$\star = -2\sum_{i=1}^{d} a_{ii}$$

$A = [a_{i,j}(x)]_{i,j=1}^{d}$ has positive eigenvalues. $\implies A(x)$ is positive definite.
$\implies z^t A(x) z > 0$ for $\neq 0$ $\implies a_{ii} = e_i^t A(x) e_i > 0$
Proceed as in the first case $f < 0$ to obtain a contradiction. $\square$

corollary 1.5. *(Minimum principle) If $\mathcal{L}u = f \geq 0$ in Ω, then u attains its minimum on the boundary.*

Proof. Apply the maximum principle to $-u$. $\square$

corollary 1.6 (Comparison principle)**.** *If $\mathcal{L}u \leq \mathcal{L}v$ in Ω and $u \leq v$ on $\partial\Omega$ then $u \leq v$ in $\overline{\Omega}$.*

Proof. Set $w = u - v$ and apply the maximum principle. $\square$

corollary 1.7. *Uniqueness There is at most 1 solution to*

$$\begin{cases} \mathcal{L}u = f & \in \Omega \\ u = g & \in \partial\Omega \end{cases}$$

Proof. Exercise. $\square$

remark 1.8. *We have not (yet) shown existence of solutions.*

corollary 1.9 (Contiuous depedence on the boundary data)**.** *The solution to*

$$\begin{cases} \mathcal{L}u = f & \in \Omega \\ u = g & \in \partial\Omega \end{cases}$$

depends continuously on the boundary data, i.e.

$$\max_{x\in\Omega} |u_1(x) - u_2(x)| \leq \max_{x\in\partial\Omega} |g_1(x) - g_2(x)|$$

Proof. Exercise. □

definition 1.10. *The second order partial differential operator $\mathcal{L}$ from (1.13) is called* ***uniformly elliptic*** *if there is an $\alpha > 0$ s.t.*

$$z^t A(x) z > \alpha \|z\|_2^2, z \neq 0.$$

α is called the ellipticity constant of $\mathcal{L}$.

corollary 1.11 (Contiuous dependence on the right-handed side)**.** *Let $\mathcal{L}$ be uniformly elliptic. Then there is a constant $c = c(\Omega, \alpha)$, s.t. for all solutions $u \in C^2(\Omega) \cap C(\overline{\Omega})$ it holds*

$$|u(x)| \leq \max_{z\in\Gamma} |\underbrace{u(z)}_{=g(z)}| + c \sup_{z\in\Omega} |\underbrace{\mathcal{L}u(z)}_{=f(z)}|$$

remark 1.12. *This tells us that small changes in f imply small changes in u.*

Proof. Let $R > 0$ s.t. $\Omega \subset B_R(0)$. Set

$$w(x) = R^2 - \|x\|_2^2 \geq 0.$$

Note that $\frac{\partial^2}{\partial x_i \partial x_j} = -2\delta_{ij}$.

$$(\mathcal{L}u)(x) = -\sum_{i,j=1}^{d} a_{ij}(x) \frac{\partial^2}{\partial x_i \partial x_j} w(x) = 2 \sum_{i=1}^{d} \underbrace{a_{ij}}_{\geq\alpha}$$

because of $z^t A(x) z \geq \alpha \|z\|_2^2$.
Now, set

$$v(t) = \max_{z\in\Gamma} |u(z)| + \frac{w(x)}{2} \sup_{z\in\Omega} |(\mathcal{L}u)(z)|$$

This yields:

$$(\mathcal{L}v)(x) = \frac{(\mathcal{L}w)(x)}{2} \sup_{z\in\Omega} |(\mathcal{L}u)(z)| \geq \sup_{z\in\Omega} |(\mathcal{L}u)(z)| \geq |(\mathcal{L}u)(x)|$$

Moreover:

$$\begin{aligned} geqv(x) \geq \sup_{z\in\Gamma} |u(z)| &\geq ||u(x)||, x \in \Omega \\ &\geq \pm u(x) \end{aligned}$$

Apply the comparison principle twice to u, v and $-u, v \implies \pm u \leq v \implies |u| \leq v$ (both in $\overline{\Omega}$).

$\implies |u(x)| \leq \max_{z\in\Gamma} |u(z)| + \underbrace{\overbrace{\frac{w(x)}{2}}^{\leq R^2}} \frac{R^2}{2\alpha} \sup_{z\in\Omega} |(\mathcal{L}u)(z)|$

□

2 Finite difference method

2.1 Poisson equation

Problem: Let $\Omega \subset \mathbb{R}^d$ bounded domain, $\Gamma = \partial\Omega$.
$f \in C(\Omega), g \in C(\Gamma)$. We look for $u \in C^2(\Omega) \cap C(\overline{\Gamma})$ s.t.

$$\begin{cases} \Delta u = f & \text{in } \Omega \\ u = g & \text{on } \Gamma \end{cases}.$$

definition 2.1. *A solution $u \in C^2(\Omega) \cap C(\overline{\Gamma})$ is called a **classical solution**. For $f = 0$, we say that u is harmonic.*

In this chapter we say solution, but refer to classical solutions.
Question: How can we solve (2.1) for rather general domains Ω?

definition 2.2. *Let $f \in C(\mathbb{R}^d)$, $1 \leq i \leq d$. We define for $h > 0$*

- *the **forward (finite) difference** as*

$$\partial_j^{+h} f = \frac{f(x + he_j) - f(x)}{h}$$

- *the **backward (finite) difference** as*

$$\partial_j^{-h} f = \frac{f(x - he_j) - f(x)}{-h}$$

- *the **central (finite) difference** as*

$$\partial_j^{h} \frac{f(x + he_j) - f(x - he_j)}{2h}$$

lemma 2.3. *Let $f \in C^4(\mathbb{R}^d)$ it holds*

$$\frac{\partial f}{\partial x_j}(x) = \partial_j^{\pm h} f(x) + R_1^{\pm} \leq \frac{h}{2} \|F\|_{C^2(\mathbb{R}^d)}$$

$$\frac{\partial f}{\partial x_j}(x) = \partial_j^{h} f(x) + R_2, R_2 \leq \frac{h^2}{6} \|f\|_{C^3(\mathbb{R}^d)}$$

$$\frac{\partial^2 f}{\partial x_i \partial x_j}(x) = (\partial_j^{+h} \partial_j^{-h} f)(x + R_3)$$

$$= \frac{f(x + he_j) - 2f(x) + f(x - he_j)}{h^2} + \underbrace{R_3}_{||\leq \frac{h^2}{12}} \|f\|_{C^4(\mathbb{R}^d)}$$

where $\|f\|_{C^k(\mathbb{R}^d)} = \sum_{|\alpha| \leq k} \sup_{x \in \mathbb{R}^d} |\partial^\alpha f(x)|$

Proof. Exercise. □

———————————————End of lecture 3 (17.10.2023)———————————————
———————————————Start of lecture 4 (19.10.2023)———————————————

Idea: For $x \in \Omega$, we have

$$\Delta u(x) = -\sum_{i=1}^{d} (\partial_i^{+h} \partial_i^{-h} u)(x) + O(h^2)$$

Idea: Introduce a equally spaced grid on Ω: Discrete Domain $\Omega_h = \{x \in \Omega : x = hk, k \in \mathbb{Z}^d\}$.

Discrete Boundary $\Gamma_h = \{x \in \Gamma : \exists 1 \leq i \leq d : x_i = hk_i, k_i \in \mathbb{Z}\}$.
Set $\overline{\Omega}_h = \Omega_h \cup \Gamma_h$, $\overline{\Omega}_h \setminus \Gamma_h$ interior points.
Observation: If Ω is a disjoint union of equal cubes, then we can modify (2.1) to

$$\begin{cases} \Delta_h u_h(x) = f(x) & \in \overline{\Omega}_h \setminus \Gamma_h \\ u_h(x) = g(x) & x \in \Gamma_h \end{cases}$$

This corresponds to a system of linear equations!

example 2.4. $\Omega = (0,1)^2, n \in \mathbb{N}, h = \frac{1}{n}, y_{ij} h(i,j), i,j = 0, \dots, n$
Assume: $g = 0$, *Abbreviate* $u_{ij} \coloneqq u(x_{ij})$, *then*

$$\begin{aligned} \Delta_h u_h(x_{ij}) &= \frac{4u_{ij} - u_{i-1j} - u_{i+1j} - u_{ij-1} - u_{ij+1}}{h^2} \\ &= \frac{1}{h^2} \begin{bmatrix} & -1 & \\ -1 & 4 & -1 \\ & -1 & \end{bmatrix} u(x_{ij}) \end{aligned}$$

This is called the ***5-point finite difference stencil****. Set* $f_{ij} \coloneqq f(x_{ij})$.

$$\begin{aligned} \implies \frac{4u_{ij} - u_{i-1j} - u_{i+1j} - u_{ij-1} - u_{ij+1}}{h^2} &= f_{ij} i = 1, \dots, n-1 \\ u_{ij} &= 0 i = \{0,1\}, j \in \{0,1\}. \end{aligned}$$

We cna write this in matrix form as

$$\frac{1}{h^2} \begin{bmatrix} A & -I & & & \\ -I & A & -I & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & -I \\ & & & -I & A \end{bmatrix} \begin{bmatrix} u_1 \\ \vdots \\ \vdots \\ u_{n-1} \end{bmatrix} = \begin{bmatrix} f_1 \\ \vdots \\ \vdots \\ f_{n-1} \end{bmatrix}$$

where

$$A = \begin{bmatrix} 4 & -1 & & & & \\ -1 & \ddots & \ddots & & & \\ & \ddots & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & & & \ddots & \ddots & -1 \\ & & & & -1 & 4 \end{bmatrix} u_i = \begin{bmatrix} u_{i,1} \\ \vdots \\ u_{i,n-1} \end{bmatrix} f_i = \begin{bmatrix} f_{i,1} \\ \vdots \\ f_{i,n-1} \end{bmatrix}$$

remark 2.5. *The same approach can be applied to more partial differential operators, but a few technicalities need to be considered.*

remark 2.6. *More general domains (non-cuboids) can be dealt with by modifying the stencils close to the boundary. However in general, this will only lead to* $O(h)$ *approximations, rather than* $O(h^2)$

Question: Are the systems of linear equations uniquely solvable?

2.2 The discrete maximum principle

Observation: Applying a finite difference stencil amounts to computing a weighted average of functions values. The value of the stencil can not be larger as the maximum of the values where it is applied to.

lemma 2.7 (Star lemma). *Let $k > 0$ and consider numbers $\alpha_0, \dots, \alpha_k$ with $\alpha_1, \dots, \alpha_k < 0$ and $p_0, \dots, p_k$ such that*

$$\sum_{l=0}^{k} \alpha_l \geq 0, \sum_{l=0}^{k} \alpha_l p_l \leq 0.$$

Assume that $p_0 \geq 0$ or $\sum_{l=0}^{k} \alpha_l = 0$, then if $p_0 \geq \max_{1 \geq l \geq k} p_l$, it holds that

$$p_0 = p_1 = \cdots = p_k$$

Proof.

$$0 \geq \sum_{k=0}^{l} \alpha_l p_l - p_0 \sum_{l=0}^{k} \alpha_l$$

$$= \sum_{l=0}^{k} \alpha_l (p_l - p_0) = \sum_{l=1}^{k} \underbrace{\underbrace{\alpha_l}_{<0} \underbrace{(p_l - p_0)}_{\geq 0}}_{\geq 0} \geq 0$$

which implies the assertion. □

theorem 2.8 (Discrete maximum principle). *Let u_h be the solution to $\Delta_h u_h = f$, with $f \leq 0$ and assume that Ω_h is (discretely) connected. Then it holds*

$$\max_{x \in \overline{\Omega}_h \setminus \Gamma_h} u_h(x) \leq \max_{x \in \Gamma_h} u_h(x).$$

Proof. Assume that the maximum is attained at $y \in \overline{\Omega}_h \setminus \Gamma_h$, set $p_0 = u_h(y)$. Identify $p_1, \dots, p_k$ with the values of u_h on the neighboring grid cells, and $\alpha_0, \dots, \alpha_k$ with the weights of the stencil.

$$0 \geq f(y) = (\Delta_h u_h)(y) = \sum_{l=0}^{k} \alpha_l p_l.$$

$$\overset{\text{Star lemma}}{\Longrightarrow} p_0 = \cdots = p_k$$

i.e., $u_h(y)$ at points in eastern, western, southern and northern direction is equal to u_h.
Proceed iteratively by marching to the boundary. □

All implications of the continuous case transfer to the discrete case. Most importantly:

corollary 2.9. *Under the assumptions of (last theorem), the solution of (2.2) is unique.*

———————————————End of lecture 4 (19.10.2023)———————————————

———————————————Start of lecture 5 (24.10.2023)———————————————

2.3 Convergence of the finite difference method

Notation:

$$\|v_h\|_{\Omega_h} = \max_{x \in \Omega_h} |v_h(x)|, \|v_h\|_{\overline{\Omega}_h} = \max_{x \in \overline{\Omega}} |v_h(x)|$$

definition 2.10. *Let $\mathcal{L}_h$ denote the finite difference approximation of $\mathcal{L}$ from (1.12). The corresponding finite difference method is called*

- ***convergent*** *of order p, if the solution to the PDE satisfies*

$$\|u-h_h\|_{\overline{\Omega}_h}=O(h^p).$$

- ***consistent*** *of order p, if*

$$\|\mathcal{L}u-\mathcal{L}_h u\|_{\overline{\Omega}_h}=O(h^p)$$

- ***stable****, if there exists $C_s>0$ s.t. for all*

$$u_h:\Omega_h\to\mathbb{R}$$

  with $u_h|_{\Gamma_h}=0$ it holds

$$\|u_h\|_{\overline{\Omega}_h}\leq C_s\left\|\mathcal{L}_h u_h\right\|_{\Omega_n}$$

remark 2.11. *The 5-point stencil yields consistency order $p=2$.*

added remark. *stability means that our solution depends continuously on our data.*

remark 2.12. *Let v_h be the coefficient vector of $v_h:\Omega_h\to\mathbb{R}$. Let $w_h=A_h v_h$ be the coefficient vector to $w_h=\mathcal{L}_h v_h$.*
$\implies \underbrace{\|v_h\|_\infty}_{=\|v_h\|}{}_{\overline{\Omega}_h}=\left\|A_h^{-1}w_h\right\|_\infty$

$$\|v_h\|_\infty\overset{stability}{\leq}C_s\left\|\mathcal{L}_h v_h\right\|_{\Omega_h}=C_s\left\|A_h v_h\right\|_\infty=C_s\left\|w_n\right\|_\infty,$$

i.e. A_h is boundedly invertible and has the same continuity constant for all $h>0$.

theorem 2.13. *If a finite difference scheme is stable and consistent of order p, then it is also convergent of order p.*

Proof.

$$\|u-u_h\|_{\overline{\Omega}_h}\overset{\text{stability}}{\leq}C_s\left\|\mathcal{L}_h(u-u_h)\right\|_{\Omega_h}=C_s\left\|\mathcal{L}_h u-\underbrace{\mathcal{L}_h u_h}_{=f=\mathcal{L}u}\right\|_{\Omega_h}=C_s\left\|\mathcal{L}_h u\mathcal{L}u\right\|_{\Omega_h}=O(h^p)$$

.

□

Observation: We need to show stability of (2.2). Then the last theorem yields convergence.
Idea: Stability is nothing else than continuous dependence on the right-hand side. Adpot the proof of Corollary 1.11 to the discrete setting.

corollary 2.14. *Let Ω be given as a disjoint union of cubes of equal size and assume $u\in C^4(\overline{\Omega})$ and satisfies 2.1. Then the finite difference approximation u_h converges with*

$$\|u-u_h\|_{\overline{\Omega}_h}=O(h^2)$$

Proof. Corollary of the following lemma. □

lemma 2.15. *Let $R>0$ s.t. $\Omega\subset B_R(0)$ and let $u_h:\Omega_h\to R$ with $u_h|_{\Gamma_h}=0$. Then it holds*

$$\|u_h\|_{\overline{\Omega}_h}\leq\frac{R^2}{2d}\left\|\Delta_h u_h\right\|_{\overline{\Omega}_h},$$

i.e., the finite difference approximation is stable.

Proof. Exercise □

Problem.

- We are restricted to very specific domains.
- Strong smoothness requirements
- Special treatment of more involved differential operators required.

End of lecture 5 (24.10.2023)