Scientific Computing 1

Manuel Hinz

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Contents

1 Partial differential equations **2**
1.1 Laplace equation 2
1.2 Heat equation 3
1.3 Wave equation 4
1.4 Helmholz equation 5
1.5 Characterization of partial differential equations 6
1.6 Maximum principle 7

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.

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

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

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

Summarizing, u needs to satisfy

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

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

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

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

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**

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

End of lecture 1 (10.10.2023)

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.
$\Longrightarrow$ $A(y)$ is symmetric and has positive, real eigenvalues.
$\Longrightarrow$ 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.

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

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

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

Observation: y is an extremal point of u

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

$f(y) = (\mathcal{L}u)(y) = -\sum_{i=1}^{d} \left(QA(y)Q^t\right)_{ii} \frac{\partial^2}{\partial \zeta_i^2} u(y) \geq 0$
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)——————————