CHAPTER 1

Mathematical modelling using partial differential equations

Many PDE models come from a basic balance or conservation law, which states that a particular measurable property of an isolated physical system does not change as the system evolves. Any particular conservation law is a mathematical identity to certain symmetry of a physical system. Here are some examples

- conservation of mass (states that the mass of a closed system of substances will remain constant)
- conservation of energy (states that the total amount of energy in an isolated system remains constant, first law of thermodynamics)
- conservation of linear momentum (states that the total momentum of a closed system of objects – which has no interactions with external agents – is constant)
- conservation of electric charge (the total electric charge of an isolated system remains constant)

1.1 Mass balance

A mass balance (also called a material balance) is an accounting of material entering and leaving a system. Fundamental to the balance is the conservation of mass principle, i.e. that matter can not disappear or be created. Mass balances are used, for example, by designing of chemical reactors, by analysis of alternative processes to produce chemicals, in pollution dispersion models etc.

Let us assume that the mass particles are dragged by a vector field $\boldsymbol{v} : \mathbb{R}^3 \to \mathbb{R}^3$. Inflow to and outflow from $\Omega \subset \mathbb{R}^3$ is allowed – see Fig. 1.1.

Let us denote by $\boldsymbol{\nu} = \boldsymbol{\nu}(\boldsymbol{x})$ the outer normal vector to Γ. The mass flowing out from Ω during the time Δt through the boundary part $d\Gamma \subset \Gamma$ is given as – cf. Fig. 1.2

$$\text{density} \;\; \text{volume} = \rho \; \boldsymbol{v} \cdot \boldsymbol{\nu} \; \Delta t \; d\Gamma.$$

The symbol $\cdot$ stands for the scalar product in $\mathbb{R}^3$.

The total flow Q_1 (inflow and outflow) through Γ is

$$Q_1 = \int_\Gamma \rho \boldsymbol{v} \cdot \boldsymbol{\nu} \Delta t \; \mathrm{d}\Gamma = \Delta t \int_\Gamma \rho \boldsymbol{v} \cdot \boldsymbol{\nu} \; \mathrm{d}\Gamma.$$

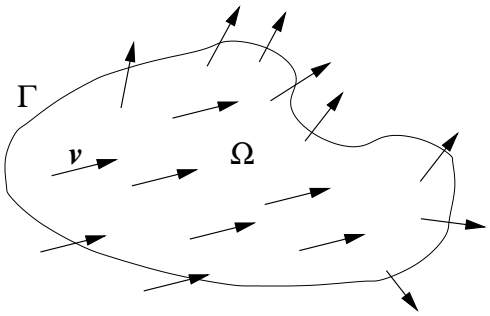

Fig. 1.1: Domain Ω with the boundary $\partial\Omega = \Gamma$ with a vector field $\boldsymbol{v}$

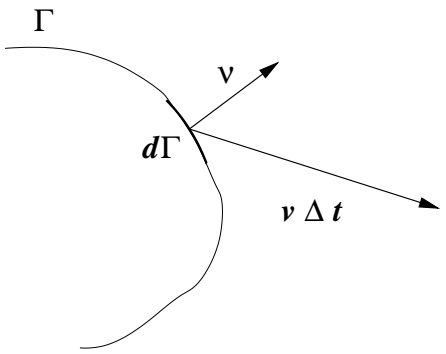

Fig. 1.2: Part of Γ with outflow

The sign of the flow is defined in such a way that outflow is positive. Therefore if Q_1 is positive then the outflow is larger than the inflow.

The total mass in the domain Ω is

$$\int_\Omega \rho \, \mathrm{d}\boldsymbol{x}.$$

Its change during the time Δt is given by

$$Q_2 = \Delta t \partial_t \int_\Omega \rho \, \mathrm{d}\boldsymbol{x}.$$

The mass balance says that the mass cannot disappear, i.e.,

$$Q_1 + Q_2 = 0.$$

The integral form of this reads as

$$\int_\Omega \partial_t \rho \, \mathrm{d}\boldsymbol{x} + \int_\Gamma \rho \boldsymbol{v} \cdot \boldsymbol{\nu} \, \mathrm{d}\Gamma = 0. \tag{1.1}$$

For the second integral we can use the integration by parts formula (the Green theorem)

$$\int_\Omega \nabla \cdot \boldsymbol{v} \, \varphi \, \mathrm{d}\boldsymbol{x} + \int_\Omega \boldsymbol{v} \cdot \nabla \varphi \, \mathrm{d}\boldsymbol{x} = \int_\Gamma \boldsymbol{v} \cdot \boldsymbol{\nu} \, \varphi \, \mathrm{d}\Gamma. \tag{1.2}$$

Here, the symbol ∇ is the "nabla operator" $\nabla\varphi = (\partial_{x_1}\varphi, \partial_{x_2}\varphi, \partial_{x_3}\varphi)$ and the symbol $\nabla\cdot$ is the "divergence operator" $\nabla \cdot \boldsymbol{v} = \sum_{i=1}^{3} \partial_{x_i} v_i$.

Thus, the relation (1.1) takes the form

$$\int_\Omega \partial_t \rho \, \mathrm{d}\boldsymbol{x} + \int_\Omega \nabla \cdot (\rho \boldsymbol{v}) \, \mathrm{d}\boldsymbol{x} = \int_\Omega \left(\partial_t \rho + \nabla \cdot (\rho \boldsymbol{v})\right) \, \mathrm{d}\boldsymbol{x} = 0.$$

This equation is valid for any domain Ω. Let us note then if a continuous function $\Phi : \mathbb{R}^3 \to \mathbb{R}$ fulfills $\int_\Omega \Phi(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} = 0$ for arbitrary Ω in $\mathbb{R}^3$, then $\Phi = 0$. Hence

$$\partial_t \rho + \nabla \cdot (\rho \boldsymbol{v}) = 0 \qquad \forall \boldsymbol{x}, t. \tag{1.3}$$

The flow field $\boldsymbol{v}$ can be time dependent. An analogous form to (1.3) is

$$\partial_t \rho + \sum_{i=1}^{3} \partial_{x_i} (\rho v_i) = 0 \qquad \forall \boldsymbol{x}, t. \tag{1.4}$$

The equation (1.3) is called the "continuity equation". It is valid for all sorts of materials. If the material under consideration has a constant density ρ then

$$\partial_t \rho = 0, \qquad \nabla \cdot (\rho \boldsymbol{v}) = \rho \nabla \cdot \boldsymbol{v}.$$

In this situation takes the continuity equation the following form

$$\nabla \cdot \boldsymbol{v} = 0 \qquad \forall \boldsymbol{x}, t. \tag{1.5}$$

Fig 1.3 shows some examples of such vector fields in $\mathbb{R}^2$.

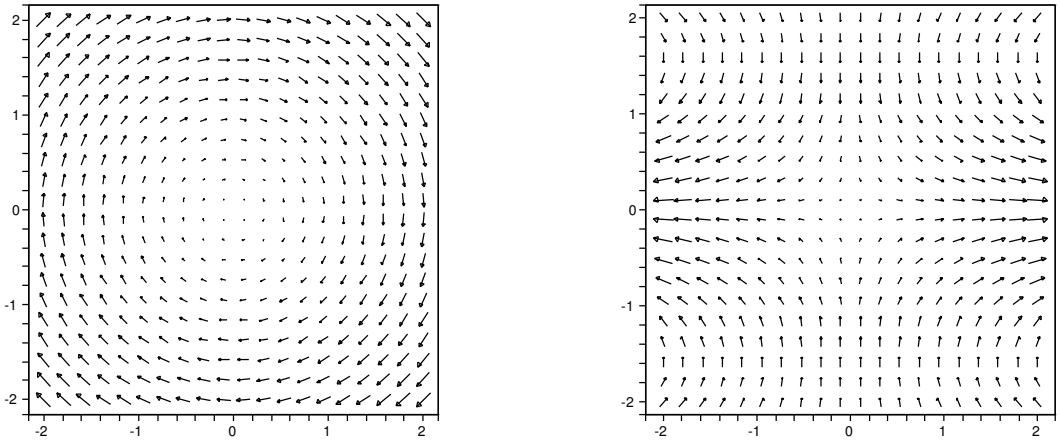

Fig. 1.3: Examples of divergence free vector fields in $\mathbb{R}^2$. Left: $\boldsymbol{v} = (x_2, -x_1)$. Right: $\boldsymbol{v} = (x_1 \cos x_2, -\sin x_2)$.

1.2 Heat transfer

Heat is a form of energy that is transferred from one body to another body. Heat transfer can occur between the places with a temperature difference. If two bodies with different temperatures are brought into contact with each other, then the heat transfers from the hotter body to the colder one. This process will continue until the temperature of the system will reach the "thermal equilibrium". The SI unit of heat is joule – 1 cal (calorie)= 4.1868 J (joule).

Heat may transfer across the boundaries of a system in both directions: either to or from the system. It occurs only when there is a temperature difference between the body and its neighborhood. Heat transfer changes the internal energy of the system. Heat is transferred by "conduction", "convection" and "radiation", which may occur separately or in combination.

Conduction heat transfer occurs only by a physical contact between bodies at different temperatures. Heat transfer through solid bodies is by conduction only.

Convection is the heat transfer within a fluid. Fluid motion may be caused by differences in density as in free convection. Density differences are a direct result of temperature differences between the fluid and the solid wall surface. In forced convection, the fluid motion is produced by external means.

Thermal radiation is the energy radiated from hot surfaces as electromagnetic waves. It does not require medium for its propagation. Heat transfer by radiation occur between solid surfaces, although radiation from gases is also possible.

Fourier's law is an empirical law based on observation. It says that the rate of heat flow through a homogeneous solid is proportional to the area of the section at right angles to the direction of heat flow, and to the temperature difference along the path of heat flow dT/dx – see Fig 1.4. Thus, the density of the heat flow can be written as

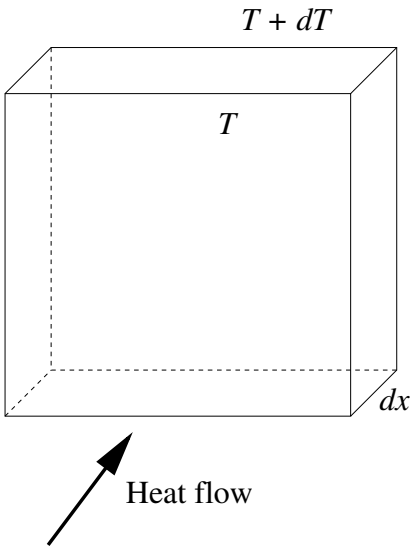

Fig. 1.4: Fourier law

$$w = -k\nabla T \cdot \boldsymbol{\nu}, \tag{1.6}$$

where $k > 0$ is the conductivity coefficient of the material. The negative sign says that the heat flow proceeds from the hotter to the colder place.

The amount of heat going through the surface Γ during the time Δt is given as

$$Q_1 = \int_\Gamma w\Delta t \ \mathrm{d}\Gamma = \Delta t \int_\Gamma w \ \mathrm{d}\Gamma.$$

The material inside the domain Ω has the density $\rho > 0$ and the specific heat capacity of a material is $c > 0$. The heat change during the time Δt inside Ω is

$$Q_2 = \int_\Omega c\rho\partial_t T\Delta t \ \mathrm{d}\boldsymbol{x} = \Delta t \int_\Omega c\rho\partial_t T \ \mathrm{d}\boldsymbol{x}.$$

Heat generated by external source f during the time Δt can be written as

$$Q_3 = \int_\Omega f\Delta t \ \mathrm{d}\boldsymbol{x} = \Delta t \int_\Omega f \ \mathrm{d}\boldsymbol{x}.$$

According to the heat balance $Q_1 + Q_2 = Q_3$ we obtain

$$\int_\Omega c\rho\partial_t T \ \mathrm{d}\boldsymbol{x} - \int_\Gamma k\nabla T \cdot \boldsymbol{\nu} \ \mathrm{d}\Gamma = \int_\Omega f \ \mathrm{d}\boldsymbol{x}.$$

When we apply the Green theorem (1.2) to the second term we arrive at

$$\int_\Omega c\rho\partial_t T \ \mathrm{d}\boldsymbol{x} - \int_\Omega \nabla \cdot (k\nabla T) \ \mathrm{d}\boldsymbol{x} - \int_\Omega f \ \mathrm{d}\boldsymbol{x} = \int_\Omega (c\rho\partial_t T - \nabla \cdot (k\nabla T) - f) \ \mathrm{d}\boldsymbol{x} = 0.$$

This is valid for any Ω. Therefore, analogously as in (1.3) we can write

$$c\rho\partial_t T - \nabla \cdot (k\nabla T) = f, \qquad \forall \boldsymbol{x}, t, \tag{1.7}$$

which is called "the heat equation".

Anisotropic materials have different conductive properties in different directions. Then k will be a tensor. For isotropic materials k is a constant.

Initial condition The heat equation is a time dependent problem. Without loss of generality we may assume that the process starts at the time $t = 0$. For the determination of $T(t, \boldsymbol{x})$ for $t > 0$ and $x \in \Omega$ we need the information about the temperature at the begin of the process. This state $T(0, \boldsymbol{x})$ for all $\boldsymbol{x} \in \Omega$ is called the initial condition.

1.2.1 Boundary conditions

If the boundary gives a value to the normal derivative of T then it is a "Neumann boundary condition"

$$-k\nabla T \cdot \boldsymbol{\nu} = \text{ given at } \Gamma.$$

For example if one end of an iron rod had a heater then energy would be added at a constant rate but the actual temperature would not be known.

If the boundary gives a value of T then it is a "Dirichlet boundary condition"

$$T = \text{ given at } \Gamma.$$

For example if one end of an iron rod has a constant temperature.

If the boundary gives a value to the linear combination of the normal derivative of T and the temperature T itself then it is a "Cauchy boundary condition"

$$-k\nabla T \cdot \boldsymbol{\nu} + \alpha T = \text{ given at } \Gamma.$$

Let us note that some authors use the name Newton or Robin instead of Cauchy.

All types of boundary conditions can be combined, e.g., Dirichlet at Γ_{Dir}, Neumann at Γ_{Neu} and Robin at Γ_{Rob}, along with the condition

$$\Gamma = \Gamma_{Dir} \cup \Gamma_{Neu} \cup \Gamma_{Rob}$$

and all boundary parts Γ_{Dir}, Γ_{Neu} and Γ_{Rob} are disjoint

$$\Gamma_{Dir} \cap \Gamma_{Neu} = \Gamma_{Neu} \cap \Gamma_{Rob} = \Gamma_{Rob} \cap \Gamma_{Dir} = \emptyset.$$

1.2.2 Steady state solution

Heat transfer is a transient (time dependent) process in a given domain Ω. We start from a given state at the begin (initial datum). The spreading of heat follows the physical laws, which are mathematically described in the heat equation. The contact with external world is described via the boundary conditions. We can observe the long time behavior of the temperature. In some situations it stabilizes, i.e., there exists

$$T(\boldsymbol{x}) = \lim_{t\to\infty} T(t, \boldsymbol{x}).$$

This limit is time-independent. Which differential equation does the limit fulfill? We recall that $T(t, \boldsymbol{x})$ fulfills (1.7). We can try to pass to the limit for $t \to \infty$ in (1.7). If we assume the existence of

$$f(\boldsymbol{x}) = \lim_{t\to\infty} f(t, \boldsymbol{x})$$

we see that $T(\boldsymbol{x})$ satisfies

$$-\nabla \cdot (k\nabla T(\boldsymbol{x})) = f(\boldsymbol{x}).$$

This equation is called "steady state heat equation" and this must be accompanied by corresponding boundary conditions under consideration.

1.3 Vibrating string

Let us consider a homogeneous elastic string with a constant density $\rho > 0$ and the length L, which is fixed between two horizontal points $x = 0$ and $x = L$. The string is in a balance and it can move only in the vertical plane. We assume that

(i) the tension T is always touching the string

(ii) only vertical movements are allowed.

We introduce the Cartesian coordinates (x, u) in the vertical plane, where the string moves. Here, x-denotes the position of a point and $u = u(t, x)$ is its vertical shifting at the time t. The string can be described as

$$\gamma(t) := \{(x, u(t, x)) \mid 0 \le x \le L\}.$$

We suppose that the function $u(t,x)$ is sufficiently smooth and the vibrations are small. The boundary conditions can be expressed as follows

$$u(t,0) = 0 = u(t,L).$$

The situation at the time t is depicted in Fig. 1.5. The part $[x,L]$ acts on the part $[0,x]$ with the

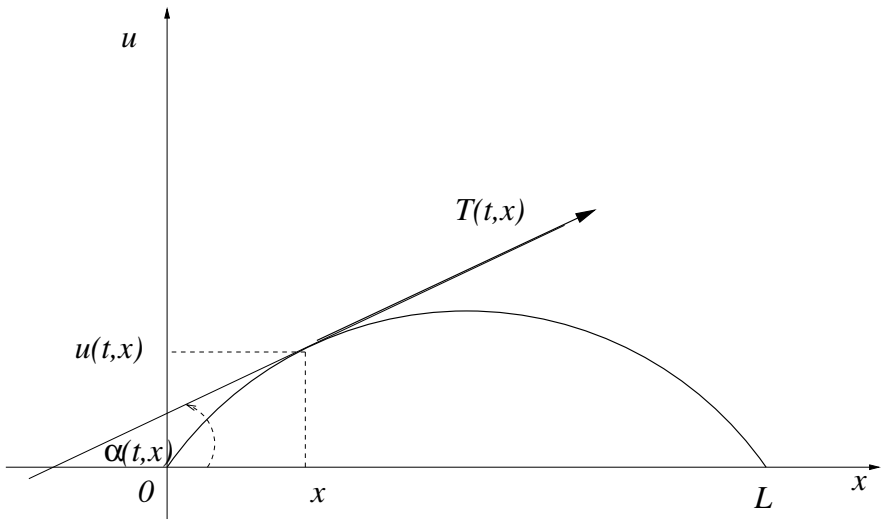

Fig. 1.5: Vibrating string

force $\boldsymbol{T}(t,x)$, $|\boldsymbol{T}(t,x)| = T(t,x)$. This force touches the curve γ – following the hypotheses (i). The angle between $\boldsymbol{T}(t,x)$ and the x-axis is denoted by $\alpha(t,x)$. The vibrations are supposed to be small, thus the length of the string remains constant

$$\int_{x_1}^{x_2} \sqrt{1+u_x^2}\ \mathrm{d}x \approx \int_{x_1}^{x_2} 1\ \mathrm{d}x = x_2 - x_1.$$

Therefore

$$\sin\alpha = \frac{u_x}{\sqrt{1+u_x^2}} \approx u_x.$$

$$\tan\alpha \approx \sin\alpha \approx u_x \qquad \text{and} \qquad \boldsymbol{T}(t,x) = T(t,x)(\cos(\alpha(t,x)), \sin(\alpha(t,x)))$$

The part $[0,x]$ acts on the part $[x,L]$ with the force $-\boldsymbol{T}(t,x)$ (action = reaction). Let us take $0 \le a < b \le L$ and $x \in [a,b]$. There is no horizontal movement, therefore

$$T(t,b)\cos(\alpha(t,b)) - T(t,a)\cos(\alpha(t,a)) = 0.$$

Thus, there exists a function $\tau(t) > 0$ for which

$$\tau(t) = T(t,x)\cos(\alpha(t,x)) = \frac{T(t,x)}{\sqrt{1+\left(u_x(t,x)\right)^2}}; \qquad \forall x \in [0,L].$$

The part of the string with $x \in [a,b]$ has the vertical change of impulse

$$p(t) = \int_a^b \rho\, u_t(t,x)\ \mathrm{d}x.$$

According the the Newton second law (Theorem of impulse and momentum) is the impulse $p_t(t) = \int_a^b \rho u_{tt}(t,x)\,dx$ equal to the sum of all vertical forces at the time t. The vertical forces consist from

(i) vertical tension forces

$$\begin{aligned} T(t,b)\sin(\alpha(t,b)) - T(t,a)\sin(\alpha(t,a)) &= \tau(t)\left[\tan\left(\alpha(t,b)\right) - \tan\left(\alpha(t,a)\right)\right] \\ &= \tau(t)\left[u_x(t,b) - u_x(t,a)\right] \\ &= \int_a^b \tau(t) u_{xx}(t,x)\ \mathrm{d}x; \end{aligned}$$

(ii) gravity force

$$-g\rho(b-a) = -g\rho \int_a^b\ \mathrm{d}x,$$

where g is the gravity constant

(iii) external forces

$$\rho \int_a^b f(t,x)\ \mathrm{d}x$$

(iv) friction forces caused by the movement through a medium. We assume that this force is proportional to the velocity with the opposite direction

$$-\rho k \int_a^b u_t(t,x)\,dx,$$

with some friction coefficient $k > 0$.

Hence it holds

$$\rho \int_a^b u_{tt}(t,x)\ \mathrm{d}x = \tau(t) \int_a^b u_{xx}(t,x)\ \mathrm{d}x + \rho \int_a^b (f(t,x) - g)\ \mathrm{d}x - \rho k \int_a^b u_t(t,x)\ \mathrm{d}x.$$

This is valid for all a, b with $0 \le a < b \le L$. We apply the mean-value theorem to the all terms, divide by $b-a$ and then we pass to the limit for $b \to a$. We obtain (a has been replaced by x)

$$u_{tt}(t,x) + k u_t(t,x) = c^2(t) u_{xx}(t,x) + h(t,x), \tag{1.8}$$

with

$$c(t) := \sqrt{\frac{\tau(t)}{\rho}} \qquad \text{and} \qquad h(t,x) := f(t,x) - g.$$

The relation (1.8) is called **damped wave equation** in 1D. The damping term is given by the friction forces. If $k = 0$ then we get the **non-homogeneous wave equation**

$$u_{tt}(t,x) = c^2(t) u_{xx}(t,x) + h(t,x). \tag{1.9}$$

Omitting the external and the gravity forces, i.e. $h(t,x) \equiv 0$, we obtain the 1D **wave equation**

$$u_{tt}(t,x) = c^2(t) u_{xx}(t,x). \tag{1.10}$$

Frequently is $c(t)$ constant. Then $\tau(t) = \tau$ and the tension $T(t,x)$ is given as

$$T(t,x) = \tau \sqrt{1 + (u_x(t,x))^2} = \tau\, s_x(t,x), \tag{1.11}$$

with

$$s(t,x) := \int_0^x \sqrt{1 + (u_x(t,\xi))^2}\, d\xi$$

the length of the part $[0,x]$ of the string.

Besides the boundary conditions $u(t,0) = u(t,L) = 0$ we also need some information about the initial state and initial velocity. These can be formulated as follows

$$u(0,x) = f(x) \quad \text{and} \quad u_t(0,x) = g(x), \qquad \forall x \in [0,L].$$

Up to now we have considered homogeneous Dirichlet boundary conditions $u(t,0) = u(t,L) = 0$ for all t. We can also prescribe the vertical motion at the boundary as

$$u(t,0) = \varphi(x) \quad \text{and} \quad u(t,L) = \psi(t), \qquad \forall t \in \mathbb{R},$$

where $\varphi(t)$ and $\psi(t)$ are given functions. This assumption on the boundary is called non-homogeneous Dirichlet boundary condition.

We consider now an another situation at the boundary. We assume that an external force $F(t)$ acts on the left point $x = 0$, which can move vertically. Let $\Delta x > 0$ be sufficiently small. We take the part $[0, \Delta x]$ of the string. There are two forces acting on this part (if we neglect friction and gravity): the external force $F(t)$ and the vertical component $\tau u_x(t, \Delta x)$ of the tension force. We determine the acceleration (= force / mass) of this part of the string

$$\begin{aligned} \lim_{\Delta x \to 0^+} \frac{\tau u_x(t,\Delta x) + F(t)}{\rho \Delta x} &= \lim_{\Delta x \to 0^+} \left[\frac{\tau}{\rho} \frac{u_x(t,\Delta x) - u_x(t,0)}{\Delta x} + \frac{F(t) + \tau u_x(t,0)}{\rho \Delta x} \right] \\ &= a^2 u_{xx}(t,0) + \lim_{\Delta x \to 0^+} \left[\frac{F(t) + \tau u_x(t,0)}{\rho \Delta x} \right]. \end{aligned}$$

If we want to guarantee the existence of the acceleration, we need $F(t) + \tau u_x(t,0) = 0$, i.e.,

$$u_x(t,0) = -\tau^{-1} F(t), \qquad \forall t \in \mathbb{R},$$

which is called non-homogeneous Neumann boundary condition. In the case $F(t) = 0$ (the point $x = 0$ is free to move) we get the homogeneous Neumann boundary condition

$$u_x(t,0) = 0, \qquad \forall t \in \mathbb{R}.$$

At the end of this section we determine the total energy of the string at the time t. We consider a part of the string $[x, x + \Delta x]$ with the mass $\rho \Delta x$ and the velocity $u_t(t,x)$. Its kinetic energy is given by $\frac{1}{2} \rho u_t^2(t,x) \Delta x$. The total energy of the string is

$$\frac{\rho}{2} \int_0^L u_t^2(t,x)\ \mathrm{d}x.$$

Now we determine the potential energy. The length r of the string corresponding with $[x, x + \Delta x]$ can be approximated by $\Delta s = \sqrt{1 + (u_x(t,x))^2} \Delta x$. Then the tension is equal to $\tau r / \Delta x$. The potential energy of this part is

$$\tau \int_{\Delta x}^{\Delta s} \frac{r}{\Delta x}\, dr = \frac{\tau}{2 \Delta x} \left[\Delta s^2 - \Delta x^2 \right] = \frac{\tau}{2}\, u_x^2(t,x) \Delta x.$$

And the total potential energy is

$$\frac{\tau}{2}\int_0^L u_x^2(t,x)\ \mathrm{d}x.$$

The total energy of the string will be

$$E(t) := \int_0^L \left(\frac{\rho}{2}\,u_t^2(t,x) + \frac{\tau}{2}\,u_x^2(t,x)\right)\ \mathrm{d}x = \frac{1}{2}\,\rho\int_0^L \left(u_t^2(t,x) + a^2u_x^2(t,x)\right)\ \mathrm{d}x. \qquad (1.12)$$

Exercise 1.1 Find the steady state (time independent) solution of

$$\begin{cases} u_{tt}(t,x) = a^2u_{xx}(t,x) - g, & \text{for } t\in\mathbb{R} \text{ and } 0\le x\le L,\\ u(t,0) = u(t,L) = 0, & \text{for } t\ge 0. \end{cases}$$

What is the meaning of this solution?

Exercise 1.2 Let $u(t,x)$ be a solution of the wave equation $u_{tt} = c^2u_{xx}$. Consider the following transformation of t and x:

$$\begin{cases} \tau &= \cosh(\omega)\,t + c^{-1}\sinh(\omega)\,x,\\ \xi &= c\sinh(\omega)\,t + \cosh(\omega)\,x, \end{cases} \iff \begin{cases} t &= \cosh(\omega)\,\tau - c^{-1}\sinh(\omega)\,\xi,\\ x &= -c\sinh(\omega)\,\tau + \cosh(\omega)\,\xi; \end{cases}$$

for any $\omega\in\mathbb{R}$. Define

$$v(\tau,\xi) := u\left(\cosh(\omega)\,\tau - c^{-1}\sinh(\omega)\,\xi, -c\sinh(\omega)\,\tau + \cosh(\omega)\,\xi\right).$$

Show that the function v solves the wave equation $v_{\tau\tau}(\tau,\xi) = c^2v_{\xi\xi}(\tau,\xi)$.

The last exercises shows the invariance of the wave equation with respect to the considered transformation. If c denotes the light velocity and

$$\cosh(\omega) = \frac{1}{\sqrt{1-v^2/c^2}}, \qquad \text{with } |v|<c,$$

then

$$\sinh(\omega) = \pm\frac{v}{c\sqrt{1-v^2/c^2}}.$$

Thus the wave equation $u_{tt} = c^2u_{xx}$ is invariant to the **Lorenz transform**.

1.4 Porous media flow

A porous medium consists of a matrix with a large amount of microscopic pores and throats which are typically narrow tubes where fluid can pass through. Soil and sand are both examples of porous media and fluid flow in a porous medium can be considered as pouring a cup of water over soil and letting the water flow into the soil due to the gravitational forces.

The description of flow in porous media is extremely difficult because of the complexity of the medium. Even though flow in a single tube is given by simple equations, the network of the tubes is impossible to know in details.

The characteristic length of a reservoir containing water and oil may be about 1km, thus reservoir engineers are usually not interested in the behavior at pore scale. Instead it is often sufficient

to average the physical properties over many pores inside different sections of the reservoir. The size of the sections may typically be of about 1m, causing variations in the fluid flow on length scales less than 1m to be neglected.

There are two important quantities describing the properties of a porous medium: the porosity θ and the permeability K. The porosity of a porous medium is defined as:

$$\theta = \frac{\text{pore volume}}{\text{matrix volume}},$$

where the pore volume denotes the total volume of the pore space in the matrix and the matrix volume is the total volume of the matrix including the pore space. Thus, $0 \leq \theta \leq 1$. The porosity has to be averaged over many pores and the considered matrix volume must be larger than the pore size. Often the porosity can be chosen as constant for the whole medium.

The permeability K describes the ability of the fluid to flow through the porous medium. K is often called the absolute permeability and is a quantity depending on the geometry of the medium only.

The fluid flowing in the pore space is characterized by the dynamical viscosity μ . The viscosity indicates the resistance in the fluid due to shear and angular deformations. At microscopic level there are friction forces in the fluid caused by the interchange of momentum in collisions between the molecules. The strength of the friction forces sets the viscosity of the fluid. Another expression for the viscosity which is often used, is the kinematic viscosity $\nu = \frac{\mu}{\rho}$, where ρ is the density of the fluid. Moreover, the viscosity of incompressible Newtonian fluids is assumed to be isotropic, thus, such fluids are characterized by only one viscosity coefficient μ.

Fluid flow trough a porous medium is often given by the phenomenological Darcy equation.

1.4.1 Darcy's law

Henry Darcy investigated the flow of water in a vertical homogeneous sand filter in 1856. He has discovered that the flow rate Q (i.e., volume of water per unit time) is

1. proportional to $h_1 - h_2$
2. proportional to the cross-sectional area A
3. inversely proportional to the length L

where the symbols h_1, h_2, A, L are defined in Figure 1.6.

Combining these conclusions one can arrive at the 1-D Darcy's law

$$Q = \frac{KA(h_1 - h_2)}{L}. \tag{1.13}$$

Defining the gradient $\boldsymbol{J} = \frac{h_1 - h_2}{L}$ and the specific discharge vector $\boldsymbol{q} = \frac{Q}{A}$, i.e., the volume of water flowing through a unit cross-sectional area normal to the flow direction per unit time, we can write

$$\boldsymbol{q} = K\boldsymbol{J}. \tag{1.14}$$

The proportionality coefficient K, appearing in Darcy's law, is called *hydraulic conductivity* of the porous medium. Sometimes it is also called *permeability coefficient*. K depends on the properties of the fluid and the porous matrix.

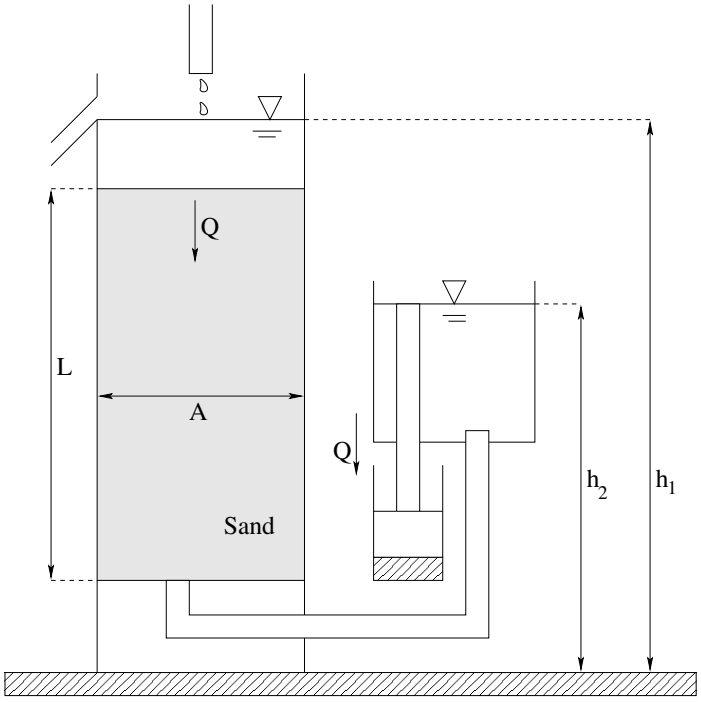

Fig. 1.6: Darcy's experiment

The experimentally derived Darcy's equation (1.13) is limited to the 1-D flow of a homogeneous incompressible fluid. The 3-D generalization of (1.13) for a homogeneous isotropic porous medium reads as

$$\boldsymbol{q} = K\boldsymbol{J} = -K\nabla\phi, \tag{1.15}$$

where ϕ is the piezometric head, $\nabla\phi$ is the hydraulic gradient. When the flow takes place through a non-homogeneous medium, Darcy's law has the form

$$\boldsymbol{q} = -\frac{k}{\mu}(\nabla p - \rho\mathbf{g}), \tag{1.16}$$

where ρ is the density of the fluid, $\mathbf{g}$ is the gravity acceleration vector directed downward, p is the pressure, k is the permeability of the medium and μ is the dynamic viscosity.

Range of validity

The relation between the specific discharge $\boldsymbol{q}$ and the hydraulic gradient ∇p expressed by Darcy's law (1.16) is linear indicating laminar flow conditions. On the other hand, rapid flow through large pore spaces may became turbulent. Hence, such a case cannot be described by Darcy's laminar flow law. The validity of Darcy's law may be expressed using a dimensionless $Reynolds\ number$. For flow through sand or gravel layers, the Reynolds number can be defined as

$$Re_{soil} = \frac{D|\boldsymbol{q}|}{\nu},$$

where $D\ [m]$ is the average grain diameter, ν is the kinematic viscosity and $\boldsymbol{q}$ the specific discharge. Practically all evidence indicates that Darcy's law is valid as long as the Reynolds number lies between 1 and 10.

1.4.2 Flow equation

The general equation for flow in porous medium is derived from the mass conservation principle

$$\frac{\partial}{\partial t}(\rho\theta) + \nabla \cdot (\rho \boldsymbol{q}) = f, \tag{1.17}$$

where $\rho \left[\frac{kg}{m^3}\right]$ is the density, θ $[-]$ is the porosity, $\boldsymbol{q}$ $\left[\frac{m}{s}\right]$ is the Darcy velocity, f $\left[\frac{m^3}{kg\ s}\right]$ is the spatially distributed source/sink, and t $[s]$ denotes the time.

1.4.3 Van Genuchten's model

p	$[m]$	pressure head
θ	[-]	water content
θ_s	[-]	saturated value of the soil-water content
θ_r	[-]	residual value of the soil-water content
K	$\left[\frac{m}{s}\right]$	hydraulic conductivity
K_s	$\left[\frac{m}{s}\right]$	hydraulic conductivity of the saturated zone

Table 1.1: Notation for van Genuchten's model

A relative simple equation for the soil-water content-pressure head curve is based on the Mualem theory (cf. Mualem [16]). The following equation was derived by Mualem (for notations see Table 1.1)

$$K_r = S^{\frac{1}{2}} \left[\frac{\int_0^S \frac{1}{p}}{\int_0^1 \frac{1}{p}} \right]^2,$$

where $S = \frac{\theta - \theta_r}{\theta_s - \theta_r}$ is a scaled dimensionless water content.

Van Genuchten has introduced an attractive class of S functions in the form $S(p) = [1 + |\alpha p|^n]^m$ (cf. van Genuchten [20]) and he has presented the model

$$\begin{cases} \theta(p) &= \begin{cases} \theta_r + \dfrac{\theta_s - \theta_r}{(1 + |\alpha p|^n)^m} & \text{for } p \le 0 \\ \theta_s & \text{for } p \ge 0 \end{cases} \\ K(\psi) &= K_s S^{\frac{1}{2}} \left[1 - \left(1 - S^{\frac{1}{m}}\right)^m\right]^2, \\ S &= \dfrac{\theta - \theta_r}{\theta_s - \theta_r} \end{cases} \tag{1.18}$$

with coefficients α, n and $m = 1 - \frac{1}{n}$. The typical behavior of the $\theta(p)$ curve is shown in Figure 1.7 and $K(\theta)$ in Fig. 1.8.

Let us define for a moment the function (this is the so-called Kirchhoff transformation)

$$\beta(p) = \int_{-\infty}^{p} K(\theta(s))\ ds.$$

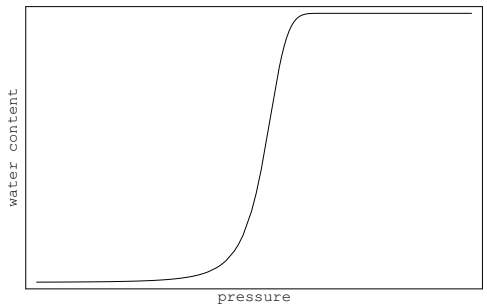

Fig. 1.7: Soil-water retention curve using van Genuchten's model

Then we can write

$$K(\theta(p))\nabla p = \nabla\beta(p).$$

The behavior of the function β is depicted in Figure 1.9.

1.4.4 Some properties of flow through porous media

Let us consider a simple Cauchy problem

$$u_t = (u^m)_{xx} \qquad \text{in } (0,\infty)\times\mathbb{R}, \tag{1.19}$$

where u_0 is a given bounded continuous non-negative initial function. We suppose $m > 1$. This equation is known as *porous media equation* (however there exist other models which are widely used in applications). Oleinik, Kalashnikov and Chzou [17] have defined a class of weak solutions of problem (1.19). They have also studied some properties of solutions. Since this pioneering paper has appeared, some hundreds of papers have been devoted to the study of flows through porous media (cf., e.g., Hornung [13], Fila and Filo [12] for a detailed bibliography).

A physical relevant case is $m \geq 2$. Let $I = (a, b)$ be a bounded open interval in $\mathbb{R}$, where

$$u_0 > 0 \quad \text{on } I, \qquad u_0 = 0 \quad \text{on } \mathbb{R}\setminus I. \tag{1.20}$$

It is well-known that the Cauchy problem (1.19) together with (1.20) admits a generalized (not classical) solution. Kalashnikov [14] has shown that for $m \geq 2$ there exist points of discontinuity of u_x in $(\varepsilon,\infty)\times\mathbb{R}$ for arbitrary $\varepsilon > 0$, even if the initial data $u_0 \in C^\infty(\mathbb{R})$. Further, Kalashnikov has shown that for $m > 1$ the solution has a finite speed of propagation, i.e., the set

$$\{(t, x) \in (0,\infty)\times\mathbb{R} : u(t, x) > 0\}$$

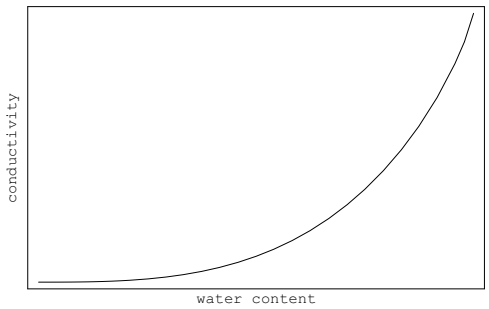

Fig. 1.8: Hydraulic conductivity versus water content using van Genuchten's model

is bounded for arbitrary fixed t and the interfaces (boundaries between $u(t,x) > 0$ and $u(t,x) = 0$) are monotone functions of time. The left interface $\xi_1(t)$ is a continuous monotone non-increasing curve through $(0,a)$ and the right interface $\xi_2(t)$ is a continuous monotone non-decreasing curve through $(0,b)$. The physical interpretation of this is clear, because the equation (1.19) obeys Darcy's law and the interface can move with limiting velocity. Aronson [4] has characterized the behavior of the interface in terms of the solution

$$\xi_i'(t) = -\frac{m}{m-1} \lim_{x \to \xi_i(t)} (u^{m-1})_x(t,x)$$

for $i = 1, 2$.

Remark 1 Let us note that solutions of linear parabolic equations have *infinite speed of propagation* which is not physical. Further, the smoothing effect for linear parabolic equations is well-known, i.e., the solution becomes infinitely smooth even if the initial data is *rough*. □

The interface can stay constant for a moment and then it begins to move or it moves from the beginning. The time, while the interface is constant, is called *waiting time*. Aronson [3] has shown a very interesting example. He has considered the Cauchy problem (1.19) together with

$$u_0(x) = \cos^2(x).$$

He has proved that

- $u^{m-1}(t, x_j) = 0$ in $[0,T)$ for all $j \in \mathbb{Z}$ and $u^{m-1}(t,x) > 0$ in $[0,T) \times \left(\mathbb{R} \setminus \bigcup_j \{x_j\}\right)$, where $x_j = \dfrac{(2j-1)\pi}{2}$ and $T = \dfrac{m-1}{2m(m+1)}$,

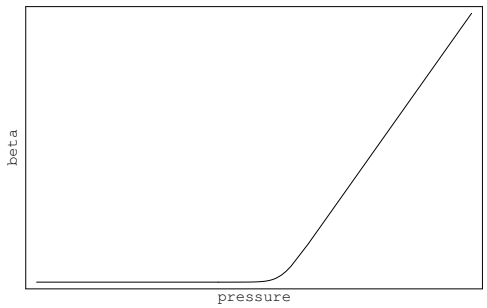

Fig. 1.9: Kirchhoff transformation using van Genuchten's model

- $u^{m-1}(t,x) \in C^\infty([0,T) \times \mathbb{R})$,
- $(u^{m-1})_{xx}(t,x_j) = \frac{2T}{T-t}$ on $[0,T)$ for all $j \in \mathbb{Z}$.

Here, the interface at each x_j stays constant on $[0,T)$, later it disappears. Similar results hold when the initial data has a compact support.

Aronson, Caffarelli and Kamin [5] have derived some upper and lower estimates for the waiting time and they have given a condition, which is sufficient to guarantee that the interface begins to move in a smooth manner. Lipschitz continuity of the interface for the porous medium equation in the d-dimensional case was shown by Caffarelli, Vazquez and Wolanski [8]. Angenent [2] has proved the analyticity of the interface (in the one-dimensional case) after the waiting time. Vazquez [21] has proved the conservation of mass for (1.19), i.e., $\int u(t,x)\ dx\ = \int u_0(x)\ dx$. Further, he has shown, that the x-coordinate $\frac{\int xu(t,x)\ dx}{\int u(t,x)\ dx}$ of the barycenter remains constant in time.

1.4.5 Multiphase flow

The multiphase approach allows to describe the simultaneous transport in different physical forms. Equations describing the whole system are based on the conservation of mass principle by application of volume averaging techniques incorporating various constitutive relations and approximations.

Transport in porous media (see Fig. 1.10) is usually multi-component (soil, air, water and volatile contaminant capable of crossing phase boundaries) and multiphase (solid, liquid, gas and

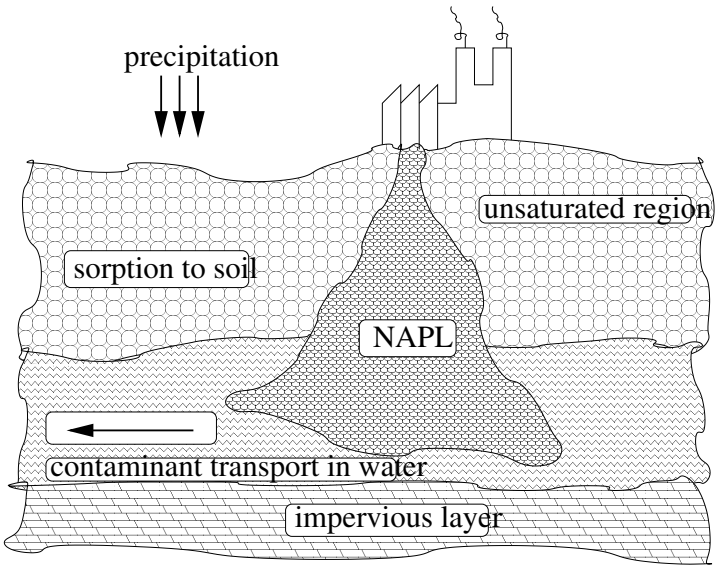

Fig. 1.10: Contaminant transport in the soil

contaminant). The macroscopic mass balance for component i in phase α can be written as (cf. Abriola and Pinder [1])

$$\partial_t(\rho^\alpha \varepsilon^\alpha \omega_i^\alpha) + \nabla \cdot (\rho^\alpha \boldsymbol{q}^\alpha \omega_i^\alpha) - \nabla \cdot \boldsymbol{J}_i^\alpha = \rho^\alpha \varepsilon^\alpha \left[f_i^\alpha + e_i^\alpha\right] \tag{1.21}$$

where $\rho^\alpha \left[\frac{kg}{m^3}\right]$ is the mass density of the phase α; ε^α [1] is the volume fraction occupied by the phase α; $\boldsymbol{q}^\alpha \left[\frac{m}{s}\right]$ is Darcy's velocity of the phase α; ω_i^α [1] is the mass fraction of component i in the α phase; $\boldsymbol{J}_i^\alpha \left[\frac{kg}{m^2 s}\right]$ is the flux vector representing the diffusive flux of component i in the phase α; $f_i^\alpha \left[\frac{1}{s}\right]$ is the source of component i in the phase α; $e_i^\alpha \left[\frac{1}{s}\right]$ is the gain of mass of component i due to phase change.

Equation (1.21) is considered under the following constraints

$$\begin{cases} \sum_i \omega_i^\alpha = 1 & \text{definition of the relative mass fraction,} \\ \sum_\alpha \varepsilon^\alpha = 1 & \text{definition of the relative volume fraction,} \\ \sum_\alpha \rho^\alpha \varepsilon^\alpha e_i^\alpha = 0 & \text{change of mass due to phase change.} \end{cases} \tag{1.22}$$

1.5 Classification of PDEs

What is a partial differential equation? A partial differential equation (PDE) is a relation involving an unknown function of several independent variables and its partial derivatives with respect to those variables. If this relation is linear we speak about linear PDEs otherwise we speak about nonlinear PDEs.

Partial differential equations are used to formulate and solve problems that involve unknown functions of several variables, such as the propagation of sound or heat, electrostatics, electrodynamics, fluid flow, elasticity, or more generally any process that is distributed in space, or distributed in space and time. Completely different physical problems may have identical or similar mathematical formulations.

Let us consider a domain $\Omega \subset \mathbb{R}^d$ and a $k \in \mathbb{N}$-times differentiable function $u : \mathbb{R}^d \to \mathbb{R}$. A d-dimensional vector

$$\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_d), \qquad \alpha_i \geq 0, \quad \alpha_i \in \mathbb{Z}$$

is called a multiindex. Its length is given by

$$|\boldsymbol{\alpha}| = \sum_{i=1}^{d} \alpha_i.$$

We introduce the following notation for

$$D^{\boldsymbol{\alpha}} u = \frac{\partial^{|\boldsymbol{\alpha}|} u}{\partial x_1^{\alpha_1} \ldots \partial x_d^{\alpha_d}}.$$

Definition 1.1 (PDE) *An expression of the form*

$$F\left(\boldsymbol{x}, D^{(k,0,\ldots,0)}u, \ldots, D^{\boldsymbol{\alpha}}u \ldots, D^{(0,0,\ldots,0)}u, \right) = 0 \qquad \boldsymbol{x} \in \Omega$$

with $|\boldsymbol{\alpha}| \leq k$ is called a PDE of the order $k \in \mathbb{N}$.

Definition 1.1 is rather general. There exist more specific forms of PDEs as follows.

Definition 1.2 *(i) A PDE is linear if it takes the following form*

$$\sum_{|\boldsymbol{\alpha}| \leq k} a_{\boldsymbol{\alpha}} D^{\boldsymbol{\alpha}} u = 0 \qquad \boldsymbol{x} \in \Omega.$$

(ii) A PDE is semilinear if it takes the following form

$$F\left(\boldsymbol{x}, D^{\boldsymbol{\beta}} u\right) + \sum_{|\boldsymbol{\alpha}| = k} a_{\boldsymbol{\alpha}} D^{\boldsymbol{\alpha}} u = 0 \qquad \boldsymbol{x} \in \Omega$$

with $|\boldsymbol{\beta}| \leq k - 1$.

(iii) A PDE is quasilinear if it takes the following form

$$F\left(\boldsymbol{x}, D^{\boldsymbol{\beta}} u\right) + \sum_{|\boldsymbol{\alpha}| = k} a_{\boldsymbol{\alpha}} \left(\boldsymbol{x}, D^{\boldsymbol{\beta}} u\right) D^{\boldsymbol{\alpha}} u = 0 \qquad \boldsymbol{x} \in \Omega$$

with $|\boldsymbol{\beta}| \leq k - 1$.

There is no general theory known concerning the solvability of general PDEs. Such an theory probably cannot exist due to the large variety of problems coming from the real world applications. Therefore one has to develop different strategies for solving specific types of problems. We give some very important examples of PDEs.

1.5.1 Examples of PDEs

Single linear PDEs

Laplace's equation

$$\Delta u = \sum_{i=1}^{d} \partial_{x_i x_i} u = 0.$$

Solutions of Laplace's equation are called harmonic functions.

Linear transport equation describes the transport of a conserved scalar u in a velocity field $\boldsymbol{q} = (q_1, \ldots, q_d)$

$$\partial_t u + \nabla \cdot (\boldsymbol{q} u) = \partial_t u + \sum_{i=1}^{d} \partial_{x_i}(q_i u) = 0.$$

Heat equation

$$\partial_t u - \Delta u = f.$$

Wave equation

$$\partial_{tt} u - \Delta u = f.$$

Euler-Tricomi's equation is used in the investigation of transonic flow

$$u_{xx} = x u_{yy}.$$

Plate equation governs the small transverse (out-of-plane) displacement u of a thin plate

$$\Delta^2 u = f.$$

Single nonlinear PDEs

Porous media equation describes diffusion in porous materials

$$\partial_t u - \Delta u^\alpha = f.$$

Minimal surface equation

$$\nabla \cdot \left(\frac{1}{\sqrt{1 + |\nabla u|^2}} \nabla u \right) = 0.$$

Burger's equation is a model problem for fluid dynamical systems

$$u_t + u\ u_x = 0.$$

Korteweg-de Vries equation describes nonlinear shallow water waves

$$u_t + u\ u_x + u_{xxx} = 0.$$

Reaction diffusion equation

$$u_t - \Delta u = f(u).$$

Linear systems of PDEs

Maxwell's equations are the set of four fundamental equations governing electromagnetism

$$\begin{aligned} \boldsymbol{E}_t - \nabla \times \boldsymbol{B} &= \mathbf{0}, \\ \boldsymbol{B}_t + \nabla \times \boldsymbol{E} &= \mathbf{0}, \\ \nabla \cdot \boldsymbol{B} &= 0 \\ \nabla \cdot \boldsymbol{E} &= 0. \end{aligned}$$

Reaction diffusion system can be found, e.g., by reductive biodegradation of chlorinated solvents

$$\begin{aligned} \partial_t c_1 - \Delta c_1 + k_1 c_1 &= 0 \\ \partial_t c_n - \Delta c_n + k_n c_n &= k_{n-1} c_{n-1}, \qquad n \geq 2, \end{aligned}$$

Nonlinear systems of PDEs

Maxwell's + Landau-Lifshitz's system is frequently used in micro- electromagnetism, e.g., by storing of information on a magnetic medium (hard disc)

$$\begin{aligned} \boldsymbol{E}_t - \nabla \times \boldsymbol{H} &= \mathbf{0}, \\ \boldsymbol{B}_t + \nabla \times \boldsymbol{E} &= \mathbf{0}, \\ \nabla \cdot \boldsymbol{B} &= 0 \\ \nabla \cdot \boldsymbol{E} &= 0 \\ \boldsymbol{B} &= \boldsymbol{H} + \boldsymbol{M} \\ \boldsymbol{M}_t + \boldsymbol{M} \times (\Delta \boldsymbol{M} + \boldsymbol{H}) + \boldsymbol{M} \times (\boldsymbol{M} \times (\Delta \boldsymbol{M} + \boldsymbol{H})) &= \mathbf{0}. \end{aligned}$$

Reaction diffusion system

$$\boldsymbol{u}_t + \nabla \cdot \boldsymbol{F}(\boldsymbol{u}) = \mathbf{0}.$$

Navier-Stokes equations describe the motion of a non-turbulent, Newtonian fluid

$$\begin{aligned} \boldsymbol{u}_t + \boldsymbol{u} \cdot \nabla \boldsymbol{u} - \Delta \boldsymbol{u} &= \nabla p, \\ \nabla \cdot \boldsymbol{u} &= 0. \end{aligned}$$

1.5.2 Well-posedness

A mathematical problem is said to be well posed in the sense of Hadamard[1] if

- the solution exists
- the solution is unique
- the solution depends continuously on the data (boundary, conditions, coefficients,...)

Examples of well-posed problems include the Dirichlet problem for Laplace's equation, and the heat equation with specified initial conditions.

Problems that are not well-posed on the sense of Hadamard are termed ill-posed. Inverse problems are often ill-posed. By an inverse problem one usually has to determine an unknown

[1] J. S. Hadamard (1865 – 1963) was a French mathematician best known for his proof of the prime number theorem in 1896.

coefficient in the PDE from the additional measurements inside the observed domain or on its boundary. A typical example is the computed axial tomography (CAT or CT scan). CT provides clinically relevant anatomic and functional information, is relatively noninvasive, and has very low short- and long-term risks (if the well-known potential hazards are avoided).

The existence and uniqueness of solutions of ordinary differential equations (ODEs) has a very satisfactory answer in the Picard-Lindelöf theorem, that is far from the case for PDEs. There are examples of PDEs which do not have solution with desired properties. The classical solutions to many PDEs fail to exist in finite time even if the initial data are smooth. Classical examples include the porous media equation $\partial_t u - \Delta u^\alpha = 0$. There exists a finite blow-up time, i.e., the time where the solution or its derivative blows-up.

An another issue is the uniqueness of a solution. There exist examples of problems with many solutions, e.g., The Neumann problem for the Laplace equation

$$\begin{aligned} \Delta u &= 0 \quad \text{in } \Omega \\ \nabla u \cdot \boldsymbol{\nu} &= 0 \quad \text{on } \partial\Omega. \end{aligned}$$

The continuous dependence of the solution on auxiliary data is frequently related to the uniqueness of the solution. In numerical models this can pose a problem because a non-continuous dependence of the solution on the data (boundary, initial or boundary conditions,...) implies that small errors in data will cause large changes in the solution. Since a numerical method is not arbitrary exact it is not clear, which of the possible approximate solutions is a good one.

1.5.3 Classification of linear PDEs of second order

A general form of a linear PDE of a second order in $\Omega \subset \mathbb{R}^d$ has the following form

$$\sum_{i,j=1}^{d} a_{ij}(\boldsymbol{x}) \frac{\partial^2 u(\boldsymbol{x})}{\partial x_i \partial x_j} + \sum_{i=1}^{d} b_i(\boldsymbol{x}) \frac{\partial u(\boldsymbol{x})}{\partial x_i} + c(\boldsymbol{x}) u(\boldsymbol{x}) = f(\boldsymbol{x}), \tag{1.23}$$

along with the given coefficient functions $a_{ij}, b_i, c, f : \Omega \to \mathbb{R}$. The equation is called

homogeneous if $f = 0$

non-homogeneous if $f \neq 0$

with constant coefficient if all coefficients are constant.

The main part of this equation is called the part containing the highest derivatives of the unknown function u, namely

$$\sum_{i,j=1}^{d} a_{ij}(\boldsymbol{x}) \frac{\partial^2 u(\boldsymbol{x})}{\partial x_i \partial x_j}.$$

In this multidimensional case the character of the PDE (1.23) is determined by the eigenvalues (EVs) of the matrix $\mathrm{A} = (a_{ij})_{i,j=1\ldots d}$.

Definition 1.3 *The PDE (1.23) is called*

parabolic *if any EV is 0*

elliptic *if all EVs are $\neq 0$ and all have the same sign*

hyperbolic *if all EVs are* $\neq 0$ *and all but one have the same sign.*

Let us note that there are cases, where the classification is not straightforward, e.g., if all EVs are nonzero but several have a different sign.

Now, we give some examples according this classification. Assume that the matrix A is symmetric. Then the spectrum of A is real and we can say

- $-\Delta u(\boldsymbol{x}) = f(\boldsymbol{x})$ is an elliptic PDE
- $u_t(\boldsymbol{x}) - \Delta u(\boldsymbol{x}) = f(\boldsymbol{x})$ is a parabolic PDE
- $u_{tt}(\boldsymbol{x}) - \Delta u(\boldsymbol{x}) = f(\boldsymbol{x})$ is a hyperbolic PDE.