Chapter 1.

Modelling with Partial Differential Equations

MANY practical applications involve the description of the state of a solid body, a fluid (in continuum mechanics no distinction is made between fluids and gases) or just any region of space. As examples consider the gravity field of an inhomogeneous body, the temperature of a solid body, the flow of water in the subsurface, the flow of gases in a complicated duct, the propagation of sound or water waves or the mechanical stress in a bridge. In this chapter, we will derive the equations of mathematical physics that describe all these phenomena.

1.1. Gravitation

Newton's famous law of gravitation

$$F(x,y) = G\frac{mM}{\|y-x\|^2}\frac{y-x}{\|y-x\|} \qquad (x \neq y) \tag{1.1}$$

gives the force vector acting on a point mass m at position $x \in \mathbb{R}^3$ excerted by another point mass M located at a point $y \in \mathbb{R}^3$ and G is the gravitational constant with the approximate value $6.67 \cdot 10^{-11}$ N m^2 kg^{-2} (there is some debate about the value – it is difficult to measure). Newton's law is stated for point masses as it has first been applied to the sun and the planets in the solar system. But how does it act in a cloud of gas of varying density? Since there are so many atoms (or molecules) in the gas it would be overwhelmingly expensive to compute all the forces ($O(N^2)$ effort for N particles).

We now wish to derive a new form of Newton's law in the form of a PDE that is usable in this case. First we rewrite Newton's law a little bit by introducing the function

$$\psi(x,y) = -\frac{GM}{\|y-x\|} \tag{1.2}$$

which is called the gravitational *potential* of a point mass in physics. In mathematics $1/\|y-x\|$ is called *singularity function*. It has the following interesting properties:

$$\nabla_x \psi(x,y) = -\frac{GM(y-x)}{\|y-x\|^3}, \qquad \Delta_x \psi(x,y) = \sum_{i=1}^{3} \partial^2_{x_i^2} \psi(x,y) = 0 \qquad (x \neq y).$$

Using it we can rewrite Newton's law as

$$F(x,y) = ma(x,y), \qquad a(x,y) = -\nabla_x \psi(x,y).$$

Note that the acceleration $a(x,y)$ is independent of the mass m (equivalence principle).

Now consider an arbitrary domain $\omega \subset \mathbb{R}^3$ (open and connected set of points) with sufficiently smooth boundary $\partial\Omega$, a point $y \notin \partial\omega$ and compute the

$$\int_{\partial\omega} a(x,y) \cdot n(x)\, ds_x = -\int_{\partial\omega} \nabla_x \psi(x,y) \cdot n(x)\, ds_x \tag{1.3}$$

where $n(x)$ denotes the exterior unit outer normal vector to ω. By ds_x we indicate that the surface integral is done with respect to the variable x and not y. For the evaluation of the integral we need to consider two cases:

i) $y \notin \omega$. By applying Gauss' integral theorem $\int_\omega \nabla \cdot u\, dx = \int_{\partial\omega} u \cdot n\, ds$ we get

$$-\int_{\partial\omega} \nabla_x \psi(x,y) \cdot n(x)\, ds_x = -\int_\omega \Delta_x \psi(x,y)\, dx = 0$$

since $\Delta_x \psi(x,y) = 0$ for any $x \in \omega$ since y is outside ω.

ii) $y \in \omega$. Now the trick from case I can not be done so easily because ψ has a singularity for $x = y$ but it can be modified. Let $B_\epsilon(y) = \{x \in \mathbb{R}^3 : \|x - y\| < \epsilon\}$ be the open ball of radius ϵ around y. Then again applying Gauss' theorem we get

$$0 = \int_{\omega \setminus B_\epsilon(y)} \Delta_x \psi(x,y)\, dx = \int_{\partial\omega} \nabla_x \psi(x,y) \cdot n(x)\, ds_x - \int_{\partial B_\epsilon(y)} \nabla_x \psi(x,y) \cdot n(x)\, ds_x$$

The left hand side integral is zero and the minus sign is due to the fact the normal to $\omega \setminus B_\epsilon(y)$ points *into* the ball $B_\epsilon(y)$. The second integral on the right hand side can be computed directly as

$$\int_{\partial B_\epsilon(y)} \nabla_x \psi(x,y) \cdot n(x)\, ds_x = 4\pi G M$$

independent of ϵ.

So we get the following result:

$$\int_{\partial\omega} a(x,y) \cdot n(x)\, ds_x = \begin{cases} -4\pi G M & y \in \omega \\ 0 & \text{else} \end{cases}. \tag{1.4}$$

Now we extend this to a distributed mass by introducing the density function $\rho : \mathbb{R}^3 \to \mathbb{R}$ with units kg m^{-3}. For any domain $\omega \subset \mathbb{R}^3$ then $M_\omega = \int_\omega \rho\, dx$ gives the mass contained in ω. We further assume that the density distribution is such that the integral $\int_{\mathbb{R}^3} \rho\, dx$ exists. Then the acceleration experienced at a point x excerted by the mass distribution ρ can be computed by subdividing the mass into an infinite number of infinitesimal pieces V_i at position y_i (superposition principle):

$$a(x) = \lim_{N\to\infty} \sum_{i=1}^{N} G\rho(y_i) V_i \nabla_x \left(\frac{1}{\|y - x\|} \right) = G \int_{\mathbb{R}^3} \rho(y) \nabla_x \left(\frac{1}{\|y - x\|} \right) dy. \tag{1.5}$$

One can check that this integral is well defined despite the singularity, i.e. it holds also for a point x *inside* a body with mass distribution ρ (transform to spherical coordinates around x).

Now being very careful with evaluating integrals one finds that for this acceleration and any suitable $\omega \subset \mathbb{R}^3$

$$\int_{\partial\omega} a(x) \cdot n(x)\, ds = -4\pi G \int_{\omega} \rho(x)\, dx$$

(only the mass inside ω plays a role). Applying again Gauss' theorem on the left hand side we find

$$\int_{\omega} \nabla \cdot a(x)\, dx = -4\pi G \int_{\omega} \rho(x)\, dx.$$

If a is sufficiently smooth the fact that ω can be chosen arbitrarily implies that the equality also holds for the integrands themselves (see e.g. [Smirnow, 1981, § 74]) and we arrive at

$$\nabla \cdot a(x) = -4\pi G \rho(x) \qquad (x \in \mathbb{R}^3). \tag{1.6}$$

The final piece is the observation that all fundamental forces in nature are conservative (a basic principle that is assumed to hold by physicists). In a conservative force field the path integral $w(a, b) = \int_a^b F(s) \cdot t(s)\, ds$ (t is the unit tangential vector) does only depend on the points a, b but not on the particular path taken from a to b. Conservativity of the force is a consequence of conservation of energy because otherwise it would be possible to generate energy in a force field by taking different paths back and forth. With an arbitray reference point r_0 we then have $w(a, b) = w(a, r_0) + w(r_0, b) = w(r_0, b) - w(r_0, a) = w'(b) - w'(a)$ where $w'(x) = w(r_0, x)$ is now only a function with a single argument, called the *gravitational potential*. Invoking the main theorem of calculus in its multi-dimensional form

$$\int_a^b \nabla\Psi(s) \cdot t(s)\, ds = \Psi(b) - \Psi(a) \tag{1.7}$$

we see that a force is conservative if and only if it can be represented as the gradient of a potential. The potential is only unique up to a constant as can be seen from (1.7).

Since $m a(x)$ with $a(x)$ from (1.6) is the gravitational force experienced by a point mass m at position x and the gravitational force is supposed to be conservative we conclude that there must exist a scalar function $\Psi(x)$ such that $a(x) = -\nabla\Psi(x)$. Inserting this into (1.6) we obtain

$$\nabla \cdot \nabla\Psi(x) = \Delta\Psi(x) = 4\pi G \rho(x) \qquad (x \in \mathbb{R}^3). \tag{1.8}$$

This equation is called *Poisson* equation. As stated Ψ is assumed to be twice continuously differentiable, which requires ρ to be at least continuous. This is practically very restrictive since, for example, the density function of the moon (having no atmosphere) might be very well approximated by a discontinuous function. It is an important part of PDE theory to give equation (1.8) a precise mathematical meaning also in this sense. The potential is determined by Equation (1.8) up to a constant. To fix the constant, an additional condition for the behaviour of Ψ for $x \to \infty$ can be imposed.

1.2. Fluid Mechanics

1.2.1. Continuum Hypothesis and Scales

Materials such as solids or fluids are made up of atoms or molecules with void space in between (we do not consider quantum effects, although, also there, partial differential equations do play

a role). Practical problems often involve excessively large numbers of atoms as we are interested in the behaviour of the material on a length scale that is very large compared to the average distance of the atoms. We call this scale of interest the macroscopic scale and the scale of the discrete particles the microscopic scale.

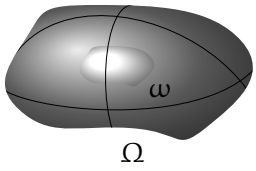
In continuum mechanics, the properties of the material are assumed to be (piecewise) continuous (or even differentiable) functions in the mathematical sense. The discrete particles are not considered, instead macroscopic properties (e.g. velocity) are defined as appropriate averages of the microscopic properties. By averaging, new quantities (such as density, temperature or pressure) arise that have no equivalent on the microscopic scale. The validity of this continuum hypothesis depends on the number of atoms (so that averages are representative) and whether the micro- and macroscale are sufficiently separated (a property called scale separation).

The laws on the microscale give now rise to new (effective) laws on the macroscale that connect the macroscopic variables. Current research is very much interested in so-called multiscale problems where the effective macroscopic laws (or coefficients in these laws) are not easily determined from the micoscopic scale (such as porous medium problems) or where there is no scale separation (e.g. turbulence).

In this chapter, fluids are considered while in the next chapter the deformation of elastic solid bodies is considered.

1.2.2. Conservation Principle

Conservation of mass, linear and angular momentum as well as energy are basic empirical law of physics (throughout this text we consider only classical mechanics where mass and energy are distinct quantities). Conservation states that the total amount of such an extensive state variable in a closed system remains constant over time. In an open system, the total amount of the quantity can vary through exchange with the environment. We are now about to state the principle of conservation in mathematical form.



We consider a compressible fluid material that fills a domain $\Omega \subseteq \mathbb{R}^n$, $n = 1, 2, 3$, which is open and connected. The domain $\omega \subset \Omega$ is chosen arbitrarily within Ω (see figure). For the subsequent derivation, ω and Ω are fixed in space and do not depend on time (an assumption to be relaxed when solids are considered). The function $\rho(x, t)$ gives the mass density in units[1] kg m^{-3} for any point $x \in \Omega$ at time t (other units, such as mol m^{-3} may be appropriate depending on the problem). The total mass $M_\omega(t)$ (in kg) contained in ω at time t is then given by

$$M_\omega(t) = \int_\omega \rho(x, t)\, dx \ .$$

The principle of conservation now states that over time the mass in ω can change only due to flow of material over the boundary $\partial\omega$ or due to injection or extraction of material into or from ω. To formulate this precisely, the velocity of the material $v(x, t)$ in m s^{-1} and the source function $f(x, t)$ in kg m^{-3} is given. For an arbitrary time interval, Δt the we can state:

$$M_\omega(t + \Delta t) - M_\omega(t) = \int_t^{t+\Delta t} \left\{ \int_\omega f(x, r)\, dx - \int_{\partial\omega} \rho(x, r) v(x, r) \cdot n(x)\, ds \right\} dr \ . \qquad (1.9)$$

[1] We always state units in the MKS (meter kilogram second) system.

The volume integral gives the contribution from sources and sinks with $f > 0$ denoting a source and $f < 0$ denoting a sink. In the surface integral, $n(x)$ denotes the exterior unit normal vector at $x \in \partial\omega$ and therefore $v \cdot n > 0$ results in a reduction of the mass in ω.

Using $\int_t^{t+\Delta t} g(r)\,dr = \Delta t\, g(t) + O(\Delta t^2)$ for sufficiently smooth g, passing to the limit $\Delta t \to 0$ and applying Gauß' theorem $\int_\omega \nabla \cdot u\,dx = \int_{\partial\omega} u \cdot n\,ds$ we obtain from (1.9) the integro-differential form of the conservation law:

$$\partial_t \int_\omega \rho(x,t)\,dx + \int_\omega \nabla \cdot (\rho(x,t)v(x,t))\,dx = \int_\omega f(x,t)\,dx \qquad \text{(for any } \omega\text{)}. \tag{1.10}$$

For sufficiently smooth functions, the fact that (1.10) holds for any ω implies the final differential form of the mass conservation law (see e.g. [Smirnow, 1981, § 74]):

$$\partial_t \rho(x,t) + \nabla \cdot (\rho(x,r)v(x,r)) = f(x,t), \qquad x \in \Omega. \tag{1.11}$$

If the fluid is incompressible then $\rho(x,t) = \text{const}$ implies

$$\nabla \cdot v(x,t) = f(x,t), \qquad x \in \Omega \tag{1.12}$$

which further reduces to $\nabla \cdot v = 0$ when there are no sources and sinks present (i.e the velocity field of an incompressible fluid without sources and sinks is divergence free).

The other conserved quantities energy and momentum can be imagined as being attached to mass. In the case of energy we set $e(x,t) = \rho(x,t)u(x,t)$, where e is the energy density with units J m^{-3} and u is the specific energy with units J kg^{-1}. We can compute the energy stored in the material occupying the volume ω as

$$E_\omega(t) = \int_\omega e(x,t)\,dx = \int_\omega \rho(x,t)u(x,t)\,dx\ .$$

Repeating the reasoning given above with ρ replaced by ρu yields the energy conservation equation

$$\partial_t(\rho(x,t)u(x,t)) + \nabla \cdot q(x,t) = f(x,t), \qquad x \in \Omega, \tag{1.13}$$

where $q(x,t)$ is now the energy density flux vector. If energy is simply flowing with the fluid (e.g. no conductive heat transport) we have $q = \rho u v$.

Similarly the (linear) momentum density (having units momentum per volume) is defined as ρv. Integration over an arbitrary volume ω gives the total momentum in ω:

$$P_\omega(t) = \int_\omega \rho(x,t)v(x,t)\,dx\ .$$

Note however, that $P(x,t)$ is a vector-valued function! For each component ρv_i of the momentum density vector we obtain the conservation equation

$$\partial_t(\rho(x,t)v_i(x,t)) + \nabla \cdot j_i = f_i(x,t), \qquad x \in \Omega,\ i = 1,\dots,d,$$

where j_i is the momentum density flux vector for the given component. If momentum is only transported with the fluid (as in inviscid flow, see § 1.2.4) we have $j_i = \rho v_i v$.

By defining the j_i to be the rows of the matrix J and defining $\nabla \cdot J$ as applying the divergence to each row (yielding a vector, see § A.2.3) one can write the momentum conservation law in compact form as

$$\partial_t(\rho(x,t)v(x,t)) + \nabla \cdot J = f(x,t), \qquad x \in \Omega. \tag{1.14}$$

In the case of inviscid flow we then have $J = \rho v v^T$. The term $\partial_t(\rho v)$ on the left hand side is rate of change of momentum density which is a force density (units N m^{-3}). Equation (1.14) is Newton's second law generalized to spatially extended bodies.

1.2.3. Heat Transfer

As an application of conservation laws we consider the flow of heat in a solid or fluid filling the bounded domain $\Omega \subset \mathbb{R}^3$. The conserved quantity is the thermal energy. Its density e is assumed to be proportional to temperature

$$e = \rho c T$$

where c is the specific heat capacity in J kg^{-1} K^{-1}, ρ is the mass density of the material in kg m^{-3} and the absolute temperature T is given in Kelvin K.

In fluids and solids the flow of thermal energy is modelled as

$$q_d = -\lambda \nabla T$$

which is known as *Fourier's law* or *diffusive flux*. It states that flow is in direction of the steepest descent of temperature. The constant of proportionality is the heat conductivity $\lambda > 0$ with units J s^{-1} m^{-1} K^{-1}. Heat conductivity may depend on position and time (e.g. in a fluid with varying composition).

In a fluid thermal energy is also transported with the fluid velocity v which gives rise to a *convective flux*

$$q_c = ev = \rho c T v.$$

The total flux is then the sum of convective and diffusive flux. Inserting all this into the conservation law (1.13) (now with $u = cT$) we obtain the *convection-diffusion equation*

$$\partial_t(\rho c T) + \nabla \cdot (\rho c T v - \lambda \nabla T) = f \qquad \text{in } \Omega \tag{1.15}$$

which is a scalar linear second-order PDE. In order to fully determine the temperature $T(x,t)$ for $x \in \Omega$ and $t > 0$, boundary conditions

$$T(x,t) = g(x,t) \qquad (x \in \Gamma \subseteq \partial\Omega,\ t > 0,\ \textit{Dirichlet}), \tag{1.16a}$$

$$(\rho c T v - \lambda \nabla T)(x,t) \cdot n(x) = j(x,t) \qquad (x \in \partial\Omega \setminus \Gamma,\ t > 0,\ \textit{Neumann}) \tag{1.16b}$$

and the initial condition

$$T(x,0) = T_0(x) \qquad (x \in \Omega) \tag{1.17}$$

must be given.

The right hand side f with units J s^{-1} m^{-3} of equation (1.15) models sources and sinks. In a solid this rate is usually known. In a fluid the source/sink term depends on the temperature of the fluid going in or out of the domain. It can be modelled as $f = rcT$ where r in kg s^{-1} m^{-3} is the amount of fluid entering or leaving the domain. When $r > 0$ fluid (and with it thermal energy) is going in and the temperature of this fluid is known. When $r < 0$ fluid is going out and the temperature of this fluid is unknown and must be computed. This leads to the final form, the so-called *convection-diffusion-reaction equation*:

$$\partial_t(\rho c T) + \nabla \cdot (\rho c T v - \lambda \nabla T) + rcT = f \qquad \text{in } \Omega. \tag{1.18}$$

Note that in this equation all coefficient functions may depend on position and time. Several important simplifications of this equation can be stated:

a) No convective flux (*reaction-diffusion equation*):

$$\partial_t(\rho c T) - \nabla \cdot (\lambda \nabla T) + r c T = f \qquad \text{in } \Omega.$$

b) No diffusive flux (*first-order PDE*):

$$\partial_t(\rho c T) + \nabla \cdot (\rho c T v) + r c T = f \qquad \text{in } \Omega.$$

c) Stationary heat flow (all coefficients are independent of time):

$$\nabla \cdot (\rho c T v - \lambda \nabla T) + r c T = f \qquad \text{in } \Omega.$$

d) Stationary heat flow in a solid:

$$-\nabla \cdot (\lambda \nabla T) + r c T = f \qquad \text{in } \Omega. \tag{1.19}$$

e) Stationary heat flow with constant conductivity and no sinks (*Poisson equation*):

$$-\nabla \cdot (\nabla T) = -\Delta T = f \qquad \text{in } \Omega.$$

Example 1.1. Figure 1.1 illustrates the solution for a three-dimensional heat transfer problem. The domain is $\Omega = (0,3) \times (0,3) \times (0,1)$ and the parameters were $v = 0$ (no convective flux), $\rho = 1$, $c = 1$, $\lambda = 1$, $r = 0$ and $f = 0$. The lateral boundaries and the region $(1,2) \times (1,2) \times \{1\}$ on the top boundary were isolated, i.e. $\nabla T \cdot n = 0$, the bottom boundary was held at constant temperature $T = 8$ and at the remaining part of the top boundary a Dirichlet condition oscillating in space and time was given. Practically one can imagine a piece of subsurface that is heated periodically from the top and that is held at constant temperature from below. The Figure shows that the oscillations are quickly dampened by the diffusion, a fact that is also observed in nature. □

Another important feature of the solution of the heat transfer problem without sources and sinks and divergence free velocity field v is that the maximum (minimum) temperature in the interior of the domain Ω does not exceed (go below) the maximum (minimum) temperature at the boundary and initial condition. This is called a maximum principle. For details we refer to [Hackbusch, 1986] or [Evans, 2010].

Multiscale Problems

Multiscale problems are problems with highly oscillating coefficient functions. Imagine a heterogeneous solid composed of two materials with different heat conductivity coefficient. The two materials occupy different regions of space and are arranged in a periodic fashion with periodicity ϵ in all directions:

$$\lambda_\epsilon(x) = \hat{\lambda}\left(\frac{x}{\epsilon}\right), \qquad \hat{\lambda}(x + e_i) = \hat{\lambda}(x) \quad (i = 1, \dots, n) \tag{1.20}$$

(e_i being the ith cartesian unit vector). The 1-periodic coefficient function $\hat{\lambda}$ taken in $\Omega = (0,1)^n$ defines the "unit cell". Then we consider the family of stationary heat transfer problems

$$-\nabla \cdot (\lambda_\epsilon(x) \nabla T_\epsilon) = f \qquad \text{in } \Omega \tag{1.21}$$

depending on the parameter $\epsilon > 0$ together with appropriate boundary conditions.

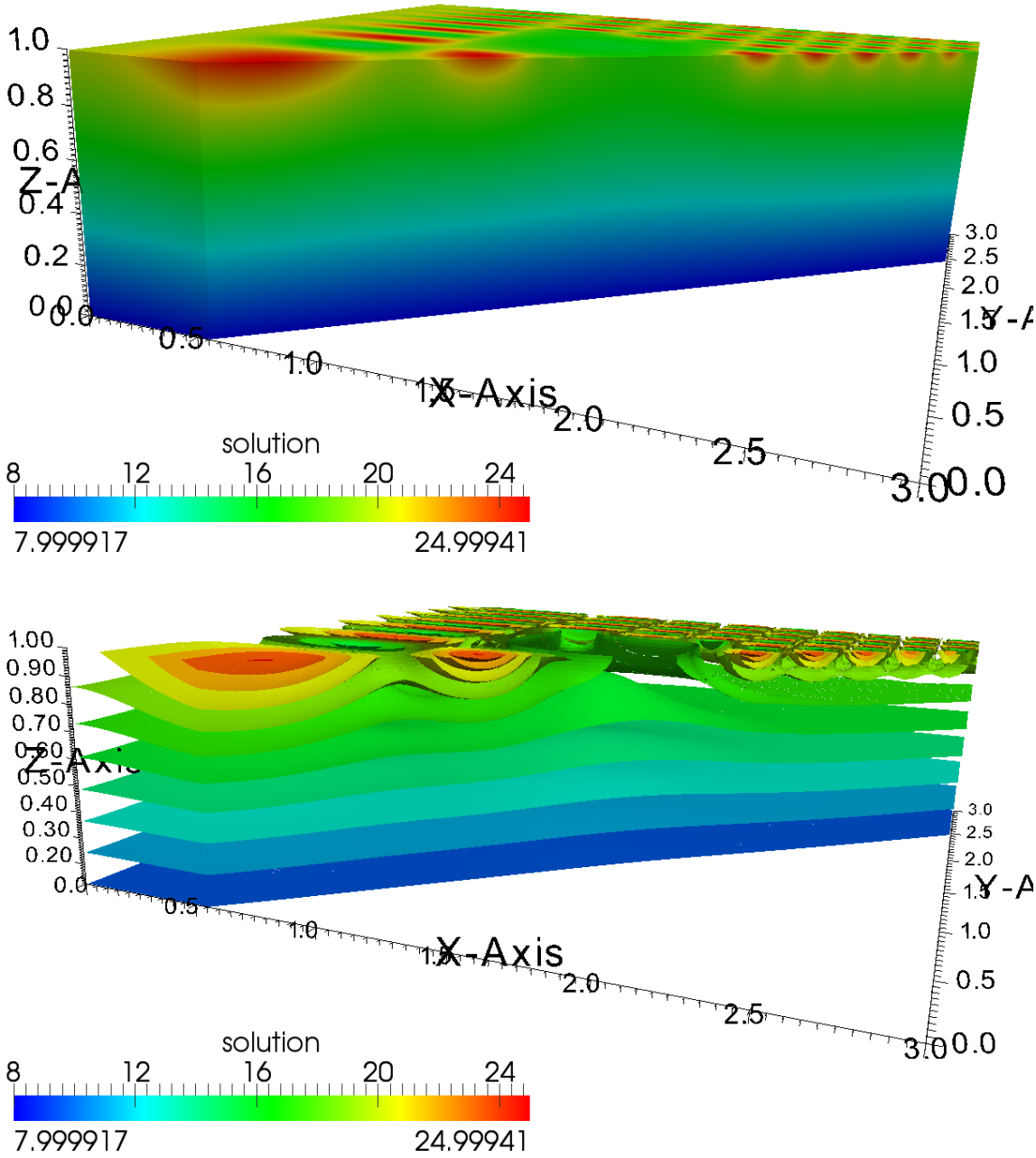


Figure 1.1.: Solution of a 3d heat transfer problem (details given in the text).

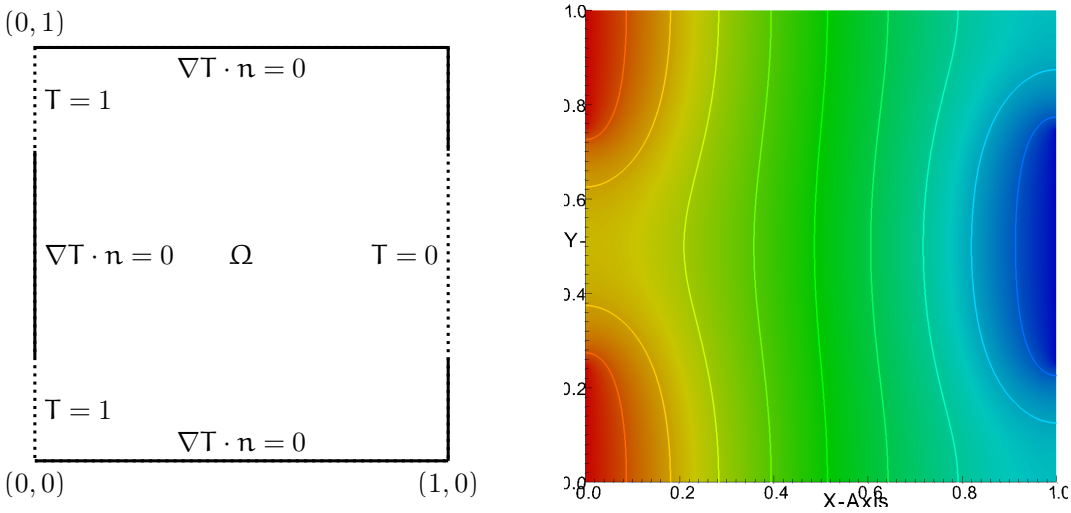


Figure 1.2.: Setup and solution for homogenous coefficient in the multiscale example.

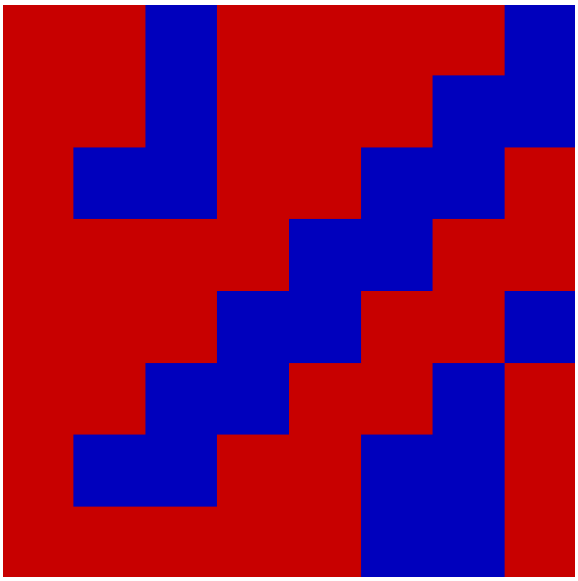


Figure 1.3.: Conductivity distribution in the unit cell.

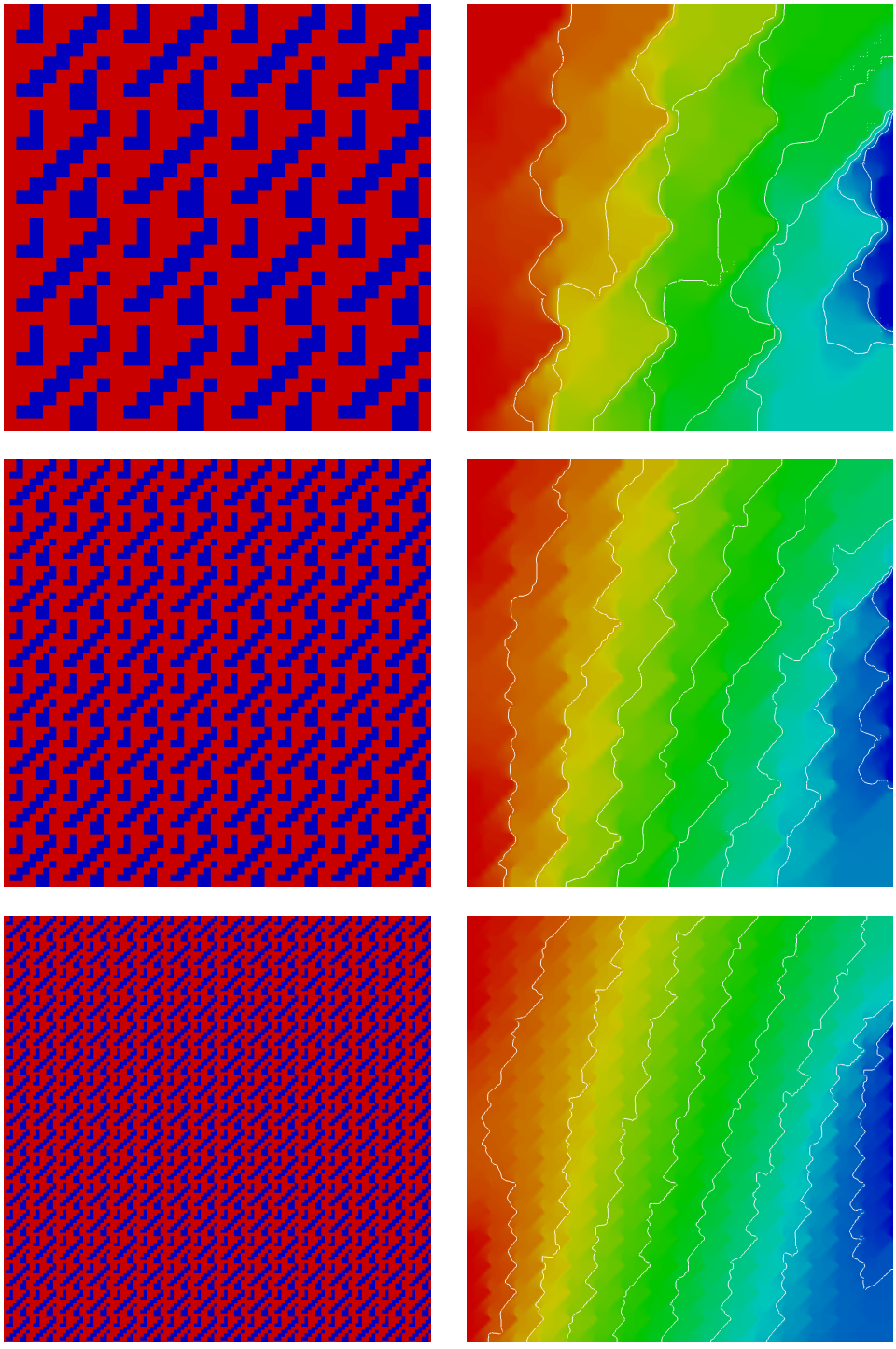


Figure 1.4.: Example of a multiscale problem in 2d (details given in the text).

Example 1.2. We consider an example of a multiscale problem in two space dimensions. Figure 1.2 on the left shows the setup of the macroscopic problem and the image to the right shows the solution to this problem with a homogeneous conductivity coefficient. Now we solve a problem with the same boundary conditions and a heterogeneous periodic coefficient as defined above. The conductivity distribution in the unit cell is shown in Figure 1.3 and in Figure 1.4 the solution for $\epsilon = 1/4$, $\epsilon = 1/8$ and $\epsilon = 1/16$ is shown. The solutions suggest that for $\epsilon \to 0$ the solution T_ϵ converges to a smooth function. For finite $\epsilon > 0$ the solution has small oscillations of the order ϵ. □

In practical applications $\epsilon \ll 1$ and computing T_ϵ is prohibitively expensive. Moreover one is only interested in the macroscopic behaviour and not in the behaviour on the scale ϵ. Homogenization theory, see e.g. [Kozlov et al., 1994], shows that the limit solution $T = \lim_{\epsilon \to 0} T_\epsilon$ can be computed as the solution of a homogeneous heat transfer problem

$$-\nabla \cdot (\Lambda \nabla T) = f \qquad \text{in } \Omega$$

where the *effective coefficient* $\Lambda \in \mathbb{R}^{n \times n}$ is a symmetric and positive definite matrix that only depends on the conductivity distribution in the unit cell and is therefore cheap to compute. From example 1.2 it becomes clear that the effective coefficient cannot just be a scalar as in this case the solution would be symmetric around $y = 1/2$ as in Figure 1.2. Instead, the contour lines are tilted to the right because the material conducts better in the direction $(1, 1)$ than in the direction $(1, -1)$.

The discussion so far involved only two scales, the macroscopic scale of interest and the scale ϵ (actually there is a third scale, the atomistic scale that has has already been eliminated by deriving the heat transfer equation). In practice, there might be more than two scales involved. For an effective solution it is important that the macroscopic scale of interest and the small scales (one is not really interested in) are clearly separated.

Another situation arises when the precise arrangenment of the materials is unknown, as is often the case with natural materials (such as e.g. rock). Then a stochastic approach may be appropriate leading to the field of stochastic partial differential equations.

1.2.4. Inviscid Fluid Flow

The flow of a gas is a very interesting and important problem. It has applications e.g.in weather and climate prediction or in star formation and the development of galaxies in astronomy. Figure 1.5 shows an image of the Cone Nebula in the galaxy NGC 2264 which is just a pillar of gas and dust. It is supposed to be a region where new stars are formed. In this section, we consider the flow of a gas ignoring the effect of internal friction. Besides the conserved quantities density, linear momentum and energy an additional concept is needed to derive the governing equations.

Pressure

In a gas that is macroscopically at rest the molecules still perform a random motion at the microscopic level. The molecules hitting the walls of the container excert a macroscopic force that must be counterbalanced by the rigid wall. This force per unit area is called pressure with units N m^{-2}. Through experiment one finds that the force per unit area excerted by the gas (at constant pressure) is always the same regardless of the shape of the wall. Therefore, the

Figure 1.5.: Cone Nebula (NASA/ESA image taken with the Hubble Space Telescope. For more information see `http://www.spacetelescope.org/images/heic0206c/`).

(scalar) pressure is the magnitude of a force (per unit area) that acts always perpendicular to the wall of the container (i.e. in the exterior normal direction).

If we would suddenly introduce a new (infinitely thin) wall inside the container (imagine a test volume ω) a force (per unit area) would be exerted at every point from each side of the wall that has equal magnitude and opposite direction so that it cancels out. We can therefore imagine pressure to be a (scalar) quantity that is defined everywhere in the gas.

The effect of pressure (being a force per unit area) needs to be considered in the momentum balance equation (1.14). If we consider a small test volume ω then the total force (including the direction) acting on the surface is given by

$$-\int_{\partial\omega} p n \, ds = -\int_{\omega} \nabla \cdot (pI) \, dx = -\int_{\omega} \nabla p \, dx. \tag{1.22}$$

This term is part of the right hand side of the integral version of equation (1.14) and I denotes the identity matrix. Note how the force always acts in negative normal direction. The sign can be understood as follows. Imagine the test volume to be a cuboid and consider e.g. the x-direction with the two faces located at x_1, x_2 with $x_1 < x_2$ and corresponding normal directions $n_1 = (-1, 0, 0)^T$ and $n_2 = (1, 0, 0)^T$. Then x- momentum must increase when pressure acts at the face at x_1 and it must decrease when pressure acts at the face at x_2. Note also, that equal pressure at x_1 and x_2 does have a zero net effect for the x-momentum in the test volume (so it is pressure difference that does have an effect).

The pressure contribution is sometimes called an interior force to distinguish it from exterior forces (such as e.g. gravity) which are only present in open systems.

Energy

In a macroscopic body of gas the total energy consists of two different forms of energy, the internal energy (translation, rotation and vibration of the molecules on the microscopic level) and the macroscopic kinetic energy due to the movement of the fluid that is macroscopically observed. Using the concept of densities we write this as

$$e = \rho u + \rho \|v\|^2/2 \tag{1.23}$$

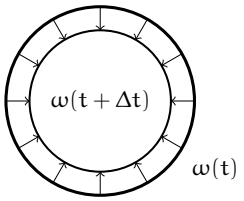
with e the total energy density in J m^{-3} and u the specific internal energy in J kg^{-1}. According to the theory of gases an algebraic relation, called an "equation of state" (depending on the type of gas), of the form

$$u = u(\rho, p) \tag{1.24}$$

relating specific internal energy, density and pressure can be derived. A well-known example is the ideal gas law $p = \bar{R}\rho T$ (here the internal energy is proportional to temperature). See below for another popular example.

Total energy e is a conserved quantity that is transported with the fluid with a flux $q = ev$. On the right hand side of the energy balance equation (1.13) internal work done in the fluid has to be considered. This internal work is known as "volume changing work" and can be experienced when using a bicycle pump: when a gas is compressed (i.e. its volume is decreased), it heats up.

We can derive the expression for volume changing work as follows: Imagine a set of molecules occupying the volume $\omega(t)$ at time t (see figure to the right). The same particles are contained in $\omega(t + \Delta t) \subset \omega(t)$ at small time interval Δt later. Subdividing $\partial\omega(t)$ into small surface elements Δs_i the work done against pressure of the gas in the time interval Δt is to first order



$$\Delta W_\omega(t) = -\lim_{N\to\infty} \sum_{i=1}^{N} \underbrace{p(x_i, t)ds_i}_{\text{normal force}} \underbrace{v(x_i) \cdot n_i \Delta t}_{\text{distance}} = -\Delta t \int_{\partial\omega(t)} pv \cdot n \, ds = -\Delta t \int_{\omega(t)} \nabla \cdot (pv) \, dx.$$

The sign is chosen such that compression ($v \cdot n < 0$) results in a positive value.

Euler Equations

Considering the internal forces due to pressure in the momentum balance law and the volume change work in the energy balance law we obtain the famous nonlinear system of partial differential equations known as the Euler equations of gas dynamics in conservative form

$$\partial_t \rho + \nabla \cdot (\rho v) = m, \tag{1.25a}$$

$$\partial_t (\rho v) + \nabla \cdot (\rho v v^T + pI) = f, \tag{1.25b}$$

$$\partial_t e + \nabla \cdot ((e + p)v) = w, \tag{1.25c}$$

which together with the thermodynamical relation

$$p = p(\rho, e) = (\gamma - 1)(e - \rho\|v\|^2/2) \tag{1.26}$$

and appropriate boundary and initial conditions describe the flow of a polytropic ideal gas. The functions m, f and w denote the mass source term, the external forces and the energy source term. Equation (1.26) is a consequence of the equation of state $u = p/((\gamma-1)\rho)$ and the definition of total energy (1.23). The constant γ is the adiabatic exponent and depends on the type of gas. For more details, see [Leveque, 2002, § 14.4]. Pressure is considered a dependent variable in (1.25) which can be eliminated using (1.26) resulting in a system of five equations for the five unknown functions ρ, v_1, v_2, v_3 and e in three space dimensions. It is interesting to note that we can combine all the equations (1.25) into a single equation for the unknown vector function $w = (\rho, \rho v, e)^T$:

$$\partial_t w + \nabla \cdot F(w) = g \tag{1.27}$$

with

$$F(w) = \begin{pmatrix} \rho v_1 & \rho v_2 & \rho v_3 \\ \rho v_1 v_1 + p(\rho, e) & \rho v_1 v_2 & \rho v_1 v_3 \\ \rho v_2 v_1 & \rho v_2 v_2 + p(\rho, e) & \rho v_2 v_3 \\ \rho v_3 v_1 & \rho v_3 v_2 & \rho v_3 v_3 + p(\rho, e) \\ (e + p(\rho, e))v_1 & (e + p(\rho, e))v_2 & (e + p(\rho, e))v_3 \end{pmatrix}. \tag{1.28}$$

An equation of the general form (1.27) is called a (nonlinear) conservation law. Yet another often encountered form is obtained by writing out the divergence:

$$\partial_t w + \sum_{j=1}^{n} \partial_{x_i} F_j(w) = g \tag{1.29}$$

where $F_j(w)$ is the j-th column of $F(w)$. Various other forms of the Euler equations can be found in the literature, most notably the nonconservative formulation. But (1.25) is the most general form that is also valid e.g. in the case of strong density contrasts.

1.2.5. Propagation of Sound Waves

Sound waves are small variations in pressure (and correspondingly density) that move through the gas. In order to derive an equation for the propagation of these variations we start with the Euler equations (1.25). We write all quantities as a constant background value (indicated by the bar) plus a small variation depending on space and time (indicated by the tilde):

$$\rho = \bar{\rho} + \tilde{\rho}, \qquad p = \bar{p} + \tilde{p}, \qquad v = \bar{v} + \tilde{v}.$$

The background velocity is actually assumed to be zero, $\bar{v} = 0$, and the temperature of the gas is assumed to be constant throughout the domain. Due to constant temperature we have $p = c^2\rho$ from the ideal gas law with $c = \sqrt{RT}$ the speed of sound and therefore $\bar{p} = c^2\bar{\rho}$ and $\tilde{p} = c^2\tilde{\rho}$.

Now the mass and momentum equations are linearized around the background state (all terms at least quadratic in variations are dropped, note especially that $v = \tilde{v}$ and vv^T can be dropped!) which results (with no external sources) in

$$\begin{aligned} \partial_t \tilde{\rho} + \bar{\rho}\nabla \cdot \tilde{v} &= 0, \\ \bar{\rho}\partial_t \tilde{v} + \nabla \tilde{p} &= 0. \end{aligned}$$

Using $\tilde{\rho} = \tilde{p}/c^2$ the density variation is eliminated and we obtain the equations of linear acoustics:

$$\partial_t \tilde{p} + c^2 \bar{\rho} \nabla \cdot \tilde{v} = 0, \tag{1.30a}$$
$$\bar{\rho} \partial_t \tilde{v} + \nabla \tilde{p} = 0. \tag{1.30b}$$

Taking the temporal derivative of the first equation and applying the divergence to the second the velocity variation can be eliminated from this system and we obtain the so-called wave equation:

$$\partial_t^2 \tilde{p} - c^2 \Delta \tilde{p} = 0. \tag{1.31}$$

In the analysis of the wave equation, (1.31) is often reduced to a first order system by setting $u = \partial_t \tilde{p}$ and $w = -\nabla \tilde{p}$. Together with the identities $\partial_{x_i} \partial_t \tilde{p} = \partial_t \partial_{x_i} \tilde{p}$ we obtain the system

$$\partial_t u + c^2 \nabla \cdot w = 0,$$
$$\partial_t w + \nabla u = 0,$$

which is equivalent to (1.30) (simply use the transformation $w = \bar{\rho}\tilde{v}$). It should be noted that it is the first order system that is derived from the physics and not the scalar second order wave equation, see also [Leveque, 2002, § 2.7].

Solid bodies are also able to support a propagation of waves an example being earthquakes. In the one-dimensional situation we may imagine a string of beads connected by springs with each other. One type of wave consists of small displacements of a bead in the direction of the string resulting in displacements of the neighbouring beads. This type of wave is called a compression wave or P-wave and it is similar to the sound waves in a gas. Another type of wave results from displacements of a bead in a direction perpendicular to the string which also results in the propagation of a wave in the direction of the string. This is called S-wave which usually travels slower than a P-wave. In the one-dimensional situation both types of waves are described by the one-dimensional wave equation $\partial_t^2 u - c^2 \partial_x^2 u = 0$ (A derivation of the P-wave is in [Eriksson et al., 1996, § 17.2] and the S-wave can be found in [Smirnow, 1981, § 176]). In a multi-dimensional solid both types of waves interact and more complicated equations result (see [Leveque, 2002, § 2.12] for some discussion). At the surface or at internal boundaries surface waves can be observed.

1.2.6. Viscous Fluid Flow

In many real fluids the effect of internal friction cannot be neglected. In a Newtonian fluid the stress tensor describing the additional flux of linear momentum is proportianal to gradients of velocity. The result is the system of *compressible Navier-Stokes equations*:

$$\partial_t \rho + \nabla \cdot (\rho v) = m, \tag{1.32a}$$
$$\partial_t (\rho v) + \nabla \cdot (\rho v v^T + pI - \tau(v)) = f, \tag{1.32b}$$
$$\partial_t e + \nabla \cdot ((e + p)v - \tau(v)v - \lambda \nabla T(e, \rho, v)) = w, \tag{1.32c}$$

with the *stress tensor*

$$\tau(v) = 2\mu \left[D(v) - \frac{1}{3}(\nabla \cdot v) I \right] \tag{1.33}$$

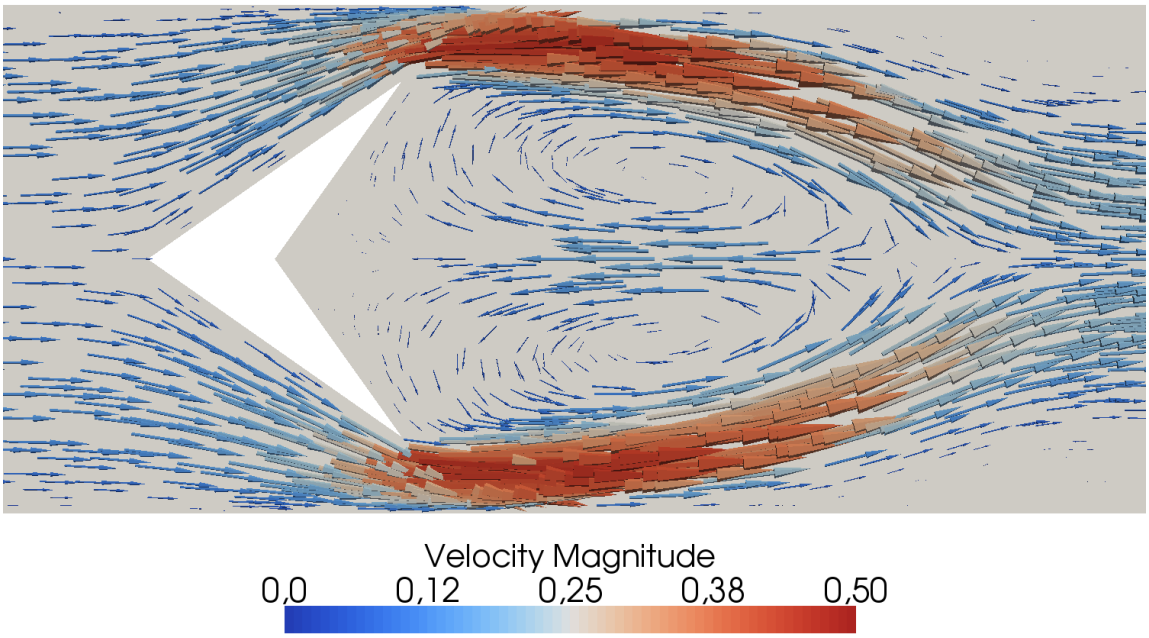


Figure 1.6.: Incompressible viscous flow in a channel with obstacle (image provided by Felix Heimann).

where shear viscosity μ is a parameter of the fluid and the *rate of strain tensor*

$$D(v) = \frac{1}{2}\left(\nabla v + (\nabla v)^T\right). \tag{1.34}$$

There are three new terms in the Navier-Stokes equations (1.32) compared to the Euler equations (1.25). The last term on the right hand side of the momentum equation describes the forces due to internal friction. The term $\tau(v)v$ in the energy equation describes the energy flux due to internal friction and $-\lambda\nabla T$ describes the heat conduction (Temperature T is a function of the state variables). Depending on the application, e.g. in star formation, heat transfer might also include the effect of radiation.

A full derivation of the new terms in the Navier-Stokes equations is beyond the scope of these lecture notes, we refer e.g. to [Chung, 1996] for details. Note however, that all the new terms involve second derivatives, i.e. the Navier-Stokes equations are a second-order system of PDEs.

Incompressible Viscous Flow

In many applications the fluid can be regarded as *incompressible* which means that density is independent of pressure. If temperature variations are also insignificant it is a constant. Neglecting also the energy equation (because temperature is assumed to have no effect on the fluid) and assuming that the fluid enters and leaves the domain only via the boundary ($m = 0$)

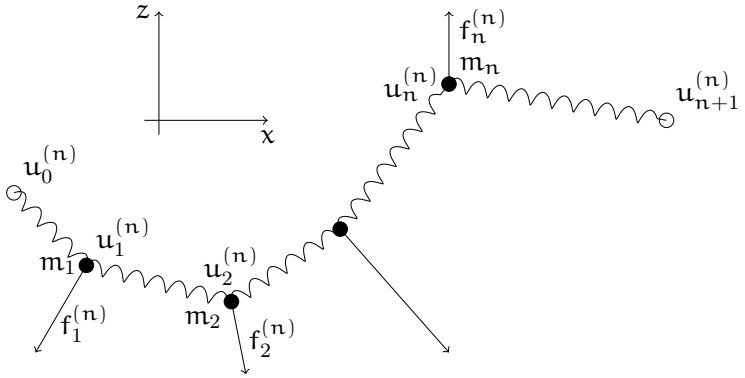


Figure 1.7.: Discrete mass-spring system.

results in the system of equations known as the *incompressible Navier-Stokes equations*:

$$\nabla \cdot v = 0, \tag{1.35a}$$

$$\partial_t v + \nabla \cdot (vv^T) - \nu \Delta v + \nabla p = f, \tag{1.35b}$$

with the kinematic viscosity $\nu = \mu/\rho$. Here p (which has been rescaled by $1/\rho$) is now an independent variable to be determined. In order to derive the momentum equation (1.35b) the incompressibility constraint $\nabla \cdot v = 0$ has been applied twice: once to simplify the stress tensor τ and a second time to conclude $\nabla \cdot D(u) = \Delta u$.

Figure 1.6 shows an example of incompressible, laminar flow around an obstacle in a two-dimensional channel.

1.3. Calculus of Variations

In this section we present a general approach that is used to study many mechanical and geometrical problems. For simplicity it will be illustrated by modelling the deflection of an elastic string where it leads to a two-point boundary value problem in ordinary differential equations. The general principle, however, applies to the multi-dimensional situation and is essential to understand the finite element method for the numerical solution of partial differential equations.

1.3.1. Equilibrium Principle

We are interested in modelling the deflection of an elastic string under a load. As an example consider a string where cloth is put on for drying. The property of elasticity means that after the load is removed the string returns exactly to its unloaded position without any lasting effect. In order to derive the model we will first consider systems of finitely many straight and ideal springs connected together. Then we will to a continuum by an appropriate limit process.

Discrete Spring System

Figure 1.7 shows the system of $n \in \mathbb{N}$ point masses $m_1, \ldots, m_n$ located at the positions $u_0^{(n)}, \ldots, u_n^{(n)}$ and connected by springs. Assuming all forces are applied in a plane we have

$u_i^{(n)} \in \mathbb{R}^2$. Spring i, $0 \leqslant i \leqslant n$, is elongated from position $u_i^{(n)}$ to position $u_{i+1}^{(n)}$ with the two endpoints

$$u_0^{(n)} = \begin{pmatrix} x_a \\ z_a \end{pmatrix}, \qquad u_{n+1}^{(n)} = \begin{pmatrix} x_b \\ z_b \end{pmatrix} \tag{1.36}$$

held fixed. All interior positions to be determined are collected in a big vector

$$u^{(n)} = (u_1^{(n)}, \dots, u_n^{(n)})^T \in \mathbb{R}^{2n}$$

which completely describes the state of the system. At each position $u_i^{(n)}$, $1 \leqslant i \leqslant n$, a force given by the vector $f_i^{(n)} \in \mathbb{R}^2$ is applied.

In order to place the system in the state $u^{(n)}$ work has to be done against the forces excerted by the springs and the forces f_i. This work is stored as elastic energy $J_{el}^{(n)}$ and potential energy $J_f^{(n)}$ (in physics elastic energy is also a form of potential energy but for ease of writing we stick to these names). We now consider both energies separately.

The magnitude of the force excerted by a single spring extended to length l is given by *Hooke's law*

$$F(l) = \kappa(l - l_0)$$

where κ is the spring constant with units N m^{-1} and l_0 the length of the unloaded spring. The work done when extending the spring from length l_0 to l is then

$$W_{el}(l) = \int_{l_0}^{l} F(s)\,ds = \int_{l_0}^{l} \kappa(s - l_0)\,ds = \left[\frac{\kappa}{2}(s - l_0)^2\right]_{l_0}^{l} = \frac{\kappa}{2}(l - l_0)^2.$$

Then the total elastic energy in all springs in state $u^{(n)}$ is

$$J_{el}^{(n)}(u^{(n)}) = \frac{1}{2}\sum_{i=0}^{n} \kappa_i(\|u_{i+1}^{(n)} - u_i^{(n)}\| - l_i)^2 \tag{1.37}$$

where κ_i and l_i are the individual spring parameters.

The work done to bring a mass m to position u against the exterior force f is given by the path integral

$$W_f(u) = -\int_0^u f \cdot t\,ds = -\|u - 0\|\frac{u - 0}{\|u - 0\|} \cdot f = -f \cdot u.$$

Here we used 0 as the reference point but any other position is also in order. Note that when $u \cdot f$ is negative (e.g. the mass is lifted *up* in the gravity field $f = (0, -mg)^T$ pointing *down*) then the potential energy increases. The potential energy of all mass points is then

$$J_f^{(n)}(u^{(n)}) = -\sum_{i=1}^{n} f_i^{(n)} \cdot u_i^{(n)} \tag{1.38}$$

and the total (potential) energy stored in the system at state $u^{(n)}$ is

$$J^{(n)}(u^{(n)}) = J_{el}^{(n)}(u^{(n)}) + J_f^{(n)}(u^{(n)}) = \frac{1}{2}\sum_{i=0}^{n} \kappa_i(\|u_{i+1}^{(n)} - u_i^{(n)}\| - l_i)^2 - \sum_{i=1}^{n} f_i^{(n)} \cdot u_i^{(n)}. \tag{1.39}$$

The *equilibrium principle* in mechanics says that the state $u_*^{(n)}$ attained by the system at equilibrium is the state of minimal (potential) energy:

$$J^{(n)}(u_*^{(n)}) \leqslant J^{(n)}(u) \quad \forall u \in \mathbb{R}^{2n}.$$

A short notation of the same statement is

$$u_*^{(n)} = \operatorname*{argmin}_{u \in \mathbb{R}^{2n}} J^{(n)}(u). \tag{1.40}$$

Note that problem (1.40) does in general not have a unique solution. An example for nonuniquess is the case $f_i^{(n)} = 0$ for all i and $\sum_{i=0}^{n} l_i > \|u_{n+1}^{(n)} - u_0^{(n)}\|$ where infinitely many solutions exist. When the endpoints of the string are sufficently far apart, however, one can prove that the functional $J^{(n)}(u)$ can be bounded from below, i.e.

$$J^{(n)}(u) \geqslant C \qquad \forall u \in \mathbb{R}^{2n} \tag{1.41}$$

and that it is convex, i.e.

$$J^{(n)}(\theta u + (1-\theta)v) \leqslant \theta J^{(n)}(u) + (1-\theta)J^{(n)}(v) \qquad \forall u, v \in \mathbb{R}^{2n}, \theta \in [0,1]. \tag{1.42}$$

By analogy with functions in one variable we may conclude that the problem has a unique global minimum. We will prove such a result later in a related context.

Continuum Limit

We now aim at describing the position of the string by a continuous curve $u : I = [0,1] \to \mathbb{R}^2$. The parameter interval I is in principle arbitrary and the equations to be derived should not depend on the particular parametrization. A number $\xi \in I$ is used to "label" a point on the string and is called *material coordinate*. The space $\mathbb{R}^2$ of positions is called the *configuration space* in this context.

To go from the discrete to the continuum model we introduce for every $n \in \mathbb{N}$ a discretization of the parameter interval

$$\xi_i^{(n)} = \frac{i}{n+1}$$

with the idea that $u(\xi_i^{(n)})$ corresponds to position $u_i^{(n)}$ of the discrete spring model. Furthermore we assume that the total length of the unloaded and unclamped string is given by L and set the lengths of the individual strings to

$$l_i^{(n)} = \frac{L}{n+1}.$$

With the abbreviation $\xi_{i\pm1/2}^{(n)} = \frac{1}{2}(\xi_i^{(n)} + \xi_{i\pm1}^{(n)})$ the other parameters of the discrete system are

$$\kappa_i^{(n)} = \kappa(\xi_{i+1/2}^{(n)}), \qquad\qquad f_i^{(n)} = \int_{\xi_{i-1/2}^{(n)}}^{\xi_{i+1/2}^{(n)}} f(\xi)\, d\xi$$

where $\kappa : I \to \mathbb{R}$ is a given continuous function describing the elastic properties of the string and $f : I \to \mathbb{R}^2$ is an integrable function giving the load density with units N m^{-1}. Inserting

these definitions into Equation (1.37) for the discrete elastic energy yields (with slight abuse of notation):

$$\begin{aligned} J_{\mathrm{el}}^{(n)}(u) &= \frac{1}{2}\sum_{i=0}^{n} \kappa_i (\|u(\xi_{i+1}^{(n)}) - u(\xi_i^{(n)}\| - l_i)^2 \\ &= \frac{1}{2}\sum_{i=0}^{n} \kappa_i \left(\frac{\|u(\xi_{i+1}^{(n)}) - u(\xi_i^{(n)}\|}{\xi_{i+1}^{(n)} - \xi_i^{(n)}} (\xi_{i+1}^{(n)} - \xi_i^{(n)}) - \frac{L}{n+1} \right)^2 \\ &= \frac{1}{2}\sum_{i=0}^{n} \kappa_i \, (\xi_{i+1}^{(n)} - \xi_i^{(n)})^2 \left(\left\| \frac{u(\xi_{i+1}^{(n)}) - u(\xi_i^{(n)}}{\xi_{i+1}^{(n)} - \xi_i^{(n)}} \right\| - L \right)^2 \end{aligned} \tag{1.43}$$

where we used $\xi_{i+1}^{(n)} - \xi_i^{(n)} = 1/(n+1)$. At this point we need to reconsider the spring "constant" κ. It has units N m^{-1} and depends on the length of the spring. This becomes important as the length of the individual springs now decreases as n increases. Mechanics tells us that a spring with cross-sectional area A_i, modulus of elasticity E_i and length l_i has a spring "constant"

$$\kappa_i = \frac{A_i E_i}{l_i} = \frac{A_i E_i}{L/(n+1)} = \frac{\tilde{\kappa}(\xi_{i+1/2}^{(n)})}{L(\xi_{i+1}^{(n)} - \xi_i^{(n)})}.$$

Note that the new material property function $\tilde{\kappa}(\xi)$ has units N and is now independent of the length of the string. Inserting this expression into Equation (1.43) yields

$$J_{\mathrm{el}}^{(n)}(u) = \frac{1}{2}\sum_{i=0}^{n} \frac{\tilde{\kappa}_i}{L} \left(\left\| \frac{u(\xi_{i+1}^{(n)}) - u(\xi_i^{(n)}}{\xi_{i+1}^{(n)} - \xi_i^{(n)}} \right\| - L \right)^2 (\xi_{i+1}^{(n)} - \xi_i^{(n)})$$

where we can now pass to the limit

$$J_{\mathrm{el}}(u) = \lim_{n\to\infty} J_{\mathrm{el}}^{(n)}(u) = \int_0^1 \frac{\tilde{\kappa}(\xi)}{2L} \left(\|u'(\xi)\| - L \right)^2 \, d\xi. \tag{1.44}$$

Hereby we assumed that the derivative $u'(\xi)$ is well defined, i.e. $u \in \left(C^1([0,1])\right)^2$.

Now the potential energy is

$$J_{\mathrm{f}}^{(n)}(u) = -\sum_{i=1}^{n} f_i^{(n)} \cdot u(\xi_i^{(n)}) = -\sum_{i=1}^{n} \int_{\xi_{i-1/2}^{(n)}}^{\xi_{i+1/2}^{(n)}} f(\xi) \cdot u(\xi_i^{(n)})$$

and passing to the limit gives

$$J_{\mathrm{f}}(u) = \lim_{n\to\infty} J_{\mathrm{f}}^{(n)}(u) = -\int_0^1 f(\xi) \cdot u(\xi).$$

As in the discrete case we have

$$J(u) = J_{\mathrm{el}}(u) + J_{\mathrm{f}}(u) = \int_0^1 \frac{\tilde{\kappa}(\xi)}{2L} \left(\|u'(\xi)\| - L \right)^2 - f(\xi) \cdot u(\xi) \, d\xi. \tag{1.45}$$

Application of the equilibrium principle now results in a minimization problem in *function space*

$$u_* = \operatorname*{argmin}_{u \in V} J(u) \tag{1.46}$$

where the space of all admissible functions V is

$$V = \left\{ v \in \left(C^1([0,1])\right)^2 : v(0) = \begin{pmatrix} x_a \\ z_a \end{pmatrix}, v(1) = \begin{pmatrix} x_b \\ z_b \end{pmatrix} \right\} \tag{1.47}$$

since $u'(\xi)$ turns up in the energy functional. This now raises the question how to solve a minimization problem in function space?

1.3.2. Variational Approach

To find the minimum of a function $g(x)$ in one real variable one searches for stationary points $g'(x_*) = 0$ and then checks whether x_* really is a minimum. Transfering this idea to minimization problems in function space such as (1.46) is the central idea of the *calculus of variations*. As in the case of a function in one variable the search for stationary points of the functional $J(u)$ results only in a necessary condition for a minimum.

To start let us rewrite the minimization property as:

$$u_* = \operatorname*{argmin}_{u \in V} J(u) \qquad \Leftrightarrow \qquad J(u_*) \leqslant J(u_* + tv) \quad \forall t \in \mathbb{R}, \forall v \in V_0$$

where

$$V_0 = \left\{ v \in \left(C^1([0,1])\right)^2 : v(0) = v(1) = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \right\}. \tag{1.48}$$

The function v is called a *variation* or *test function* and the definition of V_0 ensures that the function $u_* + tv$ always satisfies the given boundary conditions which are already incorporated in u_*. The energy functional $J(u)$ to be minimized is called *Lagrangian* in the calculus of variations and the function spaces V and V_0 are called *trial space* and *test space* respectively.

Now the function $\phi(t) = J(u_* + tv)$ is an ordinary function in one variable for a fixed $v \in V_0$. If $\frac{d\phi}{dt}$ exists then we have

$$J(u_*) \leqslant J(u_* + tv) \quad \forall t \in \mathbb{R}, \forall v \in V_0 \qquad \Rightarrow \qquad \frac{d\phi}{dt}(0) = 0 \ \ \forall v \in V_0. \tag{1.49}$$

The reverse conclusion can also be shown if the minimizer exists. Now let us compute the *configurational derivative* $\frac{d\phi}{dt}$. For any given $u \in V$, $v \in V_0$ we get

$$\frac{d}{dt} J_f(u + tv) = \frac{d}{dt} \left[-\int_0^1 f(\xi) \cdot (u(\xi) + tv(\xi)) \, d\xi \right] = -\int_0^1 f(\xi) \cdot v(\xi) \, d\xi$$

and so

$$\frac{d}{dt} J_f(u + tv)\Big|_{t=0} = -\int_0^1 f(\xi) \cdot v(\xi) \, d\xi.$$

For the more complicated elastic part we get

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{dt}}J_{\mathrm{el}}(u+tv) &= \frac{\mathrm{d}}{\mathrm{dt}}\int_0^1 \frac{\tilde\kappa(\xi)}{2L}\left(\|u'(\xi)+tv'(\xi)\|-L\right)^2 \\ &= \int_0^1 \frac{\tilde\kappa(\xi)}{L}\left(\|u'(\xi)+tv'(\xi)\|-L\right)\frac{[u'(\xi)+tv'(\xi)]\cdot v'(\xi)}{\|u'(\xi)+tv'(\xi)\|}\,\mathrm{d}\xi\end{aligned}$$

where we have used $\frac{\mathrm{d}}{\mathrm{dt}}\|x+ty\| = (x+ty)\cdot y/\|x+ty\|$ for any two vectors $x, y \in \mathbb{R}^n$ and the Euclidean scalar product and norm. By setting $t=0$ we get

$$\frac{\mathrm{d}}{\mathrm{dt}}J_{\mathrm{el}}(u+tv)\Big|_{t=0} = \int_0^1 \frac{\tilde\kappa(\xi)}{L}\frac{\|u'(\xi)\|-L}{\|u'(\xi)\|}u'(\xi)\cdot v'(\xi)\,\mathrm{d}\xi.$$

Putting both parts together results in the necessary condition for u (we refrain from writing u_* for the minimum from now on!) being a minimizer of the functional $J(u)$:

$$\int_0^1 \frac{\tilde\kappa(\xi)}{L}\frac{\|u'(\xi)\|-L}{\|u'(\xi)\|}u'(\xi)\cdot v'(\xi) - f(\xi)\cdot v(\xi)\,\mathrm{d}\xi = 0 \qquad \forall v \in V_0. \tag{1.50}$$

This equation is called a (nonlinear) *variational equation.*

Abstract Variational Problem

For a general Lagrangian of the form

$$J(u) = \int_0^1 F(u'(\xi), u(\xi))\,\mathrm{d}\xi$$

we get by applying the chain rule the variational equation

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{dt}}J(u+tv)\Big|_{t=0} &= \frac{\mathrm{d}}{\mathrm{dt}}\left[\int_0^1 F(u'(\xi)+tv'(\xi), u(\xi)+tv(\xi))\,\mathrm{d}\xi\right]\Bigg|_{t=0} \\ &= \int_0^1 \partial_1 F(u'(\xi), u(\xi))v'(\xi) + \partial_2 F(u'(\xi), u(\xi))v(\xi)\,\mathrm{d}\xi = 0 \qquad \forall v \in V_0\end{aligned} \tag{1.51}$$

where $\partial_1 F$, $\partial_2 F$ denote the partial derivatives of F with respect to the first and second argument. Note that the variation v always enters *linearly* in this equation! Therefore, the general variational equation has the abstract form:

$$\text{Find } u \in V: \quad r(u, v) = 0 \quad \forall v \in V_0 \tag{1.52}$$

where $r : V \times V_0 \to \mathbb{R}$ is linear in v, i.e.

$$r(u, v_1 + v_2) = r(u, v_1) + r(u, v_2), \qquad r(u, kv) = kr(u, v)$$

but possibly nonlinear in u. In the applications the test space V_0 is a real vector space of functions and V is an affine space $V = u_0 + V_0 = \{u : u = u_0 + v, v \in V_0\}$ incorporating the boundary conditions.

A note on the requirement of the differentiability of u and v. The minimization problem as well as the variational problem were derived under the assumption that $u, v \in \left(C^1([0,1])\right)^2$. It will turn out that this function space is neither appropriate for proving the existence of a solution nor practical for the applications (consider for example a pointwise load on the string).

Differential Equation

Integrating by parts the first term in Equation (1.51) gives

$$\begin{aligned}\int_0^1 \partial_1 F(u'(\xi), u(\xi))v'(\xi) + \partial_2 F(u'(\xi), u(\xi))v(\xi)\,d\xi \\ = \int_0^1 -\frac{d}{d\xi}\left(\partial_1 F(u'(\xi), u(\xi))\right)v(\xi) + \partial_2 F(u'(\xi), u(\xi))v(\xi)\,d\xi \\ + \left[\partial_1 F(u'(\xi), u(\xi))v(\xi)\right]_0^1\end{aligned}$$

where the boundary term vanishes due to the boundary condition on v! In order to do the integration by parts it is necessary to assume that F is now twice differentiable with respect to each variable and also that $u \in \left(C^2([0,1])\right)^2$. This leads then to the following variant of the variational equation

$$\int_0^1 \left[-\frac{d}{d\xi}\partial_1 F(u'(\xi), u(\xi)) + \partial_2 F(u'(\xi), u(\xi))\right] v(\xi)\,d\xi = 0 \qquad \forall v \in V_0.$$

Now the fundamental lemma of the calculus of variation states that if this equation is true for all test functions v then the function in square brackets must vanish pointwise:

$$-\frac{d}{d\xi}\partial_1 F(u'(\xi), u(\xi)) + \partial_2 F(u'(\xi), u(\xi)) = 0 \qquad (\xi \text{ in } (0,1)). \tag{1.53}$$

Equation (1.53) is a nonlinear two-point boundary value problem called the *Euler-Lagrange equation* for the variational problem (1.51). Note the similarity to the reasoning in §1.2.2 when going from Equation (1.10) to (1.11). There we applied Gauss' theorem to the arbitrary domain $\omega \subseteq \Omega$ which can be interpreted as a special case of integration by parts with a piecewise constant function (the characteristic function of ω).

Setting up the Euler-Lagrange equation for our string example, i.e. applying integration by parts to Equation (1.50), results in the nonlinear second-order ordinary differential equation

$$-\frac{d}{d\xi}\left[\frac{\tilde{\kappa}(\xi)}{L}\frac{\|u'(\xi)\| - L}{\|u'(\xi)\|}u'(\xi)\right] = f(\xi) \qquad (\xi \text{ in } (0,1))$$

with boundary values

$$u(0) = \begin{pmatrix} x_a \\ z_a \end{pmatrix}, \qquad u(1) = \begin{pmatrix} x_b \\ z_b \end{pmatrix}.$$

Note that for this equation to make sense for us at the moment we require $\tilde{\kappa} \in C^1([0,1])$ and $u \in \left(C^2([0,1])\right)^2$.

In summary, we now have the following situation

(I) *Minimization problem*	⇒	(II) *Variational problem*	⇒	(III) *Differential equation*
$u = \underset{v \in V}{\operatorname{argmin}} J(v)$		Find $u \in V$ such that $r(u, v) = 0 \quad \forall v \in V_0$		Solve BVB $g(u, u', u'') = 0 \quad \text{in } \Omega$ u given on $\partial\Omega$

For step (I)→(II) we introduced the concept of the configurational derivative. We will later see that (I) follows also from (II) provided that the minimum exists. For the step (II)→(III) we applied integration by parts and had to assume additional smoothness for the solution and coefficient functions. In general, a solution of problem (II) need not be a solution of problem (III) therefore. By taking the perspective of the differential equation the variational problem (II) is called the *weak formulation* of the boundary value problem.

1.3.3. Taut String Approximation

In this paragraph we are interested in the situation where the length L of the string with zero elastic energy is much shorter than the distance of the two points where it is clamped to, i.e.

$$L \ll \|u(1) - u(0)\|.$$

Under this assumption we get

$$L \ll \|u(1) - u(0)\| = \left\| \int_0^1 u'(\xi)\, d\xi \right\| \leqslant \int_0^1 \|u'(\xi)\|\, d\xi.$$

With this the energy functional (1.45) simplifies to

$$\begin{aligned} J(u) &= \int_0^1 \frac{\tilde{\kappa}(\xi)}{2L} \left(\|u'(\xi)\| - L\right)^2 - f(\xi) \cdot u(\xi)\, d\xi \\ &\approx \int_0^1 \frac{\tilde{\kappa}(\xi)}{2L} \|u'(\xi)\|^2 - f(\xi) \cdot u(\xi)\, d\xi =: \tilde{J}(u). \end{aligned}$$

Now $\tilde{J}(u)$ is a *quadratic functional* in u. The associated variational problem is

$$u \in V: \quad \int_0^1 \frac{\tilde{\kappa}(\xi)}{2L} u'(\xi) v'(\xi) - f(\xi) \cdot v(\xi)\, d\xi = 0 \qquad \forall v \in V_0 \tag{1.54}$$

which is now a *linear* variational problem in u. The related differential equation is then also linear and reads

$$-\frac{d}{d\xi}\left(\frac{\tilde{\kappa}(\xi)}{L}\frac{du}{d\xi}\right) = f \qquad \text{in } (0,1) \tag{1.55}$$

which decouples into two seperate equations for $x(\xi)$ and $z(\xi)$.

Let us assume now the special situation where there is only a vertical load $f(\xi) = (0, f_z(\xi))^T$. Naming the components $u(\xi) = (x(\xi), z(\xi))^T$ and $v(\xi) = (\phi(\xi), \psi(\xi))^T$ the variational problem (1.54) reads

$$\begin{aligned} u \in V: \quad & \int_0^1 \frac{\tilde{\kappa}(\xi)}{2L}(x'(\xi)\phi'(\xi) + z'(\xi)\psi'(\xi)) - f_z(\xi)\psi(\xi)\, d\xi \\ = & \int_0^1 \frac{\tilde{\kappa}(\xi)}{2L} x'(\xi)\phi'(\xi)\, d\xi + \int_0^1 \frac{\tilde{\kappa}(\xi)}{2L} z'(\xi)\psi'(\xi)) - f_z(\xi)\psi(\xi)\, d\xi = 0 \qquad \forall \phi, \psi \in C_0^1([0,1]). \end{aligned}$$

The equation for $x(\xi)$ can be solved analytically by solving the corresponding differential equation and we find:

$$x(\xi) = x_a + (x_b - x_a)\frac{\int_0^\xi \frac{L}{\tilde{\kappa}(s)}\, ds}{\int_0^1 \frac{L}{\tilde{\kappa}(s)}\, ds}.$$

Since L and $\tilde{\kappa}$ are strictly positive quantities the function $\xi \to x(\xi)$ is strictly increasing and therefore has an inverse $x \to x^{-1}(x)$.

We now want to write the second component $z(\xi)$ as a function of $x(\xi)$ instead of ξ. Therefore we define the new function $\hat{z}(x)$ and use the chain rule:

$$z(\xi) = \hat{z}(x(\xi)) \qquad \Rightarrow \qquad \frac{dz}{d\xi}(\xi) = \frac{d\hat{z}}{dx}(x(\xi))\frac{dx}{d\xi}(\xi).$$

The same applies for the test function $\psi(x) = \hat{\psi}(x(\xi))$. Recalling the transformation theorem for integrals $\int_a^b g(s)ds = \int_{a'}^{b'} g(\mu(t))|\frac{d\mu}{dt}(t)|\,dt$ with $\mu : [a', b'] \to [a, b]$ a differentiable map, we obtain for the variational problem for the second component $z(\xi)$:

$$\begin{aligned}
&\int_0^1 \frac{\tilde{\kappa}(\xi)}{2L}\frac{\hat{z}}{dx}(x(\xi))\frac{dx}{d\xi}(\xi)\frac{\hat{\psi}}{dx}(x(\xi))\frac{dx}{d\xi}(\xi) - f_z(\xi)\hat{\psi}(x(\xi))\,d\xi \\
&= \int_{x_a}^{x_b} \left[\frac{\tilde{\kappa}(x^{-1}(x))}{2L}\frac{d\hat{z}}{dx}(x)\left(\frac{dx}{d\xi}(x^{-1}(x))\right)^2\frac{d\hat{\psi}}{dx}(x) - f_z(x^{-1}(x))\hat{\psi}(x)\right]\frac{1}{\left|\frac{dx}{d\xi}(x^{-1}(x))\right|}\,dx \\
&= \int_{x_a}^{x_b} \underbrace{\frac{\tilde{\kappa}(x^{-1}(x))}{2L}\left|\frac{dx}{d\xi}(x^{-1}(x))\right|}_{\hat{\sigma}(x)}\frac{d\hat{z}}{dx}(x)\frac{d\hat{\psi}}{dx}(x) - \underbrace{\frac{f_z(x^{-1}(x))}{\left|\frac{dx}{d\xi}(x^{-1}(x))\right|}}_{\hat{f}(x)}\hat{\psi}(x)\,dx = 0 \qquad \forall \psi \in C_0^1([x_a, x_b]).
\end{aligned}$$

The corresponding linear second-order *scalar* differential equation for the function $\hat{z}$ now in "physical coordinates" reads:

$$-\frac{d}{dx}\left(\hat{\sigma}(x)\frac{d\hat{z}}{dx}\right) = \hat{f}(x) \qquad \text{in } (x_a, x_b)$$

with boundary conditions

$$\hat{z}(x_a) = z_a, \qquad \hat{z}(x_b) = z_b.$$

In two space dimensions the equation

$$-\nabla \cdot (\sigma(x)\nabla u) = f \qquad \text{in } \Omega \subset \mathbb{R}^2$$

with boundary conditions

$$u = g \qquad \text{on } \partial\Omega \tag{1.56}$$

is a model for the vertical position of a thin sheet of rubber under vertical load that is clamped at the boundary. Figure 1.8 shows an example for the two-dimensional case. Note that $\|\nabla u\|$ can become very large near so-called "reentrant corners" of the domain.

1.3.4. Linear Elasticity and Plate Problem

The considerations of this Section can be generalized to a small deformations of a three-dimensional elastic material experiencing both tension and compression. The resulting energy functional for the *linear elasticity problem* is

$$J(u) = \int_\Omega \frac{1}{2}\left\{\lambda(\nabla \cdot u)^2 + 2\mu D(u) : D(u)\right\} - f \cdot u\,dx \tag{1.57}$$

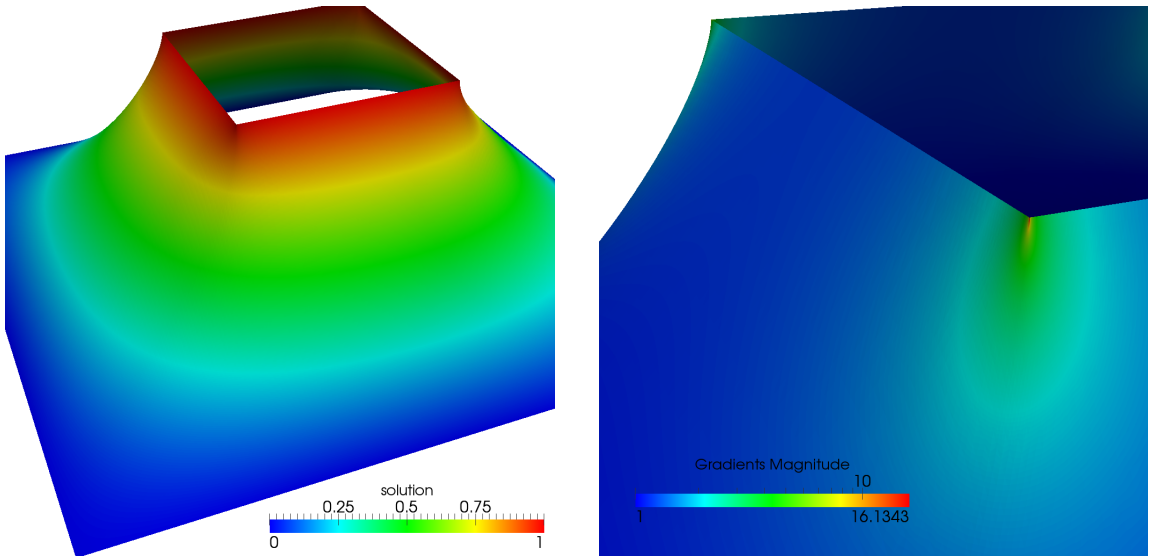


Figure 1.8.: A thin rubber sheet over the region $\Omega = (0,3)^2 \setminus (1,2)^2$ clamped to height 1 at the inner boundary and to 0 at the outer boundary. Left image shows rubber sheet colored by height and right image shows rubber sheet colored by the norm of the gradient in logarithmic (!) scale.

where $u \in \left(C^1(\Omega)\right)^3$ is the unknown *displacement* of the of the material from its unloaded configuration (i.e. $x + u(x)$ is the position of the material point $x \in \Omega$ under load). Then $D(u) = \frac{1}{2}(\nabla u + (\nabla u)^T)$ is the strain tensor from (1.34), λ, μ are the *Lamé coefficients* of the material and f are volume forces. The boundary condition

$$u(x) = g(x) \qquad \text{on } \partial\Omega$$

models clamping of the material at the boundary. The Euler-Lagrange equation corresponding to the variational formulation of (1.57) is now a linear second-order *system* of partial differential equations. For details we refer to [Braess, 2003, §3] and [Ciarlet, 2002, §1.2].

If we are interested in the deflection of a thin plate of elastic material with constant thickness, a well established model is the *plate problem* with the energy functional

$$J(u) = \int_\Omega \frac{1}{2}\left\{|\Delta u|^2 + 2(1-\sigma)((\partial_{x_1 x_2} u)^2 - \partial^2_{x_1} u\, \partial^2_{x_2} u)\right\} - fu\, dx \tag{1.58}$$

with $\sigma = \lambda/(2(\lambda+\mu))$ the *Poisson coefficent* computed from the Lamé coefficients. Here u is again a scalar function giving the vertical displacement of the plate out of the planar reference configuration. As boundary conditions we consider $u = 0$ on $\partial\Omega$. Note that the functional (1.58) involves second derivatives of u! The corresponding Euler-Lagrange equation of the variational formulation is now a *fourth-order* partial differential equation

$$\partial^4_{x_1} u + \partial^4_{x_2} = \Delta^2 u = f \qquad \text{in } \Omega \tag{1.59}$$

with boundary conditions $u = \partial_n u = 0$ on $\partial\Omega$. We refer to [Ciarlet, 2002, §1.2] or [Hackbusch, 1986, §5.3].

1.3.5. Hamilton's Principle

So far we considered stationary problems where the state attained by the system is a minimizer of potential energy (equilibrium principle). The energy functional (Lagrangian) is convex and bounded from below which ensures that a solution of the corresponding variational problem (which determines stationary points of the Lagrangian) is the globally unique minimizer.

In the dynamic case the energy functional involves kinetic and potential energy and is typically not convex any more. It turns out, that for certain systems the state can still be determined by finding stationary points of the energy functional, i.e. solving the corresponding variational problem. This principle is called *Hamilton's principle* and the energy functional is called a *Hamiltonian* in this case. For more information and some examples we refer to [Eriksson et al., 1996, §11.2].

1.4. Type Classification and Model Problems

1.4.1. Basic Mathematical Questions

So far we have derived several different PDEs by physical reasoning without mentioning a word about their solvability. From other types of mathematical equations, most notably ordinary differential equations, it is clear that we have to ask the following questions:

a) *Existence*: Does a given PDE problem have a solution?

b) *Uniqueness*: Is this solution the only one?

c) *Stability*: How does the data influence the solution?

A PDE problem is informally called *well-posed* (in the sense of Hadamard) if

a) it has a solution,

b) this solution is unique and

c) it depends continuously on the data.

If any of these conditions is not fullfilled it is called *ill-posed*. The discovery of chaos theory in the 20th century tells us that a problem need not be well-posed to be physically meaningful. Even the existence of solutions to many practically relevant problems such as the Euler or Navier-Stokes equations is open. In fact, a proof of the existence (and regularity, see below) of a solution to the incompressible Navier-Stokes equations in three space dimensions (this is important) is one of the millenium prize problems[2].

The informal definition of a well-posed problem needs to be made mathematically precise. The first question is what a solution should be. A natural assumption for an equations such as

$$\partial_x^2 u + \partial_y^2 u + \partial_z^2 u = f \qquad (x \in \Omega)$$

would be that u is twice continuously differentiable with respect to each variable. We say that a function is a *classical solution* of a PDE problem if it has continuous derivatives up to the required order and it satisfies the PDE for every $x \in \Omega$.

[2]The precise description of the task can be found here: `http://www.claymath.org/millennium/Navier-Stokes_Equations/`

The number of derivatives of a function is called its *regularity*. If a solution to a PDE problem possesses higher derivatives than required by the PDE it is said to have "additional regularity". This is important to assess the (speed of) convergence of numerical schemes. It turns out that also functions that *do not have* the derivatives required by the PDE may be called "solutions" in an appropriate sense (so-called weak solutions). A particular example is the conservation law

$$\partial_t u + \partial_x u = 0 \qquad (x \in \mathbb{R}, t > 0)$$

where also discontinuous functions $u(x,t)$ do make sense, as we will show below.

Unfortunately there is no theory that covers the solvability of PDEs in general and it is unlikely that such a theory exists. Instead techniques have been developed that can be used to analyze certain classes of PDEs. Similarly, there are no general numerical methods that can be applied successfully to any PDE but the development of numerical schemes follows the different classes introduced for the analysis. Below we will introduce the following important classes of PDEs:

a) Second-order scalar elliptic equation.

b) Second-order scalar hyperbolic equation.

c) Second-order scalar parabolic equation.

d) First-order hyperbolic systems.

1.4.2. Second-order Scalar Equations

Type Classification

Our aim is now to sort second-order scalar equations into different classes. We restrict ourselves to linear equations (nonlinear equations are classified after linearization). From the viewpoint of physical applications the independent variables are characterized as "time" and "space". In the following definition this distinction is not made, i.e. $x = (x_1, \dots, x_n)^T$ denotes just a vector of n independent variables where one of them may be time.

The general linear second-order scalar PDE has one of the two forms

$$Lu = -\sum_{i,j=1}^{n} \partial_{x_j}(a_{ij}(x)\partial_{x_i} u) + \sum_{i=1}^{n} \partial_{x_i}(b_i(x)u) + c(x)u = f \qquad \text{in } \Omega \tag{1.60}$$

or

$$Lu = -\sum_{i,j=1}^{n} a_{ij}(x)\partial_{x_j}\partial_{x_i} u + \sum_{i=1}^{n} b_i(x)\partial_{x_i} u + c(x)u = f \qquad \text{in } \Omega \tag{1.61}$$

where L is called a linear *differential operator* and Ω is some domain. The specificiation of boundary conditions to obtain a well-posed problem is intentionally omitted as it depends on the given coefficent functions.

We say that the PDE is in *divergence form* if it is given by (1.60). This is the form that arises when deriving the equation from a conservation principle. This also explains the minus sign in the second-order terms which reminds us that some flow in direction of the negative gradient is modelled. If the coefficients are continuously differentiable we can rewrite the form (1.60) into the form (1.61) and vice versa using the product rule. Doing this results in new coefficients

$\tilde{b}_i(x)$ and $\tilde{c}(x)$ but the coefficients $a_{ij}(x)$ remain the same. Moreover, since $\partial_{x_i}\partial_{x_j}u = \partial_{x_j}\partial_{x_i}u$ we may assume without loss of generality that

$$a_{ij}(x) = a_{ji}(x) \qquad (i, j = 1, \dots, n, x \in U).$$

Either form (1.60) or (1.61) may be more appropriate for different purposes. In the following we will consider only form (1.61), tacitly assuming that both forms are equivalent.

Definition 1.3. For every point $x \in U$ define the real symmetric $n \times n$ matrix $(A(x))_{ij} = a_{ij}(x)$ and the column vector $b(x) = (b_1(x), \dots, b_n(x))^T$. Then the *partial differential operator* L (or Equation (1.61)) is called

a) *elliptic* in x if all eigenvalues of $A(x)$ are nonzero and have the same sign,

b) *hyperbolic* in x if all eigenvalues are nonzero, $n-1$ eigenvalues have the same sign and the remaining eigenvalue has the opposite sign,

c) *parabolic* in x if one eigenvalue is zero, the remaining eigenvalues have the same sign and the $n \times (n+1)$ matrix $(A(x), b(x))$ has full rank.

The operator (or the equation) is called elliptic (hyperbolic, parabolic) if it is elliptic (hyperbolic, parabolic) in every point $x \in U$. □

The names elliptic, hyperbolic and parabolic are taken from the two-dimensional case where a level set of the quadratic form $q(x_1, x_2) = a_{11}x_1^2 + 2a_{12}x_1x_2 + a_{22}x_2^2$ is either an ellipse, a hyperbola or a parabola. In the case $n = 2$ the classification is complete, i.e. every linear second-order PDE is either elliptic, hyperbolic or parabolic or it is not a PDE (this case is excluded by the rank condition in the parabolic case). For $n > 2$ there are PDEs that are neither elliptic, parabolic or hyperbolic. Moreover, there are useful PDEs that have different types in different parts of the domain. Note also that the type of the operator depends only on the coefficients of the second-order terms, the so-called *leading part*.

Characteristics

In the initial value problem for a second-order ordinary differential equation the solution u and its derivative du/dt are prescribed at some t_0 in order to determine the solution at later times $t > t_0$. We can transfer this process to partial differential equation in the following way: Given u on a surface Γ in $\mathbb{R}^n$ together with its derivative in direction normal to the surface, can we determine the second derivative in normal direction, and with it the solution in the neighborhood of the surface, from the given data and the PDE (1.61)? This problem is generally called the *Cauchy problem* for (1.61). Points $x \in \Gamma$ where the Cauchy problem can *not* be solved are called *characteristic points* and if it is not solvable in any point of a given surface the surface itself is called a *characteristic surface*. On a characteristic surface the solution of the PDE or its normal derivative may not be continuous although the coefficients (and the surface) are smooth. Therefore the existence of characteristic surfaces for a differential operator gives important information.

In order to answer this question about characteristic points and surfaces we assume the surface Γ to be smooth and denote by $q_1(x), \dots, q_n(x)$ a system of orthonormal vectors in $x \in \Gamma$ such that $q_1(x), \dots, q_{n-1}(x)$ are tangential to the surface and $q_n(x)$ points in direction normal to the surface. Since Γ is smooth and u as well as its normal derivative ∂_{q_n} are given

on all of Γ also $\partial_{q_i} u$ and $\partial_{q_i}\partial_{q_n} u$ for $1 \leqslant i < n$ are given. So the task is to compute the single derivative $\partial^2_{q_n} u$ from the given data and the PDE.

In order to do that we introduce the coordinate transformation $x(s) = Q(y)s + y$ for an arbitrary $y \in \Gamma$ and $Q(y) = [q_1(y), \dots, q_n(y)]$ the column matrix of tangential and normal vectors. We now want to derive a PDE for the new function

$$v(s) = u(x(s)) = u(Q(y)s + y)$$

locally around $y \in \Gamma$. Employing the chain rule we obtain for the gradient and the Hessian

$$\begin{aligned} \partial_{s_j} v(s) &= q_j^T \nabla_x u(x(s)) && \Rightarrow && \nabla_s v(s) = Q^T \nabla_x u(x(s)) \\ \partial_{s_i}\partial_{s_j} v(s) &= q_j^T \nabla_x^2 u(x(s)) q_i && \Rightarrow && \nabla_s^2 v(s) = Q^T \nabla_x^2 u(x(s)) Q. \end{aligned}$$

Note that $\partial^2_{s_n} v(s) = q_n^T \nabla_x^2 u(x(s)) q_n = q_n^T \nabla_x (q_n^T \nabla_x u(x(s))) = \partial^2_{q_n} u(x(s))$ is the second derivative in normal direction. Since Q is orthogonal we get

$$\nabla_x u(x(s)) = Q \nabla_s v(s) \qquad\qquad \nabla_x^2 u(x(s)) = Q \nabla_s^2 v(s) Q^T$$

which we insert into the PDE:

$$-A(x(s)) : (Q \nabla_s^2 v(s) Q^T) + b(x(s)) \cdot (Q \nabla_s v(s)) + c(x(s)) = f(x(s)).$$

Here we used the notation $A : B = \sum_{i,j=1}^n (A)_{i,j} B_{i,j}$. Using the identity $A : (QBQ^T) = (Q^T A Q) : B$, see appendix A.3.1, we obtain the transformed PDE for $v(s)$:

$$-(Q^T A(x(s)) Q) : \nabla_s^2 v(s) + (Q^T b(x(s)))^T \cdot \nabla_s v(s) + c(x(s)) = f(x(s)).$$

Writing out components in the leading order part we find

$$- q_n^T A q_n \partial^2_{s_n} v - \sum_{i,j=1 (i \neq j)}^{n} q_i^T A q_j \partial_{s_i}\partial_{s_j} v + (Q^T b)^T \cdot \nabla_s v + c = f. \tag{1.62}$$

From this we see that the missing derivative $\partial^2_{s_n} v(s) = \partial^2_{q_n} u(x(s))$ can be computed from the given data if and only if

$$q_n^T A q_n \neq 0. \tag{1.63}$$

The matrix A is always symmetric and therefore diagonalizable, i.e. it has n real eigenvalues $\lambda_1, \dots, \lambda_n$ together with a set of orthonormal eigenvectors $r_1, \dots, r_n$. With the column matrix $R = [r_1, \dots, r_n]$ we have $R^T A R = \Lambda = \operatorname{diag}(\lambda_1, \dots, \lambda_n)$. We now discuss the condition (1.63) depending on the type of equation:

i) The PDE (1.61) is of elliptic type. Then all eigenvalues of A are either positive or negative, i.e. $q_n^T A q_n \neq 0$ for any $q_n \neq 0$. Therefore the desired derivative $\partial^2_{q_n} u(x(s))$ can always be computed for any surface Γ. We conclude that an elliptic PDE does not have characteristic surfaces. This also means that the solution and its gradient are smooth as long as the coefficients of the equation are smooth enough.

ii) The PDE (1.61) is of parabolic type. Then A has one zero eigenvalue and all others are nonzero and have the same sign. Without loss of generality let $\lambda_n = 0$ with corresponding eigenvector r_n. Now

$$q_n A q_n = 0 \quad \Leftrightarrow \quad q_n = \alpha_n r_n$$

for any α_n, meaning that $\partial^2_{q_n} u(x(s))$ can *not* be computed at a point on the surface when the normal to points in direction of the eigenvector r_n. Characteristic surfaces have normal direction $r_n(y)$ in every $y \in \Gamma$. In fact this does not explain why all nonzero eigenvalues need to have the same sign.

iii) The PDE (1.61) is of hyperbolic type. Then A has $n-1$ eigenvalues of the same sign and one with the opposite sign. Without loss of generality let λ_n be this eigenvalue. Decomposing $q_n = \alpha_n r_n + \sum_{i=1}^{n-1} \alpha_i r_i$ we get

$$q_n A q_n = \alpha_n^2 \lambda_n + \sum_{i=1}^{n-1} \alpha_i^2 \lambda_i = 0 \quad \Leftrightarrow \quad \alpha_n = \pm \sqrt{\sum_{i=1}^{n-1} -\frac{\lambda_i}{\lambda_n} \alpha_i^2}.$$

Note that the radicand is always nonnegative due to the sign condition in the definition of hyperbolicity. Now

$$q_n = \pm \sqrt{\sum_{i=1}^{n-1} -\frac{\lambda_i}{\lambda_n} \alpha_i^2} r_n + \sum_{i=1}^{n-1} \alpha_i r_i$$

are all the surface normal directions for which the derivative $\partial^2_{q_n} u(x(s))$ can not be computed. For any choice of $\alpha_1, \ldots, \alpha_{n-1}$ we get *two* possible directions. Since q_n is a direction it can be scaled arbitrarily. Therefore in the case $n = 2$ we can fix $\alpha_1 = 1$ and there are exactly two directions:

$$q_n = r_1 \pm \sqrt{-\frac{\lambda_1}{\lambda_2}}\, r_2.$$

If $n > 2$, there is an $n-2$ dimensional set of directions.

Characteristic surfaces are closely related to the Cauchy-Kovalevskaya theorem, see [Renardy and Rogers, 1993, §2.2], which asserts the local existence of solutions of a system of PDEs in the neighborhood of noncharacteristic surfaces. It is not of much practical use because the data and the surface are required to be analytic and it is indifferent to well-posed and ill-posed problems. Although it turns out that the choice of boundary and initial conditions that lead to a well-posed problem strongly depends on the type of the equation this question can not be answered with the techniques given so far. In the following we will give boundary and initial conditions that lead to well-posed problems for the different types with proofs given later in the text or in the literature. Ill-posedness of certain problems will be shown by the way of counter examples.

Elliptic Equations

The condition for ellipticity results in $A(x)$ being either positive or negative definite. Since the sign can be changed arbitrarily by multiplying the equation by -1 the convention is to require

that $A(x)$ is positive definite (then $A(x)$ models a permeability tensor). From §1.2.3 we learn that elliptic equations model e.g. the stationary flow of heat in a solid or fluid material.

The "simplest" elliptic equation is obtained by setting $A = I$, $b = 0$, $c = 0$:

$$-\Delta u = f \qquad \text{in } \Omega \tag{1.64}$$

and is called *Poisson equation*. If also $f = 0$ the equation is called *Laplace equation* or *potential equation*. In §1.1 we have seen that the Poisson equation describes e.g. the gravitational potential.

Now we turn to the question of boundary conditions on $\partial\Omega$. The analysis of the Cauchy problem above suggests that the solution in the neighborhood of the boundary can be determined from u and $\partial_n u$ given on the boundar, where n denotes by convention the direction of the unit outer normal to $\partial\Omega$. The following counter example shows that such boundary data may not lead to a well-posed problem.

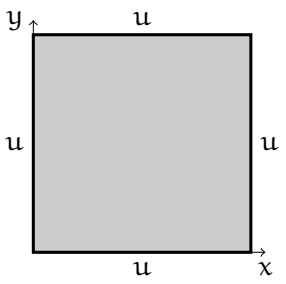
Example 1.4. [Rannacher, 2006, §1.2]. Consider $n = 2$ and $\Omega = \{(x, y) \in \mathbb{R}^2 : x > 0\}$. On the curve $\Gamma = \{(0, y) \in \mathbb{R}^2\}$ we prescribe the Cauchy data $u(0, y) = u_0^0(y) = 0$ and $\partial_x u(0, y) = u_0^1 = 0$. Clearly the function $u(x, y) = 0$ solves the Laplace equation $\Delta u = 0$ with this boundary data. Now we chose $\epsilon > 0$ and set the boundary data to

$$u_\epsilon^0(y) = 0, \qquad\qquad u_\epsilon^1(y) = \epsilon \sin(y/\epsilon).$$

One verifies that

$$u_\epsilon(x, y) = \epsilon^2 \sinh(x/\epsilon) \sin(y/\epsilon), \qquad\qquad \sinh(z) = \frac{1}{2}(e^z - e^{-z})$$

solves $\Delta u = 0$ in Ω and satisfies the given boundary data. Now we have on the one hand $\lim_{\epsilon\to 0} u_\epsilon^1 = u_0^1$ but on the other hand $\lim_{\epsilon\to 0} u_\epsilon \neq u$. Another way formulate the result is that the ratio $(\sup_{(x,y)\in\Omega} |u_\epsilon(x, y)|)/(\sup_{(0,y)\in\Gamma} |u_\epsilon^1(y)|)$ grows without bound. This means that the solution in the interior does not depend continuously on the data and therefore the problem is not well-posed. □



It turns out that on every point of the boundary only *one* of the following conditions

$$u = g \qquad \text{(Dirichlet)}, \tag{1.65a}$$

$$\partial_n u = g \qquad \text{(Neumann)}, \tag{1.65b}$$

$$\partial_n u + \alpha u = g \qquad \text{(Robin)}, \tag{1.65c}$$

can be prescribed. That these prescriptions actually lead to well-posed problems for the general elliptic equation will be shown later as part of the convergence theory. Note also, that the Neumann condition requires a compatibility condition with the right hand side f in order to be solvable and the solution is only unique up to a constant. The boundary conditions can be mixed, i.e. on different parts of the boundary, different conditions can be given.

Parabolic Equations

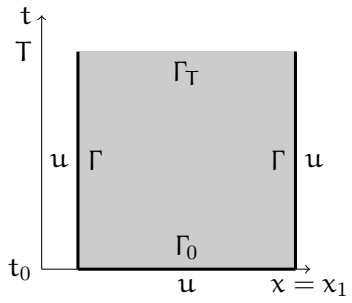
In the parabolic case one eigenvalue is zero. We assume that this eigenvalue is λ_n and rename the variable x_n to t. The "simplest" parabolic equation is obtained by setting $A = \left(\begin{smallmatrix} \lambda I & 0 \\ 0 & 0 \end{smallmatrix}\right)$ with some constant $\lambda > 0$, $b = 0$ and $c = 0$ which leads to the equation

$$\partial_t u - \lambda \sum_{i=1}^{n-1} \partial^2_{x_i} u = \partial_t u - \lambda \Delta u = f \qquad \text{in } U. \tag{1.66}$$

Second derivatives are taken only with respect to the "spatial" variables $x_1, \ldots, x_{n-1}$. From §1.2.3 we learn that this equation models instationary heat flow in a homogeneous solid body with heat conductivity λ. The equation with $\lambda = 1$ and $f = 0$

$$\partial_t u = \Delta u \qquad \text{in } U \tag{1.67}$$

is generally referred to as *heat equation* in the mathematical literature.



Parabolic equations are typically solved in a space-time cylinder $U = \Omega \times \Sigma$ with Ω the spatial domain and $\Sigma = (t_0, t_0 + T)$ a time interval. For the boundary conditions we identify the boundaries $\Gamma = \{(x,t) \in U : x \in \partial\Omega, t \in \Sigma\}$, $\Gamma_0 = \{(x,t) \in U : x \in \Omega, t = t_0\}$ and $\Gamma_T = \{(x,t) \in U : x \in \Omega, t = T\}$. This is illustrated for one spatial dimension in the figure to the left. Since $-\Delta$ is an elliptic operator on the $n-1$ spatial variables the same boundary conditions as in the elliptic case (with g now depending on time as well), i.e. those in (1.65), can be applied on Γ. The surfaces Γ_0 and Γ_T are characteristic since the normal direction $(0, \ldots, 0, 1)^T$ points in direction of the eigenvector corresponding to the zero eigenvalue. But the equation is only first order in that direction the prescription of the solution on either Γ_0 or Γ_T is sufficient. We now show by way of a counter example that a prescription of u on Γ_T ("at the end of the time interval") may lead to an ill-posed problem.

Example 1.5. [Braess, 2003]. Consider $n = 2$, $U = \Omega \times \Sigma = (0,1) \times [-1, 0)$. We prescribe the condition $u(0,t) = u(1,t) = 0$ on Γ and the condition

$$u(x,0) = \frac{1}{k} \sin(k\pi x) \qquad (k \in \mathbb{N})$$

for $t = 0$ which corresponds to Γ_T above. One verifies that

$$u(x,t) = \frac{1}{k} e^{-k^2\pi^2 t} \sin(k\pi x)$$

solves the heat equation $\partial_t u = \partial^2_x u$ in U and satisfies the boundary data. We observe that for $k \to \infty$ $\sup_{x \in \Omega} |u(x,0)| \to 0$ but $\sup_{(x,t) \in U} |u(x,t)| \to \infty$. On the other hand $u(x,y) = 0$ solves the heat equation for $u(x,0) = 0$. So again the solution does not depend continuously on the data. Observe, however, that changing U to $U = (0,1) \times (0,1]$ and the same data at $t = 0$ which now corresponds to Γ_0 (!) in the notation introduced above. we get $|u(x,t)| \to 0$ for $k \to \infty$. □

From the example we motivate that a conditions on Γ and Γ_0 do lead to a well-posed problem. On Γ_T no condition is necessary. The conditions on Γ are referred to as boundary conditions while the condition on Γ_0 is referred to

Hyperbolic Equations

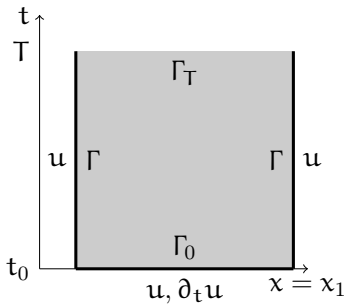
In the hyperbolic case $n-1$ eigenvalues have the same sign and one eigenvalue has the opposite sign. We assume without loss of generality that $\lambda_n < 0$, $\lambda_i > 0$, $1 \leqslant i \leqslant n-1$ and rename the variable x_n to t. The "simplest" hyperbolic equation is obtained by setting $A = \left(\begin{smallmatrix} \kappa I & 0 \\ 0 & -1 \end{smallmatrix}\right)$ with some constant $\kappa > 0$, $b = 0$ and $c = 0$ which leads to the equation

$$\partial_t^2 u - \kappa \sum_{i=1}^{n-1} \partial_{x_i}^2 u = \partial_t^2 u - \kappa \Delta u = f \qquad \text{in } U. \tag{1.68}$$

As in the parabolic case second derivatives are taken only with respect to the "spatial" variables $x_1, \ldots, x_{n-1}$. From §1.2.5 we learn that this equation models the propagation of sound waves in a gas with $\sqrt{\kappa}$ the speed of sound. The equation with $\kappa = 1$ and $f = 0$

$$\partial_t^2 u = \Delta u \qquad \text{in } U \tag{1.69}$$

is generally referred to as *wave equation* in the mathematical literature.



Hyperbolic equations are typically solved in a space-time cylinder $U = \Omega \times \Sigma$ with Ω the spatial domain and $\Sigma = (t_0, t_0 + T)$ a time interval. For the boundary conditions we identify the boundaries $\Gamma = \{(x,t) \in U : x \in \partial\Omega, t \in \Sigma\}$, $\Gamma_0 = \{(x,t) \in U : x \in \Omega, t = t_0\}$ and $\Gamma_T = \{(x,t) \in U : x \in \Omega, t = T\}$. This is illustrated for one spatial dimension in the figure to the left. In the hyperbolic case no boundary surface is characteristic. Since the operator $-\Delta u$ is elliptic an elliptic operator with respect to the $n-1$ spatial variables the same boundary conditions (1.65) as in the elliptic case, with g now depending as well on time, can be applied on Γ. On Γ_0, it turns out, the prescription of the initial conditions u and $\partial_t u$ does lead to a well-posed problem. If such a condition is prescribed on Γ_0 no condition on Γ_T can be given.

However, in contrast to the parabolic case, the role of Γ_0 and Γ_T can be reversed without leading to an ill-posed problem. This can be seen as follows: Suppose $u^+(x,t)$ is a solution of the wave equation in $U^+ = \Omega \times (0, T]$ with initial data prescribed at $t = 0$. Then the function $u^-(x,t) = u^+(x,-t)$ is a solution of the wave in $U^- = \Omega \times [-T, 0)$ with "final data" prescribed at $t = 0$ and boundary data $u^-(x,t) = u^+(x,-t), x \in \partial\Omega, t \in [-T, 0)$. So when the problem in U^+ is well posed also the "reflected problem" in U^- is well-posed.

We now turn to the question whether supplying u on Γ_0 *and* Γ_T instead of $u, \partial_t u$ on either Γ_0 *or* Γ_T leads to a well-posed problem. The following counter example shows that this is in general not the case.

Example 1.6. [Hackbusch, 1986, §1.4]. Consider $U = \Omega \times \Sigma = (0,1) \times (0, 1/\pi]$. We prescribe the data $u(x,0) = u(0,t) = u(1,t) = 0$ and $u(x, 1/\pi) = \sin(k\pi x)$ for $k \in \mathbb{N}$. One verifies that

$$u(x,t) = \sin(k\pi x) \frac{\sin(k\pi t)}{\sin k}$$

solves the wave equation in U and satisfies the given data. Now for $k \to \infty$ we have $|u(x, 1/\pi)| \leqslant 1$ but $\sup\{1/\sin \nu : \nu \in \mathbb{N}\} = \infty$. Again, the solution does not depend continuously on the data. □

In the following, we consider therefore the wave equation with boundary conditions (1.65) on Γ and initial conditions $u, \partial_t u$ on Γ_0.

Extensions

Sometimes the partial differential operator $L(\epsilon)$ depends on a parameter $\epsilon \geqslant 0$. Then the PDE is called *singularly perturbed* if the type of $L(0)$ is different from the type $L(\epsilon)$ for $\epsilon > 0$. As an example consider the equation

$$\partial_t u - \epsilon \Delta u + b \cdot \nabla u = 0.$$

For any $\epsilon > 0$ the equation is second-order parabolic but for $\epsilon = 0$ the equation is first-order (hyperbolic).

We now turn to the type classification of nonlinear partial differential equations. The most general form of a scalar second-order nonlinear PDE in n variables is

$$F(\partial^2_{x_1} u, \partial_{x_1}\partial_{x_2} u, \dots \partial^2_{x_n} u, \partial_{x_1} u, \dots, \partial_{x_n} u, u, x) = 0 \qquad (x \in U)$$

with F a function in $n(n-1)/2 + 2n + 1$ variables which we may name

$$z = (z_{11}, z_{12}, \dots, z_{nn}, z_1, \dots, z_n, z_0)^T.$$

A linearization of the PDE around the state $\bar{u}(x)$ is obtained by decomposing $u(x) = \bar{u}(x) + \tilde{u}(x)$ and applying Taylor expansion:

$$F(\partial^2_{x_1} u, \dots, u, x) \doteq \sum_{j=1}^{n} \sum_{i \geqslant j} \partial_{z_{ij}} F \, \partial_{x_j}\partial_{x_i} \tilde{u} + \sum_{i=1}^{n} \partial_{z_i} F \, \partial_{x_i} \tilde{u} + \partial_{z_0} F \, \tilde{u} + \bar{F} = 0.$$

This is a linear PDE in $\tilde{u}$ with coefficients $a_{ij}(x) = \partial_{z_{ij}} F(\partial^2_{x_1} \bar{u}, \dots, \bar{u}, x)$. The type classification is then applied to this linear a PDE for a given state $\bar{u}$.

As an example consider the *porous medium equation*

$$\partial_t u - \Delta u^p = \partial_t u - \nabla \cdot (u^{p-1} \nabla u) = 0 \tag{1.70}$$

with $p > 1$ and where we assume that boundary and initial conditions are such that $u \geqslant 0$ is ensured. This equation is called *degenerate parabolic* as it is parabolic at points where $u(x) > 0$ and it degenerates into an ordinary differential equation at points where $u(x) = 0$.

1.4.3. First-order Hyperbolic Systems

Method of Characteristics

We will consider the linear scalar conservation law

$$\partial_t u + \nabla \cdot (v u) = 0 \qquad \text{in } \mathbb{R}^n \times \mathbb{R}^+ \tag{1.71}$$

with initial conditions

$$u(x, 0) = u^0(x) \qquad \text{on } \mathbb{R}^n. \tag{1.72}$$

Here $v : \mathbb{R}^n \times \mathbb{R}^+ \to \mathbb{R}^n$ is a given time-dependent velocity field assumed sufficiently smooth. The extension to a bounded domain Ω is straightforward. The nonlinear case is treated in [Evans, 2010, § 3.2]. The following Theorem gives an explicit solution formula for this equation.

Theorem 1.7. Let $u \in C^1(\mathbb{R}^n \times \mathbb{R}_0^+)$ solve (1.71) for a smooth velocity field $v \in [C^1(\mathbb{R}^n \times \mathbb{R}^+)]^n$. For any point $x^0 \in \mathbb{R}^n$ define the *characteristic curve* $(\hat{x}(t), t)$ by

$$\frac{d\hat{x}}{dt}(t) = v(\hat{x}(t), t), \ t > 0, \qquad \hat{x}(0) = x^0 \ . \tag{1.73}$$

Then the solution of (1.71) at any point along the curve (1.73) is given by

$$u(\hat{x}(t), t) = u^0(x^0) \exp\left(-\int_0^t (\nabla \cdot v)(\hat{x}(s), s)\, ds \right) \quad . \tag{1.74}$$

Proof. Differentiating u along the curve gives

$$\begin{aligned} \frac{d}{ds} u(\hat{x}(s), s) &= \partial_t u(\hat{x}(s), s) + \sum_{i=1}^n \partial_{x_i} u(\hat{x}(s), s) \frac{d\hat{x}_i}{ds}(s) \\ &= \partial_t u(\hat{x}(s), s) + \nabla u(\hat{x}(s), s) \cdot v(\hat{x}(s), s) \\ &= \partial_t u(\hat{x}(s), s) + \nabla \cdot (v(\hat{x}(s), s) u(\hat{x}(s), s)) - (\nabla \cdot v(\hat{x}(s), s)) u(\hat{x}(s), s) \end{aligned}$$

where we have used the definition of the characteristic curve and the product rule $\nabla \cdot (vu) = v \cdot \nabla u + (\nabla \cdot v)u$. The first two terms vanish since u solves (1.71) and we are left with the linear homogeneous ordinary differential equation

$$\frac{d}{ds} u(\hat{x}(s), s) = -(\nabla \cdot v(\hat{x}(s), s)) u(\hat{x}(s), s) \tag{1.75}$$

which has the solution stated in the Theorem. □

The characteristic curves defined in the Theorem are the paths followed by particles in the flow. A special case is given when v is divergence free, $\nabla \cdot v = 0$. Then Theorem 1.7 states that the solution is constant along any characteristic curve. In particular $v = \text{const}$ is a divergence free velocity field and the corresponding characteristic curves $(\hat{x}(t), t) = (x^0 + vt, t)$ are straight lines in space-time. The solution at any point is then given by $u(x, t) = u^0(x - vt)$.

As a further specialization consider now the special initial data $u^0(x) = \phi(y \cdot x)$ where y is an arbitrary vector of modulus 1 and ϕ is a strictly monotone scalar function. Since $\nabla \phi(y \cdot x) = \phi(y \cdot x) y$ the level sets of $u^0(x)$ are hyperplanes in $\mathbb{R}^n$ which are perpendicular to the given direction y. For this special initial data the solution of (1.71) with $v = \text{const}$ is given by $u(x, t) = \phi(y \cdot (x - vt)) = \phi(y \cdot x - ty \cdot v)$. Thus the level contours move with velocity $y \cdot v$ in the direction y. This explains the fact that solutions of (1.71) support the propagation of *waves* (without a formal definition of a wave). More specifically, solutions of the form $\phi(y \cdot x - ty \cdot v)$ are called *plane waves* and they play a role in the generalization to systems of equations.

Using the explicit solution formula from Theorem 1.7 we can analyze the regularity of the solution. Clearly, when the velocity field is smooth enough (e.g. Lipschitz continuous in x) and the initial data u^0 is continuously differentiable then also $u(x, t)$ will be continuously differentiable. However, the solution formula makes also sense when the initial data is discontinuous (which might be a perfectly good approximation for a density or a concentration)!

Example 1.8. Consider the one-dimensional case with $v = 1$ and the step initial condition

$$u^0(x) = \begin{cases} 2 & x \leqslant 0 \\ 1 & x > 0 \end{cases} \quad .$$

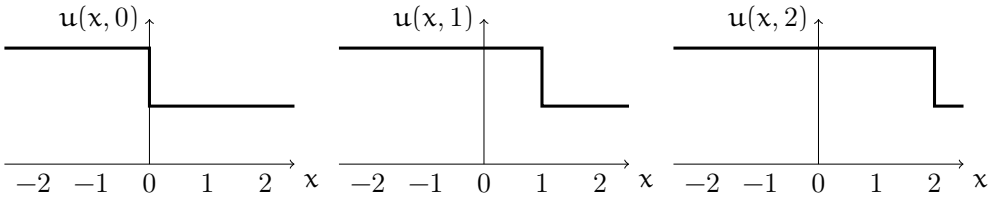


Figure 1.9.: Solution of the equation $\partial_t u + \partial_x u = 0$ with a step initial condition.

The solution according to the method of characteristic $u(x,t) = u^0(x-t)$ is then also discontinuous and is illustrated in Figure 1.9 for the times $t = 0, 1, 2$. □.

This example illustrates that requiring a solution of a kth order PDE to be k times continuously differentiable might be too restrictive. The question is then to give such "generalized" solutions lacking the required regularity a precise mathematical sense.

One-dimensional Systems

We now turn, as an intermediate step, to the case of a vector-valued function $u(x,t) = (u_1(x,t), \ldots, u_m(x,t))^T$ in one spatial dimension and consider the system of equations

$$\partial_t u + B\partial_x u = 0 \qquad \text{in } \mathbb{R}^n \times \mathbb{R}^+ \tag{1.76}$$

where B is a constant $m \times m$ matrix. One idea to solve this equation is to require B to be real diagonalizable, i.e. B has m real eigenvalues $\lambda_1, \ldots, \lambda_m$ and a corresponding set of eigenvectors $r_1, \ldots, r_m$ that form a basis of $\mathbb{R}^m$. In that case there exists an orthogonal matrix Q with $QBQ^T = D$, $D = \operatorname{diag}(\lambda_1, \ldots, \lambda_m)$. Using the transformation $w = Qu$ we can transform the system (1.76) into the equivalent system

$$\partial_t w + D\partial_x w = 0 \qquad \text{in } \mathbb{R}^n \times \mathbb{R}^+ \quad .$$

In the transformed system all components decouple and each component can be solved independently using the method of characteristics. Note that the velocities are the eigenvalues λ_k which might be different for each component. Each component of the solution of the original system $u = Q^T w$ is then a linear combination of these "simple" waves w_j.

We can also ask whether a system of the form (1.76) can have plane wave solutions. To find them we make the ansatz

$$u(x,t) = \phi(\gamma x - \sigma t)$$

where the "direction" γ is now reduced to a scalar, $\phi : \mathbb{R} \to \mathbb{R}^m$ is now a vector-valued function in one argument and the scalar factor σ is to be determined. Inserting this ansatz into the PDE (1.76) results in

$$\frac{d\phi}{ds}(\gamma x - \sigma t)(-\sigma) + A\frac{d\phi}{ds}(\gamma x - \sigma t)\gamma = (-\sigma I + \gamma A)\frac{d\phi}{ds}(\gamma x - \sigma t) = 0 \quad .$$

This equation can not be satisfied by any profile function ϕ in contrast to the scalar case. However, if we assume A to be diagonalizable we can require that $\frac{d\phi}{ds}$ is equal to an eigenvector:

$$\frac{d\phi}{ds} = r_k \qquad \Rightarrow \qquad \phi(s) = s r_k + \phi_k \quad (k = 1, \ldots, m).$$

Then our equation reduces to

$$(-\sigma + y\lambda_k)r_k = 0 \qquad \Leftrightarrow \qquad \sigma = \lambda_k \quad (k = 1, \dots, m).$$

Thus we can conclude that equation (1.76) supports m plane wave solutions that have the form

$$u_k(x,t) = (yx - y\lambda_k t)r_k + \phi_k \qquad (k = 1, \dots, m)$$

with arbitrary ϕ_k provided A is diagonalizable. Since y has the meaning of a direction we may assume $y = 1$ and so the possible velocities $\sigma = \lambda_k$ are just the eigenvalues of A.

It turns out that the diagonalizability of A is not just a nice mathematical structure that allows one to solve the system (1.76) but that such systems are also practically relevant!

Multi-dimensional Systems

We now turn to the linear system of m equations in n space dimensions of the form

$$\partial_t u + \sum_{j=1}^{n} B_j \partial_{x_j} u = f \qquad \text{in } \mathbb{R}^n \times \mathbb{R}^+ \tag{1.77}$$

with the initial condition

$$u(x,0) = u^0(x) \qquad \text{on } \mathbb{R}^n \tag{1.78}$$

where $u : \mathbb{R}^n \times \mathbb{R}_0^+ \to \mathbb{R}^m$ is the unknown function and $B_j : \mathbb{R}^n \times \mathbb{R}_0^+ \to \mathbb{R}^{m\times m}$, $f : \mathbb{R}^n \times \mathbb{R}_0^+ \to \mathbb{R}^m$ are given functions that may depend on position and time.

This system can not be transformed into a decoupled system for the individual components by a transformation $w = Qu$ because the matrices B_j are, in general, not simultaneously diagonalizable. However, we can still ask for the existence of plane wave solutions. As in the one-dimensional case we make the ansatz $u(x,t) = \phi(y \cdot x - \sigma t)$ where $y \in \mathbb{R}^n$ is now a given direction, ϕ is a vector-valued function in one variable and the B_j are assumed to be constant matrices. Inserting this ansatz into the PDE (1.77) yields

$$\left(-\sigma I + \sum_{j=1}^{n} y_j B_j\right) \frac{d\phi}{ds}(y \cdot x - \sigma t) = 0 \quad .$$

If we now assume that the matrix $B(y) = \sum_{j=1}^{n} y_j B_j$ is diagonalizable for any $y \in \mathbb{R}^n$ with m eigenvalues $\lambda_k(y)$ and corresponding eigenvectors $r_k(y)$we can set again $\frac{d\phi}{ds} = r_k(y)$ and the system reduces to

$$(-\sigma + \lambda_k(y))\, r_k(y) = 0 \quad .$$

Consequently we will have plane the m wave solutions of the form

$$u_k(x,t) = (y \cdot x - \lambda_k(y)t)r_k(y) + \phi_k \qquad (k = 1, \dots, m)$$

with arbitrary ϕ_k. This motivates now the following definition.

Definition 1.9 (Hyperbolic linear first-order systems)**.** The system of equations (1.77) is called *hyperbolic* if for each $x, y \in \mathbb{R}^n$ and $t \geqslant 0$ the $m \times m$ matrix

$$B(x,t;y) = \sum_{j=1}^{n} y_j B_j(x,t) \tag{1.79}$$

is real diagonalizable, i.e. it has m real eigenvalues $\lambda_1(x,t;y), \dots, \lambda_m(x,t;y)$ and its corresponding eigenvectors $r_1(x,t;y), \dots, r_m(x,t;y)$ form a basis of $\mathbb{R}^m$. In addition there are two special cases:

i) The system is called *symmetric hyperbolic* if $B_j(x,t)$ is symmetric for every $x \in \mathbb{R}^n$, $t \geqslant 0$ and $j = 1, \dots, m$.

ii) The system is called *strictly hyperbolic* if for $x, y \in \mathbb{R}^n$, $y \neq 0$ and $t \geqslant 0$ the matrix $B(x,t;y)$ has m distinct real eigenvalues. □

Example 1.10 (Linear Acoustics)**.** We consider the system of linear acoustics in three space dimensions given in Equation (1.30). Setting $u = (\tilde{p}, \tilde{v}_1, \tilde{v}_2, \tilde{v}_3)$ this system can be written as

$$\partial_t u + \sum_{j=1}^{n} B_j \partial_{x_j} u = 0$$

with

$$B_1 = \begin{pmatrix} 0 & c^2\bar{\rho} & 0 & 0 \\ 1/\bar{\rho} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad B_2 = \begin{pmatrix} 0 & 0 & c^2\bar{\rho} & 0 \\ 0 & 0 & 0 & 0 \\ 1/\bar{\rho} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad B_3 = \begin{pmatrix} 0 & 0 & 0 & c^2\bar{\rho} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1/\bar{\rho} & 0 & 0 & 0 \end{pmatrix}.$$

For any $y \in \mathbb{R}^3$ we therefore have

$$B(y) = \sum_{j=1}^{3} y_j B_j = \begin{pmatrix} 0 & y_1 c^2\bar{\rho} & y_2 c^2\bar{\rho} & y_3 c^2\bar{\rho} \\ y_1/\bar{\rho} & 0 & 0 & 0 \\ y_2/\bar{\rho} & 0 & 0 & 0 \\ y_3/\bar{\rho} & 0 & 0 & 0 \end{pmatrix}.$$

With the transformation matrix $T = \operatorname{diag}(\bar{\rho}c, 1, 1, 1)$ we see that $B(y)$ is similar to the symmetric matrix

$$T^{-1}B(y)T = \begin{pmatrix} 0 & y_1 c & y_2 c & y_3 c \\ y_1 c & 0 & 0 & 0 \\ y_2 c & 0 & 0 & 0 \\ y_3 c & 0 & 0 & 0 \end{pmatrix}$$

and therefore is diagonalizable with eigenvalues

$$\lambda_{1,2} = \pm c\|y\| \qquad \text{and} \qquad \lambda_{3,4} = 0.$$

Since y is a direction vector we may assume $\|y\| = 1$ and therefore the system supports two wave solutions with velocities $\pm c$ (explaining that c is the speed of sound). □

Definition 1.9 can be extended to the slightly more general system

$$B_0 \partial_t u + \sum_{j=1}^{n} B_j \partial_{x_j} u = 0 \qquad \text{in } \mathbb{R}^n \times \mathbb{R}^+ \tag{1.80}$$

where B_0 is a constant symmetric positive definite matrix. This system is also called hyperbolic provided the matrix $B(x,t;y)$ defined in (1.79) is diagonalizable. This can be shown as follows. By assumption there exists an orthogonal matrix Q such that $QBQ^T = D = \operatorname{diag}(\mu_1, \ldots, \mu_m)$, $\mu_k > 0$. With the transformation $w = D^{1/2}Qu$ the system (1.80) is equivalent to

$$\partial_t w + \sum_{j=1}^{n} D^{1/2} Q B_j Q^T D^{-1/2} \partial_{x_j} w = 0 \qquad \text{in } \mathbb{R}^n \times \mathbb{R}^+.$$

For this transformed system and any $y \in \mathbb{R}^n$

$$\sum_{j=1}^{n} y_j D^{1/2} Q B_j Q^T D^{-1/2} = D^{1/2} Q \left(\sum_{j=1}^{n} y_j B_j \right) Q^T D^{-1/2} = D^{1/2} Q B(x,t;y) Q^T D^{-1/2}$$

so the diagonalizability of $B(x,t;y)$ also implies the hyperbolicity of the transformed system.

We now establish a connection of first-order hyperbolic systems to second-order scalar hyperbolic equations. We only consider the case $b \equiv 0$, $c \equiv 0$ in (1.61). With the vector-valued function $v = (v_1, \ldots, v_n, v_{n+1})^T = (\partial_{x_1} u, \ldots, \partial_{x_n} u, \partial_t u)^T$ we obtain the system of $n+1$ equations

$$\begin{aligned} \sum_{j=1}^{n} a_{ij} \partial_t v_j - \sum_{j=1}^{n} a_{ij} \partial_t v_{n+1} &= 0 \qquad (i = 1, \ldots, n), \\ \partial_t v_{n+1} - \sum_{j=1}^{n} \sum_{i=1}^{n} a_{ij} \partial_{x_j} v_i &= f. \end{aligned}$$

Here the first n equations are a consequence of the n identities $\partial_t \partial_{x_i} u = \partial_{x_i} \partial_t u$ and the fact that the rows of $A(x,t)$ are linearly independent. The last equation is our second-order hyperbolic PDE. Now this system can be written as first-order system of the form (1.80) with the matrices

$$B_0 = \begin{pmatrix} a_{11} & \ldots & a_{1n} & 0 \\ \vdots & & \vdots & \vdots \\ a_{n1} & \ldots & a_{nn} & 0 \\ 0 & \ldots & 0 & 1 \end{pmatrix}, \qquad B_j = \begin{pmatrix} 0 & \ldots & 0 & -a_{1j} \\ \vdots & & \vdots & \vdots \\ 0 & \ldots & 0 & -a_{nj} \\ -a_{1j} & \ldots & -a_{nj} & 0 \end{pmatrix}.$$

The positive definiteness of $A(x,t)$ ensures the positive definiteness of B_0 and since the B_j are symmetric any combination $\sum_{j=1}^{n} y_j B_j$ is diagonalizable. Thus we have shown that a scalar second-order hyperbolic PDE can be written as a (symmetric) hyperbolic first-order system. This also implies that (appropriately generalized) solutions of a scalar second-order hyperbolic PDE may be discontinuous.

Definition 1.9 is extended to the case of a nonlinear conservation law (1.27) (such as the Euler equations) as follows. We rewrite the conservation law using the chain rule (assuming F to be sufficiently smooth):

$$\partial_t u + \sum_{j=1}^{n} \partial_{x_j} F_j(u) = \partial_t u + \sum_{j=1}^{n} \nabla F_j(u) \partial_{x_j} u$$

(∇F_j denotes the Jacobian matrix). Then the nonlinear system is called hyperbolic if the matrix

$$B(x, t; y) = \sum_{j=1}^{n} y_j \nabla F_j(u(x, t))$$

is diagonalizable for any $y \in \mathbb{R}^n$ and possible state $u(x, t)$.

1.5. Model Problems

In order to summarize this chapter we give a list of problems (including boundary and initial conditions) which will serve as model problems in the rest of the text and which we will be able to solve numerically in the course of the lecture. In the following $\Omega \subset \mathbb{R}^n$ is a (spatial) domain, $\Sigma = (0, T]$ is a time interval and $u : \Omega \to \mathbb{R}$ or $u : \Omega \times \Sigma \to \mathbb{R}$ denotes the unknown scalar function.

a) Transport problem (first-order hyperbolic).

$$\begin{aligned} \partial_t u + \cdot(\nu u) &= f && \text{in } \Omega \\ u &= g && \text{on } \Gamma = \{x \in \partial\Omega \,:\, \nu(x) \cdot n(x) < 0\}. \end{aligned}$$

b) Laplace equation (Dirichlet problem, second-order elliptic).

$$\begin{aligned} -\Delta u &= 0 && \text{in } \Omega \\ u &= g && \text{on } \partial\Omega. \end{aligned}$$

c) Poisson equation (Neumann problem, second-order elliptic).

$$\begin{aligned} -\Delta u &= f && \text{in } \Omega \\ -\nabla u \cdot n &= g && \text{on } \partial\Omega. \end{aligned}$$

In order for a solution to exist the compatibility condition $\int_\Omega f \, dx = \int_{\partial\Omega} g \, ds$ is required. The solution is unique up to a constant.

d) Heat equation (second-order parabolic).

$$\begin{aligned} \partial_t u - \Delta u &= f && \text{in } \Omega \times \Sigma \\ u &= g && \text{on } \partial\Omega \times \Sigma \\ u &= u_0 && \text{on } \Omega \times \{0\}. \end{aligned}$$

e) Wave equation (second-order hyperbolic).

$$\begin{aligned} \partial_t^2 u - \Delta u &= f && \text{in } \Omega \times \Sigma \\ u &= g && \text{on } \partial\Omega \times \Sigma \\ u = u_0, \partial_t u &= u_1 && \text{on } \Omega \times \{0\}. \end{aligned}$$