1 Introduction to mathematical modelling and numerical simulation

1.1 General introduction

This chapter is an introduction to two distinct, but closely linked, aspects of applied mathematics: **mathematical modelling** and **numerical simulation**. A mathematical model is a representation or an abstract interpretation of physical reality that is amenable to analysis and calculation. Numerical simulation allows us to calculate the solutions of these models on a computer, and therefore to simulate physical reality. In this book, the models we shall study will be partial differential equations (or PDEs), that is, differential equations in several variables (time and space, for example).

For the moment we shall put aside a third fundamental aspect of applied mathematics, that is, the mathematical analysis of models to which we shall return in a little more depth in later chapters. We need, in some way, to both motivate and justify this necessary intrusion of mathematical analysis. We shall see that the numerical calculation of the solutions of these physical models sometimes has some unpleasant surprises which can only be explained by a sound understanding of their mathematical properties. Once again we recall the fundamental multidisciplinary character of applied mathematics, and therefore of numerical simulation, which combines mathematics, computer science, and engineering.

Although most of the problems and applications which motivate applied mathematics are fundamentally **nonlinear** (see, for example, [12], [27]), we confine ourselves

in this work to linear problems for simplicity. Likewise, we only consider deterministic problems, that is, with no random or stochastic components. Finally, in order for this chapter to be introductory and easily accessible, we shall often be a little imprecise in our mathematical arguments. The more rigorous reader can be reassured that we shall return to the concepts introduced in this way more carefully in the following chapter.

The plan of this chapter is the following. Section 1.2 is devoted to an elementary example of modelling which leads to **the heat flow equation**. Section 1.3 is a quick review of the principal PDEs that we meet in the usual models in mechanics, physics, or engineering sciences. Section 1.4 is an informal introduction to numerical analysis and the **finite difference** method. Finally, in the Section 1.5 we give the definition of a **well-posed problem** as well as a (brief) classification of PDEs.

1.2 An example of modelling

Modelling represents a considerable part of the work of an applied mathematician and requires a thorough knowledge, not only of applied mathematics, but also of the scientific discipline to which it is applied. In fact, in many cases the mathematical model may not yet be established, or we must select the pertinent one from among several possibilities, or we must simplify known models which are too complex. However, in an introductory presentation of the discipline it is not possible to do justice to this step of the modelling process: we must begin by learning the basic properties of applied mathematics! This is why we limit ourselves to describing the derivation of a well-known classical physical model, and we refer the reader who wishes to know more to more specialised works.

The model which we shall describe is known as the **heat flow equation**, or the diffusion equation.

Let us consider a domain Ω in N space dimensions (denoted by $\mathbb{R}^N$, with in general $N = 1, 2$, or 3) which we assume is occupied by a homogeneous, isotropic material which conducts heat. We denote the space variable by x, that is a point of Ω, and the time variable by t. The heat sources in Ω (possibly nonuniform in time and space) are represented by a given function $f(x, t)$, while the temperature is an unknown function $\theta(x, t)$. The quantity of the heat is proportional to the temperature θ and is therefore $c\theta$ where c is a physical constant (which depends on the material) called the specific heat. To calculate the temperature θ, we write down the **law of conservation of energy** or of heat. In an elementary volume V contained in Ω, the variation in time of the amount of heat is the balance of that produced by the sources and that which leaves or returns through the element boundaries. In other words,

$$\frac{d}{dt}\left(\int_V c\theta \, dx\right) = \int_V f \, dx - \int_{\partial V} q \cdot n \, ds, \tag{1.1}$$

where ∂V is the boundary of V (with surface element ds), n is the outward unit

normal from V, and q is the heat flux vector. If we apply Gauss's theorem we obtain

$$\int_{\partial V} q \cdot n \, ds = \int_V \mathrm{div} q \, dx.$$

Gathering together the different terms in (1.1) and using the fact that the elementary volume V is independent of time, we deduce the energy conservation equation

$$c\frac{\partial \theta}{\partial t} + \mathrm{div} q = f \tag{1.2}$$

which holds at every point $x \in \Omega$ and for all time t. We recall that the divergence operator is defined by

$$\mathrm{div} q = \sum_{i=1}^{N} \frac{\partial q_i}{\partial x_i} \text{ with } q = (q_1, \ldots, q_N)^T.$$

We must now link the heat flow to the temperature, by what is called a **constitutive law**. In this case, we use Fourier's law which says that the heat flux is proportional to the temperature gradient

$$q = -k \nabla \theta T \tag{1.3}$$

where k is a positive constant (which depends on the material) called the thermal conductivity. Remember that the gradient operator is defined by

$$\nabla \theta = \left(\frac{\partial \theta}{\partial x_1}, \ldots, \frac{\partial \theta}{\partial x_N} \right)^T.$$

By combining the conservation law (1.2) and the constitutive law (1.3), we obtain an equation for the temperature θ

$$c\frac{\partial \theta}{\partial t} - k\Delta\theta = f,$$

where $\Delta = \mathrm{div}\nabla$ is the Laplacian operator given by

$$\Delta\theta = \sum_{i=1}^{N} \frac{\partial^2 \theta}{\partial x_i^2}.$$

This equation is valid in the entire domain Ω and we must add another relation, called a **boundary condition**, which describes what happens at the boundary $\partial\Omega$ of the domain, and another relation which describes the initial state of the temperature. By convention, we choose the instant $t = 0$ to be the initial time, and we impose an **initial condition**

$$\theta(t = 0, x) = \theta_0(x), \tag{1.4}$$

where θ_0 is the function giving the initial distribution of the temperature in the domain Ω. The type of boundary condition depends on the physical context. If the domain is

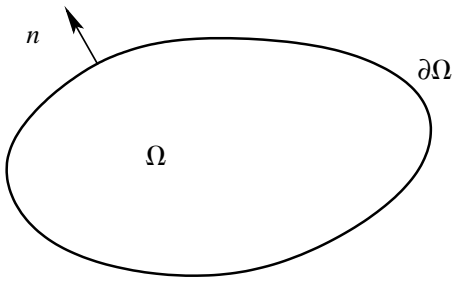

Figure 1.1. Unit normal vector oriented to the exterior.

surrounded by a region of constant temperature, then, by rescaling the temperature, the temperature satisfies the Dirichlet boundary condition

$$\theta(t,x) = 0 \quad \text{for all } x \in \partial\Omega \text{ and } t > 0. \tag{1.5}$$

If the domain is assumed to be adiabatic or thermally isolated from the exterior, then the heat flux across the boundary is zero and the temperature satisfies the Neumann boundary condition

$$\frac{\partial\theta}{\partial n}(t,x) \equiv n(x)\cdot\nabla\theta(t,x) = 0 \quad \text{for all } x \in \partial\Omega \text{ and } t > 0, \tag{1.6}$$

where n is the unit outward normal to Ω (see Figure 1.1). An intermediate situation can happen: the heat flux across the boundary is proportional to the jump in temperature from the exterior to the interior, and the temperature satisfies the Fourier (or Robin) boundary condition

$$\frac{\partial\theta}{\partial n}(t,x) + \alpha\theta(t,x) = 0 \quad \text{for all } x \in \partial\Omega, \text{ and } t > 0 \tag{1.7}$$

where α is a positive constant. As we must choose a boundary condition (as one of the steps in the modelling), we shall take the Dirichlet boundary condition (1.5). Finally, gathering together the equation, the initial value, and the boundary condition satisfied by the temperature, we obtain the heat equation

$$\begin{cases} c\dfrac{\partial\theta}{\partial t} - k\Delta\theta = f & \text{for } (x,t) \in \Omega \times \mathbb{R}_*^+ \\ \theta(t,x) = 0 & \text{for } (x,t) \in \partial\Omega \times \mathbb{R}_*^+ \\ \theta(t=0,x) = \theta_0(x) & \text{for } x \in \Omega \end{cases} \tag{1.8}$$

Problem (1.8) therefore comprises a PDE equipped with boundary conditions and an initial value. Because of the boundary conditions, we say that (1.8) is a **boundary value problem**, but we also say that it is a **Cauchy problem** because of the initial value.

Remark 1.2.1 In this model of heat propagation we must make the physical units precise: the temperature θ is expressed in degrees Kelvin (K), the specific heat c in Joules per kilogram per degree Kelvin ($J/(kg \times K)$), the thermal conductivity (per unit of mass) k in Joules metre squared per kilogramme per degree Kelvin per second ($Jm^2/(kg \times K \times s)$). From a mathematical point of view, we shall frequently neglect these units, and also assume that the constants c and k are equal to 1 (this is equivalent to making the physical quantities nondimensional). •

Remark 1.2.2 We have mentioned three types of boundary condition, Dirichlet, Neumann, and Fourier (but there are others) which hold on the entire boundary $\partial\Omega$. Of course, we can easily imagine situations where the boundary conditions are mixed: Dirichlet on $\partial\Omega_{\mathrm{D}}$, Neumann on $\partial\Omega_{\mathrm{N}}$, and Fourier on $\partial\Omega_{\mathrm{F}}$, with $\partial\Omega_{\mathrm{D}}, \partial\Omega_{\mathrm{N}}, \partial\Omega_{\mathrm{F}}$ being a partition of the boundary $\partial\Omega$. •

Remark 1.2.3 The heat flow equation (1.8) is **linear** in the sense that its solution θ depends linearly on the data (f, θ_0). In physics, this property is often described in terms of a superposition principle: a linear combination of data (f, θ_0) leads to a solution θ which is the same linear combination of solutions corresponding to each term of the decomposition of data. From a physical point of view, linearity is only one hypothesis among many. Indeed, for problems with a strong variation in temperature, Fourier's law is false, and it should be corrected by assuming that the thermal conductivity k depends on the temperature θ and its gradient $\nabla\theta$ (which makes the problem nonlinear). Even worse, for very rapid phenomena (explosions, for example) it is necessary to abandon the assumption of the proportionality of the heat flux q to the temperature gradient $\nabla\theta$. Indeed, this hypothesis (which initially appears 'natural') leads to the following paradox: the heat propagates with infinite velocity in the domain Ω. We shall see later (see Remark 1.2.9) how to reach this paradox. Let us remember for the moment that modelling is making hypotheses and describing their domain of validity. •

Remark 1.2.4 Problem (1.8) is not just a model of heat propagation. In fact it has a universal character, and we find it in many unrelated phenomena (we simply change the names of the variables). For example, (1.8) is also known as **the diffusion equation**, and models the diffusion or migration of a density or concentration across the domain Ω (imagine a pollutant diffusing in the atmosphere, or a chemical species migrating in a substrate). In this case, θ is the concentration or the density in question, q is the mass flux, k is the diffusivity, and c is the volume density of the species. Likewise, the conservation law (1.2) is a mass balance, while the constitutive law (1.3) is called Fick's law. •

Remark 1.2.5 Problem (1.8) also occurs in finance where it is called the **Black–Scholes model**. A variant of (1.8) allows us to find the value of an option to buy (or call option) a stock, which is initially worth x, for price k at some time in the future T.

This value is the solution u of

$$\begin{cases} \dfrac{\partial u}{\partial t} - ru + 1/2rx\dfrac{\partial u}{\partial x} + 1/2\sigma^2 x^2 \dfrac{\partial^2 u}{\partial x^2} = 0 & \text{for } (x,t) \in \mathbb{R} \times (0,T) \\ u(t=T,x) = \max(x-k,0) & \text{for } x \in \mathbb{R} \end{cases} \tag{1.9}$$

More precisely, $u(0,x)$ is the value at time $t=0$ of the call option with exercise price k at the exercise time $T>0$, and with value x at $t=0$. The volatility is denoted by σ and the interest rate by r. We remark that (1.9) is a final value and not an initial value problem, but that the sign of the second space derivative is opposite to that in (1.8). Consequently, after reversing the time, (1.9) is a parabolic equation. •

Numerous variants of the heat equation (1.8) exist, some of which we shall now explore. Up until now we have assumed that heat propagates in a fixed medium, or at least a still medium. Let us now assume that it propagates in a moving medium, for example, a fluid moving with velocity $V(x,t)$ (a vector valued function in $\mathbb{R}^N$). Then, we must now change the constitutive law since the heat flux is the sum of a diffusive flux (as before) and a convective flux (proportional to the velocity V), and proceeding similarly to the arguments above leads us to the **convection–diffusion** problem

$$\begin{cases} c\dfrac{\partial \theta}{\partial t} + cV \cdot \nabla\theta - k\Delta\theta = f & \text{in } \Omega \times \mathbb{R}_*^+ \\ \theta = 0 & \text{on } \partial\Omega \times \mathbb{R}_*^+ \\ \theta(t=0,x) = \theta_0(x) & \text{in } \Omega \end{cases} \tag{1.10}$$

The difference between (1.8) and (1.10) is the appearance of a convection term. We measure the balance between this new convection term and the diffusion term by a dimensionless number called the **Péclet number**, defined by

$$\mathrm{Pe} = \frac{cVL}{k}, \tag{1.11}$$

where L is a characteristic length of the problem (for example, the diameter of the domain Ω). If the Péclet number is very small then the diffusive effects dominate the convective effects, and model (1.8) is sufficient to describe the phenomenon. If the Péclet number is neither small nor large (we say that it is the order of unity), then model (1.10) is more realistic than (1.8). On the other hand, if the Péclet number is very large, we can simplify (1.10) by removing the diffusion term. We then obtain the equation known as the **advection** equation

$$\begin{cases} c\dfrac{\partial \theta}{\partial t} + cV \cdot \nabla\theta = f & \text{in } \Omega \times \mathbb{R}_*^+ \\ \theta(t,x) = 0 & \text{for } (x,t) \in \partial\Omega \times \mathbb{R}_*^+ \text{ if } V(x) \cdot n(x) < 0 \\ \theta(t=0,x) = \theta_0(x) & \text{in } \Omega \end{cases} \tag{1.12}$$

We note the difference in the boundary condition of (1.12) with respect to that of (1.10): we no longer impose that the temperature θ is zero everywhere on the boundary $\partial\Omega$ but only on those parts of the boundary where the velocity V is re-entrant.

We have therefore described three models of heat propagation by convection and diffusion, (1.8), (1.10), (1.12), which have different regimes of validity depending on different values of the Péclet number. Of course, the analytical or numerical solution of these three problems is very different. This is reflected in the current state of mathematical modelling: there are several competing models and we must choose the 'best'.

In order to understand better the fundamental differences which exist between these models, we temporarily restrict ourselves to the case where $\Omega = \mathbb{R}$ the whole real line (which rids us of the question of the boundary conditions), where the source term f is zero, and where the velocity V is constant. We can then explicitly calculate solutions of these models. For example, (1.10) becomes

$$\begin{cases} \dfrac{\partial \theta}{\partial t} + V \dfrac{\partial \theta}{\partial x} - \nu \dfrac{\partial^2 \theta}{\partial x^2} = 0 & \text{for } (x,t) \in \mathbb{R} \times \mathbb{R}_*^+ \\ \theta(t=0,x) = \theta_0(x) & \text{for } x \in \mathbb{R} \end{cases} \tag{1.13}$$

with $\nu = k/c$, which has solution

$$\theta(t,x) = \frac{1}{\sqrt{4\pi\nu t}} \int_{-\infty}^{+\infty} \theta_0(y) \exp\left(-\frac{(x - Vt - y)^2}{4\nu t} \right) dy. \tag{1.14}$$

A solution of (1.8) is easily obtained by setting $V = 0$ in the expression (1.14).

Exercise 1.2.1 We assume that the initial condition θ_0 is continuous and uniformly bounded in $\mathbb{R}$. Verify that (1.14) is a solution of (1.13).

With the same simplifying hypotheses, the advection equation becomes

$$\begin{cases} \dfrac{\partial \theta}{\partial t} + V \dfrac{\partial \theta}{\partial x} = 0 & \text{for } (x,t) \in \mathbb{R} \times \mathbb{R}_*^+ \\ \theta(t=0,x) = \theta_0(x) & \text{for } x \in \mathbb{R} \end{cases} \tag{1.15}$$

We verify that

$$\theta(t,x) = \theta_0(x - Vt) \tag{1.16}$$

is a solution of the equation (1.15).

Exercise 1.2.2 We assume that the initial data θ_0 is differentiable and uniformly bounded over $\mathbb{R}$. Verify that (1.16) is a solution of (1.15). Show that (1.16) is the limit of (1.14) as the parameter ν tends to zero.

Remark 1.2.6 If we solve the heat flow equation (1.8) on a bounded interval (and not in the whole space), we can also calculate an explicit solution by using Fourier analysis (see [4], [38]). This solution would be a little less 'explicit' than (1.14) as it is defined as the sum of an infinite series. We remark that it was precisely to solve the heat flow equation that Fourier invented the analysis which takes his name. •

Remark 1.2.7 The role of time is fundamentally different in equations (1.8) and (1.12). Indeed, assuming that the source term is zero, $f = 0$, if we change the sign of time t and that of the velocity, the advection equation (1.12) is unchanged (when we change the time we change the current). Conversely, a change in the sign of time in the heat flow equation (1.8) cannot be compensated by any variation in the sign of the data. This is obvious in the explicit form of the solution: (1.16) is invariant by changing the sign of t and V, whereas (1.14) (with $V = 0$) decreases in time, indicating the 'arrow' of time. We say that the advection equation is **reversible** in time, while the heat flow equation is **irreversible** in time. This mathematical observation is confirmed by physical intuition: some phenomena are reversible in time, others are not (like the diffusion of a drop of milk in a cup of tea). •

Remark 1.2.8 Another fundamental difference between equations (1.8) and (1.12) lies with the property of **invariance with respect to change of scale**. Let us assume that the source term is zero, $f = 0$. It is easy to see that if $\theta(x, t)$ is a solution of the heat flow equation (1.8), then, for all $\lambda > 0$, $\theta(x/\lambda, t/\lambda^2)$ is also a solution of the same equation (for a different initial value). Likewise, assuming that the velocity V is constant, if $\theta(x, t)$ is a solution of the advection equation (1.12), then $\theta(x/\lambda, t/\lambda)$ is also a solution. We see that the scaling of time is not the same in both cases. We also remark that, in both cases, the equations are invariant under translation in space and in time. •

Remark 1.2.9 A surprising property (from the physical point of view) of the heat flow equation (1.8) is that the solution in (x, t) depends on all the initial values in $\mathbb{R}$ (see formula (1.14)). In particular, in the case of (1.13), if the initial data is positive with compact support, then for all time $t > 0$ (no matter how small) the solution is strictly positive over all $\mathbb{R}$: in other words, the heat propagates 'instantaneously' to infinity. We say that the heat **propagates with an infinite velocity** (which is clearly a limitation of the model). On the other hand, in the advection equation (1.15) the initial data is convected with velocity V (see formula (1.16)): therefore there is a **finite velocity of propagation**. •

Remark 1.2.10 Thanks to the explicit formulas (1.14) and (1.16), we easily verify that the solutions of the convection–diffusion equation (1.13) and of the advection equation (1.15) satisfy the property

$$\min_{x\in\mathbb{R}} \theta_0(x) \leq \theta(x,t) \leq \max_{x\in\mathbb{R}} \theta_0(x) \quad \text{for all } (x,t) \in \mathbb{R} \times \mathbb{R}^+,$$

which is called the **maximum principle**. This property (which is equally important from the point of view of both mathematics and physics) extends to more general forms of the convection–diffusion equation (1.10) and of the advection equation (1.12). We shall study it more carefully later. •

1.3 Some classical models

In this section we shall quickly describe some classical models. Our goal is to present the principal classes of PDEs which we shall study later, and to show that these equations play a very important role in diverse scientific areas. From now on, we shall nondimensionalize all the variables, which will allow us to set the constants in the models equal to 1.

1.3.1 The heat flow equation

As we have seen, the heat flow equation appears as a model in many problems in science and engineering. It is written

$$\begin{cases} \dfrac{\partial u}{\partial t} - \Delta u = f & \text{in } \Omega \times \mathbb{R}_*^+ \\ u = 0 & \text{on } \partial\Omega \times \mathbb{R}_*^+ \\ u(t=0) = u_0 & \text{in } \Omega. \end{cases} \tag{1.17}$$

This equation is first order in time and second order in space (the order is that of the highest partial derivatives). We shall say that this equation is parabolic (see Section 1.5.2). We have already seen some properties of this equation: irreversibility in time, propagation with infinite velocity, and the maximum principle.

Exercise 1.3.1 We shall find a property of exponential decrease in time (see formula (1.14)) of the solution of the heat flow equation (1.17) in a bounded domain. In one space dimension, we set $\Omega = (0,1)$ and we assume that $f = 0$. Let $u(t,x)$ be a regular solution of (1.17). Multiplying the equation by u and integrating with respect to x, establish the equality

$$\frac{1}{2}\frac{d}{dt}\left(\int_0^1 u^2(t,x)\,dx\right) = -\int_0^1 \left|\frac{\partial u}{\partial x}(t,x)\right|^2 dx.$$

Show that every continuously differentiable function $v(x)$ on $[0,1]$, such that $v(0) = 0$, satisfies the Poincaré inequality

$$\int_0^1 v^2(x)\,dx \leq \int_0^1 \left|\frac{dv}{dx}(x)\right|^2 dx.$$

From this, deduce the exponential decrease in time of $\int_0^1 u^2(t,x)\,dx$.

1.3.2 The wave equation

The wave equation models propagation of waves or vibration. For example, in two space dimensions it is a model to study the vibration of a stretched elastic membrane (like the skin of a drum). In one space dimension, it is also called the vibrating cord equation. At rest, the membrane occupies a plane domain Ω. Under the action of

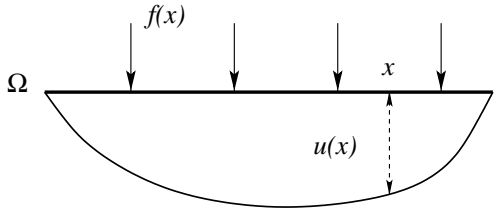

Figure 1.2. Displacement of an elastic cord.

a force normal to the plane with intensity f, it deforms and its normal displacement is denoted by u (see Figure 1.2). We assume that it is fixed at the boundary, which gives a Dirichlet boundary condition. The wave equation with solution u is given by

$$\begin{cases} \dfrac{\partial^2 u}{\partial t^2} - \Delta u = f & \text{in } \Omega \times \mathbb{R}_*^+ \\ u = 0 & \text{on } \partial\Omega \times \mathbb{R}_*^+ \\ u(t=0) = u_0 & \text{in } \Omega \\ \dfrac{\partial u}{\partial t}(t=0) = u_1 & \text{in } \Omega \end{cases} \tag{1.18}$$

We note that this equation is second order in time and that we therefore need two initial conditions for u. We say that this equation is hyperbolic (see Section 1.5.2).

Exercise 1.3.2 We work in $N = 1$ space dimensions. We assume that the initial data u_0 and u_1 are regular functions, and that $f = 0$ with $\Omega = \mathbb{R}$. We note that U_1 is a primitive of u_1. Verify that

$$u(t,x) = \frac{1}{2}\left(u_0(x+t) + u_0(x-t)\right) + \frac{1}{2}\left(U_1(x+t) - U_1(x-t)\right), \tag{1.19}$$

is the unique solution of (1.18) in the class of regular functions.

The wave equation shares, with the advection equation (1.12), the important property of **propagation with finite velocity**. Indeed, exercise 1.3.3 shows that the solution at a point (x,t) does not depend on all the initial data but only on the values in a restricted interval called the **domain of dependence** (or light cone; see Figure 1.3). We recall that this property is not shared by the heat flow equation since it is clear, from formula (1.14), that the solution in (x,t) depends on all the values of the initial data.

Another property of the wave equation is its invariance under the change of direction of time. If we change t to $-t$, the form of the equation does not change. We can therefore 'integrate' the wave equation in the positive or negative time directions in the same way. We say that the wave equation is **reversible in time**.

Exercise 1.3.3 Verify that the solution (1.19) at the point (x,t) only depends on the values of the initial data u_0 and u_1 in the segment $[x-t, x+t]$. Verify also that $u(-t,x)$ is a solution of (1.18) in $\Omega \times \mathbb{R}_*^-$ if we change the sign of the initial velocity $u_1(x)$.

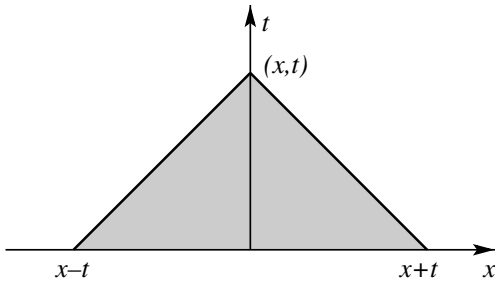

Figure 1.3. Domain or cone of dependence of the wave equation.

Exercise 1.3.4 We propose showing a principle of conservation of energy for the wave equation (1.18) without using the explicit formula (1.19). In one space dimension, we set $\Omega = (0,1)$ and we assume $f = 0$. Let $u(t,x)$ be a regular solution of (1.18). Multiplying the equation by $\partial u/\partial t$ and integrating with respect to x, establish the energy equality

$$\frac{d}{dt}\left(\int_0^1 \left|\frac{\partial u}{\partial t}(t,x)\right|^2 dx + \int_0^1 \left|\frac{\partial u}{\partial x}(t,x)\right|^2 dx\right) = 0.$$

Compare this with what happens for the heat equation.

1.3.3 The Laplacian

For certain choices of source term f, the solution of the heat flow equation (1.17) reaches a **steady** (or stationary) state, that is, $u(t,x)$ tends to a limit $u_\infty(x)$ as time t tends to infinity. Often, it is interesting to calculate this steady state directly. In this case, for a source term $f(x)$ which is independent of time, we solve an equation which is second order in space

$$\begin{cases} -\Delta u = f & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega, \end{cases} \tag{1.20}$$

which we call the Laplacian or Laplace's equation. We say that this equation is elliptic (see Section 1.5.2). We remark that the Laplacian is also the stationary version of the wave equation (1.19). The Laplacian also occurs in numerous fields of science and engineering. For example, (1.20) models the vertical displacement of an elastic membrane subjected to a normal force f and fixed around its boundary.

1.3.4 Schrödinger's equation

Schrödinger's equation describes the evolution of the wave function u of a particle subject to a potential V. Recall that $u(t,x)$ is a function of $\mathbb{R}^+ \times \mathbb{R}^N$ with values in $\mathbb{C}$ and that the square of its modulus $|u|^2$ is interpreted as the probability that the particle is found at the point (t,x). The potential $V(x)$ is a real-valued function. The wave function is a solution of

$$\begin{cases} i\dfrac{\partial u}{\partial t} + \Delta u - Vu = 0 & \text{in } \mathbb{R}^N \times \mathbb{R}_*^+ \\ u(t=0) = u_0 & \text{in } \mathbb{R}^N \end{cases} \tag{1.21}$$

There are no boundary conditions in (1.21) since the equation holds over the whole of space (which has no boundary). Nevertheless, we shall see that a 'reasonable' choice of function space in which to look for the solution implies *de facto* a condition of decay to infinity of u which can be interpreted as a boundary condition at infinity.

Exercise 1.3.5 We propose to show principles of energy conservation for Schrödinger's equation (1.21). Let $u(t,x)$ be a regular solution of (1.21) in one space dimension which decreases to zero (as does $\partial u/\partial x$) as $|x| \to +\infty$. Show that for every differentiable function $v(t)$ we have

$$\mathcal{R}\left(\frac{\partial v}{\partial t}\overline{v}\right) = \frac{1}{2}\frac{\partial |v|^2}{\partial t},$$

where $\mathcal{R}$ denotes the real part and $\overline{v}$ the complex conjugate of v. Multiplying the equation by $\overline{u}$ and integrating with respect to x, establish the energy equality

$$\int_{\mathbb{R}} |u(t,x)|^2 \, dx = \int_{\mathbb{R}} |u_0(x)|^2 \, dx.$$

Multiplying the equation by $\partial\overline{u}/\partial t$, show that

$$\int_{\mathbb{R}} \left(\left| \frac{\partial u}{\partial x}(t,x) \right|^2 + V(x) \, |u(t,x)|^2 \right) dx = \int_{\mathbb{R}} \left(\left| \frac{\partial u_0}{\partial x}(x) \right|^2 + V(x) \, |u_0(x)|^2 \right) dx.$$

1.3.5 The Lamé system

The Lamé system is a particular case of the linearized stationary elasticity equations which model deformations of a solid under the assumption of small deformations and of small displacements (see Section 5.3.1 for further details on the modelling). To obtain the Lamé system, we assume that the solid is homogeneous and isotropic and that it is fixed at the boundary. The principal difference from the preceding models is that here we have a **system** of equations, that is, several coupled equations. The solid at rest occupies the domain Ω of the space $\mathbb{R}^N$. Under the action of a force f

it deforms, and each point x moves to $x + u(x)$. The force $f(x)$ is a vector-valued function of Ω in $\mathbb{R}^N$, as is the displacement $u(x)$. This is a solution of

$$\begin{cases} -\mu\Delta u - (\mu+\lambda)\nabla(\mathrm{div}u) = f & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega \end{cases} \tag{1.22}$$

where λ and μ are two constants, the Lamé constants, which are characteristics of the homogeneous, isotropic material which comprises the solid. For mechanical reasons these constants satisfy $\mu > 0$ and $2\mu + N\lambda > 0$. The Dirichlet boundary condition for u reflects the fact that the solid is assumed fixed and immovable at its boundary. $\partial\Omega$.

The system (1.22) has been written in vector notation. If we denote by f_i and u_i, for $1 \le i \le N$, the components of f and u in the canonical basis of $\mathbb{R}^N$, (1.22) is equivalent to

$$\begin{cases} -\mu\Delta u_i - (\mu+\lambda)\dfrac{\partial(\mathrm{div}u)}{\partial x_i} = f_i & \text{in } \Omega \\ u_i = 0 & \text{on } \partial\Omega \end{cases}$$

for $1 \le i \le N$. We remark that, if $(\mu+\lambda) \neq 0$, then the equations for each component u_i are coupled by the divergence term. Obviously, in $N = 1$ dimension, the Lamé system has only one equation and reduces to the Laplacian.

1.3.6 The Stokes system

The Stokes system models the flow of a viscous incompressible fluid with small velocity. We assume that the fluid occupies a domain Ω and that it adheres to the boundary, that is, its velocity is zero at the boundary (which leads to a Dirichlet boundary condition). Under the action of a force $f(x)$ (a function of Ω in $\mathbb{R}^N$), the velocity $u(x)$ (a vector) and the pressure $p(x)$ (a scalar) are solutions of

$$\begin{cases} \nabla p - \mu\Delta u = f & \text{in } \Omega \\ \mathrm{div}u = 0 & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega \end{cases} \tag{1.23}$$

where $\mu > 0$ is the fluid viscosity. We note that there are a further N equations $\nabla p - \mu\Delta u = f$ (corresponding to the **conservation of momentum**), and one other equation $\mathrm{div}u = 0$ called the **incompressibility condition** (which corresponds to **conservation of mass**). If the space dimension is $N = 1$, the Stokes system is uninteresting as we easily see that the velocity is zero and the pressure is a primitive of the force. On the other hand, in dimensions $N \ge 2$, the Stokes system makes good sense: in particular, there exist nontrivial incompressible velocity fields (take, for example, a curl).

1.3.7 The plate equations

We consider small elastic deformations of a thin plane plate (which is negligible in its other dimensions). If we denote by Ω the average surface of the plate, and $f(x)$

(a function of Ω in $\mathbb{R}$) the resultant normal of the forces, then the normal component of the displacement $u(x)$ (a scalar) is the solution of the thin plate equation

$$\begin{cases} \Delta(\Delta u) = f & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega \\ \dfrac{\partial u}{\partial n} = 0 & \text{on } \partial\Omega \end{cases} \tag{1.24}$$

where we denote by $\frac{\partial u}{\partial n} = \nabla u \cdot n$ with n the outward unit normal vector to $\partial\Omega$. We remark that this is a partial differential equation which is fourth order in space (also called the bi-Laplacian). This is why it is necessary to have two boundary conditions. These boundary conditions represent the clamping of the plate (there is neither displacement nor rotation of the edge of the plate).

We remark that it is possible to justify the plate equation (1.24) asymptotically from the Lamé system (1.22) by letting the thickness of the plate to tend to zero. This is an example of mathematical modelling.

1.4 Numerical calculation by finite differences

1.4.1 Principles of the method

Apart from some very particular cases, it is impossible to calculate explicitly the solutions of the different models presented above. It is therefore necessary to have recourse to numerical calculation on a computer to estimate these solutions both qualitatively and quantitatively. The principle of all methods for the numerical solution of PDEs is to obtain discrete numerical values (that is, a finite number) which **'approximate'** (in a suitable sense, to be made precise) the exact solution. In this process we must be aware of two fundamental points: first, we do not calculate exact solutions but approximate ones; second, we **discretize** the problem by representing functions by a finite number of values, that is, **we move from the 'continuous' to the 'discrete'.**

There are numerous methods for the numerical approximation of PDEs. We present one of the oldest and simplest, called the finite difference method (later we shall see another method, called the finite element method). For simplicity, we limit ourselves to one space dimension (see Section 2.2.6 for higher dimensions). For the moment, we shall only consider the practical principles of this method, that is, the construction of what we call the **numerical schemes**. We reserve the theoretical justification of these schemes for Chapter 2, that is, the study of their convergence (in what way the approximate discrete solutions are close to the exact continuous solutions).

To discretise the spatio-temporal continuum, we introduce a **space step** $\Delta x > 0$ and a **time step** $\Delta t > 0$ which will be the smallest scales represented by the numerical method. We define a mesh or discrete coordinates in space and time (see Figure 1.4)

$$(t_n, x_j) = (n\Delta t, j\Delta x) \quad \text{for } n \geq 0, \;\; j \in \mathbb{Z}.$$