

# Part I

## Modelling techniques

## 1

## The basics of modelling

### 1.1 Introduction

This short introductory chapter is about mathematical modelling. Without trying to be too prescriptive, we discuss what we mean by the term, why we might want to do it and what kind of models are commonly used. Then we look at some very standard models, which you have almost certainly met before, and we see how their derivation is a blend of what are thought of as universal physical laws, such as conservation of mass, momentum and energy, with experimental observations and, perhaps, some ad hoc assumptions in lieu of more specific evidence.

One of the themes that run through this book is the applicability of all kinds of mathematical idea to ‘real-world’ problems. Some of these arise in attempts to explain natural phenomena, for example in models for water waves. We will see a number of these models as we go through the book. Other applications are found in industry, which is a source of many fascinating and non-standard mathematical problems and a big ‘end-user’ of mathematics. You might be surprised at how little is known of the detailed mechanics of most industrial processes, although when you see the operating conditions – ferocious temperatures, inaccessible or minute machinery, corrosive chemicals – you realise how expensive and difficult it would be to carry out detailed experimental investigations. In any case, many processes work just fine, having been designed by engineers who know their job. If it ain’t broke, don’t fix it; so where does mathematics come in? Some important uses are in the quality control and cost control of existing processes and in the simulation and design of new processes. We may want to understand: why does a certain

#### 4 *The basics of modelling*

type of defect occur; what is the ‘rate-limiting’ part of a process (the slowest ship, to be speeded up); how to improve efficiency, however marginally; whether a novel idea is likely to work at all and if so, how to control it.

It is in the nature of real-world problems that they are large, messy and often rather vaguely stated. It is very rarely worth anybody’s while to produce a ‘complete solution’ to a problem which is complicated and whose desired outcome is not necessarily well specified (to a mathematician). Mathematicians are usually most effective in analysing a relatively small ‘clean’ subproblem for which more broad-brush approaches run into difficulty. Very often the analysis complements a large numerical simulation which, although effective elsewhere, has trouble with this particular aspect of the problem. Its job is to provide understanding and insight in order to complement simulation, experiment and other approaches.

We begin with a chat about what models are and what they should do for us. Then we bring some simple ideas about physical conservation laws and how to use them together with the experimental evidence about how materials behave, with the aim of formulating closed systems of equations; this is illustrated with two canonical models, for heat flow and for fluid motion. There are many other models embedded elsewhere in the book, and we will deal with these as we come to them.

### 1.2 What do we mean by a model?

There is no point in trying to be too precise in defining the term ‘mathematical model’: we all understand that it is some kind of mathematical statement about a problem originally posed in non-mathematical terms. Some models are *explicative*, that is, they explain a phenomenon in terms of simpler, more basic processes. A famous example is Newton’s theory of planetary motion, whereby the whole complex motion of the solar system was shown to be a consequence of ‘force equals mass times acceleration’ and the inverse square law of gravitation. However, not all models aspire to explain. For example, the standard Black–Scholes model for the evolution of prices in stock markets, used by investment banks the world over, says that the percentage difference between tomorrow’s stock price and today’s is a lognormal random variable. Although this is a great simplification, in that it says that all we need to know are the mean and variance of this distribution, it says nothing about what will cause the price change.

All useful models, whether explicative or not, are *predictive*: they allow us to make quantitative predictions (whether deterministic or probabilistic) that can be used either to test and refine the model, should that

be necessary, or for use in practice. The outer planets were found using Newtonian mechanics to analyse small discrepancies between observation and theory,<sup>1</sup> and the Moon missions would have been impossible without this model. Every day, banks make billions of dollars worth of trades based on the Black–Scholes model; in this case, since model predictions do not always match market prices, they may use the latter to refine the basic model (here there is no simple underlying mechanism to appeal to, so adding model features in a heuristic way is a reasonable way to proceed).

Most of the models we discuss in this book are based on differential equations, ordinary or partial: in the main they are deterministic models of continuous processes. Many of them should already be familiar to you, and they are all accessible with the standard tools of real and complex analysis, partial differential equations, basic linear algebra and so on. I would like, however, to mention some kinds of models that we don't have the space to cover.

- Statistical models

Statistical models can be both explicative and predictive, in a probabilistic sense. They deal with questions of extracting information about cause and effect or making predictions in a random environment and describing that randomness. Although we touch on probabilistic models, for a full treatment see a text such as [49].

- Discrete models of various kinds

Many, many vitally important and useful models are intrinsically discrete: think, for example of the optimal scheduling of take-off slots from LHR, CDG or JFK airports, or the routing of packets of information through the mobile phone network. Discrete mathematics is a vast area with a huge range of techniques, impinging on practically every other area of mathematics, computer science, economics and so on.

- 'Black-box' models such as neural nets or genetic algorithms, and 'lumped parameter' models

The term 'model' is often used for these techniques, in which a 'black box' is trained, using observed data, to predict the output of a system

<sup>1</sup> This is a very early example of an *inverse problem*: assuming a model, and given observations of the solution determine certain model parameters, in this case the unknown positions of Uranus and Neptune. A more topical example is the problem of constructing an image of your insides from a scan or from electrical measurements taken from electrodes on your skin. Unfortunately, such problems are beyond the scope of this book; for a discussion, see [14].

6 *The basics of modelling*

given the input. The user need never know what goes on inside the black box (it is usually some form of curve fitting and/or optimisation algorithm), so while these algorithms can have some predictive capacity they can rarely be explicative. Although often useful, the philosophy behind black-box models is more or less orthogonal to that behind the models in this book; if you are interested, see [22]. Lumped-parameter models are somewhat in the same spirit: a complex system is represented by a much simpler set of ad hoc descriptions, as for example when a complicated mechanical system is modelled by a simple spring–dashpot combination.

### 1.3 Principles of modelling: physical laws and constitutive relations

Many models, especially those based on mechanics or heat flow (which includes most models in this book), are underpinned by physical principles such as the conservation of mass, momentum, energy or electric charge. We may have to think about how we interpret these ideas, especially in the case of energy, which can take so many forms (kinetic, potential, heat, chemical, . . . ) and be converted from one to another. Although they are in the end subject to experimental confirmation, the experimental evidence for these conservation principles is so overwhelming that, with care in interpretation, we can take them as assumptions.<sup>2</sup>

Work is heat and heat is work: this is loosely the first law of thermodynamics, in mnemonic form.

However, this gets us only so far. We can do very simple problems, such as the mechanics of point particles, and that's about it. Suppose, for example, that we want to derive the heat equation for heat flow in a homogeneous, isotropic, continuous solid. We can reasonably assume that at each point  $\mathbf{x}$  and time  $t$  there is an energy density  $E(\mathbf{x}, t)$  such that the internal (heat) energy inside any fixed volume  $V$  of the material is

$$\int_V E(\mathbf{x}, t) \, d\mathbf{x}.$$

We can also assume that there is a heat flux vector  $\mathbf{q}(\mathbf{x}, t)$  such that the rate of heat flow across a plane with unit normal  $\mathbf{n}$  is

$$\mathbf{q} \cdot \mathbf{n}$$

per unit area. Then we can write down the conservation of energy for  $V$  in the form

$$\frac{d}{dt} \int_V E(\mathbf{x}, t) \, d\mathbf{x} + \int_{\partial V} \mathbf{q}(\mathbf{x}, t) \cdot \mathbf{n} \, dS = 0,$$

<sup>2</sup> We are making additional assumptions that we are not dealing with quantum effects, or matter on the scale of atoms, or relativistic effects. We will deal only with models for human-scale systems.

where  $\partial V$  is the surface bounding  $V$ , on the assumption that no heat is converted into other forms of energy. Next, we use Green's theorem on the surface integral and, as  $V$  is arbitrary, the usual argument (see Section 1.4) gives us

$$\frac{\partial E}{\partial t} + \nabla \cdot \mathbf{q} = 0. \quad (1.1)$$

At this point, general assumptions fail us, and we have to bring in some experimental evidence. We need to relate both  $E$  and  $\mathbf{q}$  to the temperature  $T(\mathbf{x}, t)$ , by what are called *constitutive relations*. For many, but not all, materials, the internal energy is directly proportional to the temperature, which is written as

$$E = \rho c T,$$

where  $\rho$  is the density and  $c$  is a constant called the *specific heat capacity*. Likewise, *Fourier's law* states that the heat flux is proportional to the temperature gradient,

$$\mathbf{q} = -k \nabla T.$$

Putting these both into (1.1), we have

$$\rho c \frac{\partial T}{\partial t} = k \nabla^2 T,$$

as expected. The appearance of material properties such as  $c$  and  $k$  is a sure sign that we have introduced a constitutive relation, and it should be stressed that these relations between  $E$ ,  $\mathbf{q}$  and  $T$  are material dependent and experimentally determined. There is no a priori reason for them to have the nice linear form given above, and indeed for some materials one or other may be strongly nonlinear.<sup>3</sup>

Another set of models where constitutive relations play a prominent role is models for solid and fluid mechanics.

### 1.3.1 Example: inviscid fluid mechanics

Let us first look at the familiar Euler equations for inviscid incompressible fluid motion,

$$\rho \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p, \quad \nabla \cdot \mathbf{u} = 0.$$

Ask yourself why there is a minus sign. The second law of thermodynamics in loose mnemonic form: heat cannot flow from a cooler body to a hotter one.

'Oiler', not 'Yewler'.

<sup>3</sup> It is an experimental fact that temperature changes in most materials are proportional to the energy put in or taken out. However, both  $c$  and  $k$  may depend on temperature, especially if the material melts or freezes gradually, as for paraffin or some kinds of frozen fish. Such materials lead to nonlinear versions of the heat equation; fortunately, many common substances have nearly constant  $c$  and  $k$  values and so are well modelled by the linear heat equation.

## 8 The basics of modelling

Remember a *material volume* is one whose boundary moves with the fluid velocity, that is, it is made up of a fixed set of fluid particles.

Here  $\mathbf{u}$  is the fluid velocity and  $p$  the pressure, both being functions of position  $\mathbf{x}$  and time  $t$ , and  $\rho$  is the fluid density. The first equation is clearly ‘mass  $\times$  acceleration = force’, bearing in mind that we have to calculate the acceleration ‘following a fluid particle’ (that is, we use the convective derivative), and the second expresses mass conservation (now would be a good moment for you to do the first two exercises at the end of the chapter unless this is all very familiar material).

The constitutive relation is rather less obvious in this case. When we work out the momentum balance for a small material volume  $V$ , we are encapsulating the physical law

convective rate of change of momentum in  $V$  = net force on  $V$ .

The convective rate of change of momentum in  $V$  is given by

$$\int_V \rho \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) dV.$$

We then say that the net force on  $V$  is provided solely by the pressure and acts normally to  $\partial V$ . This is our constitutive assumption: that the internal forces in an inviscid fluid are completely described by a pressure field that acts isotropically (equally in all directions) at every point. Then, ignoring gravity, the force on  $V$  is

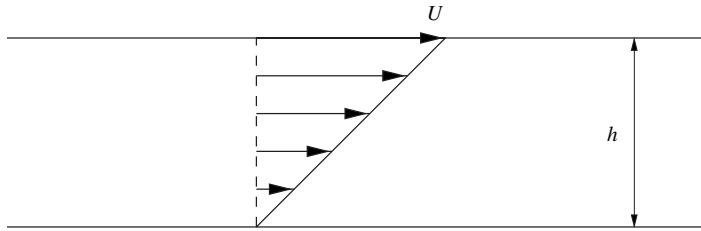
$$\int_{\partial V} -p \mathbf{n} dS = - \int_V \nabla p dV,$$

by a standard vector identity, and since  $V$  is arbitrary we do indeed retrieve the Euler equations.

### 1.3.2 Example: viscous fluids

Things are a little more complicated for a *viscous* fluid, namely one whose ‘stickiness’ generates internal forces which resist the motion. This model will be unfamiliar to you if you have never looked at viscous flow. If this is so, you can do one or more of the following.

- Just ignore it; you will then miss out on some nice models for thin fluid sheets and fibres in Chapter 20, but that’s about all.
- Go with the flow: trust me that the equations are not only believable (an informal argument is given below, and in any case I am assuming you know about the inviscid part of the model) but indeed correct. As is so often necessary in real-world problems, see what the mathematics has to say and let the intuition grow.
- Go away and learn about viscous flow; try the books [43] or [2].



**Figure 1.1** Drag on two parallel plates in shear, a configuration known as Couette flow. The upper plate is moving relative to the lower at speed  $U$ ; the arrows indicate the velocity profile.

Viscosity is the property of a liquid that measures its resistance to shearing, which occurs when layers of fluid slide over one another. In the configuration of Figure 1.1, the force per unit area on either plate due to viscous drag is found for many liquids to be proportional to the shear rate  $U/h$  and is written  $\mu U/h$ , where the constant  $\mu$  is called the *dynamic viscosity*. Such fluids are termed *Newtonian*.

Our strategy is again to consider a small element of fluid and, using the momentum balance equation, on the left-hand side work out the rate of change of momentum,

$$\int_V \rho \frac{D\mathbf{u}}{Dt} dV,$$

while on the right-hand side we have

$$\int_{\partial V} \mathbf{F} dS,$$

the net force on the boundary of the element. Then we use the divergence theorem to turn the surface integral into a volume integral and, as  $V$  is arbitrary, we are done.

Now for any continuous material, whether a Newtonian fluid or not, it can be shown (you will have to take this on trust; see [43] for a derivation) that there is a *stress tensor*, a matrix  $\boldsymbol{\sigma}$  with entries  $\sigma_{ij}$ , having the property that the force per unit area exerted by the fluid in direction  $i$  on a small surface element with normal  $\mathbf{n} = (n_j)$  is given by  $\boldsymbol{\sigma} \cdot \mathbf{n} = (\sigma_{ij}n_j)$ ; see Figure 1.2. It can also be shown that  $\boldsymbol{\sigma}$  is symmetric:  $\sigma_{ij} = \sigma_{ji}$ . In an isotropic material (one with no built-in directionality), there are also some invariance requirements with respect to translations and rotations.

Thus far, our analysis could apply to any fluid. The force term in the equation of motion takes the form

$$\int_{\partial V} \boldsymbol{\sigma} \cdot \mathbf{n} dS, \quad \text{with components} \quad \int_{\partial V} \sigma_{ij}n_j dS$$

We are using the summation convention, where by terms with repeated indices are summed over from 1 to 3; thus for example

$$\sigma_{ii} = \sigma_{11} + \sigma_{22} + \sigma_{33}.$$

It should be clear that

$$\nabla \cdot \mathbf{u} = \partial u_i / \partial x_i$$

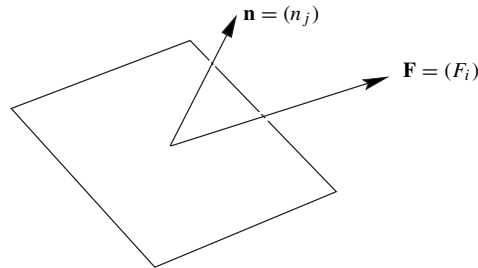
and that

$$(\nabla \cdot \boldsymbol{\sigma})_i = \frac{\partial \sigma_{ij}}{\partial x_j}.$$



10 The basics of modelling

**Figure 1.2** Force on a small surface element.



which by the divergence theorem is equal to

$$\int_{\partial V} \nabla \cdot \boldsymbol{\sigma} \, dS, \quad \text{with components} \quad \int_{\partial V} \frac{\partial \sigma_{ij}}{\partial x_j} \, dS,$$

and so we have the equation of motion

$$\frac{D(\rho \mathbf{u})}{Dt} = \nabla \cdot \boldsymbol{\sigma}. \tag{1.2}$$

We now have to say what kind of fluid we are dealing with. That is, we have to give a constitutive relation to specify  $\boldsymbol{\sigma}$  in terms of the fluid velocity, pressure etc. For an inviscid fluid, the only internal forces are those due to pressure, which acts isotropically. The pressure force on our volume element is

$$\int_{\partial V} -p \mathbf{n} \, dS$$

with corresponding stress tensor

$$\sigma_{ij} = -p \delta_{ij},$$

Which matrix has entries  $\delta_{ij}$ ?  
 Interpret  $\delta_{ij} v_j = v_i$  in matrix terms.

where  $\delta_{ij}$  is the Kronecker delta. This clearly leads to the Euler momentum-conservation equation

$$\rho \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p.$$

When the fluid is viscous, we need to add on the contribution due to viscous-shear forces. From consideration of the experiment of Figure 1.1 it is very reasonable that the new term should be linear in the velocity gradients, and it can be shown, bearing in mind the invariance requirements mentioned above, that the appropriate form for  $\sigma_{ij}$  is

$$\sigma_{ij} = -p \delta_{ij} + \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right).$$

For future reference we write out the components of  $\sigma$  in two dimensions:

$$(\sigma_{ij}) = \begin{pmatrix} -p + 2\mu \frac{\partial u}{\partial x} & \mu \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \\ \mu \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) & -p + 2\mu \frac{\partial v}{\partial y} \end{pmatrix}. \quad (1.3)$$

Substituting this into the general equation of motion (1.2), and using the incompressibility condition  $\nabla \cdot \mathbf{u} = \partial u_i / \partial x_i = 0$ , it is a straightforward *exercise* to show that the equation of motion of a viscous fluid is

The emphasis means that it is a good idea to do it.

$$\rho \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \mu \nabla^2 \mathbf{u}, \quad \nabla \cdot \mathbf{u} = 0. \quad (1.4)$$

These equations are known as the *Navier–Stokes equations*. The first contains the corresponding inviscid terms, i.e. the Euler equations, but with the new term  $\mu \nabla^2 \mathbf{u}$ , which represents the influence of viscosity. As we shall see later, this term has profound effects.

### 1.4 Conservation laws

Perhaps we should elaborate on the ‘usual argument’ that, allegedly, leads to equation (1.1). Whenever we work in a continuous framework, and we have a quantity that is conserved, we offset changes in its *density*  $P(\mathbf{x}, t)$  with equal and opposite changes in its *flux*  $\mathbf{q}(\mathbf{x}, t)$ . Taking a small volume  $V$  and arguing as above, we have

$$\frac{d}{dt} \int_V P(\mathbf{x}, t) \, d\mathbf{x} + \int_{\partial V} \mathbf{q} \cdot \mathbf{n} \, dS = 0,$$

the first term being the time rate of change in the quantity inside  $V$ , and the second the net flux of it into  $V$ . Applying Green’s theorem to this latter integral,<sup>4</sup> we have

$$\int_V \frac{\partial P}{\partial t} + \nabla \cdot \mathbf{q} \, d\mathbf{x} = 0.$$

As  $V$  is arbitrary, we conclude that

$$\frac{\partial P}{\partial t} + \nabla \cdot \mathbf{q} = 0,$$

a statement that is often referred to as a *conservation law*.<sup>5</sup>

<sup>4</sup> Needless to say, this argument requires  $\mathbf{q}$  to be sufficiently smooth, which can usually be verified *a posteriori*; in Chapter 7 we shall explore some cases where this smoothness is not present.

<sup>5</sup> Sometimes this term is reserved for cases in which  $\mathbf{q}$  is a function of  $P$  alone.