

Chapter 1

Basics of Hydrodynamics and Kinetic Theory

Abstract After reading this chapter, you will have a working understanding of the equations of fluid mechanics, which describe a fluid's behaviour through its conservation of mass and momentum. You will understand the basics of the kinetic theory on which the lattice Boltzmann method is founded. Additionally, you will have learned about how different descriptions of a fluid, such as the continuum fluid description and the mesoscopic kinetic description, are related.

While the lattice Boltzmann method (LBM) has found applications in fields as diverse as quantum mechanics and image processing, it has historically been and predominantly remains a computational fluid dynamics method. This is also the spirit of this book in which we largely develop and apply the LBM for solving fluid mechanics phenomena.

To facilitate discussions in subsequent chapters, we summarise in Sect. 1.1 the most basic theory of fluid dynamics. In particular, we will review the continuity, Navier-Stokes and energy equations which are direct consequences of conservation of mass, momentum and energy. However, fluid dynamics is a *continuum* description of fluids which treats them as continuous blobs of matter, ignoring the fact that matter is made up of individual molecules. Section 1.2 discusses various representations of a fluid, from the continuum level to the atomic level. Section 1.3 gives a basic introduction to *kinetic theory*, a finer description of a fluid where we track the evolution of its constituent molecules' *distributions* in coordinate and velocity space. The LBM springs from kinetic theory, making this description fundamental to this book.

1.1 Navier-Stokes and Continuum Theory

We give an overview of fluid dynamics, in particular the continuity equation (cf. Sect. 1.1.1), the Navier-Stokes equation (NSE, cf. Sect. 1.1.2) and the equation of state (cf. Sect. 1.1.3). This section is necessarily somewhat brief and cannot replace a proper fluid dynamics textbook, such as [1–4].

Throughout this book we utilise the index notation, using Greek indices to denote an arbitrary component of a vector or a tensor, e.g. $f_\alpha \in \{f_x, f_y, f_z\}$. Repeated indices

imply a summation, e.g. $a_\beta b_\beta = \sum_\beta a_\beta b_\beta = \mathbf{a} \cdot \mathbf{b}$. This style of notation is explained in more depth in Appendix A.1.

1.1.1 Continuity Equation

The field of fluid dynamics concerns itself with *macroscopic* phenomena of fluid motion. This implies that the fluid concept is a continuum one. Even when we speak about a fluid element, such a volume contains many molecules. This fluid element is small with respect to the system size, but is large in comparison to the size of each individual molecule and the typical distance between them. We will discuss the breakdown of this assumption in Sect. 1.2, but for most applications in fluid dynamics this is a very robust approximation.

Let us now consider a small fluid element with density ρ which occupies some stationary volume V_0 . The mass of this fluid element is simply $\int_{V_0} \rho \, dV$. If we consider the change of this mass per unit time, it must be due to fluid flow into or out of the volume element because fluid mass cannot be created or destroyed. Mathematically, this may be written as

$$\frac{\partial}{\partial t} \int_{V_0} \rho \, dV = - \oint_{\partial V_0} \rho \mathbf{u} \cdot d\mathbf{A} \quad (1.1)$$

where the closed area integral is taken over the boundary ∂V_0 of the volume element V_0 , \mathbf{u} is the fluid velocity, and we take the outward normal as the direction of $d\mathbf{A}$. The surface integral on the right-hand side of (1.1) can be transformed into a volume integral using the divergence theorem to give

$$\int_{V_0} \frac{\partial \rho}{\partial t} \, dV = - \int_{V_0} \nabla \cdot (\rho \mathbf{u}) \, dV. \quad (1.2)$$

This leads to

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (1.3)$$

since the volume V_0 is stationary and arbitrary. Equation (1.3) is the **continuity equation** in fluid dynamics. It is a partial differential equation (PDE) reflecting the conservation of mass. The vector

$$\rho \mathbf{u} = \mathbf{j} \quad (1.4)$$

is called the **momentum density** or **mass flux density**.

In the literature, the continuity equation is also sometimes written in the forms

$$\frac{\partial \rho}{\partial t} + \mathbf{u} \cdot \nabla \rho + \rho \nabla \cdot \mathbf{u} = 0 \quad \text{or} \quad \frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{u} = 0. \quad (1.5)$$

Here we have introduced the *material derivative*

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \quad (1.6)$$

which denotes the rate of change as the fluid element moves about in space, rather than the rate of change $\partial/\partial t$ at a fixed point in space.

Exercise 1.1 Fluid conservation equations can be given in two main forms: *conservation form*, as in (1.3), or *material derivative form*, as in (1.5). Using the continuity equation, (1.3), show that for a general conserved quantity λ the two forms can be related as

$$\frac{\partial(\rho\lambda)}{\partial t} + \nabla \cdot (\rho\mathbf{u}\lambda) = \rho \frac{D\lambda}{Dt}. \quad (1.7)$$

1.1.2 Navier-Stokes Equation

Similar to our analysis above, we can consider the change of momentum of a fluid element with density ρ and velocity \mathbf{u} , occupying a small volume V_0 . For a simple ideal fluid, the change of net momentum can be due to (i) flow of momentum into or out of the fluid element, (ii) differences in pressure p and (iii) external body forces \mathbf{F} . Each of these contributions is written respectively on the right-hand side of the following momentum balance equation:

$$\frac{d}{dt} \int_{V_0} \rho \mathbf{u} \, dV = - \oint_{\partial V_0} \rho \mathbf{u} \mathbf{u} \cdot d\mathbf{A} - \oint_{\partial V_0} p \, d\mathbf{A} + \int_{V_0} \mathbf{F} \, dV. \quad (1.8)$$

Here, $\mathbf{u} \mathbf{u}$ denotes the outer product with components $u_\alpha u_\beta$. Transforming the surface integrals into volume integrals using the divergence theorem, the above equation can be rewritten as

$$\int_{V_0} \frac{\partial(\rho \mathbf{u})}{\partial t} \, dV = - \int_{V_0} \nabla \cdot (\rho \mathbf{u} \mathbf{u}) \, dV - \int_{V_0} \nabla p \, dV + \int_{V_0} \mathbf{F} \, dV. \quad (1.9)$$

This leads to the **Euler equation**:

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \mathbf{F}, \quad (1.10)$$

a PDE describing the conservation of momentum for an ideal fluid.

This momentum equation can be written in a more general form, called the **Cauchy momentum equation**:

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot \boldsymbol{\Pi} = \mathbf{F}. \quad (1.11)$$

Here we have used the **momentum flux density tensor**, defined as

$$\Pi_{\alpha\beta} = \rho u_\alpha u_\beta - \sigma_{\alpha\beta}. \quad (1.12)$$

The term $\sigma_{\alpha\beta}$ is called the **stress tensor** and corresponds to the non-direct momentum transfer of the moving fluid. For simple fluids described by the Euler equation we find an isotropic stress $\sigma_{\alpha\beta} = -p\delta_{\alpha\beta}$; the stress tensor contains diagonal elements which are the same in all directions.

The momentum flux transfer in the Euler equation only includes momentum transfer which is reversible, either through the flow of mass or due to pressure forces which are conservative. For real fluids, we need to include a viscosity or internal friction term which causes dissipative and irreversible transfer of momentum from one fluid element to another, neighbouring element.

To establish the form of this *viscous stress tensor* $\boldsymbol{\sigma}'$, we first argue that such contribution must be zero when the flow is uniform, including rigid body translation and rotation. We may further argue that if the velocity gradients are small, then momentum transfer due to viscosity is well captured by terms which are proportional to the first derivatives of the velocity only [3]. A general tensor of rank two satisfying these two arguments is

$$\sigma'_{\alpha\beta} = \eta \left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} \right) + \zeta \delta_{\alpha\beta} \frac{\partial u_\gamma}{\partial x_\gamma} \quad (1.13)$$

where η and ζ are coefficients of viscosity. They are usually assumed to be isotropic and uniform, though this assumption will break down for more complex fluids.

The viscous stress tensor is often separated into a traceless *shear stress* and a *normal stress*:

$$\sigma'_{\alpha\beta} = \eta \left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} - \frac{2}{3} \delta_{\alpha\beta} \frac{\partial u_\gamma}{\partial x_\gamma} \right) + \eta_B \delta_{\alpha\beta} \frac{\partial u_\gamma}{\partial x_\gamma}. \quad (1.14)$$

The first viscosity coefficient η is usually called the *shear viscosity* while the combination $\eta_B = 2\eta/3 + \zeta$ is normally called the *bulk viscosity*.

With the total stress tensor given as the sum of the pressure and viscosity contributions,

$$\sigma_{\alpha\beta} = \sigma'_{\alpha\beta} - p\delta_{\alpha\beta}, \quad (1.15)$$

we are now ready to write down the full momentum equation for a viscous fluid. Inserting (1.14) and (1.15) into (1.11), we obtain the **Navier-Stokes equation**

$$\begin{aligned} \frac{\partial(\rho u_\alpha)}{\partial t} + \frac{\partial(\rho u_\alpha u_\beta)}{\partial x_\beta} \\ = -\frac{\partial p}{\partial x_\alpha} + \frac{\partial}{\partial x_\beta} \left[\eta \left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} \right) + \left(\eta_B - \frac{2\eta}{3} \right) \frac{\partial u_\gamma}{\partial x_\gamma} \delta_{\alpha\beta} \right] + F_\alpha. \end{aligned} \quad (1.16)$$

Assuming the viscosities are constant, this can be simplified to give

$$\rho \frac{Du_\alpha}{Dt} = -\frac{\partial p}{\partial x_\alpha} + \eta \frac{\partial^2 u_\alpha}{\partial x_\beta \partial x_\beta} + \left(\eta_B + \frac{\eta}{3} \right) \frac{\partial^2 u_\beta}{\partial x_\alpha \partial x_\beta} + F_\alpha. \quad (1.17)$$

The NSE can be simplified considerably if the flow may be regarded as incompressible with $\rho = \text{const}$, so that the continuity equation, (1.3), reduces to $\nabla \cdot \mathbf{u} = 0$. In this case, we can write the NSE in its most common form, the **incompressible Navier-Stokes equation**

$$\rho \frac{D\mathbf{u}}{Dt} = -\nabla p + \eta \Delta \mathbf{u} + \mathbf{F}. \quad (1.18)$$

Here, $\Delta = \nabla \cdot \nabla = \partial^2 / (\partial x_\beta \partial x_\beta)$ is the *Laplace operator*.

Exercise 1.2 Let us consider the steady shear flow known as *Couette flow* where an incompressible fluid is sandwiched between two parallel plates as shown in Fig. 1.1(a). The separation between the two plates is d in the y -direction. The bottom plate is held fixed such that $\mathbf{u} = (0, 0, 0)^\top$ while the top plate moves with velocity $\mathbf{u} = (U, 0, 0)^\top$. There is no external force applied to the system. Starting from the

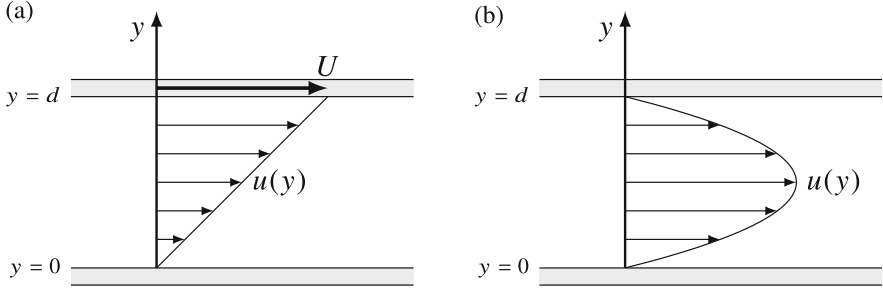


Fig. 1.1 Two fundamental steady-state flows between two plates. (a) Couette flow. (b) Poiseuille flow

incompressible NSE in (1.18), show that the velocity profile of the fluid is given by

$$u_x(y) = \frac{U}{d}y. \quad (1.19)$$

You should assume that there is no slip between the fluid and the parallel plates. In other words, the velocity of the fluid near the wall is equal to that of the wall.

Exercise 1.3 Let us now consider a steady, incompressible fluid flow commonly known as *Poiseuille flow*. The fluid is enclosed between two parallel plates and is moving in the x -direction, as shown in Fig. 1.1(b). The separation between the two plates is d along the y -axis. Poiseuille flow can in fact be driven by either (i) a constant pressure gradient or (ii) an external body force (such as gravity) in the x -direction. Assume the no-slip boundary condition between the fluid and the plates.

- (a) For a pressure gradient driven flow, show that the fluid velocity profile is given by

$$u_x(y) = -\frac{1}{2\eta} \frac{dp}{dx} y(y-d). \quad (1.20)$$

- (b) Derive the corresponding velocity profile when the flow is driven by an external body force.

1.1.3 Equations of State

At this point we have four equations that describe the behaviour of a fluid. The continuity equation, (1.3), describes the conservation of mass. The conservation of

momentum is described by the Euler equation or the Navier-Stokes equation (one equation for each of the three spatial components) in (1.10) and (1.16), respectively.¹

However, this system of equations is not closed. While we have five unknowns (density ρ , pressure p and the three velocity components u_x, u_y, u_z), we have only four equations to describe their evolution. Consequently, the system of equations is *unsolvable*, unless we can fix variables, e.g. by assuming the density to be constant.

We can add another equation to the system thanks to the *state principle* of equilibrium thermodynamics [2]. It relates the *state variables* that describe the local thermodynamic state of the fluid, such as the density ρ , the pressure p , the temperature T , the internal energy e , and the entropy s . We will defer a more detailed description of the temperature, the internal energy, and the entropy to Sect. 1.3. The state principle declares that any of these state variables can be related to any other two state variables through an *equation of state* [2].

The most famous such equation of state is the **ideal gas law**,

$$p = \rho RT. \quad (1.21)$$

It relates the pressure to the density and the temperature through the *specific gas constant* R , with units $[R] = \text{J}/(\text{kg K})$.²

Another equation of state for ideal gases expresses the pressure as a function of the density and the entropy, [2]

$$\frac{p}{p_0} = \left(\frac{\rho}{\rho_0} \right)^\gamma e^{(s-s_0)/c_V}. \quad (1.22)$$

The constants p_0, ρ_0 and s_0 refer to values at some constant reference state. This equation makes use of the heat capacities at *constant volume* c_V and *constant pressure* c_p and their ratio γ , also known as the *adiabatic index*. These are defined generally as [2]

$$c_V = \left(\frac{\partial e}{\partial T} \right)_V, \quad c_p = \left(\frac{\partial(e + p/\rho)}{\partial T} \right)_p, \quad \gamma = \frac{c_p}{c_V}. \quad (1.23)$$

In an ideal gas, the two heat capacities are related as $c_p = c_V + R$.

¹A fifth conservation equation for energy can also be derived, though we will only briefly address it later in Sect. 1.3.5 since it is less important both in fluid mechanics and in the LBM.

²The ideal gas law is expressed in many forms throughout science, often with quantities given in moles. Equation (1.21) is expressed using the state variables employed in fluid mechanics, the cost being that the specific gas constant R *varies between different gases*. Here, $R = k_B/m$, where k_B is Boltzmann's constant and m is the mass of the a gas molecule.

The attentive reader may have realised that any equation of state must introduce a *third* variable into the system of equations: for instance, (1.21) introduces the temperature T and (1.22) introduces the entropy s . Consequently, introducing the equation of state does not itself directly close the system of equations. The system can only be fully closed if an equation that describes the evolution of the third state variable is also derived from the aforementioned energy equation. However, the resulting system of equations is very cumbersome.

Instead, introducing the equation of state gives us more options to close the system of equations through suitable approximations. For example, most of acoustics is based on the assumption that s is approximately constant [2, 5]. This simplifies (1.22) to the *isentropic equation of state*

$$p = p_0 \left(\frac{\rho}{\rho_0} \right)^\gamma \quad (1.24)$$

and closes the system of equations.

In some cases we can also approximate the fluid as having a constant temperature $T \approx T_0$, which simplifies (1.21) to the **isothermal equation of state**

$$p = \rho RT_0 \quad (1.25)$$

that has a linear relationship between the pressure p and the density ρ .

Exercise 1.4 The isothermal equation of state is central to the LBM. Show that it is merely a special case of the isentropic equation of state, (1.24), with $\gamma = 1$.

Another approximation mentioned previously in Sect. 1.1.2 is the incompressible fluid of constant density $\rho = \rho_0$. In this case, an equation of state is not used since the incompressible continuity equation $\nabla \cdot \mathbf{u} = 0$ and the incompressible NSE in (1.18) are by themselves sufficient. Together, these form a closed system of four equations for the four remaining variables p , u_x , u_y and u_z .

For small deviations from a reference state, nonlinear equations of state such as (1.22) may also be approximated by linearisation. For instance, using the total differential we may linearise any equation of state $p(\rho, s)$ as also illustrated in Fig. 1.2:

$$p = p_0 + p' \approx p_0 + \left(\frac{\partial p}{\partial \rho} \right)_s \rho' + \left(\frac{\partial p}{\partial s} \right)_\rho s'. \quad (1.26)$$

Here, the derivatives are evaluated about $p = p_0$, and the primed variables represent deviations from the reference state defined by p_0 , ρ_0 , and s_0 .

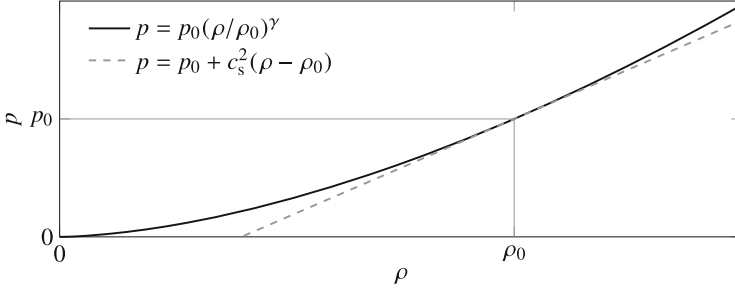


Fig. 1.2 Comparison of the isentropic equation of state in (1.24) and its linearised version in (1.27) for $\gamma = 5/3$

For the isentropic equation of state in (1.24), (1.26) is further simplified to

$$p \approx p_0 + c_s^2 \rho' \quad (1.27)$$

since the speed of sound c_s is in general given by the relation [2, 5]

$$c_s^2 = \left(\frac{\partial p}{\partial \rho} \right)_s. \quad (1.28)$$

In the case of the isentropic and isothermal equations of state in (1.24) and (1.25), we find that $c_s = \sqrt{\gamma RT_0}$ and $c_s = \sqrt{RT_0}$, respectively.

Note that the constant reference pressure p_0 is completely insignificant to the NSE as only the pressure gradient $\nabla p = \nabla(p_0 + p') = \nabla p'$ is present in the equation.³ Therefore, the isothermal equation of state, which can be expressed as

$$p = c_s^2 \rho \implies p = c_s^2 \rho_0 + c_s^2 \rho', \quad (1.29)$$

can be used to model other equations of state in the linear regime if the entropy is nearly constant: as long as the speed of sound is matched, it does not matter if the reference pressure p_0 is different.

1.2 Relevant Scales

As discussed in the previous section, the mathematical descriptions of fluid dynamics rely on the continuum assumption where we operate at length and time scales sufficiently large that the atomistic picture can be averaged out. To formalise this discussion, let us start by considering the hierarchy of length scales associated with

³While p_0 is relevant to the energy equation that we will see later in Sect. 1.3.5, this equation is usually not taken into account in LB simulations.

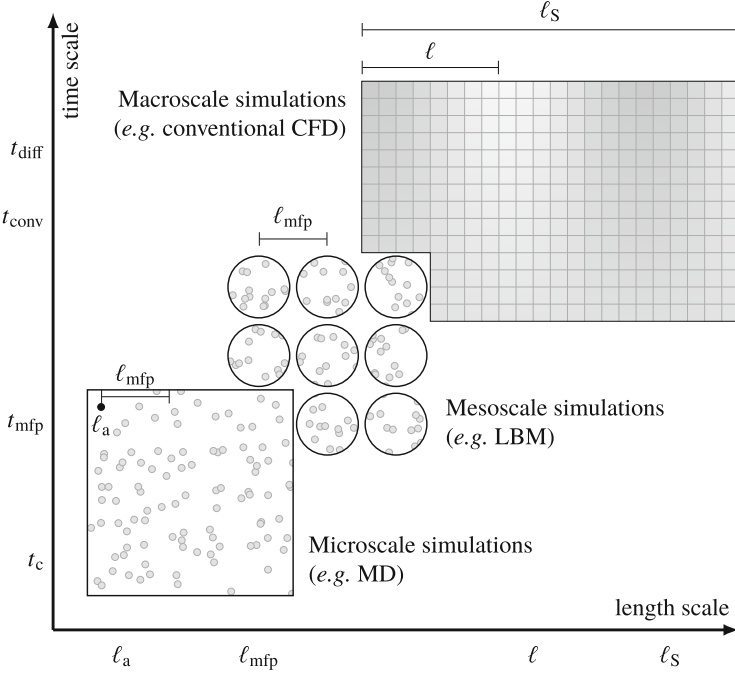


Fig. 1.3 The hierarchy of length and time scales in typical fluid dynamics problems. Depending on the level of details required, different simulation techniques are suitable

a typical fluid flow problem. If we stay within the classical mechanics picture, from small to large, we have (i) the size of the fluid atom or molecule ℓ_a , (ii) the mean free path (distance travelled between two successive collisions) ℓ_{mfp} , (iii) the typical scale for gradients in some macroscopic properties ℓ and (iv) the system size ℓ_s . The typical ordering of these length scales is $\ell_a \ll \ell_{mfp} \ll \ell \leq \ell_s$, as illustrated in Fig. 1.3.

In the context of fluids, one often refers to **microscopic**, **mesoscopic** and **macroscopic** descriptions as depicted in Fig. 1.3. In this book, “microscopic” denotes a molecular description and “macroscopic” a fully continuum picture with tangible quantities such as fluid velocity and density. Microscopic systems are therefore governed by Newton’s dynamics, while the NSE is the governing equation for a fluid continuum. In between the microscopic and macroscopic description, however, is the “mesoscopic” description which does not track individual molecules. Rather, it tracks *distributions* or *representative collections* of molecules. Kinetic theory, which we will come back to in Sect. 1.3, is the mesoscopic fluid description on which the LBM is based.

Coupled to this hierarchy of length scales is the hierarchy of time scales. At very short times, we can define the collision time $t_c \sim \ell_a/v_T$, i.e. the duration of a collision event where $v_T = (k_B T/m)^{1/2}$ is the average thermal velocity of the molecules. Within Boltzmann's standard kinetic theory, we usually assume $t_c \rightarrow 0$, i.e. collisions happen instantaneously. Note that the thermal velocity v_T is different from the macroscopic fluid velocity, $u \ll v_T$.⁴ Next we can define the mean flight time between two successive collisions, $t_{\text{mfp}} = \ell_{\text{mfp}}/v_T$. This is the time scale at which kinetic theory operates and where the system relaxes to local equilibrium through collision events. Local equilibrium, however, does not mean that the system is in global equilibrium. In fact, the opposite is often the case, and we are interested in studying these situations.

At longer time and larger length scales, there can exist hydrodynamic flow from one region of the fluid to another. Depending on whether we have advective (inertial regime) or diffusive (viscous regime) dynamics, the shortest (most relevant) time scale is either $t_{\text{conv}} \sim \ell/u$ or $t_{\text{diff}} \sim \ell^2/\nu$ where ν is the kinematic viscosity. The kinetic viscosity is related to the dynamic shear viscosity by $\eta = \rho\nu$. The ratio between these two hydrodynamic time scales is the well-known *Reynolds number*:

$$\text{Re} = \frac{t_{\text{diff}}}{t_{\text{conv}}} = \frac{u\ell}{\nu}. \quad (1.30)$$

Both high and low Reynolds number flows are of interest. High Reynolds number flows, on the one hand, are usually dominated by turbulence and are relevant for vehicle aerodynamics, building designs, and many other applications. On the other hand, there is a surge of interest in low Reynolds number flows due to their importance in microfluidics and biophysics.

Another important macroscopic time scale is the acoustic time scale, $t_{\text{sound}} \sim \ell/c_s$, where c_s is the speed of sound in the fluid. This time scale determines how fast compression waves propagate in the fluid. When the acoustic time scale is fast in comparison to the advective time scale, the fluid behaves similarly to an incompressible fluid. Otherwise, the fluid compressibility is an important factor, which provides a number of additional physics such as shock waves. The *Mach number*

$$\text{Ma} = \frac{t_{\text{sound}}}{t_{\text{conv}}} = \frac{u}{c_s} \quad (1.31)$$

defines the ratio between the acoustic and advective time scales. In practice, we can usually assume steady fluid flow with $\text{Ma} \leq 0.1$ to be incompressible.

We emphasise that there are a number of situations where the above-mentioned ordering of length and time scales is not satisfied. Examples include flows of rarified gases and nanofluidics. For the former, the mean free path becomes large enough so that it is comparable to the macroscopic length scale: $\ell_{\text{mfp}} \sim \ell$. On the other

⁴However, the thermal velocity v_T is of the order of the speed of sound c_s [2].

hand, the miniaturisation of fluidic devices makes the system size in nanofluidics comparable to the mean free path: $\ell_S \sim \ell_{\text{mfp}}$. A particularly useful parameter is therefore the *Knudsen number*

$$\text{Kn} = \frac{\ell_{\text{mfp}}}{\ell} \quad (1.32)$$

that defines the ratio between the mean free path and the representative physical length scale. For $\text{Kn} \ll 1$, the hydrodynamic picture (Navier-Stokes) is valid, whereas for $\text{Kn} \gtrsim 1$, one has to go back to the kinetic theory description. As we shall see later in Sect. 1.3.5, the Knudsen number is in fact the (small) expansion parameter used in the Chapman-Enskog theory to derive the NSE from the Boltzmann equation. The Knudsen number is also closely related to the Mach and Reynolds numbers. It was first shown by von Kármán that

$$\text{Kn} = \alpha \frac{\text{Ma}}{\text{Re}} \quad (1.33)$$

with α being a numerical constant. This relation is thus known as the *von Kármán relation*.

Dimensionless numbers such as the Reynolds, Knudsen and Mach numbers proliferate in the fluid mechanics literature. These numbers are in fact very useful. Primarily, we must appreciate that fluid flows which share the same dimensionless numbers provide the same physics upon a simple scaling by the typical length and velocity scales in the problem. This important statement is called the **law of similarity**.

To illustrate this, let us rewrite the incompressible NSE of (1.18) in its dimensionless form. We renormalise any length scale in the system by ℓ and velocity by the mean fluid velocity V , such that

$$\mathbf{u}^* = \frac{\mathbf{u}}{V}, \quad p^* = \frac{p}{\rho V^2}, \quad \mathbf{F}^* = \frac{\mathbf{F}\ell}{\rho V^2}, \quad \frac{\partial}{\partial t^*} = \frac{\ell}{V} \frac{\partial}{\partial t}, \quad \nabla^* = \ell \nabla \quad (1.34)$$

and hence

$$\frac{d\mathbf{u}^*}{dt^*} = -\nabla^* p^* + \frac{1}{\text{Re}} \Delta^* \mathbf{u}^* + \mathbf{F}^*. \quad (1.35)$$

As already mentioned before, the Reynolds number measures the relative importance of inertial to viscous terms in the NSE.

It is important to keep in mind that not all dimensionless numbers can be identical when comparing flows at smaller and larger length or time scales. Even if the

Reynolds number of two systems is the same, the Mach or Knudsen numbers are usually not. However, as long as the ordering of length and time scales is the same, their exact values often do not matter much. The key here is usually the separation of length and time scales. For example, if the Knudsen or Mach number is sufficiently small, their actual values are irrelevant for the hydrodynamic flows of interests where the Reynolds number is the key parameter. Therefore, usually it can be argued that all flows with the same Reynolds number are comparable to one another. In Chap. 7 we will get back to the non-dimensionalisation and how to take advantage of the law of similarity to convert parameters from the physical world to a simulation and back.

1.3 Kinetic Theory

Here we provide a concise summary of kinetic theory, the cornerstone of the LBM. Following the introduction in Sect. 1.3.1, we introduce the particle distribution function in Sect. 1.3.2. As we will see in later chapters, the assumption of a local equilibrium (cf. Sect. 1.3.3) is a crucial component of the LBM. Kinetic theory provides a kinetic description of gases; as such, molecular collisions play a central role. In Sect. 1.3.4 we discuss the collision operator in the Boltzmann equation. Conservation laws, such as mass and momentum conservation, follow from kinetic theory (cf. Sect. 1.3.5). Finally, we touch upon Boltzmann's \mathcal{H} -theorem in Sect. 1.3.6.

1.3.1 Introduction

As mentioned in Sect. 1.2, kinetic theory is a fluid description that lies between the *microscopic* scale where we track the motion of individual molecules and the *macroscopic* scale where we describe the fluid using more tangible quantities such as density, fluid velocity, and temperature. In the *mesoscopic* kinetic theory, we describe the *distribution* of particles in a gas, a quantity which evolves on timescales around the mean collision time t_{mfp} .

While kinetic theory can in principle be used to describe any fluid, it is most commonly applied to the simplest case of a dilute gas. There we can assume that the constituent molecules spend very little of their time actually *colliding* (i.e. $t_c \ll t_{\text{mfp}}$, using the terminology of Sect. 1.2). This is equivalent to assuming that the molecules almost always collide one-on-one, with three particles almost never simultaneously being involved in a collision. This assumption does not hold as well for dense gases where molecules are closer together and therefore spend more of their time colliding, and it does not hold at all for liquids where molecules are held close to each other by intermolecular attracting forces and thus constantly interact. While it

is possible to formulate a kinetic theory of liquids [6], this is much more difficult than for dilute gases.

For simplicity, we will constrain our discussion in this section to the kinetic theory of *dilute monatomic* gases. Single atoms collide elastically, so that all translational energy is conserved in a collision. On the other hand, molecules consisting of several atoms have inner degrees of freedom; they may contain rotational and vibrational energy. Therefore, while total energy is always conserved in collisions, a collision between two such molecules may also be *inelastic* (i.e. translational energy becomes rotational or vibrational energy) or *superelastic* (i.e. rotational or vibrational energy becomes translational energy). In addition, molecular rotation and vibration must be treated quantum mechanically. The kinetic theory of polyatomic gases can be found in the literature [7–10]. However, the macroscopic behaviour of polyatomic and monatomic gases is largely similar.

Apart from the quantisation of rotational and vibrational energy in polyatomic gases, the kinetic theory of gases can be considered to be completely classical physics, as it is a statistical description of a large number of particles. As per Bohr's correspondence principle, the quantum behaviour of a system reduces to classical behaviour when the system becomes large enough.

1.3.2 The Distribution Function and Its Moments

The fundamental variable in kinetic theory is the particle **distribution function** $f(\mathbf{x}, \boldsymbol{\xi}, t)$. It can be seen as a generalisation of density ρ which also takes the microscopic *particle velocity* $\boldsymbol{\xi}$ into account. While $\rho(\mathbf{x}, t)$ represents the density of mass in *physical* space, $f(\mathbf{x}, \boldsymbol{\xi}, t)$ simultaneously represents the density of mass in both three-dimensional *physical* space *and* in three-dimensional *velocity* space. Therefore, f has the units

$$[f] = \text{kg} \times \frac{1}{\text{m}^3} \times \frac{1}{(\text{m/s})^3} = \frac{\text{kg s}^3}{\text{m}^6}. \quad (1.36)$$

In other words, the distribution function $f(\mathbf{x}, \boldsymbol{\xi}, t)$ represents the density of particles with velocity $\boldsymbol{\xi} = (\xi_x, \xi_y, \xi_z)$ at position \mathbf{x} and time t .

Example 1.1 To demonstrate how the distribution function extends the concept of density, let us consider a gas in a box of size $V = L_x \times L_y \times L_z$, as shown in Fig. 1.4. The total mass of the gas inside the box is of course given by the integral of the density over the box, $\int_V \rho \, d^3x$. We can also calculate more specific things using the density: for instance, the mass in the *left half* of the box is $\int_{x=0}^{x=L_x/2} \rho \, d^3x$. The distribution function f would let us find even more specific things: for example, the

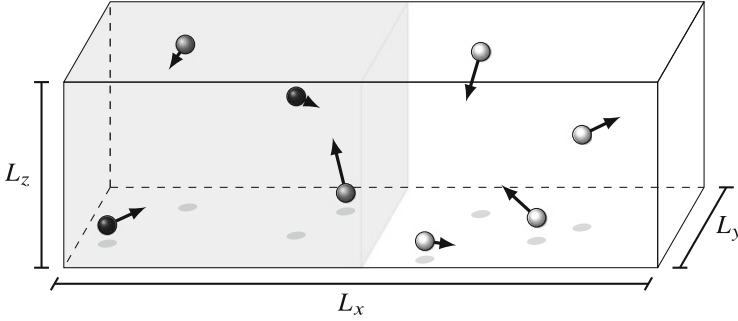


Fig. 1.4 Particles in a box. *Right-moving* particles in the *left half* of the box are marked as black. The total mass of such particles can be found from f as in (1.37)

mass of *right-moving* particles, i.e. particles with $\xi_x > 0$, in the *left half* of the box is

$$\int_{x=0}^{x=L_x/2} \int_{\xi_x > 0} f \, d^3\xi \, d^3x. \quad (1.37)$$

The distribution function f is also connected to macroscopic variables like the density ρ and the fluid velocity u from its **moments**. These moments are integrals of f , weighted with some function of ξ , over the entire velocity space. For instance, the macroscopic **mass density** can be found as the moment

$$\rho(\mathbf{x}, t) = \int f(\mathbf{x}, \xi, t) \, d^3\xi. \quad (1.38a)$$

By integrating over velocity space in this way, we are considering the contribution to the density of particles of *all possible velocities* at position \mathbf{x} and time t .

We can also consider the particles' contribution ξf to the momentum density. Again considering all possible velocities, we find the macroscopic **momentum density** as the moment

$$\rho(\mathbf{x}, t) \mathbf{u}(\mathbf{x}, t) = \int \xi f(\mathbf{x}, \xi, t) \, d^3\xi. \quad (1.38b)$$

Similarly, we can find the macroscopic **total energy density** as the moment

$$\rho(\mathbf{x}, t) E(\mathbf{x}, t) = \frac{1}{2} \int |\xi|^2 f(\mathbf{x}, \xi, t) \, d^3\xi. \quad (1.38c)$$

(continued)

This contains two types of energy; the energy $\frac{1}{2}\rho|\mathbf{u}|^2$ due to the bulk motion of the fluid and the internal energy due to the random thermal motion of the gas particles. It is also possible to find only the latter type, the macroscopic **internal energy density**, as the moment

$$\rho(\mathbf{x}, t)e(\mathbf{x}, t) = \frac{1}{2} \int |\mathbf{v}|^2 f(\mathbf{x}, \boldsymbol{\xi}, t) d^3\xi. \quad (1.38d)$$

Here we have introduced the **relative velocity** \mathbf{v} , which is the deviation of the particle velocity from the local mean velocity:

$$\mathbf{v}(\mathbf{x}, t) = \boldsymbol{\xi}(\mathbf{x}, t) - \mathbf{u}(\mathbf{x}, t). \quad (1.39)$$

These expressions for the fluid energy only consider the *translational* energy of the molecules, i.e. the energy due to the movement with their velocity $\boldsymbol{\xi}$. In the more difficult kinetic theory of polyatomic gases, the internal energy must include additional degrees of freedom, such as molecular vibrational and rotational energies.

Exercise 1.5 Consider a somewhat unrealistic spatially homogeneous gas where all particles are moving with the same velocity \mathbf{u} so that the distribution function is $f(\mathbf{x}, \boldsymbol{\xi}, t) = \rho \delta(\boldsymbol{\xi} - \mathbf{u})$. Verify from its moments that its density is ρ and its momentum density is $\rho\mathbf{u}$. Additionally, find its moments of total energy density and internal energy density.

Exercise 1.6

(a) Show that the relative velocity moment of f is

$$\int \mathbf{v} f(\mathbf{x}, \boldsymbol{\xi}, t) d^3\xi = 0. \quad (1.40a)$$

(b) Using this and the identity $|\mathbf{v}|^2 = |\boldsymbol{\xi}|^2 - 2(\boldsymbol{\xi} \cdot \mathbf{u}) + |\mathbf{u}|^2$, show that the total and internal energy densities at a given position and time are related as

$$\rho e = \rho E - \frac{1}{2}\rho|\mathbf{u}|^2. \quad (1.40b)$$

We can also find the pressure as a moment of the distribution function. There are several ways to do this. The most direct route, presented, e.g., in [11, 12], is to consider that particles impart momentum when bouncing off a surface. At higher particle velocities, more momentum is imparted, and more particles can bounce off in a given time. A closer analysis results in an expression for pressure as a moment of f .

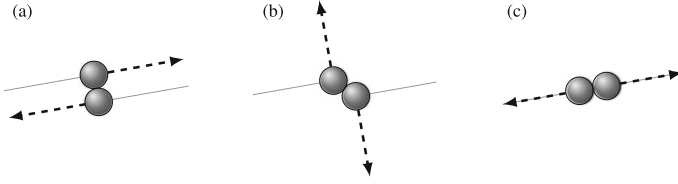


Fig. 1.5 Some collisions between hard spheres, with incoming paths shown in grey and outgoing paths in black. (a) Grazing collision. (b) Angled collision. (c) Head-on collision

A shortcut to the same expression for pressure can be made by using the equipartition theorem of classical statistical mechanics. This gives a specific internal energy density of $RT/2$ for each *degree of freedom* [2]. These degrees of freedom are typically molecular translation, vibration, and rotation. For monatomic gases, there is no inner molecular structure and there can be no vibration or rotation, leaving only the translational movement in the three spatial dimensions.

Thus, with three degrees of freedom, we can use the ideal gas law in (1.21) and find for an ideal monatomic gas that

$$\rho e = \frac{3}{2} \rho RT = \frac{3}{2} p. \quad (1.41)$$

Consequently, both the pressure and the temperature can be found proportional through the same moment as internal energy:

$$p = \rho RT = \frac{2}{3} \rho e = \frac{1}{3} \int |\mathbf{v}|^2 f(\mathbf{x}, \boldsymbol{\xi}, t) d^3 \boldsymbol{\xi}. \quad (1.42)$$

Exercise 1.7 Show from (1.41) and the heat capacity definitions in (1.23) that the specific heat capacities and the heat capacity ratio of an ideal monatomic gas are

$$c_V = \frac{3}{2} R, \quad c_p = \frac{5}{2} R \quad \implies \quad \gamma = \frac{5}{3}. \quad (1.43)$$

1.3.3 The Equilibrium Distribution Function

The outgoing directions of two elastically colliding hard spheres is highly sensitive to small variations in their initial relative positions, as illustrated in Fig. 1.5. This is not only true for hard spheres like pool balls that only really interact when they touch, but also for molecules that interact at a distance, e.g. *via* electromagnetic forces. Therefore, collisions tend to even out the angular distribution of particle velocities in a gas around the mean velocity \mathbf{u} .

Consequently, when a gas has been left alone for sufficiently long, we may assume that the distribution function $f(\mathbf{x}, \boldsymbol{\xi}, t)$ will reach an *equilibrium distribution* $f^{\text{eq}}(\mathbf{x}, \boldsymbol{\xi}, t)$ which is isotropic in velocity space around $\boldsymbol{\xi} = \mathbf{u}$: in a reference frame moving with speed \mathbf{u} , the equilibrium distribution can be expressed as $f^{\text{eq}}(\mathbf{x}, |\mathbf{v}|, t)$.

Let us perform one additional assumption: we limit our search for an equilibrium distribution to solutions of the separable form

$$f^{\text{eq}}(|\mathbf{v}|^2) = f^{\text{eq}}(v_x^2 + v_y^2 + v_z^2) = f_{1\text{D}}^{\text{eq}}(v_x^2) f_{1\text{D}}^{\text{eq}}(v_y^2) f_{1\text{D}}^{\text{eq}}(v_z^2). \quad (1.44a)$$

In other words, we assume that the 3D equilibrium distribution is the product of three 1D equilibrium distributions.

If we hold the magnitude of the velocity constant, i.e. with $|\mathbf{v}|^2 = v_x^2 + v_y^2 + v_z^2 = \text{const}$, we find that

$$f^{\text{eq}}(|\mathbf{v}|^2) = \text{const} \implies \ln f^{\text{eq}}(v_x^2) + \ln f^{\text{eq}}(v_y^2) + \ln f^{\text{eq}}(v_z^2) = \text{const}. \quad (1.44b)$$

This is fulfilled when each 1D equilibrium has a form like $\ln f_{1\text{D}}^{\text{eq}}(v_x^2) = a + b v_x^2$, with a and b being generic constants. Consequently,

$$\ln f_{1\text{D}}^{\text{eq}}(v_x) + \ln f_{1\text{D}}^{\text{eq}}(v_y) + \ln f_{1\text{D}}^{\text{eq}}(v_z) = 3a + b(v_x^2 + v_y^2 + v_z^2) = \text{const}, \quad (1.44c)$$

and the full 3D equilibrium distribution is of the form

$$f^{\text{eq}}(|\mathbf{v}|) = e^{3a} e^{b|\mathbf{v}|^2}. \quad (1.44d)$$

Since monatomic collisions conserve mass, momentum, and energy, the constants a and b can be found explicitly by demanding that f^{eq} has the same moments of density and energy as f .

Thus, the **equilibrium distribution** can be found to be

$$\begin{aligned} f^{\text{eq}}(\mathbf{x}, |\mathbf{v}|, t) &= \rho \left(\frac{3}{4\pi e} \right)^{3/2} e^{-3|\mathbf{v}|^2/(4e)} = \rho \left(\frac{\rho}{2\pi p} \right)^{3/2} e^{-p|\mathbf{v}|^2/(2\rho)} \\ &= \rho \left(\frac{1}{2\pi RT} \right)^{3/2} e^{-|\mathbf{v}|^2/(2RT)}. \end{aligned} \quad (1.45)$$

These different forms are related through (1.41).

This brief derivation follows the same lines as Maxwell's original derivation. The equilibrium distribution fulfills all the assumptions we have placed upon it, but we have not proven that it is *unique*. However, the same distribution can be

found uniquely using more substantiated statistical mechanics [11], as done later by Boltzmann. In honor of these two, this equilibrium distribution is often called the *Maxwell-Boltzmann distribution*.

Exercise 1.8 Show that the moments in (1.38), applied to the equilibrium distribution in (1.45), result in a density ρ , a fluid velocity \mathbf{u} and internal energy e . *Hint: Consider the symmetries of the integrands. If an integrand is spherically symmetric about $\mathbf{v} = \mathbf{0}$, the substitution $d^3\xi = 4\pi|\mathbf{v}|^2 d|\mathbf{v}|$ can be performed.*

1.3.4 The Boltzmann Equation and the Collision Operator

Now we know what the distribution function $f(\mathbf{x}, \boldsymbol{\xi}, t)$ represents and what we can obtain from it. But how does it evolve? We will now find the equation that describes its evolution in time. For notational clarity, we will drop explicitly writing the dependence of f on $(\mathbf{x}, \boldsymbol{\xi}, t)$.

Since f is a function of position \mathbf{x} , particle velocity $\boldsymbol{\xi}$ and time t , its total derivative with respect to time t must be

$$\frac{df}{dt} = \left(\frac{\partial f}{\partial t} \right) \frac{dt}{dt} + \left(\frac{\partial f}{\partial x_\beta} \right) \frac{dx_\beta}{dt} + \left(\frac{\partial f}{\partial \xi_\beta} \right) \frac{d\xi_\beta}{dt}. \quad (1.46)$$

Looking at each term on the right-hand side in order, we have $dt/dt = 1$, the particle velocity $dx_\beta/dt = \xi_\beta$, and from Newton's second law the specific body force $d\xi_\beta/dt = F_\beta/\rho$ which has the units of $[F/\rho] = \text{N/kg}$.

Using the common notation $\Omega(f) = df/dt$ for the total differential, we get the **Boltzmann equation**

$$\frac{\partial f}{\partial t} + \xi_\beta \frac{\partial f}{\partial x_\beta} + \frac{F_\beta}{\rho} \frac{\partial f}{\partial \xi_\beta} = \Omega(f). \quad (1.47)$$

This can be seen as a kind of advection equation: the first two terms represent the distribution function being advected with the velocity $\boldsymbol{\xi}$ of its particles. The third term represents forces affecting this velocity. On the right hand side, we have a source term, which represents the local redistribution of f due to collisions. Therefore, the source term $\Omega(f)$ is called the *collision operator*.

We know that collisions conserve the quantities of mass, momentum, and in our monatomic case, translational energy. These conservation constraints can be

represented as moments of the collision operator, similarly to those in (1.38):

$$\text{mass conservation:} \quad \int \Omega(f) d^3\xi = 0, \quad (1.48a)$$

$$\text{momentum conservation:} \quad \int \xi \Omega(f) d^3\xi = \mathbf{0}, \quad (1.48b)$$

$$\text{total energy conservation:} \quad \int |\xi|^2 \Omega(f) d^3\xi = 0, \quad (1.48c)$$

$$\text{internal energy conservation:} \quad \int |\mathbf{v}|^2 \Omega(f) d^3\xi = 0. \quad (1.48d)$$

Exercise 1.9 Show using (1.39) that the total and internal energy conservation constraints are equivalent.

Boltzmann's original collision operator is of the form of a complicated and cumbersome double integral over velocity space. It considers all the possible outcomes of two-particle collisions for any choice of intermolecular forces. However, the collision operators used in the LBM are generally based on the much simpler **BGK collision operator** [13]:

$$\Omega(f) = -\frac{1}{\tau} (f - f^{\text{eq}}). \quad (1.49)$$

This operator, named after its inventors Bhatnagar, Gross and Krook, directly captures the relaxation of the distribution function towards the equilibrium distribution. The time constant τ , which determines the speed of this equilibration, is known as the **relaxation time**. The value of τ directly determines the transport coefficients such as viscosity and heat diffusivity, as we will show later in Sect. 4.1.

Any useful collision operator must both respect the conserved quantities as expressed in (1.48) and ensure that the distribution function f locally evolves towards its equilibrium f^{eq} . The BGK operator is the simplest possible collision operator given these constraints. However, it is not as exact as Boltzmann's original operator: the BGK operator predicts a *Prandtl number*, which indicates the ratio of viscosity and thermal conduction, of $\text{Pr} = 1$. Boltzmann's original operator correctly predicts $\text{Pr} \simeq 2/3$, a value also found in lab experiments on monatomic gases [10].

Exercise 1.10 For a force-free, spatially homogeneous case $f(\mathbf{x}, \xi, t) \rightarrow f(\xi, t)$, show that the BGK operator relaxes an initial distribution function $f(\xi, t = 0)$

exponentially to the equilibrium distribution $f^{\text{eq}}(\xi)$ as

$$f(\xi, t) = f^{\text{eq}}(\xi) + (f(\xi, 0) - f^{\text{eq}}(\xi)) e^{-t/\tau}. \quad (1.50)$$

1.3.5 Macroscopic Conservation Equations

The macroscopic equations of fluid mechanics can actually be found directly from the Boltzmann equation, (1.46). We do this by taking the moments of the equation, i.e. by multiplying it with functions of ξ and integrating over velocity space.

For convenience, we introduce a general notation for the moments of f ,

$$\begin{aligned} \Pi_0 &= \int f \, d^3\xi = \rho, & \Pi_\alpha &= \int \xi_\alpha f \, d^3\xi = \rho u_\alpha, \\ \Pi_{\alpha\beta} &= \int \xi_\alpha \xi_\beta f \, d^3\xi, & \Pi_{\alpha\beta\gamma} &= \int \xi_\alpha \xi_\beta \xi_\gamma f \, d^3\xi. \end{aligned} \quad (1.51)$$

The first two moments are already known as the moments for mass and momentum density. The second-order moment $\Pi_{\alpha\beta}$ will soon be shown to be the momentum flux tensor from (1.12). As we can see from their definitions, these moments are not altered if their indices are reordered.

To deal with the force terms, we need to know the moments of the force term, which we can find directly using multidimensional integration by parts as

$$\begin{aligned} \int \frac{\partial f}{\partial \xi_\beta} \, d^3\xi &= 0, \\ \int \xi_\alpha \frac{\partial f}{\partial \xi_\beta} \, d^3\xi &= - \int \frac{\partial \xi_\alpha}{\partial \xi_\beta} f \, d^3\xi = -\rho \delta_{\alpha\beta}, \\ \int \xi_\alpha \xi_\alpha \frac{\partial f}{\partial \xi_\beta} \, d^3\xi &= - \int \frac{\partial (\xi_\alpha \xi_\alpha)}{\partial \xi_\beta} f \, d^3\xi = -2\rho u_\beta. \end{aligned} \quad (1.52)$$

1.3.5.1 Mass Conservation Equation

The simplest equation we can find from the Boltzmann equation is the *continuity equation* which describes the conservation of mass. Directly integrating the Boltzmann equation over velocity space, we find

$$\frac{\partial}{\partial t} \int f \, d^3\xi + \frac{\partial}{\partial x_\beta} \int \xi_\beta f \, d^3\xi + \frac{F_\beta}{\rho} \int \frac{\partial f}{\partial \xi_\beta} \, d^3\xi = \int \Omega(f) \, d^3\xi. \quad (1.53)$$

The integrals in each term can be resolved according to the moments in (1.38) and (1.52), in addition to the collision operator's mass conservation property in (1.48a). Thus, we find the *continuity equation* from (1.3) which describes mass conservation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_\beta)}{\partial x_\beta} = 0. \quad (1.54)$$

Note that this equation only depends on the conserved moments ρ and ρu_α . It does not depend on the particular form of f , unlike the following conservation equations.

1.3.5.2 Momentum Conservation Equation

If we similarly take the first moment of the Boltzmann equation, i.e. we multiply by ξ_α before integrating over velocity space, we find

$$\frac{\partial(\rho u_\alpha)}{\partial t} + \frac{\partial \Pi_{\alpha\beta}}{\partial x_\beta} = F_\alpha. \quad (1.55)$$

The moment $\Pi_{\alpha\beta}$ defined in (1.51) is the *momentum flux tensor*, (1.12).

Exercise 1.11 By splitting the particle velocity as $\xi = \mathbf{u} + \mathbf{v}$, show that the momentum flux tensor can be decomposed as

$$\Pi_{\alpha\beta} = \rho u_\alpha u_\beta + \int v_\alpha v_\beta f \, d^3\xi. \quad (1.56)$$

Thus, the second moment of the Boltzmann equation becomes the *Cauchy momentum equation* previously seen in (1.11):

$$\frac{\partial(\rho u_\alpha)}{\partial t} + \frac{\partial(\rho u_\alpha u_\beta)}{\partial x_\beta} = \frac{\partial \sigma_{\alpha\beta}}{\partial x_\beta} + F_\alpha. \quad (1.57)$$

However, this equation is not closed as we do not know the *stress tensor*

$$\sigma_{\alpha\beta} = - \int v_\alpha v_\beta f \, d^3\xi \quad (1.58)$$

explicitly. To approximate this stress tensor, we must somehow find an explicit approximation of the distribution function f . In Sect. 1.3.5.4 we will discuss how this may be done.

1.3.5.3 Energy Conservation Equation

Finally, we can find the energy equation from the trace of the second moment. In other words, we multiply by $\xi_\alpha \xi_\alpha$ before integrating over velocity space, resulting in

$$\frac{\partial(\rho E)}{\partial t} + \frac{1}{2} \frac{\partial \Pi_{\alpha\alpha\beta}}{\partial x_\beta} = F_\beta u_\beta. \quad (1.59)$$

We can simplify this in two steps. First, we can split the moment in the same way as for the momentum equation, giving the *total energy equation*

$$\frac{\partial(\rho E)}{\partial t} + \frac{\partial(\rho u_\beta E)}{\partial x_\beta} = \frac{\partial(u_\alpha \sigma_{\alpha\beta})}{\partial x_\beta} + F_\beta u_\beta - \frac{\partial q_\beta}{\partial x_\beta} \quad (1.60)$$

with the *heat flux* \mathbf{q} given as the moment

$$q_\beta = \frac{1}{2} \int v_\alpha v_\alpha v_\beta f \, d^3\xi. \quad (1.61)$$

Secondly, we can eliminate the bulk motion energy component $\frac{1}{2}\rho|\mathbf{u}|^2$ from the equation by subtracting (1.57) multiplied with u_α . The end result is the *internal energy equation*

$$\frac{\partial(\rho e)}{\partial t} + \frac{\partial(\rho u_\beta e)}{\partial x_\beta} = \sigma_{\alpha\beta} \frac{\partial u_\alpha}{\partial x_\beta} - \frac{\partial q_\beta}{\partial x_\beta}. \quad (1.62)$$

1.3.5.4 Discussion

Finding the macroscopic conservation equations from basic kinetic theory shows us that the mass equation is exact and invariable, while the momentum and energy equations depend on the stress tensor and the heat flux vector which themselves depend on the form of f .

At this point we do not know much about f except its value at equilibrium. It can be shown that approximating (1.58) and (1.61) by assuming $f \simeq f^{\text{eq}}$ results in the Euler momentum equation from (1.10) and a simplified energy equation sometimes known as the *Euler energy equation*. Both are shown in (1.63).

Exercise 1.12 Assume that $f \simeq f^{\text{eq}}$ for an ideal gas. From (1.58) and (1.61), show that the general momentum and internal energy conservation equations result in the Euler momentum and energy equations

$$\frac{\partial(\rho u_\alpha)}{\partial t} + \frac{\partial(\rho u_\alpha u_\beta)}{\partial x_\beta} = -\frac{\partial p}{\partial x_\alpha} + F_\alpha, \quad \frac{\partial(\rho e)}{\partial t} + \frac{\partial(\rho u_\beta e)}{\partial x_\beta} = -p \frac{\partial u_\beta}{\partial x_\beta}. \quad (1.63)$$

Both these Euler equations lack the viscous stress tensor σ' and the heat flux found in the Navier-Stokes-Fourier momentum and energy equations. We previously found the viscous stress in (1.14) while the heat flux is [2]

$$\mathbf{q} = -\kappa \nabla T, \quad (1.64)$$

κ being the fluid's thermal diffusivity.

The fact that the Euler equations are found for a particle distribution f at *equilibrium* indicates that the phenomena of viscous dissipation and heat diffusivity are connected to *non-equilibrium*, i.e. the deviation $f - f^{\text{eq}}$. How, then, can we find a more general form of f which takes this deviation into account?

The *Chapman-Enskog analysis* is an established method of connecting the kinetic and continuum pictures by finding non-equilibrium contributions to f . Its main idea is expressing f as a perturbation expansion about f^{eq} :

$$f = f^{\text{eq}} + \epsilon f^{(1)} + \epsilon^2 f^{(2)} + \dots \quad (1.65)$$

The *smallness parameter* ϵ labels each term's order in the *Knudsen number* $\text{Kn} = \ell_{\text{mfp}}/\ell$, as defined in (1.32). For $\text{Kn} \rightarrow 0$, when the fluid is dominated by collisions, the particle distribution is approximately at equilibrium, and the fluid's behaviour is described by the Euler equation.

The perturbation of f combined with a non-dimensionalisation analysis lets us explicitly find the first-order perturbation $f^{(1)}$ from the macroscopic derivatives of the equilibrium distribution f^{eq} [12, 14]. Using this perturbation to approximate the stress tensor and heat flux moments in (1.58) and (1.61), we find the same stress tensor and heat flux as in (1.14) and (1.64), respectively. The resulting transport coefficients are simple functions of τ :

$$\eta = p\tau, \quad \eta_B = 0, \quad \kappa = \frac{5}{2} R p \tau. \quad (1.66)$$

We will get back to the topic of the Chapman-Enskog analysis in Sect. 4.1.

What have we seen here? On a macroscopic scale, the **Boltzmann equation** describes the **macroscopic behaviour of a fluid**. To a zeroth-order approximation we have $f \approx f^{\text{eq}}$, giving the macroscopic equations of the *Euler model*. To a first-order approximation, $f \approx f^{\text{eq}} + \epsilon f^{(1)}$, we get the *Navier-Stokes-Fourier model* with its viscous stress and heat conduction.

It is also possible to go further; the second-order approximation $f \approx f^{\text{eq}} + \epsilon f^{(1)} + \epsilon^2 f^{(2)}$ results in the so-called *Burnett model* which in principle gives even more detailed and accurate equations for the motion of a fluid. In practice, however, the Burnett and Navier-Stokes-Fourier models are only distinguishable at high

Knudsen numbers [8], where the Burnett model predicts, e.g., ultrasonic sound propagation with a better agreement with experiments [15]. However, even higher-order approximations paradoxically give a *poorer* prediction of ultrasonic sound propagation [15]. A proposed reason for this strange result is that the Chapman-Enskog expansion is actually *asymptotic* [8], meaning that f *diverges* as more terms are added in its expansion. This also casts some doubt on the Burnett model. For the purpose of this book, we do not need to consider expansions beyond the first-order approximation $f \approx f^{\text{eq}} + \epsilon f^{(1)}$.

1.3.6 Boltzmann's \mathcal{H} -Theorem

The thermodynamic property of *entropy* can also be related to the distribution function f . The *entropy density* is denoted by ρs , with the unit of $[\rho s] = \text{J/kg m}^3$.

Boltzmann himself showed that the quantity

$$\mathcal{H} = \int f \ln f \, d^3\xi \quad (1.67)$$

can only ever decrease and that it reaches its minimum value when the distribution function f reaches equilibrium.

We can see this directly from the Boltzmann equation in (1.46). By multiplying it with $(1 + \ln f)$, using the chain rule in reverse, and taking the zeroth moment of the resulting equation, we can find

$$\frac{\partial}{\partial t} \int f \ln f \, d^3\xi + \frac{\partial}{\partial x_\alpha} \int \xi_\alpha f \ln f \, d^3\xi = \int \ln f \, \Omega(f) \, d^3\xi. \quad (1.68)$$

This equation is a balance equation for the quantity \mathcal{H} and is found as a moment of the Boltzmann equation, similarly to the mass, momentum, and energy conservation equations in Sect. 1.3.5. Thus, the quantity $\int \xi_\alpha f \ln f \, d^3\xi = \mathcal{H}_\alpha$ is the flux of the quantity \mathcal{H} that we can split into an advective component $u_\alpha \int f \ln f \, d^3\xi$ and a diffusive component $\int v_\alpha f \ln f \, d^3\xi$.

For the BGK collision operator, the right-hand side of (1.68) can be found to be non-positive:

$$\begin{aligned}
 \int \ln f \Omega(f) d^3\xi &= \int \ln\left(\frac{f}{f^{\text{eq}}}\right) \Omega(f) d^3\xi + \int \ln(f^{\text{eq}}) \Omega(f) d^3\xi \\
 &= \frac{1}{\tau} \int \ln\left(\frac{f}{f^{\text{eq}}}\right) (f^{\text{eq}} - f) d^3\xi \\
 &= \frac{1}{\tau} \int f^{\text{eq}} \ln\left(\frac{f}{f^{\text{eq}}}\right) \left(1 - \frac{f}{f^{\text{eq}}}\right) d^3\xi \leq 0.
 \end{aligned} \tag{1.69}$$

The $\ln(f^{\text{eq}})\Omega(f)$ integral can be shown to disappear by inserting f^{eq} and using the conservation constraints of the collision operator in (1.48). The last inequality follows from the general inequality $\ln x(1-x) \leq 0$ for all $x > 0$. For $x = 1$, which corresponds to the equilibrium $f = f^{\text{eq}}$, the inequality is exactly zero. This inequality can also be shown for Boltzmann's original collision operator and can be considered a necessary criterion for any collision operator in kinetic theory.

Consequently, (1.68) corresponds to the equation

$$\frac{\partial \mathcal{H}}{\partial t} + \frac{\partial \mathcal{H}_\alpha}{\partial x_\alpha} \leq 0. \tag{1.70}$$

This shows us that \mathcal{H} is not conserved in the system: it never increases, but instead it decreases, until the particle distribution reaches equilibrium. This is called the *Boltzmann \mathcal{H} -theorem*. It states that molecular collisions invariably drive the distribution function towards equilibrium.⁵

At first sight, this seems analogous to how the thermodynamic quantity of entropy always increases in a system unless the system has reached an equilibrium characterised by an entropy maximum. Indeed, for ideal gases \mathcal{H} is actually **proportional to the entropy density** ρs [10, 16]:

$$\rho s = -R\mathcal{H}. \tag{1.71}$$

⁵A more expansive and rigorous explanation of the \mathcal{H} -theorem can be found elsewhere [8, 10].

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