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1 Introduction

We live in a world out of equilibrium – a nonequilibrium world. We are surrounded by phenomena occurring in nature, in industrial and technological processes and in controlled experiments that we can only understand with the aid of a theoretical framework that encompasses nonequilibrium processes. Our understanding of these phenomena is largely based on a macroscopic theory that starts with the balance equations for the densities of mass, momentum, energy and other macroscopic quantities. To solve these equations, it is necessary to introduce relationships based on experiments that relate the observable properties of materials to the variables that define their macroscopic state. These relationships may describe equilibrium or locally equilibrium states of the material and in this case they are called equations of state. But we also need other relationships that relate the fluxes of properties to the property gradients that drive them. These are called constitutive or transport equations. The main subject of this book is the study of these transport equations and the material properties, such as the transport coefficients that account for the differences in the behaviour of different substances, using molecular dynamics simulation methods.

The molecular dynamics (MD) simulation method was developed soon after the Monte Carlo (MC) method, for the purpose of studying relaxation and transport phenomena [9]. Both MC and MD employed periodic boundary conditions, in which the system of interest is assumed to be replicated periodically in all directions, to limit (but not totally eliminate) the effects of the finite system size. At first, applications of this new technique focused on the structure, dynamics and equations of state of equilibrium systems [10–12]. The development in the 1950s of the Green–Kubo formalism, relating linear transport coefficients to equilibrium fluctuations in the corresponding fluxes [13, 14], made it possible to use equilibrium simulations to study nonequilibrium properties. However these methods, based on the computation of time correlation functions, were difficult to apply to all of the transport properties except self-diffusion due to their large computational requirements in comparison to the computing power available at that time. In addition, they could only address transport processes in the linear regime, i.e. where the flux is directly proportional to the thermodynamic driving force. These factors motivated the development of nonequilibrium molecular dynamics (NEMD) methods.

Early nonequilibrium simulations of shear flow by Lees and Edwards [15], Gosling, McDonald and Singer [16] and Ashurst and Hoover [17] set the stage for decades of innovation and advancement through the interplay of theory, experiment and simulation.

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There is no better example of this than the extraordinary growth of nonequilibrium statistical mechanics and molecular simulation as they both matured during the 1980s. For interested readers, much of the historical development of nonequilibrium molecular dynamics methods can be traced through Hoover's review and the accompanying original research articles in a special issue of *Physica* in 1983 [18], Hoover's 1993 review [19] and the book by Evans and Morriss [2].

Throughout the development of nonequilibrium simulation methodology there have emerged three distinct ways of performing nonequilibrium simulations. The first class of methods tries to model a real physical system as closely as possible and applies perturbations that are physically realistic. The Ashurst and Hoover [17] paper represents a prototype of this approach. This method has the great advantage that there is never any uncertainty regarding the relationship between the thermodynamic force applied in the simulation and the natural one. The disadvantages are that the simulated systems must always represent a tiny portion of any realistic system (unless the system that we want to mimic is actually nanoscopic), and the perturbations that are applied must be enormous compared to those existing in nature, due to the large thermal noise in the quantities being computed for small systems. This type of simulation is often called a 'boundary-driven' nonequilibrium simulation because the thermodynamic force arises due to the conditions of the momentum, heat or chemical species reservoirs attached to the system of interest. In these simulations, heat that is generated by the nonequilibrium processes occurring in the system of interest is transferred by natural thermal conduction to the boundary regions where it is removed by velocity rescaling [17] or one of the modern synthetic thermostats discussed in the following chapters. Even though the Lees and Edwards method employs periodic boundary conditions, it can be seen as a member of this class because it is the motion of the periodic images above and below the main simulation box that drives the shear flow. They therefore act as momentum reservoirs. Whereas nonperiodic reservoir methods result in spatially inhomogeneous properties, the Lees-Edwards method results in spatially homogeneous properties. This is a huge advantage for the accurate determination of transport properties.

A second class of nonequilibrium simulation method is one in which a spatially periodic (usually sinusoidal) transverse perturbation is applied through an explicit external force to drive shear flow, so that it is compatible with standard periodic boundary conditions. The method devised by Gosling, McDonald and Singer [16] is the prototype of this class. In this method, there are no reservoirs to absorb the dissipated heat. Gosling, McDonald and Singer allowed the temperature of the system to rise with time, yielding the temperature dependence of the properties during the course of the simulation. Later variants of this sinusoidal transverse force (STF) technique applied a synthetic thermostat to the fluid to allow the development of a true steady state. This method results in spatially inhomogeneous properties, because the strain rate, density and temperature all follow a sinusoidal spatial dependence.

The third method uses explicit external forces in the equations of motion, combined with periodic boundary conditions, to drive homogeneous fluxes of the desired type. This method was pioneered by Hoover, Evans and others in the early 1980s [20, 21]. Like the STF method, this method has the advantage that the perturbation is explicit

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in the equations of motion, making it possible to apply response theory to the system. Because the perturbation is spatially homogeneous, the response of the system is also homogeneous so the properties are computed at a specific, known thermodynamic state. Finally, the absence of reservoirs means that surface effects can be eliminated, without requiring excessively large systems. The transport properties can be obtained by direct averaging of the fluxes [20], by using the ‘subtraction method’ to reduce noise [22] or by forming their nonequilibrium transient time correlation functions and applying nonlinear response theory to determine their average values (the TTCF method) [23].

By the early 1990s when the first edition of the book by Evans and Morriss [2] appeared, many of the basic technical aspects of nonequilibrium molecular dynamics simulation methods were already settled. These techniques had been developed and tested using simple atomic liquids as a testbed. With the growth of computer power and increasing sophistication of algorithms and software, it became possible to embark on more ambitious investigations of nonequilibrium phenomena, and the range of applications of NEMD grew rapidly.

In this book, we have decided to restrict our attention to homogeneous NEMD methods based on the Hoover-Evans approach, STF methods based on the Gosling McDonald and Singer method and inhomogeneous NEMD methods where the inhomogeneity (i.e. the presence of interfaces in confined flows) is itself of interest. We have not discussed the wide range of very useful techniques based on reservoir methods superficially similar to the original Ashurst and Hoover simulations, but differing in important ways. This is not due to a lack of confidence in these methods on our part, but rather the simple lack of time it would take us to do justice to them, the limited space available to us, and our own lack of personal experience with them. These techniques have been successfully used to study shear flow [24], thermal conductivity and thermal diffusion [25] and we encourage the curious reader to seek further information in the vast ocean of scientific literature.

The remainder of this book is summarised as follows. In Chapter 2, we introduce the theory of nonequilibrium thermodynamics, which provides the macroscopic foundations of our description of nonequilibrium phenomena and helps us to decide which properties are worth computing. The nonequilibrium thermodynamics of the transport of mass and heat in multicomponent fluids, and the transport of spin angular momentum in molecular fluids are treated in detail.

Chapter 3 outlines the elements of nonequilibrium statistical mechanics that are necessary for an understanding of the algorithms and methods to be described later. Particular attention is paid to the development of response theory in a form that is suitable for the analysis of homogeneous nonequilibrium molecular dynamics algorithms and the TTCF method.

The statistical mechanical derivations of expressions for the temperature and fluxes are the focus of Chapter 4. Derivations of expressions for the temperature, pressure tensor and heat flux vector are carried out in detail for different circumstances in order to display to those who are new to the field some of the finer points that are often omitted from original research articles.

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The underlying theory of the SLLOD algorithm for simulating homogeneous flows of atomic fluids is discussed in Chapter 5, with a focus on shear and elongational flows. The intricate details of homogeneous thermostats for nonequilibrium systems and periodic boundary conditions that are compatible with the various flows are discussed.

Applications of the SLLOD equations of motion for atomic fluids are presented in Chapter 6. Steady and oscillatory flows are discussed for different types of deformation including shear and elongation.

Algorithms for heat and mass transport are discussed in Chapter 7. Single component and multicomponent systems are considered and the connections between the phenomenological coefficients for heat flow, diffusion and the cross-effects and their corresponding practical transport coefficients are discussed.

Chapter 8 considers nonequilibrium flows of molecular liquids. Some simple models for molecular liquids and the molecular version of the SLLOD algorithm are described. Simulation methods for different ensembles are discussed and results for a few cases of molecular liquids are described.

Simulations of inhomogeneous systems including STF, planar Couette and Poiseuille flow simulations are covered in Chapter 9. Chapter 10 extends this discussion to the increasingly important case of confined molecular liquids.

In the final chapter, we consider the implications of the breakdown of standard Navier-Stokes-Fourier hydrodynamics in the analysis of NEMD simulations of highly inhomogeneous fluids. This requires the consideration of generalised hydrodynamics, in which the stress becomes a nonlocal function of the strain rate. A proper consideration of slip, which is usually negligible in macroscopic hydrodynamics, is seen to be vitally important for nanofluidic flows.

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2 Nonequilibrium Thermodynamics and Continuum Mechanics

Molecular dynamics simulations provide us with a numerical solution to the equations of motion for all of the particles in a system. For a system of N particles, this gives us $3N$ positions and $3N$ momenta, which embody the full microscopic description of the system. By itself, this is too much information. What we require is a way to compute measurable properties from this microscopic description. Experimental studies of thermal and mechanical processes in fluids at the macroscopic and mesoscopic scales are based on coarse-grained measurements of field variables that obey the laws of continuum thermodynamics and mechanics. In this chapter, we will review some of the basic results of continuum thermodynamics and mechanics that we need to make the link between the microscopic mechanical variables and the variables of continuum thermodynamics and mechanics. Fortunately, a well-developed formalism for the unified treatment of continuum thermodynamics and mechanics already exists, namely nonequilibrium thermodynamics. Many excellent books and review articles on nonequilibrium thermodynamics are available, ranging from classical treatments of linear nonequilibrium thermodynamics [4] to more advanced treatments of nonequilibrium thermodynamics for systems that are far from equilibrium [26, 27]. Here, we will provide a simplified introduction to this vast and growing field, with an emphasis on the ideas that are pertinent to our discussion of nonequilibrium molecular dynamics simulations.

2.1 Thermodynamics

The first law of thermodynamics for a macroscopic system is expressed as

$$\Delta U = Q - W, \tag{2.1}$$

where ΔU is the internal energy change, Q is the heat absorbed by the system and W is the thermodynamic work done by the system. The second law of thermodynamics, which introduces the entropy S, expresses the entropy difference between two equilibrium states A and B in the form

$$\int_A^B \frac{dQ}{T} \leq S(B) - S(A), \tag{2.2}$$

where dQ is an infinitesimal heat transfer into the system along some arbitrary thermodynamic path and T is the temperature of the heat bath from which the heat is absorbed.

If the path is a reversible or "quasi-static" one, then the infinitesimal heat absorbed for any segment of that path is denoted as dQ_R, and the definition of an entropy change in terms of the reversible heat transfer is obtained

$$dQ_R\big/T = dS. \tag{2.3}$$

In classical thermodynamics, the second law is expressed as an equality for a reversible process, but for an arbitrary process it is an inequality. This is clearly unsatisfactory, for a number of different reasons. First, it means that the second law of thermodynamics becomes purely qualitative and it loses its ability to predict the progress of the entropy through processes that are not "quasi-static". Secondly, it results in a paradox, because common statements of the second law imply that the entropy of an arbitrary nonequilibrium state for an isolated system is defined and it increases until the system reaches its equilibrium state. Both of these issues are resolved if we adopt the local equilibrium hypothesis. When the local equilibrium hypothesis is satisfied, the local entropy density remains well defined, and the total entropy of the system is the volume integral of the local entropy density. When the local equilibrium hypothesis is not satisfied, even the existence of the entropy and the uniqueness of the temperature remain contentious.

One of the primary goals of nonequilibrium thermodynamics is to obtain an equality for the entropy change for certain types of irreversible processes. Here, we will restrict our attention to processes for which the local equilibrium hypothesis is satisfied and this goal can be achieved.

In general, the properties of a material undergoing a thermal or mechanical change will not necessarily be homogeneous in space or constant in time. Therefore, it is useful to introduce local, time-dependent quantities in place of the extensive thermodynamic variables if we want a description of the processes occurring inside the system's boundaries. For example, the volume is replaced by the specific volume, defined as the limit as the mass goes to zero of the volume per unit mass of a small but macroscopic mass element of the system,

$$v\left(\mathbf{r},t\right) = \frac{1}{\rho\left(\mathbf{r},t\right)} = \lim_{\delta m\to 0}\frac{\delta V}{\delta m}, \tag{2.4}$$

where we have also introduced the more commonly used mass density, $\rho\left(\mathbf{r},t\right)$. All of the other extensive thermodynamic variables can similarly be converted into local specific (per unit mass) field variables.

Let us consider a small but macroscopic mass element δm, undergoing a reversible thermal process. The first law of thermodynamics can be applied to find the infinitesimal internal energy change $d(\delta U)$ due to any combination of a reversible infinitesimal heat transfer where the differential of the heat absorbed is given by $d(\delta Q_R) = Td(\delta S)$, and an infinitesmal reversible compression or expansion where the differential of the work done by the material is $d(\delta W_R) = pd(\delta V)$, as

$$d(\delta U) = Td(\delta S) - pd(\delta V). \tag{2.5}$$

Now we can substitute $\delta U = u\left(\mathbf{r},t\right)\delta m$, $\delta S = s\left(\mathbf{r},t\right)\delta m$ and $\delta V = \delta m/\rho\left(\mathbf{r},t\right)$, take the limit as the mass approaches zero, and rearrange the result to obtain the reversible part

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of the change in the entropy due to changes in the thermodynamic fields,

$$T(\mathbf{r},t)ds(\mathbf{r},t) = du(\mathbf{r},t) - \frac{p(\mathbf{r},t)}{\rho^2(\mathbf{r},t)}d\rho(\mathbf{r},t). \tag{2.6}$$

This is the local form of the Gibbs equation. The Gibbs equation and its generalisations are central to classical and extended treatments of nonequilibrium thermodynamics. Note that although the specific internal energy, entropy and volume are very useful thermodynamic field variables, it is often more convenient to work with their densities. For example, the internal energy density (internal energy per unit volume) is equal to the specific internal energy multiplied by the mass density, $\rho(\mathbf{r},t)\,u(\mathbf{r},t)$.

2.2 Continuum Mechanics

The basic principles of continuum mechanics can be found in any one of a large number of excellent books. Treatments with an emphasis on fluids include those by Bird *et al.* [28, 29], Tanner [30], Phan-Thien and Huilgol [31] and Truesdell [32]. Our aim here is to introduce some basic concepts that we will use later in our development of nonequilibrium thermodynamics and our interpretations of molecular dynamics simulations.

2.2.1 Pressure Tensor

The forces acting on a small element of fluid can be classified as either short-ranged, in which case they are regarded as contact forces acting on the surface of the element, or long-ranged, where they are regarded as acting throughout the entire element. Continuum mechanics treats contact forces as contributions to the pressure tensor, whereas forces that act throughout a fluid are treated as body forces. Of course, the distinction between these two types of force is not always clear, particularly if we consider a very small volume element with a size approaching the range of the "short-ranged" forces, but it is usually the case that intermolecular forces fall into the short-ranged category and external gravitational and electric fields can be regarded as long-ranged.

Consider an element of surface area on a closed surface in the fluid. The element of surface area has an orientation defined by the outward pointing normal vector at that point on the surface. The total force $d\mathbf{F}$ acting on the oriented surface element $d\mathbf{A}$ due to the pressure tensor arising from molecular motion and intermolecular interactions within the material is given by

$$d\mathbf{F} = -\mathbf{P}^T \cdot d\mathbf{A}. \tag{2.7}$$

This is the mechanical definition of the pressure tensor. In an isotropic equilibrium fluid, the pressure tensor is isotropic, $\mathbf{P} = p\mathbf{1}$, where $\mathbf{1}$ is the second-rank isotropic tensor (the unit tensor) and p is the scalar pressure of the equilibrium fluid, $p = (1/3)\,\mathrm{Tr}\,(\mathbf{P})$. In the context of fluid mechanics, it is often preferred to separate the equilibrium and nonequilibrium parts of the pressure tensor and define the nonequilibrium part of the pressure tensor as $\mathbf{\Pi} = \mathbf{P} - p\mathbf{1}$ and the stress as $\boldsymbol{\sigma} = -\mathbf{\Pi}^T$. Note that the transpose in

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this relationship is required because stress is defined in terms of the force exerted by the surrounding medium on a fluid element, $d\mathbf{F} = \boldsymbol{\sigma} \cdot d\mathbf{A}$ whereas the pressure tensor is defined as the diffusive transport of momentum through the surface. This distinction is discussed in more detail by Bird *et al.* [28]. In many cases, the pressure tensor is symmetric, but in situations where the intrinsic angular momentum density of the material plays a role, the pressure tensor may possess an antisymmetric component.

2.2.2 Deformation

In continuum mechanics, we can characterise the kinematics of material deformation in terms of the motion of a set of material points which are defined by their positions at a certain time. For example, a point $\mathbf{r}'$ could represent the position of a certain material element at time $t = 0$, and the label $\mathbf{r}'$ can be used to identify this point at all future times, regardless of the motion that the material may undergo. The trajectory of a material point is given by its path function $\mathbf{r} = \mathbf{M}(\mathbf{r}', t)$ [31] and the deformation gradient tensor is defined as $\mathsf{F} = (\partial\mathbf{r}/\partial\mathbf{r}')^T$, where the superscript T denotes the transpose. The relative deformation gradient $\mathsf{F}_t(\tau) = (\partial\mathbf{r}''/\partial\mathbf{r})$ is defined as the derivative of the position at some intermediate time τ with respect to its position at another time t. In general, neither of these times need be equal to $t = 0$. Deformation can be defined in terms of the "right relative Cauchy-Green strain tensor", which is given by

$$\mathsf{C}_t(\tau) = \mathsf{F}_t(\tau)^T \mathsf{F}_t(\tau). \tag{2.8}$$

As the name implies, this measure of strain is not unique. In particular, for finite strains, as distinct from infinitesimal strains, different strain measures are not identical. The differences between these different measures of strain arise from different possible choices of the reference state. Alternative definitions of strain can be found in many of the previously mentioned books on theoretical rheology or continuum mechanics [28, 30–32]. For our current purposes, it is sufficient to choose a commonly used definition and develop our treatment consistently with this definition.

Standard treatments of rheology discuss fluid deformation in terms of the "rheologically simple fluid" model. A "rheologically simple fluid" is defined as one for which the stress is given by a spatially local functional of the strain history. For a "rheologically simple fluid" the deformation can also be expressed in terms of the Rivlin-Ericksen tensors, which are defined as the material (streaming) derivatives of the strain tensor, given by

$$\left.\frac{d^n}{d\tau^n}\mathsf{C}_t(\tau)\right|_{\tau=t} = \mathbf{A}_n(t), \tag{2.9}$$

where $n = 0, 1, 2, \ldots$. This can also be expressed in terms of the velocity gradient tensor $\mathbf{L} = \nabla\mathbf{v}$ and its transpose. Using the results for the material derivative of the relative deformation gradient and its transpose, $\dot{\mathsf{F}} = \mathbf{L}\mathsf{F}$ and $\dot{\mathsf{F}}^T = \mathsf{F}^T\mathbf{L}^T$, the rate of change of the strain is found to be

$$\begin{aligned}\frac{d}{d\tau}\mathsf{C}_t(\tau) &= \frac{d}{d\tau}\left(\mathsf{F}_t(\tau)^T\,\mathsf{F}_t(\tau)\right)\\ &= \mathsf{F}_t^T\cdot\mathbf{L}\cdot\mathsf{F}_t+\mathsf{F}_t^T\cdot\mathbf{L}^T\cdot\mathsf{F}_t.\end{aligned}\tag{2.10}$$

Evaluating this at time $t=\tau$ results in $\mathsf{F}_t^T=\mathsf{F}_t=\mathbf{1}$ which then gives

$$\mathbf{A}_1(t)=\left.\frac{d}{d\tau}\mathsf{C}_t(\tau)\right|_{\tau=t}=\mathbf{L}+\mathbf{L}^T\tag{2.11}$$

for the rate of strain. This reflects the fact that the rate of strain is related to only the symmetric part of the velocity gradient tensor. In the standard continuum mechanics treatment, the higher-order time derivatives are defined in terms of the gradients of the particle accelerations and higher derivatives as

$$\mathbf{L}_n=\left.\frac{d^n}{d\tau^n}\mathsf{F}_t(\tau)\right|_{\tau=t}=\nabla\frac{d^n\mathbf{r}}{dt^n}=\nabla\frac{d^{n-1}\mathbf{v}}{dt^{n-1}}\tag{2.12}$$

and the Rivlin-Eriksen tensors are then given by

$$\mathbf{A}_n(t)=\left.\frac{d^n}{d\tau^n}\mathsf{C}_t(\tau)\right|_{\tau=t}=\sum_{r=0}^{n}\binom{n}{r}\mathbf{L}_{n-r}^T\mathbf{L}_r,\tag{2.13}$$

where $\binom{n}{r}=\frac{n!}{r!(n-r)!}$, $\mathbf{L}_1=\mathbf{L}$ and $\mathbf{L}_0=\mathbf{1}$. A recursion relation due to Oldroyd [31] can be used to generate the $(n+1)^{th}$ Rivlin-Eriksen tensor from the n^{th},

$$\mathbf{A}_{n+1}=\frac{d}{dt}\mathbf{A}_n+\mathbf{A}_n\cdot\mathbf{L}+\mathbf{L}^T\cdot\mathbf{A}_n.\tag{2.14}$$

These results will be used later when simulation results for the stress tensor in shear and planar elongational flows are described in terms of some standard continuum mechanical constitutive equations.

2.3 Nonequilibrium Thermodynamics

The equations of change for the thermal and mechanical fields, i.e. the density, the streaming velocity and the internal energy, are derived from basic physical principles – conservation of mass, Newton's second law of motion and conservation of the total energy. In keeping with our simplified approach, which we hope will most clearly display the underlying physical ideas, we will apply these principles to the motion of a mass element and derive the balance equations for the density, velocity and specific internal energy fields.

2.3.1 Mass Balance

We begin our derivation of the balance equation for the mass with the assumption that our small but macroscopic subsystem is defined as a cuboidal element of the continuum

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that maintains a constant mass while it undergoes thermal and mechanical changes.[1] Thus, we can write

$$\frac{d(\delta m)}{dt} = \frac{d}{dt}(\rho \delta V) = \rho \frac{d(\delta V)}{dt} + \delta V \frac{d\rho}{dt} = 0. \tag{2.15}$$

The volume of the mass element can only change if the velocities of the fluid at opposing faces of the cuboid are different, so the term containing the rate of change of the volume can be written as

$$\frac{1}{\delta V}\frac{d(\delta V)}{dt} = \frac{1}{\delta x \delta y \delta z}\frac{d}{dt}(\delta x \delta y \delta z) = \frac{1}{\delta x}(\delta v_x) + \frac{1}{\delta y}\left(\delta v_y\right) + \frac{1}{\delta z}(\delta v_z), \tag{2.16}$$

which becomes $\nabla \cdot \mathbf{v}$ in the limit as the size of the mass element approaches zero. Thus, we obtain the equation of change for the local fluid density,

$$\frac{d\rho}{dt} = -\rho \nabla \cdot \mathbf{v}. \tag{2.17}$$

2.3.2 Momentum Balance

Applying Newton's second law of motion to the small mass element, we obtain

$$\delta m \frac{d\mathbf{v}}{dt} = \delta \mathbf{F}^t, \tag{2.18}$$

where $\delta \mathbf{F}^t$ is the total force acting on the material element. We will consider two types of force that may act on the mass element. The first is the force due to interactions with the surrounding fluid (via the pressure tensor, Equation (2.7)), and the second is the body force due to an external field $\mathbf{F}^e$, which we will write as $\delta \mathbf{F} = \delta m \mathbf{F}^e$. This explicitly nominates the external field as a gravitational field, since it couples to the mass, but the body forces due to electric and other fields can be written in a similar way, by altering the variable to which the field couples. The explicit form of the x-component of the total force due to the stresses on all six faces of the cuboid and the external body force is

$$\begin{aligned} \delta F_x^t = & -\delta y \delta z \left[P_{xx}(x+\delta x) - P_{xx}(x)\right] - \delta z \delta x \left[P_{yx}(y+\delta y) - P_{yx}(y)\right] \\ & - \delta x \delta y \left[P_{zx}(z+\delta z) - P_{zx}(z)\right] + \delta m F_x^e \end{aligned} \tag{2.19}$$

and the other components are similar. Figure 2.1 shows some of these forces schematically. Substituting Equation (2.19) and the corresponding equations for the y and z components of the force into Equation (2.18) and then dividing both sides by the volume of the mass element $\delta V = \delta x \delta y \delta z$ and taking the continuum limit, we find

$$\rho \frac{d\mathbf{v}}{dt} = -\nabla \cdot \mathbf{P} + \rho \mathbf{F}^e. \tag{2.20}$$

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[1] A cuboid is a parallelepiped with rectangular faces.