0. General introduction to the course

The lattice-Boltzmann method (LBM) is an interesting way of doing simulations of fluid flow and related transport processes and a useful addition to more mainstream computational fluid dynamics (CFD) methods based on finite volumes, finite differences or finite elements. There are many reasons for using LBM, and many reasons for not using it, mainly dependent on the applications you are interested in. An understanding of the LBM will help you in deciding if your application could benefit from it and – if so – will hopefully get you a quick start.

The course will be divided in five two-hour lectures. For each lecture I will compile a set of Lecture Notes. The current notes (*LN01*) deal with kinetic theory which forms the basis of the LBM. *LN02* explain the LBM in quite some detail. *LN03* discuss practical aspects such as boundary conditions, how to translate real (physical) flow systems in an LBM simulation, and what an actual LBM code could look like. *LN04* and *LN05* discuss a number of more specialized topics: collision operators, body forces, immersed boundary method, implementations for multiphase flow and for turbulence.

After I completed a first draft of all five sets of Lecture Notes I realized that the first two sets are quite theoretical / mathematical. Please bear with me in the first two lectures if your main interest is applying the LBM, the last three lectures will be much more applied.

These course notes are partly based on the book "The lattice Boltzmann method – principles and practice" by Krüger et al (Springer, ISBN 978-3-319-44647-9). I decided not to provide literature references in the lecture notes. Eighty percent can be found back in the above book (albeit sometimes in different notation); feel free to consult me for the remaining twenty percent.

1. Kinetic theory

1.1 Introduction
Matter consists of molecules. In a gas they fly around thereby colliding with one another. In a classical molecular dynamics description of a gas we follow individual molecules by solving their Newtonian equations of motion that include interaction forces between the molecules. Simulating this on a computer is called Molecular Dynamics (MD). In a continuum approach the discrete (molecular) nature of matter is abandoned to make place for a description in terms of functions describing properties (pressure, density, velocity, temperature) that continuously depend on (three-dimensional) location in space and time. Kinetic theory is a description in between molecular and continuous; a *mesoscopic* description.

1.2 Distribution function
Starting point of kinetic theory is the notion of a *distribution function*. Since distribution functions are also fundamental to the lattice-Boltzmann method it is worthwhile to go over some of the concepts and results from kinetic theory. To keep things relatively simple, we will consider a dilute, monoatomic gas with the molecules having no internal degrees of freedom (such as vibration or rotation) and the molecules colliding elastically.

The distribution function is denoted as $f(\mathbf{x}, \boldsymbol{\xi}, t)$ with $\mathbf{x}$ space vector, $\boldsymbol{\xi}$ velocity vector, and t time. It can be seen as a generalization of the density $\rho(\mathbf{x}, t)$, now also taking into account

velocity. It is the density of molecules in physical space as well as in *velocity space*. The SI units of the distribution function are $[f] = \text{kg} \cdot \dfrac{1}{\text{m}^3} \cdot \dfrac{1}{(\text{m/s})^3}$. Density, momentum and energy follow from integrations over velocity space:

$$\rho(\mathbf{x},t) = \iiint f(\mathbf{x},\boldsymbol{\xi},t) d^3\xi \tag{1.1}$$

$$\rho(\mathbf{x},t)\mathbf{u}(\mathbf{x},t) = \iiint \boldsymbol{\xi} f(\mathbf{x},\boldsymbol{\xi},t) d^3\xi \tag{1.2}$$

$$\rho(\mathbf{x},t)E(\mathbf{x},t) = \tfrac{1}{2} \iiint |\boldsymbol{\xi}|^2 f(\mathbf{x},\boldsymbol{\xi},t) d^3\xi \tag{1.3}$$

As we will see, it is useful to make a distinction between random thermal motion (with velocity $\mathbf{v}(\mathbf{x},t)$) and bulk motion of molecules (with velocity $\mathbf{u}(\mathbf{x},t)$ as identified in Eq. 1.2): $\mathbf{v}(\mathbf{x},t) \equiv \boldsymbol{\xi}(\mathbf{x},t) - \mathbf{u}(\mathbf{x},t)$. The energy associated to $\mathbf{v}(\mathbf{x},t)$ is

$$\rho(\mathbf{x},t)e(\mathbf{x},t) = \tfrac{1}{2} \iiint |\mathbf{v}|^2 f(\mathbf{x},\boldsymbol{\xi},t) d^3\xi \tag{1.4}$$

is called internal energy. We note that only translational kinetic energy is considered in the above expressions. This is due to us dealing with monoatomic gases that do not have rotational or vibrational degrees of freedom.

A quick way of finding an expression for pressure goes via the ideal gas law and the equipartition theorem. The latter relates internal energy per translational degree of freedom with temperature: $e_{dof} = \tfrac{1}{2}RT$ for each degree of freedom. With three degrees of freedom this gets $\rho e = \tfrac{3}{2}\rho RT$. The usual way of writing the ideal gas law in fluid dynamics is $p = \rho RT$ so that

$$p = \rho RT = \tfrac{2}{3}\rho e = \tfrac{1}{3} \iiint |\mathbf{v}|^2 f(\mathbf{x},\boldsymbol{\xi},t) d^3\xi \tag{1.5}$$

It is useful to check units at this stage. When we write $p = \rho RT$ then R is not the (universal) molar based gas constant $R_{molar} = 8.31 \text{ J}/(\text{mol} \cdot \text{K})$; instead, $R = R_{molar}/m$ with m the molar mass of the gas. Molar mass has units kg/mol so that R has units $\text{J}/(\text{kg} \cdot \text{K}) = \text{m}^2/(\text{s}^2 \cdot \text{K})$ which should be given $e = \tfrac{3}{2}RT$ and e having units m^2/s^2 (the latter from the way e is defined in Eq. 1.4).

1.3 Equilibrium distribution function
If a gas is left alone for sufficiently long time and molecules have undergone many collisions thereby exchanging momentum one can imagine that the distribution of velocities of the molecules reaches an equilibrium. This equilibrium is expected to be isotropic in velocity space. We assume – without lack of generality – the average velocity $\mathbf{u}$ equal to zero so that $\mathbf{v}(\mathbf{x},t) \equiv \boldsymbol{\xi}(\mathbf{x},t)$. Isotropy in velocity space then means that only the velocity magnitude (not the direction) matters for the equilibrium distribution function: $f^{eq}(\mathbf{x},|\mathbf{v}|,t)$. An important result of statistical mechanics is that the equilibrium distribution has the following form:

$$f^{eq}\left(\mathbf{x},|\mathbf{v}|,t\right)=\rho\left(\frac{1}{2\pi RT}\right)^{3/2}e^{-|\mathbf{v}|^2/(2RT)}$$ (1.6)

Equation 1.6 goes by the name Maxwell-Boltzmann distribution. It shows, as an example, that increasing temperature will get you a wider distribution function.

1.4 Evolution of distribution function

If we take the total derivative of the distribution function with respect to time we get

$$\frac{df}{dt}=\frac{\partial f}{\partial t}\frac{dt}{dt}+\frac{\partial f}{\partial x_\beta}\frac{dx_\beta}{dt}+\frac{\partial f}{\partial\xi_\beta}\frac{d\xi_\beta}{dt}$$ (1.7)

Where we use index notation for the location (x_β) and velocity (ξ_β) vector components and the summation convention: sum over repeated Greek indices (for example $\frac{\partial f}{\partial x_\beta}\frac{dx_\beta}{dt}=\frac{\partial f}{\partial x}\frac{dx}{dt}+\frac{\partial f}{\partial y}\frac{dy}{dt}+\frac{\partial f}{\partial z}\frac{dz}{dt}$). In Eq. 1.7, $\frac{dt}{dt}=1$, $\frac{dx_\beta}{dt}=\xi_\beta$, $\frac{d\xi_\beta}{dt}$ is an acceleration per unit volume and therefore $\frac{d\xi_\beta}{dt}=\frac{F_\beta}{\rho}$. Collisions are a reason for change of the distribution function since they re-distribute momentum. Combining these notions leads to the Boltzmann equation

$$\frac{\partial f}{\partial t}+\xi_\beta\frac{\partial f}{\partial x_\beta}+\frac{F_\beta}{\rho}\frac{\partial f}{\partial\xi_\beta}=\Omega(f)$$ (1.8)

where $\Omega(f)$ is the collision operator. It depends on the distribution function, i.e. on the way mass is distributed over physical and velocity space. The Boltzmann equations (Eq. 1.8) can be interpreted as an advection equation with forces and collisions as source terms. In a molecular collision, mass is not lost so that a property of the collision operator is

$$\iiint\Omega(f)d^3\xi=0$$ (1.9)

If we also assume that total momentum and total energy is conserved in collisions this implies.

$$\iiint\boldsymbol{\xi}\,\Omega(f)d^3\xi=\mathbf{0}$$ (1.10)

$$\iiint|\boldsymbol{\xi}|^2\Omega(f)d^3\xi=0$$ (1.11)

A lot of physics goes into the collision operator as it involves a wide spectrum of collision scenarios and intermolecular forces. To avoid (too much) complexity, simple heuristic approaches have been proposed that prove remarkably useful. Respect for conservation laws and the notion that collisions will eventually drive a system to equilibrium have led to the Bhatnagar, Gross & Krook (BGK) collision operator:

$$\Omega(f) = -\frac{1}{\tau}\left(f - f^{eq}\right) \tag{1.12}$$

The time constant τ determines how fast we relax to equilibrium; e.g. for a force-free, homogeneous system $f(\xi,t) = f^{eq}(\xi) + \left[f(\xi,t=0) - f^{eq}(\xi)\right]e^{-t/\tau}$. As expected and as we will see when discussing the lattice-Boltzmann method, τ determines the transport coefficients, most importantly – for fluid mechanics – the viscosity. Thinking of a heat transfer example, if we have a volume of gas with non-uniform temperature and leave it alone, temperature differences will even out and eventually the temperature will become uniform. In a physical sense, the time scales on which this happens will depend on the thermal diffusion coefficient (symbol a) and the size of the system. In a BGK sense they will be determined by the relaxation time τ. Hence the connection between τ and a.

1.5 Transport equations

It is time to relate the somewhat esoteric concept of distribution function with concepts more familiar to fluid dynamics. This we do by deriving transport equations from the Boltzmann equation (Eq. 1.8).

In the first place, we integrate Eq. 1.8 over velocity space:

$\frac{\partial}{\partial t}\iiint f d^3\xi + \frac{\partial}{\partial x_\beta}\iiint \xi_\beta f d^3\xi + \frac{F_\beta}{\rho}\iiint \frac{\partial f}{\partial \xi_\beta} d^3\xi = \iiint \Omega(f) d^3\xi$. We quickly realize that (Eq.

1.1) $\iiint f d^3\xi = \rho$; also (Eq. 1.2) $\iiint \xi_\beta f d^3\xi = \rho u_\beta$; and (Eq. 1.9) $\iiint \Omega(f) d^3\xi = 0$. The

term with the force ($\frac{F_\beta}{\rho}\iiint \frac{\partial f}{\partial \xi_\beta} d^3\xi$) is a little less straightforward. We argue that this term is

equal to zero based on integration by parts. As a reminder, consider two functions h and g that

have derivatives h' and g'. Then $\int hg' = hg\big|_{-\infty}^{\infty} - \int h'g$. Applying this

$\iiint 1 \cdot \frac{\partial f}{\partial \xi_\beta} d^3\xi = 1 \cdot f\big|_{-\infty}^{\infty} - 0 = 0$. As a result, integration of the Boltzmann equation over

velocity space gets us the continuity equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_\beta)}{\partial x_\beta} = 0 \tag{1.14}$$

(one more time: we are here using the summation convention so that Eq. 1.14 actually reads

$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_x)}{\partial x} + \frac{\partial(\rho u_y)}{\partial y} + \frac{\partial(\rho u_z)}{\partial z} = 0$)

A momentum balance equation is obtained when we multiply the Boltzmann equation by ξ_α and then integrate over velocity space:

$\frac{\partial}{\partial t}\iiint \xi_\alpha f d^3\xi + \frac{\partial}{\partial x_\beta}\iiint \xi_\alpha \xi_\beta f d^3\xi + \frac{F_\beta}{\rho}\iiint \xi_\alpha \frac{\partial f}{\partial \xi_\beta} d^3\xi = \iiint \xi_\alpha \Omega(f) d^3\xi$. First term on the

left-hand side: $\frac{\partial \rho u_\alpha}{\partial t}$; the integral in the second term we will call – for reasons that will

hopefully become clear later – the momentum flux tensor: $\Pi_{\alpha\beta} \equiv \iiint \xi_\alpha \xi_\beta f d^3\xi$ so that the second term gets $\dfrac{\partial \Pi_{\alpha\beta}}{\partial x_\beta}$; the integral in the third term is

$$\iiint \xi_\alpha \frac{\partial f}{\partial \xi_\beta} d^3\xi = \xi_\alpha f \big|_{-\infty}^{\infty} - \iiint \frac{\partial \xi_\alpha}{\partial \xi_\beta} f d^3\xi = -\rho \delta_{\alpha\beta} \text{ with } \delta_{\alpha\beta} \text{ the Kronecker delta}$$

($\delta_{\alpha\beta} = 1$ if $\alpha{=}\beta$; $\delta_{\alpha\beta} = 0$ if $\alpha \neq \beta$). The right-hand side is zero given Eq. 1.10 (momentum conservation in collisions). Eventually the momentum balance has the form

$$\frac{\partial \rho u_\alpha}{\partial t} + \frac{\partial \left(\Pi_{\alpha\beta}\right)}{\partial x_\beta} = F_\alpha \tag{1.15}$$

(for the last time: Eq. 1.15 uses the summation convention; writing out the x-component of Eq. 1.15: $\dfrac{\partial \rho u_x}{\partial t} + \dfrac{\partial \left(\Pi_{xx}\right)}{\partial x} + \dfrac{\partial \left(\Pi_{xy}\right)}{\partial y} + \dfrac{\partial \left(\Pi_{xz}\right)}{\partial z} = F_x$)

In Section 1.2 we hinted at splitting the velocity of molecules in average and thermal velocities: $\boldsymbol{\xi}(\mathbf{x},t) = \mathbf{u}(\mathbf{x},t) + \mathbf{v}(\mathbf{x},t)$, component wise: $\xi_\alpha = u_\alpha + v_\alpha$. Then

$\Pi_{\alpha\beta} = \iiint (u_\alpha + v_\alpha)(u_\beta + v_\beta) f d^3\xi = u_\alpha u_\beta \iiint f d^3\xi + u_\alpha \iiint v_\beta f d^3\xi + u_\beta \iiint v_\alpha f d^3\xi + \iiint v_\alpha v_\beta f d^3\xi$

; $u_\alpha u_\beta \iiint f d^3\xi = \rho u_\alpha u_\beta$; $u_\alpha \iiint v_\beta f d^3\xi = 0$; $u_\beta \iiint v_\alpha f d^3\xi = 0$. The last term we define as the stress tensor: $\iiint v_\alpha v_\beta f d^3\xi = -\sigma_{\alpha\beta}$. Putting this all together results in what is known as the *Cauchy momentum equation*:

$$\frac{\partial \rho u_\alpha}{\partial t} + \frac{\partial \left(\rho u_\alpha u_\beta\right)}{\partial x_\beta} = \frac{\partial \sigma_{\alpha\beta}}{\partial x_\beta} + F_\alpha \tag{1.16}$$

The stress tensor is usually written as the sum of viscous stress and pressure: $\sigma_{\alpha\beta} = \sigma'_{\alpha\beta} - p\delta_{\alpha\beta}$. Interestingly, if we would assume the fluid to be an ideal gas in equilibrium ($f = f^{eq}$ the Maxwell-Boltzmann distribution Eq. 1.6), evaluating the integral $\iiint v_\alpha v_\beta f^{eq} d^3\xi$ results in $\rho R T \delta_{\alpha\beta}$ which is equal to the pressure. Therefore, for an ideal gas in equilibrium, $\sigma_{\alpha\beta} = -p\delta_{\alpha\beta}$. As a consequence, viscous stresses are the result of non-equilibrium effects.

Viscous stresses are *modelled* in terms of fluid deformation: $\sigma'_{\alpha\beta} = \mu\left(\dfrac{\partial u_\alpha}{\partial x_\beta} + \dfrac{\partial u_\beta}{\partial x_\alpha}\right) + \zeta \delta_{\alpha\beta} \dfrac{\partial u_\gamma}{\partial x_\gamma}$

where μ and ζ are (material-related) coefficients. It is more common to write this as

$$\sigma'_{\alpha\beta} = \mu\left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} - \frac{2}{3}\delta_{\alpha\beta}\frac{\partial u_\gamma}{\partial x_\gamma}\right) + \mu_b \delta_{\alpha\beta}\frac{\partial u_\gamma}{\partial x_\gamma} \tag{1.17}$$

The term with the coefficient μ (which is viscosity) is a traceless stress tensor (*deviatoric* stress); the term with μ_b (which is called bulk viscosity) contains normal viscous stresses due

to volume changes (expansion and contraction). It should be clear that the bulk viscosity μ_b is related to the parameters μ and ζ: $\mu_b = \frac{2}{3}\mu + \zeta$.

With the notions regarding the stress tensor (its division in pressure and viscous stress, the latter divided in a deviatoric part and a normal part) the Cauchy momentum equation (Eq. 1.16) can be written as the Navier-Stokes equation:

$$\frac{\partial \rho u_\alpha}{\partial t} + \frac{\partial \left(\rho u_\alpha u_\beta \right)}{\partial x_\beta} = -\frac{\partial p}{\partial x_\alpha} + \frac{\partial}{\partial x_\beta} \left[\mu \left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} \right) + \left(\mu_b - \frac{2}{3}\mu \right) \delta_{\alpha\beta} \frac{\partial u_\gamma}{\partial x_\gamma} \right] + F_\alpha \quad (1.18)$$

In most fluids related research at the School of Engineering of UAberdeen, fluids are incompressible, i.e. have constant density. This implies that the continuity (Eq. 1.14) reduces to $\frac{\partial u_\beta}{\partial x_\beta} = 0$. As a consequence, the incompressible Navier-Stokes equation is a bit simpler than its general form:

$$\rho \frac{\partial u_\alpha}{\partial t} + \rho u_\beta \frac{\partial u_\alpha}{\partial x_\beta} = -\frac{\partial p}{\partial x_\alpha} + \frac{\partial}{\partial x_\beta} \left[\mu \left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} \right) \right] + F_\alpha \quad (1.19)$$

In the next set of Lecture Notes (LN02) the above notions from kinetic theory will proof useful for understanding the lattice-Boltzmann method. An important take-home message is that viscous stresses relate to fluids being off-equilibrium. A potentially confusing issue is compressibility. In the lattice-Boltzmann method, fluids are compressible. The main application of the method is, however, for incompressible fluids. This and more will be discussed in the upcoming lectures.