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FROM BOLTZMANN EQUATION TO NAVIER-STOKES

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Purpose: The objective of this article is to present a detailed derivation of the N-S system of equations from the more general Boltzmann equation.
Design/methodology/approach: This paper presents a derivation of general conservation equations based on the Boltzmann equation. It collates essential information from statistical mechanics and mathematical analysis. As previously stated, the objective is to collate all the requisite derivations of the NS equations from the Boltzmann equation to provide a comprehensive foundation for further study and to address frequently omitted steps. Such derivations can be found in existing literature, but they are often less detailed or are scattered across extensive studies where a single subsection is devoted to them. Conversely, a comprehensive grasp of the interconnections between the two equations facilitates a profound comprehension of the fundamental tenets of LBM. Furthermore, it illuminates the methodology for employing the solution of the Boltzmann equation to simulate fluid dynamics, a technique that can prove invaluable in the development of novel LBM applications.
Findings: A comprehensive set of assumptions and derivations which is often absent from the literature on this topic.
Originality/value: The manner in which the material is presented is original or challenging to locate, according to the authors' knowledge.
Keywords: mathematics, statistical mechanics, computational fluid mechanics.
Category of the paper: Mathematical Physics, Theoretical Fluid Dynamics.

1. Introduction

The Navier-Stokes (N-S) equations are equations that mathematically express the balance of momentum and conservation of mass for moving Newtonian fluid. Sometimes the N-S equations are accompanied by equations of state relating to pressure, temperature, and density.

In essence, the N-S equations are a set of partial differential equations that describe the changes in velocity, pressure, and density at any point in a fluid depending on the forces (gravity, viscosity, external forces) acting on the fluid at that point.

The N-S equations include in case of compressible and viscid flow:

- The equation of continuity (describing the principle of conservation of mass):

$$\frac{\partial \rho}{\partial t} + \nabla \circ (\rho \vec{u}) = 0 \tag{1}$$

  which states that the mass of the system must remain constant over time.

- Momentum equations (a set of equations describing the principle of conservation of momentum in j-th geometric direction):

$$\frac{\partial (\rho\, u_j)}{\partial t} + \nabla \circ \left(\rho\, \vec{u} u_j + \vec{P_j} - \vec{\pi_j}\right) - F_j = 0 \tag{2}$$

  expressing the fact that the rate of change of momentum the of the fluid element is caused only by the mass forces F_j and stresses $\vec{P_j} - \vec{\pi_j}$.

- Internal energy equation:

$$\frac{\partial E}{\partial t} + \vec{u} \circ \nabla E = -P \nabla \circ \vec{u} + \Psi - \nabla \circ \vec{\Phi} \tag{3}$$

  denoting that in any process change in internal energy is caused by pressure, viscous dissipation and changes of heat conduction flux.

The Navier-Stokes equations are still difficult to solve analytically, especially for complex geometries and boundary conditions, so they are usually solved numerically using computational fluid dynamics (CFD) techniques. For some time, another approach to solving the equations of conservation of mass, momentum and energy involving the use of the so-called Lattice Boltzmann Method has been gaining popularity.

The Lattice Boltzmann Method (LBM) is a method derived from the Boltzmann density equation, introduced by Hardy et al. in 1973 as a simplified approach to solving fluid dynamics problems (Cf. Hardy, 1973a, 1973b). Compared to traditional methods for solving Navier-Stokes equations, the LBM method has several advantages, including simplicity, efficiency, and the ability to handle complex geometries and boundary conditions.

Like any other method, LBM is not fully universal, and some difficulties are encountered when using it. A significant complication is problems requiring the construction of adaptive lattices and defining boundary conditions on the edges of areas with curved geometry and geometry not matched to a discrete lattice. The still unsolved problem is the use of LBM to model flows with large heat gradients and fully compressible flow. Modeling of thermoacoustic effects is still a matter of active research. Various proposals for solving these difficulties can be found in the literature (Zhao, 2020; Basu, 2020; Li, 2016), which does not change the fact that the development of LBM for various applications is a current and interesting research problem.

It should be noted that the Boltzmann equation and the Navier-Stokes equations describe different aspects of fluid dynamics and are not directly comparable in generality. The Boltzmann equation is a more fundamental description of the flow because it considers the behavior of individual fluid molecules and their collisions. It is a statistical equation that describes the change in the probability distribution of molecules with a fixed velocity in a fixed area.

The Navier-Stokes equations, on the other hand, are used to describe the continuum of fluid dynamics. They describe the macroscopic behavior of a fluid, such as its velocity, pressure, and density, and are more suitable for describing fluid flow at larger scales. One needs to reduce the amount of information coming from the Boltzmann equation to obtain the solution of Navier-Stokes equations. This is done by computing moments of the Boltzmann equation and will be covered in this work.

According to the idea, the Lattice Boltzmann Method does not numerically solve the equations of conservation of macroscopic properties such as mass, momentum, and energy (as it is in CFD), but models a fluid consisting of fictitious mesoscopic populations that move along a discrete grid called a lattice. The distribution of the populations in the grid is described by a set of discrete probability distribution functions that evolve over time according to a simplified version of the Boltzmann equation. In LBM, the Navier-Stokes equations are therefore not solved directly. However, their solutions are reconstructed from the solution of the Boltzmann equation. This apparent complication makes it possible to create a flow modeling procedure that is surprisingly simple to implement. This approach is possible since, under certain assumptions, the N-S equations can be derived from the more general Boltzmann equation.

In the literature, one can often find the statement that the Boltzmann equation is a more general equation than the N-S equation. On the other hand, it is difficult to find a detailed derivation of the relationship between these equations. This paper undertakes to show step-by-step how to derive from the Boltzmann equation all three equations representing the conservation law of mass, momentum, and energy.

It may be noted that much of the literature encountered leads ultimately to a series of articles written in the late 1940s by Harold Grad. These deal with the theoretical derivation of the N-S equations from the Boltzmann equation (Grad, 1949a) and also give a number of useful properties of Hermite polynomials, which are used in the discretization of the Boltzmann equation (Grad, 1949b). The paper also uses some of the designations and transitions from (Shu, 1991). Historically, Boltzmann's lattice method was first derived more experimentally from so-called lattice gas automata. More recent overview of applications can be found in (Li, 2020). An overview of the development of this theory up to 2000 with early examples of calculations can be found in (Li-Shi, 2000). Nowadays, methods based on LBM allow calculations of, for example, flows related to combustion and thermoacoustic phenomena (Miled, 2020; Bhairapurada, 2022; Taileb, 2022) it can also be applied to microfluidic phenomena (cf. Xu, 2021).

In most works dealing with LBM, it is emphasized that the LBM method uses the fact that instead of solving the N-S equations, the Boltzmann equation is solved, which, although more general, is better suited for discretization. The very derivation of the relationships between the Boltzmann and N-S equations is often incomplete or omitted in literature. Meanwhile, a full understanding of the relationship between the two descriptions helps to thoroughly understand the essence of LBM and indicate how to use the solution of the Boltzmann equation to model flow phenomena, including those caused by thermal phenomena.

This article aims to present a very detailed derivation of the equations of continuity, N-S equations, and the energy equation from the more general Boltzmann equation. We believe that the description using the language of mathematics helps in the development of methods for describing physical phenomena and the development of simulation methods.

2. Boltzmann equation

The Boltzmann equation is a partial differential equation that describes the behavior of a gas at the molecular level. It describes how the distribution of molecules changes over time because of collisions between them. The basic concept used here is the distribution function f that describes the distribution of molecules in phase space. This function tells the number of molecules (in other formulations mass of molecules) at a given point of 7-dimensional phase space – three spatial coordinates, three velocity components and temporal coordinate. It is worth noting that $\mathrm{f} = \mathrm{f}(\vec{x}, \vec{v}, \mathrm{t})$.

The change occurring with respect to time in the value of the function f is described by the total derivative[1]: $\frac{df}{dt}$. Since the redistribution of molecules occurs only because of their collision, it can be written that:

$$\frac{df}{dt} = \Omega(f) \tag{4}$$

Where the occurring on the right-hand side of the source term Ω is the so-called *collision operator*. The original form of the collision operator given by Boltzmann is expressed by an integral that considers different collision angles. Due to its complex form, the operator in this form is not suitable for simulations, so the standard approach is to use approximations of it with much simpler operators. The typical approach is to use the BGK collision operator. In this formulation, the distribution function tends exponentially to the equilibrium distribution function.

[1] In engineering science, the total derivative is often called the substantial derivative and uses the symbol $\frac{Df}{Dt}$.

From the physical interpretation of derivatives:

$$v_i = \frac{dx_i}{dt},\ a_i = \frac{dv_i}{dt}$$

it follows that the equation (4) describing changes in the distribution function takes the form:

$$\frac{\partial f}{\partial t} + \sum_{i=1}^{3}\left(v_i \frac{\partial f}{\partial x_i} + \frac{F_i}{\rho}\frac{\partial f}{\partial v_i}\right) = \Omega(f). \tag{5}$$

This equation is called the Boltzmann equation.

In the equation (5), according to Newton's second law of dynamics $a_i = F_i/m$, the acceleration is written in terms of the external force $\vec{F} = (F_1, F_2, F_3)$, where F_i denotes the force in the i-th direction per unit volume. The variable ξ_i means velocity in the appropriate direction in the velocity space[2].

Solving the Boltzmann equation in the general case is a difficult task due to the complexity of the collision operator, especially for systems with many molecules. For this reason, practical applications usually use an approximation of the Ω operator by the so-called BGK collision operator (proposed by Bhatnagar, Gross and Krook in (Bhatnagar, 1954)) of the form

$$\Omega(f) = -\frac{1}{\tau}(f - f^{eq}), \tag{6}$$

where τ denotes the relaxation time, and f^{eq} is the so-called equilibrium solution.

The equation (5) with the collision operator taken in this way is called the simplified Boltzmann equation.

The function f^{eq} is an equilibrium distribution function representing the steady state of the system in which the fluid is in equilibrium. This interpretation means that f^{eq} takes the form of the Maxwell-Boltzmann distribution, which is expressed in the three-dimensional case by the following formula:

$$f^{eq}(\vec{x}, \vec{v}, t) = \left(\frac{m}{2\pi k_B T}\right)^{\frac{3}{2}} \exp\left(-m\,\frac{|\vec{v} - \vec{u}|^2}{2k_B T}\right), \tag{7}$$

where:

m - denotes mass of molecule,

k_B - Boltzmann constant,

T - temperature,

$\vec{v}$ - intrinsic molecule velocity,

$\vec{u}$ - macroscopic fluid velocity (hence $\vec{w} = \vec{v} - \vec{u}$ is the velocity fluctuation of the molecule).

[2] Since the considerations are carried out with respect to a unit volume, the mass m can be replaced by the density of the fluid ρ.

3. From Boltzmann equation to conservation laws

The fact that the Boltzmann equation is more general than the N-S equations means that its solution (in selected cases) is the solution of the equations of fluid dynamics (a system including the equations (1), (2), (3)).

From the form of the collision operator, it follows that f tends exponentially to the Maxwell-Boltzmann distribution f^{eq} and locally conserves mass, momentum and energy. Note also that it follows from the definition of the function f that[3]:

$$\rho(\vec{x},t) = \int_{\mathcal{V}} m \cdot f(\vec{x},\vec{v},t)\, d^3v, \tag{8}$$

where:

m - the mass of the molecule,

$\mathcal{V}$ - the set of all velocities in all possible directions.

3.1. From Boltzmann to continuity equation

The continuity equation (1) is a relation derived from the principle of conservation of mass. Multiply Boltzmann's equation (5) by the mass of the molecule m and integrate over all possible velocities (i.e., over d^3v). We get:

$$\underbrace{\int_{\mathcal{V}} m \cdot \frac{\partial f}{\partial t}\, d^3v}_{(\mathrm{B1}_1)} + \underbrace{\int_{\mathcal{V}} m \cdot \sum_{i=1}^{3} v_i \frac{\partial f}{\partial x_i}\, d^3v}_{(\mathrm{B1}_2)} + \underbrace{\int_{\mathcal{V}} m \cdot \sum_{i=1}^{3} \frac{F_i}{\rho} \frac{\partial f}{\partial v_i}\, d^3v}_{(\mathrm{B1}_3)} = \underbrace{0}_{\mathrm{B1}_4}.$$

where:

$(\mathrm{B1}_1)$

$$\int_{\mathcal{V}} m \cdot \frac{\partial f}{\partial t}\, d^3v = \frac{\partial}{\partial t} \underbrace{\int_{\mathcal{V}} m \cdot f\, d^3v}_{\rho(\vec{x},t)} = \frac{\partial \rho}{\partial t}$$

$(\mathrm{B1}_2)$ note that[4]:

$$\int_{\mathcal{V}} m \cdot v_i \frac{\partial f}{\partial x_i}\, d^3v = \frac{\partial}{\partial x_i} \underbrace{\int_{\mathcal{V}} v_i \cdot mf\, d^3v}_{u_i \rho(\vec{x},t)} = \frac{\partial (u_i \rho)}{\partial x_i}$$

Thus:

$$\int_{\mathcal{V}} m \cdot \sum_{i=1}^{3} v_i \frac{\partial f}{\partial x_i}\, d^3v = \sum_{i=1}^{3} \int_{\mathcal{V}} m \cdot v_i \frac{\partial f}{\partial x_i}\, d^3v = \frac{\partial (u_1\rho)}{\partial x_1} + \frac{\partial (u_2\rho)}{\partial x_2} + \frac{\partial (u_3\rho)}{\partial x_3}$$

$$= \left[\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \frac{\partial}{\partial x_3}\right] \circ [\rho u_1, \rho u_2, \rho u_3] = \nabla \circ (\rho \vec{u})$$

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[3] To simplify the notation, it was assumed that the integral in (8) means $\iiint_{\mathcal{V}} m \cdot f(\vec{x},\vec{v},t)\, dv_1\, dv_2\, dv_3$

[4] v_i is the component of the molecule's own velocity, and u_i is the component of the molecules' average velocity (macroscopic velocity) in the fluid region.

(B1$_3$) because of:

$$\int_v m \cdot \frac{\partial f}{\partial v_i}\frac{F_i}{\rho}\, d^3v = \frac{\partial}{\partial v_i}\frac{F_i}{\rho}\underbrace{\int_v m \cdot f\, d^3v}_{\rho(\vec{x},t)} = \frac{\partial F_i}{\partial v_i} = 0,$$

we obtain:

$$\sum_{i=1}^{3}\int_v m \cdot \frac{\partial f}{\partial v_i}\frac{F_i}{\rho}\, d^3v = m\sum_{i=1}^{3}\frac{\partial F_i}{\partial v_i} = 0$$

The zeroing of the derivative of the external force after the velocities is because the force does not depend on the velocity of the molecules in the fluid.

(B1$_4$) According to the principle of conservation of mass, the right-hand side of the equation disappears, since molecules neither appear nor disappear because of collisions.

In view of the above, it is easy to see how the continuity equation (5) follows from the Boltzmann equation (1):

$$\begin{array}{ccccccc} \dfrac{\partial f}{\partial t} & + & \displaystyle\sum_{i=1}^{3} v_i \frac{\partial f}{\partial x_i} & + & \displaystyle\sum_{i=1}^{3} \frac{F_i}{\rho}\frac{\partial f}{\partial v_i} & = & \Omega(f) \\ \Downarrow & & \Downarrow & & \Downarrow & & \Downarrow \\ \dfrac{\partial \rho}{\partial t} & + & \nabla \circ (\rho \vec{u}) & + & 0 & = & 0 \end{array}$$

3.2. From Boltzmann to momentum equations

Momentum equations are derived from the principle of conservation of momentum. Let us consider a certain quantity connected with a molecule, such as mass m or momentum in a certain direction mv_i. For short let us denote such quantity with C.Then, the integral

$$\int_v C\, f\, d^3v = \langle C \rangle$$

denotes the value of C averaged with respect to velocity. Assume, for the purposes of the calculations in this subsection, that we are considering the direction j. Boltzmann's equation (5) multiplied by the momentum of the molecule mv_j and integrated over all velocities has the form:

$$\underbrace{\int_v m\, v_j \cdot \frac{\partial f}{\partial t}\, d^3v}_{(\mathrm{B2}_1)} + \underbrace{\int_v m\, v_j \cdot \sum_{i=1}^{3} v_i \frac{\partial f}{\partial x_i}\, d^3v}_{(\mathrm{B2}_2)} + \underbrace{\int_v m\, v_j \cdot \sum_{i=1}^{3} \frac{F_i}{\rho}\frac{\partial f}{\partial v_i}\, d^3v}_{(\mathrm{B2}_3)} = \underbrace{0}_{(\mathrm{B2}_4)}.$$

We get:

(B2$_1$)

$$\int_v m v_j \cdot \frac{\partial f}{\partial t}\, d^3v = \frac{\partial}{\partial t}\underbrace{\int_v v_j \cdot mf\, d^3v}_{u_j \cdot \rho(\vec{x},t)} = \frac{\partial(\rho u_j)}{\partial t}.$$

(B2$_2$) from:

$$\vec{v} = \underbrace{\vec{u}}_{\text{global fluid velocity}} + \underbrace{\vec{w}}_{\text{molecule's velocity fluctuation}}$$

it follows that:

$$\int_{\mathcal{V}} m\, v_j \cdot v_i \frac{\partial \mathrm{f}}{\partial x_i}\, d^3v = \frac{\partial}{\partial x_i}\int_{\mathcal{V}} \underbrace{v_j v_i}_{(w_j+u_j)(w_i+u_i)}\, \mathrm{mf}\, d^3\mathrm{v}$$

$$= \frac{\partial}{\partial x_i}\int_{\mathcal{V}} \left(w_j w_i + w_j u_i + u_j w_i + u_j u_i\right) \cdot mf\; d^3\mathrm{v}$$

$$= \frac{\partial}{\partial x_i}\int_{\mathcal{V}} u_j\, u_i \cdot mf\; d^3v + \frac{\partial}{\partial x_i}\int_{\mathcal{V}} w_j\, u_i \cdot mf\; d^3 + \frac{\partial}{\partial x_i}\int_{\mathcal{V}} u_j w_i \cdot mf\; d^3v$$

$$+ \frac{\partial}{\partial x_i}\int_{\mathcal{V}} ww_{ij} \cdot mf\; d^3v = \frac{\partial\left(u_j u_i \rho\right)}{\partial x_i} + \frac{\partial\left(\langle w_j u_i\rangle \rho\right)}{\partial x_i} + \frac{\partial\left(\langle w_i u_j\rangle \rho\right)}{\partial x_i} + \frac{\partial\left(\langle w_i w_j\rangle \rho\right)}{\partial x_i} = (*)$$

where $\langle x\rangle$ denotes expected value of unknown x.

Note that $\langle u_j u_i\rangle = u_j u_i$ and $\langle w_j u_i\rangle = \langle w_i u_j\rangle = 0$, because the velocity of the chaotic motion of the molecules cancels out (as long as it is in the first power). Hence:

$$(*) = \frac{\partial\left(u_j u_i \rho\right)}{\partial x_i} + \frac{\partial\left(\langle w_i w_j\rangle \rho\right)}{\partial x_i}$$

The expression $\langle w_i w_j\rangle$ is an element of second order tensor

$$\vec{\mathrm{w}} \otimes \vec{\mathrm{w}} = \begin{bmatrix} \langle \mathrm{w}_1\, \mathrm{w}_1\rangle & \langle \mathrm{w}_1\, \mathrm{w}_2\rangle & \langle \mathrm{w}_1\, \mathrm{w}_3\rangle \\ \langle \mathrm{w}_2\, \mathrm{w}_1\rangle & \langle \mathrm{w}_2\, \mathrm{w}_2\rangle & \langle \mathrm{w}_2\, \mathrm{w}_3\rangle \\ \langle \mathrm{w}_3\, \mathrm{w}_1\rangle & \langle \mathrm{w}_3\, \mathrm{w}_2\rangle & \langle \mathrm{w}_3\, \mathrm{w}_3\rangle \end{bmatrix} \tag{9}$$

The random velocities are **almost** uncorrelated, so the off-diagonal elements of the $\vec{w} \otimes \vec{w}$ tensor are close to 0. Let's separate the effects of this tensor into those related to pressure and viscosity:

$$P = \frac{1}{3}\rho(\langle w_1^2\rangle + \langle w_2^2\rangle + \langle w_3^2\rangle) \quad \text{(pressure)}$$

$$\pi_{ij} = P\delta_{ij} - \rho\langle w_i w_j\rangle \quad \text{(viscous stress tensor)}$$

With these symbols:

$$\rho\langle w_i w_j\rangle = P\delta_{ij} - \pi_{ij} \tag{10}$$

that gives:

$$\int_{\mathcal{V}} m\, v_j \cdot v_i \frac{\partial f}{\partial x_i}\, d^3v = \frac{\partial\left(u_j u_i \rho\right)}{\partial x_i} + \frac{\partial}{\partial x_i}\left(P\delta_{ij} - \pi_{ij}\right) \tag{11}$$

Henceforth:

$$\sum_{i=1}^{3}\left(\int_{\mathcal{V}} m\, v_j \cdot v_i \frac{\partial f}{\partial x_i}\, d^3v\right) = \sum_{j=1}^{3}\left(\frac{\partial\left(u_j u_i \rho\right)}{\partial x_i} + \frac{\partial}{\partial x_i}\left(P\delta_{ij} - \pi_{ij}\right)\right)$$

$$= \frac{\partial\left(u_1 u_j \rho\right)}{\partial x_1} + \frac{\partial\left(u_2 u_j \rho\right)}{\partial x_2} + \frac{\partial\left(u_3 u_j \rho\right)}{\partial x_3} + \frac{\partial\left(P\delta_{1j} - \pi_{1j}\right)}{\partial x_1} + \frac{\partial\left(P\delta_{2j} - \pi_{2j}\right)}{\partial x_2} + \frac{\partial\left(P\delta_{3j} - \pi_{3j}\right)}{\partial x_3}$$

$$= \left[\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \frac{\partial}{\partial x_3}\right] \circ \left(\left[\rho u_1 u_j, \rho u_2 u_j, \rho u_3 u_j\right] + \left[P\delta_{1j} - \pi_{1j}, P\delta_{2j} - \pi_{2j}, P\delta_{3j} - \pi_{3j}\right]\right)$$

$$= \nabla \circ \left(\rho \vec{u} u_j + \overrightarrow{P_j} - \overrightarrow{\pi_j}\right)$$

(B2$_3$) Note that from the derivative $\frac{\partial(v_j f)}{\partial v_i}$ it follows that[5]:

$$v_j \frac{\partial f}{\partial v_i} = \frac{\partial\left(v_j f\right)}{\partial v_i} - \frac{\partial v_j}{\partial v_i} \cdot f$$

Hence:

$$\int_{\mathcal{V}} m\, v_j \cdot \frac{\partial f}{\partial v_i} \frac{F_i}{\rho}\, d^3v = \frac{mF_i}{\rho} \int_{\mathcal{V}} v_j \frac{\partial f}{\partial v_i}\, d^3v =$$

$$= \frac{mF_i}{\rho} \int_{\mathcal{V}} \left(\frac{\partial\left(v_j f\right)}{\partial v_i} - \frac{\partial v_j}{\partial v_i} \cdot f\right) d^3v = \frac{mF_i}{\rho} \int_{\mathcal{V}} \left(-\delta_{ij} f\right)\, d^3v$$

because[6]:

$$\frac{mF_i}{\rho} \int_{\mathcal{V}} \frac{\partial\left(f v_j\right)}{\partial v_i}\, d^3v = \frac{\partial}{\partial v_i} \frac{F_i}{\rho} \underbrace{\int_{\mathcal{V}} v_j f\, m\, d^3v}_{u_j \cdot \rho(\vec{x},t)} = \frac{\partial\left(F_i u_j\right)}{\partial v_i} = 0$$

And:

$$\frac{\partial v_j}{\partial v_i} = \delta_{ij} = \begin{cases} 1, i = j \\ 0, i \neq j \end{cases}$$

Finally

$$\sum_{i=1}^{3}\left(\int_{\mathcal{V}} m\, v_j \cdot \frac{\partial f}{\partial v_i} \frac{F_i}{\rho}\, d^3v\right) = \sum_{i=1}^{3} \frac{mF_i}{\rho} \int_{\mathcal{V}} \left(-\delta_{ij} f\right)\, d^3v = -\sum_{i=1}^{3} \frac{F_i}{\rho} \delta_{ij} \underbrace{\int_{\mathcal{V}} m\, f\, d^3v}_{\rho(\vec{x},t)} = -F_j$$

(B2$_4$) As in the case of continuity of mass, the principle of conservation of momentum guarantees that the right-hand side of the equation disappears because the molecules do not change the total momentum in the area because of collisions.

[5] Derivative $\frac{\partial(v_j f)}{\partial v_i} = \frac{\partial v_j}{\partial v_i} \cdot f + v_j \frac{\partial f}{\partial v_i}$.

[6] The average velocity of the fluid does not depend on the velocity of the molecule.

In effect, the Boltzmann equation results in the (2) equation. the N-S equation (for j-th variable):

$$\begin{array}{ccccccc} \dfrac{\partial f}{\partial t} & + & \displaystyle\sum_{i=1}^{3} v_i \frac{\partial f}{\partial x_i} & + & \displaystyle\sum_{i=1}^{3} \frac{F_i}{\rho}\frac{\partial f}{\partial v_i} & = & \Omega(f) \\ \Downarrow & & \Downarrow & & \Downarrow & & \Downarrow \\ \dfrac{\partial(\rho\, u_j)}{\partial t} & + & \nabla \circ \left(\rho\, \vec{u}\mathrm{u_j} + \vec{\mathrm{P}_\mathrm{j}} - \vec{\pi_\mathrm{j}}\right) & + & -F_j & = & 0 \end{array}$$

4. From Boltzmann to energy equation

The following discussion will use the concept of internal energy per unit volume:

$$E = \int_v \frac{mw^2}{2} f d^3v = \left\langle \frac{w^2}{2}\rho \right\rangle \tag{12}$$

As in the subsections above, we multiply the Boltzmann equation (5) by the kinetic energy of the molecule $\frac{mv^2}{2} = \frac{m}{2}(v_1^2 + v_2^2 + v_3^2)$ and we integrate over velocities. Hence:

$$\underbrace{\int_v \frac{mv^2}{2}\cdot\frac{\partial f}{\partial t}\, d^3v}_{(\mathrm{B3}_1)} + \sum_{i=1}^{3} \underbrace{\int_v \frac{mv^2}{2} v_i \cdot \frac{\partial f}{\partial x_i}\, d^3v}_{(\mathrm{B3}_2)} + \underbrace{\sum_{i=1}^{3} \int_v \frac{mv^2}{2}\frac{F_i}{\rho}\cdot\frac{\partial f}{\partial v_i}\, d^3v}_{(\mathrm{B3}_3)} = \underbrace{0}_{(\mathrm{B3}_4)} \tag{13}$$

(B3$_1$)

$$\int_v \frac{mv^2}{2}\cdot\frac{\partial f}{\partial t}\, d^3v = \frac{\partial}{\partial t}\int_v \left(\frac{u^2}{2} + \vec{u}\circ\vec{w} + \frac{w^2}{2}\right) mf\; d^3v = \frac{\partial}{\partial t}\left(\frac{u^2}{2}\rho + \underbrace{\left\langle \frac{w^2}{2}\rho \right\rangle}_{E}\right)$$

because $\int_v \vec{u}\circ\vec{w}\, mf\, d^3v = \langle uw\rho\rangle = 0$

(B3$_2$) Considerations will be made for i −th component.

$$\int_v \frac{mv^2}{2} v_i \cdot \frac{\partial f}{\partial x_i}\, d^3v = \frac{\partial}{\partial x_i}\left(\int_v \frac{m}{2}\sum_{k=1}^{3}(u_k + w_k)^2(u_i + w_i)\cdot f\, d^3v\right) =$$

$$= \frac{\partial}{\partial x_i}\left(\frac{\rho}{2}\left\langle \sum_{k=1}^{3}(u_k + w_k)^2(u_i + w_i)\right\rangle\right) =$$

$$= \frac{\partial}{\partial x_i}\left(\frac{\rho}{2}\left\langle \sum_{k=1}^{3}(u_i u_k^2 + 2u_i u_k w_k + u_i w_k^2 + w_i u_k^2 + 2u_k w_k w_i + w_i w_k^2)\right\rangle\right)$$

The expected value of the expressions in which the velocity of the chaotic motion of the molecules $\vec{w}$ occurs in the first power is 0:

$$\frac{\partial}{\partial x_i}\left(\frac{\rho}{2}\left\langle\sum_{k=1}^{3}(u_i u_k^2 + u_i w_k^2 + 2u_k w_k w_i + w_i w_k^2)\right\rangle\right) =$$

$$= \frac{\partial}{\partial x_i}\frac{\rho}{2}\left(\sum_{k=1}^{3}(u_i u_k^2 + \langle u_i w_k^2\rangle + 2\langle u_k w_k w_i\rangle + \langle w_i w_k^2\rangle)\right) =$$

$$= \frac{\partial}{\partial x_i}\frac{\rho}{2}\left(u_i u^2 + \langle u_i w^2\rangle + 2\sum_{k=1}^{3} u_k\langle w_k w_i\rangle + \langle w_i w^2\rangle\right) =$$

$$= \frac{\partial}{\partial x_i}\left(\frac{\rho u^2}{2}u_i + \underbrace{\left\langle\frac{\rho w^2}{2}\right\rangle}_{E}u_i + \sum_{k=1}^{3}\underbrace{\rho\langle w_k w_i\rangle}_{P\delta_{ik}-\pi_{ik}}u_k + \underbrace{\frac{\rho\langle w^2 w_i\rangle}{2}}_{\Phi_i}\right) =$$

$$= \frac{\partial}{\partial x_i}\left(\frac{\rho u^2}{2}u_i + Eu_i + \sum_{k=1}^{3}(P\delta_{ik} - \pi_{ik})u_k + \Phi_i\right)$$

where:

$P\delta_{ik} - \pi_{ik}$ is defined as in (10),

Φ_i – denotes conduction heat flux.

(B3$_3$) From the formula for the derivative of the product:

$$\frac{\partial(fv^2)}{\partial v_i} = \frac{\partial\left(f\cdot(v_1^2+v_2^2+v_3^2)\right)}{\partial v_i} = \frac{\partial f}{\partial v_i}\cdot v^2 + 2v_i f$$

it follows that:

$$\frac{\partial f}{\partial v_i}\cdot v^2 = \frac{\partial(fv^2)}{\partial v_i} - 2v_i f.$$

Thus:

$$\sum_{i=1}^{3}\int_{\mathcal{V}}\frac{mv^2}{2}\frac{F_i}{\rho}\cdot\frac{\partial f}{\partial v_i}\,d^3v = \sum_{i=1}^{3}\int_{\mathcal{V}}\frac{F_i}{2\rho}\cdot\left(m\frac{\partial(fv^2)}{\partial v_i} - 2mv_i f\right)d^3v =$$

$$= \frac{F_i}{2\rho}\int_{\mathcal{V}}\left(\nabla_{\vec{v}}mfv^2 - \sum_{i=1}^{3}2mv_i f\right)d^3v = \frac{F_i}{2\rho}\int_{\mathcal{V}}\nabla_{\vec{v}}\,mfv^2\,\mathrm{d}^3v - \sum_{i=1}^{3}\frac{F_i}{\rho}\int_{\mathcal{V}}mv_i f\,\mathrm{d}^3v =$$

$$= \frac{F_i}{2m}\underbrace{\oiint_{\partial\mathcal{V}} fv^2\vec{n}\,\mathrm{d}S}_{\text{Divergence Theorem}} - \sum_{i=1}^{3}\frac{F_i}{\rho}\rho u_i = -\sum_{i=1}^{3}F_i u_i$$

Integral $\oiint_{\partial\mathcal{V}} fv^2\mathcal{V}\vec{n}\,\mathrm{d}S = 0$ since there is no outflow of molecules from the $\mathcal{V}$ region (in phase space). Hence, the total energy equation, derived from the Boltzmann equation, takes the form:

$$\frac{\partial}{\partial t}\left(\frac{u^2}{2}\rho + E\right) + \sum_{i=1}^{3}\frac{\partial}{\partial x_i}\left(\frac{\rho u^2}{2}u_i + Eu_i + \sum_{k=1}^{3}(P\delta_{ik} - \pi_{ik})u_k + \Phi_i\right) = \sum_{i=1}^{3}F_i\,u_i \qquad (14)$$

To express the above equation in a form that includes only quantities related to the internal motion of the molecules, let us return to the momentum equation:

$$\frac{\partial}{\partial t}(\rho u_i) + \sum_{k=1}^{3} \frac{\partial}{\partial x_k}(\rho u_i u_k + P\delta_{ik} - \pi_{ik}) = F_i$$

Calculating the derivatives of the products, the equation above, one can write:

$$\underline{u_i \frac{\partial \rho}{\partial t}} + \rho \frac{\partial u_i}{\partial t} + \sum_{k=1}^{3} \left(\frac{\partial \rho u_k}{\partial x_k} u_i + \underline{\frac{\partial u_i}{\partial x_k} \rho u_k} \right) + \sum_{k=1}^{3} \frac{\partial}{\partial x_k}(P\delta_{ik} - \pi_{ik}) = F_i$$

The underlined components, according to the continuity equation (2), add up to 0. Therefore:

$$\rho \frac{\partial u_i}{\partial t} + \sum_{k=1}^{3} \left(\frac{\partial \rho u_i}{\partial x_k} u_k \right) = F_i - \sum_{k=1}^{3} \frac{\partial}{\partial x_k}(P\delta_{ik} - \pi_{ik}) . \tag{15}$$

Let us revisit the momentum equation again, this time multiplying it by the velocity u_i:

$$u_i \frac{\partial}{\partial t}(\rho u_i) + \sum_{k=1}^{3} u_i \frac{\partial}{\partial x_k}(\rho u_i u_k + P\delta_{ik} - \pi_{ik}) = F_i u_i$$

Using the derivative of the product $\frac{\partial(\rho u_i)}{\partial t}$, this equation can be written in the form:

$$\frac{\partial \rho u_i^2}{\partial t} - \underline{\rho u_i \frac{\partial u_i}{\partial t}} + \sum_{k=1}^{3} \left(\frac{\partial \rho u_i^2 u_k}{\partial x_k} - \underline{\rho u_i u_k \frac{\partial u_i}{\partial x_k}} \right) + \sum_{k=1}^{3} u_i \frac{\partial}{\partial x_k}(P\delta_{ik} - \pi_{ik}) = F_i u_i .$$

As a result of adding equation above to equation (15) multiplied by u_i underlined components will cancel out. Finally, we get:

$$\frac{\partial \rho u_i^2}{\partial t} + \sum_{k=1}^{3} \frac{\partial \rho u_i^2 u_k}{\partial x_k} = 2F_i u_i - 2\sum_{k=1}^{3} u_i \frac{\partial}{\partial x_k}(P\delta_{ik} - \pi_{ik}).$$

Finally:

$$\frac{\partial}{\partial t}\left(\frac{\rho u_i^2}{2} \right) + \sum_{k=1}^{3} \frac{\partial}{\partial x_k}\left(\frac{\rho u_i^2 u_k}{2} \right) = F_i u_i - \sum_{k=1}^{3} u_i \frac{\partial}{\partial x_k}(P\delta_{ik} - \pi_{ik}) \tag{16}$$

Summing up the variants of the equation (16) corresponding to each direction, we get:

$$\frac{\partial}{\partial t}\left(\frac{\rho(u_1^2 + u_2^2 + u_3^2)}{2} \right) + \sum_{k=1}^{3} \frac{\partial}{\partial x_k}\left(\frac{\rho(u_1^2 + u_2^2 + u_3^2)u_k}{2} \right) =$$

$$= F_1 u_1 + F_2 u_2 + F_3 u_3 - \sum_{i=1}^{3}\sum_{k=1}^{3} u_i \frac{\partial}{\partial x_k}(P\delta_{ik} - \pi_{ik}),$$

which is easily simplified to:

$$\frac{\partial}{\partial t}\left(\frac{\rho u^2}{2} \right) + \sum_{k=1}^{3} \frac{\partial}{\partial x_k}\left(\frac{\rho u^2 u_k}{2} \right) = \sum_{i=1}^{3} F_i u_i - \sum_{i=1}^{3}\sum_{k=1}^{3} u_i \frac{\partial}{\partial x_k}(P\delta_{ik} - \pi_{ik}) . \tag{17}$$

Using the product rule derivative

$$\frac{\partial\left((P\delta_{ik}-pi_{ik})u_i\right)}{\partial x_k}=u_i\frac{\partial}{\partial x_k}(P\delta_{ik}-\pi_{ik})+(P\delta_{ik}-\pi_{ik})\frac{\partial u_i}{\partial x_k}$$

we get:

$$\frac{\partial}{\partial t}\left(\frac{\rho u^2}{2}\right)+\sum_{k=1}^{3}\frac{\partial}{\partial x_k}\left(\frac{\rho u^2 u_k}{2}\right)=\sum_{i=1}^{3}F_i\,u_i-\sum_{i=1}^{3}\sum_{k=1}^{3}\left(\frac{\partial(P\delta_{ik}-\pi_{ik})u_i}{\partial x_k}-(P\delta_{ik}-\pi_{ik})\frac{\partial u_i}{\partial x_k}\right)$$

Subtracting the above equation from the equation (14) we are left with:

$$\frac{\partial E}{\partial t}+\sum_{i=1}^{3}\frac{\partial E u_i}{\partial x_i}+\sum_{i=1}^{3}\sum_{k=1}^{3}\left((P\delta_{ik}-\pi_{ik})\frac{\partial u_i}{\partial x_k}\right)+\sum_{i=1}^{3}\frac{\partial\Phi_i}{\partial x_i}=0.$$

Taking the symbol $\Psi=\sum_{i=1}^{3}\sum_{k=1}^{3}\pi_{ik}\frac{\partial u_i}{\partial x_k}$ as rate of viscous dissipation the internal energy equation is obtained:

$$\frac{\partial E}{\partial t}+\sum_{i=1}^{3}\frac{\partial E u_i}{\partial x_i}=-\sum_{i=1}^{3}\sum_{k=1}^{3}P\,\delta_{ik}\frac{\partial u_i}{\partial x_k}+\Psi-\sum_{i=1}^{3}\frac{\partial\Phi_i}{\partial x_i}$$

which can be converted to (3).

5. LBM algorithm overview

The main purpose of the considerations presented so far in the paper is to show how to obtain the Navier-Stokes equations from the Boltzmann equation. Each of the conservation laws was obtained by integrating over all velocities the Boltzmann equation, which was previously multiplied by the appropriate quantities.

The same principle also guides the idea of the Lattice Boltzmann Method. The discretization of the Boltzmann equation (in the velocity, space, and time domains) leads to the construction of an iterative procedure describing the evolution of a discrete variant of the distribution function, i.e., the flow of mesoscopic populations in the lattice.

The main idea behind LBM is to write the Boltzmann equation in a discrete form. Discretization begins with the construction of a discrete mesh (lattice) that divides the computational domain into cells. Only q directions are considered in each cell. The discrete distribution function is analogous to the continuous counterpart in the sense that from its moments we can recover density, momentum, and energy, but is only defined on a discrete finite set of velocities, positions, and time instances. The values of the distribution function defined on certain nodes at a given instance of time are called mesoscopic populations. Each of the finite number of populations has velocity in one of q allowed directions. The population assigned to node ${}_jx$ and having velocity in direction i is denoted by ${}_if({}_jx)$. The lattice model

determines how many populations with discrete velocity vectors in different directions will be assigned to a lattice node. In two-dimensional simulations, the D2Q9 lattice is most often used, in which there are 9 populations at each node. An exemplary node of the D2Q9 lattice (together with the method of numbering velocities) is shown in Fig. 1. The population with zero velocity is resting in the middle of the node. Symbolically, the fact that populations can be of different sizes is indicated by the different lengths of the corresponding arrows.

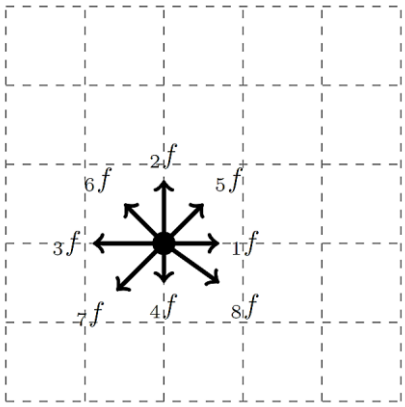

Figure 1. Example of lattice populations.

The evolution of the i-th population is described by the formula:

$$ {}_{i}f({}_{j}x + \overrightarrow{{}_{i}v}\Delta t, t + \Delta t) = {}_{i}f({}_{j}x, t) + \Omega({}_{i}f({}_{j}x, t)) \tag{18} $$

Note that since the right side of the equation (18) depends only on the values of the functions at points in the space, calculations can be carried out simultaneously for all points in space (which significantly reduces the time for performing simulations). In LBM this step in calculations is called *a collision*. The left side of the equation (18) does require knowledge of the value of the distribution function at neighboring points (*a propagation*), but since this step only involves shifting the previously calculated values to other positions, once the variables are properly arranged in the computer's memory, it does not significantly reduce computing performance. The collision and the propagation together form one iteration step for the ${}_{i}f$ population.

It should be emphasized that the equation (18) applies only to the behavior of the population inside the flow domain. A separate treatment is required for boundary conditions, which, due to the topic of the paper, will be omitted here.

If we know the values of the discrete distribution function at each node and for each direction (population), the macroscopic quantities of interest can be determined using the corresponding weighted sums.

And so:

$$ \rho({}_{j}x, t) = \sum_{i=1}^{N} {}_{i}f({}_{j}x, t) $$

$$\rho({}_j x, t)\vec{u}({}_j x, t) = \sum_{i=1}^{N} {}_i \vec{v}({}_j x, t_i) f({}_j x, t)$$

where: N is the number of populations in the adopted lattice model.

Note that in LBM, the density is obtained analogously to that in (8) by summing the discrete distributions of all populations. The momentum can be determined as the effect of multiplying the discrete values of f by the population velocities (similar to the derivation of the momentum conservation principle equations).

Just as the macroscopic variables are the corresponding moments of the distribution function f with respect to the velocity $\vec{v}$, the same quantities can be determined as sums of discrete values of f obtained by the Lattice Boltzmann Method. A detailed consideration of LBM with a discussion of the implementation of boundary conditions can be found in (Krüger, 2016).

6. Conclusions

The Boltzmann equation and the Navier-Stokes equations describe different aspects of fluid dynamics and are not directly comparable in generality. Because the Boltzmann equation considers the behavior of individual fluid molecules and their collisions, it is considered a more fundamental description of the flow.

The fact that this equation is more general than the N-S equations is one of the foundations of the Boltzmann lattice method. In LBM, instead of equations describing fluid dynamics on a macroscopic scale, a fluid consisting of fictitious mesoscopic populations is modeled, each of which is associated with a specific lattice node and has a specific velocity. Discrete values of the population density function determined in LBM are used to find quantities characteristic of fluid dynamics. Literature often emphasizes the advantages of calculations using LBM, but it is difficult to find a justification for the relationship between equations of a different nature, such as the Boltzmann equation and the equations of conservation of mass, momentum and energy.

The article presents detailed derivations of the continuity equation, the Navier-Stokes equations, and the energy equation from the Boltzmann equation. The work was aimed at systematizing and, above all, detailing the calculations showing the interrelationships between these equations. The conditions in which the more general Boltzmann equations are reduced to one of the equations describing flows on a macroscopic scale help in understanding how the results obtained in LBM are used in calculations competing with standard CFD.

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