# ON THE CONNECTION BETWEEN THE MICROSCOPIC DESCRIPTION-BASED STATISTICAL MECHANICS APPROACH AND MACROSCOPIC DESCRIPTION-BASED FLUID DYNAMICS APPROACH

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***Abstract.*** *This work is part of an ongoing research aimed at establishing a quasi-comprehensive foundation of Boltzmann equation in order to support a numerical implementation of the Lattice Boltzmann Method (LBM). It has focus on providing basis for the preliminary studies on differential equations mostly suitable to describe multiphase flow models and, at a further stage, to help foreseeing solutions to more complex flows like a particulate immersed in a fluid under the action of a magnetic field. Notwithstanding the goal stated above, this work has the sole purpose of fostering the connection by allowing an interchange of techniques consisting in applying methods of the macroscopic domain to the field of statistical physics so as to retrieve the very well known type of formula obtainable through the use of transport equations. That means transport equations commonly used under a stated principle governing experimentally observed phenomena only meaningful for applied sciences and engineering, to be used in the microscopic domain and described in terms of the phase space. This may be undertaken by establishing parallel quantities based on the similarity of roles they play in their original domains. The simplest example that could be mentioned is the Liouville equation describing the dynamical behavior of the density function along a system trajectory. It may be derived accordingly by applying the conservation principle to the number of points of a given ensemble in place of the mass of a labeled system, without mentioning any feature related to canonical transformation or joint probability density functions. Besides fostering the comparison of different approaches, the proposed method of interchanging techniques wills also bring about discussion of key issues related to fluid dynamics and statistical physics/mechanics.*

***Keywords:*** *microscopic description; macroscopic; lattice Boltzmann; statistical mechanics.*

## 1. INTRODUCTION

The most suitable way to introduce the present work is by calling the expression *the Triumph for the Mechanics*, which can be found in the textbook on classical physics written by Caruso and Oguri (2006), which embodies the conception that it is possible to explain the molecular chaos from the order and certainty. This conception is fostered by the fact that the description of the Brownian motion, for instance, consisting in random displacements of particles immersed in a liquid, can be supported by the Newton Laws applied to the collisions between the constituent particles of the liquid and those immersed.

On the other hand, the apparent order observable from a macroscophic system and its physical properties are implied by an underneath chaos, and this is easily conceived when one thinks of a steady motion of a piston as a result of the pressure the confined gas exerts on the boundaries of a cylinder, allowing us to conceive that such a steady motion results from chaotic molecular collisions, i.e. one can deduce macroscopic fluid flow and interpret the resulting effects from the microscopic models by assuming probabilities instead of certanties and partial or uncorrelated states in every part of the domain.

The two preceding paragraphs contribute to strengthen the acceptance of the underneath relationship between the concepts of the kinectic theory, a branch of statistical physics, and macrocopically observable physical phenomena. However, besides the relationship between the steady motion rendered by a macroscopic volume of gas and the associated system comprising a very large number of molecules (say, $10^{20}$) moving in a rather irregular way, connections can also be established for the interchange of principles and methods between the domains of study pertaining to Fluid Mechnics and Statistical Physics.

The last type of connection also provides hints about a suitable establishment of the Boltzmann equation aimed at achieving the optimization of the computational effort and robustness of the numerical implementation of the Lattice Boltzmann Method (LBM) which is based on the molecular theory for fluid flows.

## 2. BASIC PRINCIPLES AND RELEVANT EQUATIONS

The relevant equations for this work pertains to continuum mechanics, classical mechanics with phase space-related concepts and kinetic theory. They will be written in this order.

## 2.1 CONTINUUM MECHANICS

As this work has its focus on the comparison of kinematic features of transport equations for hydrodynamic variables of a macroscopic flow, while in the domain of continuum mechanics, and the ones for $n$-body distribution functions, while in the domain of statistical physics, the key equations will be written with no mention of any adhoc model usually applied to describe the microestructures.

### 2.1.1 Reynolds' transport equation

The Reynolds transport theorem and associated equation will be directly applied to the purpose of this work. Although this equation can be in classical textbooks like Batchelor (2006) and Slattery (1972), it will be written here for the sake convenience.

**i**) **First form**:

$$\frac{D\Psi}{Dt} = \frac{D}{Dt}\int_{vm} \psi d\vartheta = \int_{vm} \frac{\partial \psi}{\partial t} d\vartheta + \int_{sm} \psi \mathbf{u}.\mathbf{n} dS. \tag{1}$$

**ii**) **Second form (stems from the surface integral transformation)**:

$$\frac{D\Psi}{Dt} = \frac{D}{Dt}\int_{vm} \psi d\vartheta = \int_{vm} \left[\frac{\partial \psi}{\partial t} + \nabla.(\psi \mathbf{u})\right] d\vartheta. \tag{2}$$

**iii**) **Third form (stems from the development of $\nabla.(\psi\mathbf{u})$)**:

$$\frac{D\Psi}{Dt} = \frac{D}{Dt}\int_{vm} \psi d\vartheta = \int_{vm} \left[\frac{D\psi}{Dt} + \psi \nabla.\mathbf{u}\right] d\vartheta. \tag{3}$$

In these equations $D/Dt$ denotes material derivative, $\Psi$ denotes any extensive property of a selected portion of fluid, $\psi$ denotes any specific property of the fluid (the amount of $\Psi$ per unit volume of the fluid), $t$ denotes time, $\mathbf{u}$ denotes the velocity field, $vm$ denotes the material volume, $sm$ denotes the boundary of the material volume, $\mathbf{n}$ denotes the unit normal vector pointing outwards the surface element, $d\vartheta$ denotes the material volume element and $dS$ denotes the material surface element. The relationship between a given specific property $\psi$ and its corresponding intensive or local property (the amount of $\Psi$ per unit mass of the fluid) may be given by $\psi = \rho\theta$, where $\theta$ denotes the intensive property, and $\rho$ is the fluid density. Note that if $\rho$ is the selected specific quantity, then $\theta$ is unity.

### 2.1.2 Conservation laws of continuum mechanics

From Batchelor (2006) the laws of continuum mechanics state that the total amount of some extensive quantity associated with a material body of fluid is either invariant or change under the action of known external influences. This statement is mathematically written by applying a concerned principle which governs the time change rate of material integrals expressed by any of the equations (1) or (2) or (3). The resulting differential equations are obtaned by applying the fundamental Lemma of Calculus to the integrands.

**i**) **Mass conservation equation or equation of continuity**. Expresses the mathematical statement of conservation mass of a selected portion of fluid (labeled material body):

$$\frac{\partial \rho}{\partial t} + \nabla.(\rho \mathbf{u}) = \frac{D\rho}{Dt} + \rho \nabla \cdot (\mathbf{u}) = 0. \tag{4}$$

**ii**) **The equation of motion (Cauchy's equation)**. Expresses the mathematical relation equating the rate of change of momentum of a selected portion of fluid to the sum of all forces acting on that portion of fluid:

$$\rho \frac{D\mathbf{u}}{Dt} - \nabla \cdot \sigma - \rho \mathbf{b} = 0. \tag{5}$$

where $\sigma$ denotes the stress tensor and $\mathbf{b}$ denotes volume force per unit mass fo fluid. The energy equation is not relevant to the purpose of the present work.

## 2.2 CLASSICAL MECHANICS

Engineers quite often have to deal with systems discribed by a large number of coordinates. To obtain the differential equations for such systems one may employ transformation techniques for mapping the physical system onto the so-called *configuration space* comprising the minimum number of independent parameters necessary to uniquely determine the system trajectory. The resulting independent parameters are called degrees of freedom or generalized coordinates.

### 2.2.1 Lagrangian formalism

Consider $N$-particle system. The set of tranformations that maps the physical space onto the configuration space is given by:

$$\mathbf{r_i} = \mathbf{r_i}(q_1, q_2, ...., q_n, t) \qquad i = 1, ...., N, \tag{6}$$

$$\dot{\mathbf{r_i}} = \sum_{k=1}^{n} \frac{\partial \mathbf{r_i}}{\partial q_k} \dot{q_k} + \frac{\partial \mathbf{r_i}}{\partial t}, \qquad k = 1, ...., n \quad \text{and} \tag{7}$$

$$\delta \mathbf{r_i} = \sum_{k=1}^{n} \frac{\partial \mathbf{r_i}}{\partial q_k} \delta q_k. \tag{8}$$

In the equations (6), (7) and (8) $\mathbf{r_i}$ and $\dot{\mathbf{r_i}}$ denote, respectively, the radii vector and velocity vector of the $i$th particle, $\delta \mathbf{r_i}$ denotes the virtual vector displacement in actual physical space, $q_k$ labels the $k$th generalized coordinate, $\dot{q_k}$ labels the $k$th generalized velocity, $\delta q_k$ denotes the infinitesimal virtual change in the $k$th generalized coordinate and $n$ denotes the number of degrees of freedom.

The total number of defining coordinates minus the number of equations of kinematic constraints equals $n$. As the virtual change excludes time change, the time $t$ does not appear explicity in the equation (8). It must be emphasized that by virtual change one means a virtual variation in the configuration (spatial variation only) of the original system in actual physical space, compatible with force and kinematic constraints. From the equation (8), $\dot{\mathbf{r_i}}$ is a function of $q_k$ and $\dot{q_k}$.

The key principles from which the differential equations for the system can be derived are the *D'Alambert's Principle* and *Virtual Works Principle*, respectively:

$$\mathbf{F_i} + \tilde{\mathbf{F}}_\mathbf{i} - m_i \ddot{\mathbf{r}}_\mathbf{i} = \mathbf{0} \qquad i = 1, ..., N \quad \text{and} \tag{9}$$

$$\sum_{i=1}^{N} \left( \mathbf{F_i} + \tilde{\mathbf{F}}_\mathbf{i} - m_i \ddot{\mathbf{r}}_\mathbf{i} \right) \cdot \delta \mathbf{r_i} = 0. \tag{10}$$

where in the equation (9) $\mathbf{F_i}$ denotes the force applied to the $i$th particle, $\tilde{\mathbf{F}}_\mathbf{i}$ denotes the force constraining the motion of the $i$th particle and $m_i$ is the mass of the $i$th particle. Remarkable comments on the equation (9): it corresponds to another way of writing the Newton's second law (representing the so-called dynamical equilibrium), and the net force acting on each particle vanishes. The equation (10) represents the sum of virtual works done by the net force acting on each particle, emphasizing that the virtual work done by constraint force $\tilde{\mathbf{F}}_\mathbf{i}$ vanishes.

The set of differential equations (the so-called Lagrange's equations) necessary to describe the dynamics of the system is obtained by substituting the equation (8) into equation (10). An overwhelming algebraic manipulation, which can be found in books on classical mechanics like Azevedo (1976) and Meriam (1966), renders the Lagrange's equations and the generalized force for each degree of freedom:

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q_k}}\right) - \left(\frac{\partial L}{\partial q_k}\right) = Qd_k \qquad k = 1, .., n, \tag{11}$$

$$L(q_k, \dot{q_k}) = T(q_k, \dot{q_k}) - U(q_k) \ , \tag{12}$$

$$T = \frac{1}{2} \sum_{i=1}^{N} m_i \dot{\mathbf{r}}_\mathbf{i} . \dot{\mathbf{r}}_\mathbf{i}) \ , \tag{13}$$

$$Qc_k = \sum_{i=1}^{N} \mathbf{Fc_i} . \left( \frac{\partial \mathbf{r_i}}{\partial q_k} \right) = -\frac{\partial U}{\partial q_k} \quad \text{and} \tag{14}$$

$$Qd_k = \sum_{i=1}^{N} \mathbf{Fd_i} . \left( \frac{\partial \mathbf{r_i}}{\partial q_k} \right) . \tag{15}$$

In the equations (11), (12), (13), (14) and (15): $L$ denotes Lagrangian function (or kinetic potential), $T$ denotes the kinetic energy, $U$ denotes the potential energy function, $\mathbf{Fc_i}$ denotes conservative force acting on $i$th particle, $\mathbf{Fd_i}$ denotes non-conservative force acting on $i$th particle, $Qc_k$ denotes the $k$th generalized conservative force and $Qd_k$ denotes the $k$th generalized non-conservative force (both associated to the $k$th degree of freedom).

### 2.2.2 Hamiltonian formalism

A third variational principle which also provides means for finding the differential equations of motion of a dynamical system is *Hamilton's Extended Principle*. This principle, also derived from the equation (10), rewritten as follows:

$$\delta T + \overline{\delta W} = \sum_{i=1}^{N} m_i \frac{d}{dt}(\dot{\mathbf{r}}_\mathbf{i}.\delta \mathbf{r}_\mathbf{i}) \ , \tag{16}$$

which renders, after time integration from time $t_1$ to time $t_2$:

$$\int_{t_1}^{t_2} \left(\delta T + \overline{\delta W}\right) dt = 0 \ . \tag{17}$$

The equation (17) is the statement of *Hamilton's Extended Principle*. Further development from this principle with $\overline{\delta W} = -\delta U + \overline{\delta W_d}$ yields:

$$\int_{t_1}^{t_2} \delta L dt = -\int_{t_1}^{t_2} \sum_{k=1}^{n} Q d_k \delta q_k dt. \tag{18}$$

For holonimic and conservative systems ($\overline{\delta W_d} = \sum_{k=1}^{n} Q d_k \delta q_k = 0$) one gets the statement of *Hamilton's Principle*:

$$\delta I = \delta \int_{t_1}^{t_2} L dt = 0. \tag{19}$$

In the equations (16), (17), (18) and (19) $\overline{\delta W}$ denotes the sum of virtual works done by the external forces, $\overline{\delta W_d}$ denotes the sum of virtual works done by non-conservative forces and $I$ denotes the action integral. Remarkable comments on *Hamilton's Principle*: it selects the correct (optimal) dynamical path from all possible paths followed by the system in configuration space . In other words it is a *principle of least action* which renders the stationary value to $I$ as implied in the equation (19).

### 2.2.3 Hamilton's equations and phase space

Let us write the equation (11) in the form:

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q_k}}\right) = \left(\frac{\partial L}{\partial q_k}\right) + Q d_k \qquad\qquad k = 1, .., n, \tag{20}$$

and also define the quantity $p_k$:

$$p_k \equiv \left(\frac{\partial L}{\partial \dot{q_k}}\right) \ . \tag{21}$$

Thus, from the equation (20):

$$\frac{dp_k}{dt} = \left(\frac{\partial L}{\partial q_k}\right) + Q d_k. \tag{22}$$

In these equations $p_k$ represents a kind of generalized linear momentum. For the sake of presenting the building blocks of statistical physics, let us introduce the $2n$-dimensional cartesian space $(q_1, ..., q_n, p_1, ..., p_n)$, which is also called $\Gamma$-space or phase space, where the state of the system at any given instant is a single point, and the energy-related dynamical variable $\bar{H}$. Let us assign the following relationship between $\bar{H}$ and the Lagrangian function $L$:

$$\bar{H}(q_k, p_k) = \sum_{k=1}^{n} \left(\frac{\partial L}{\partial \dot{q_k}}\right) \dot{q_k} - L(q_k, \dot{q_k}) = \sum_{k=1}^{n} p_k \dot{q_k} - L(q_k, \dot{q_k}). \tag{23}$$

The differential equation for $\bar{H}$ may be derived by differentiating (23) and taking into account the equation (20), (21) and (22). Thus:

$$\frac{\partial \bar{H}}{\partial q_k} = -\dot{p_k} + Q d_k \quad \text{and} \tag{24}$$

$$\frac{\partial \bar{H}}{\partial p_k} = \dot{q_k} \ . \tag{25}$$

By adopting a similar procedure, the time rate of change of the quantity $\bar{H}$ yields:

$$\frac{d\bar{H}}{dt} = \sum_{k=1}^{n} Qd_k \dot{q_k}. \tag{26}$$

The equation (26) is a statement that if $Qd_k \neq 0$, the energy $\bar{H}$ of the system increases or decreases as the motion of the system unfolds in time and the integral $I$, as implied in the equation (19), would not assume a stationary value (extremum). On the other hand, if $Qd_k = 0$ for $k = 1, ..., n$ (conservative system) then $\bar{H} = H$ so the equations (24) and (25) are reduce to:

$$\frac{\partial H}{\partial q_k} = -\dot{p_k} \quad \text{and} \tag{27}$$

$$\frac{\partial H}{\partial p_k} = \dot{q_k}. \tag{28}$$

where $H$ is the Hamiltonian function (a constant of the motion or integral of the system), equations (27) and (28) are called Hamilton's equations and $p_k$ is called canonical momentum or momentum conjugate to the the coordinate of the system. The dynamical orbit of the system (one-dimensional locus or system trajectory) is a curve the (2$n$+1)-dimensional cartesian space $(q_1, ..., q_n, p_1, ..., p_n, t)$, which is called $\tilde{\Gamma}$-space. Integration of equations (27) (28) yields the state of the system specified by $2n$ constants of motion.

Regarding the key elements of classical mechanics so far derived the following assumptions are relevant:

**i)** the force fields are conservative ($Qd_k = 0$),

**ii)** the systems are holonimic where the equations of kinematic constraints are time independent,

**iii)** the Hamiltonian $H$ (an integral of the system) is an not an explicit function of time, and

**iv)** the Hamilton's equations are strictly kinematic and suitable to define operators in phase space.

## 3. FINDING CONNECTIONS

To achieve the intended connections the first step is to introduce the general equation of motion for a given dynamical variable $\Xi = \Xi(\mathbf{q}, \mathbf{p}, t)$ in $\tilde{\Gamma}$-space. Then we write:

$$\frac{d\Xi}{dt} = \frac{\partial \Xi}{\partial t} + \frac{\partial \Xi}{\partial \mathbf{q}} \cdot \dot{\mathbf{q}} + \frac{\partial \Xi}{\partial \mathbf{p}} \cdot \dot{\mathbf{p}} = \frac{\partial \Xi}{\partial t} + \frac{\partial \Xi}{\partial \mathbf{q}} \cdot \frac{\partial H}{\partial \mathbf{p}} - \frac{\partial H}{\partial \mathbf{q}} \cdot \frac{\partial \Xi}{\partial \mathbf{p}} = \frac{\partial \Xi}{\partial t} - L_n \Xi \quad \text{and} \tag{29}$$

$$L_n = \frac{\partial H}{\partial \mathbf{q}} \cdot \frac{\partial}{\partial \mathbf{p}} - \frac{\partial H}{\partial \mathbf{p}} \cdot \frac{\partial}{\partial \mathbf{q}} = \sum_{k=1}^{n} \left[ \frac{\partial H}{\partial q_k} \frac{\partial}{\partial p_k} - \frac{\partial H}{\partial p_k} \frac{\partial}{\partial q_k} \right]. \tag{30}$$

where the substitution of equations (27) and (28) is implied. Here $L_n$ denotes the Liouville's operator and the symbol (.) denotes the inner product suitably defined in $\tilde{\Gamma}$-space. Sometimes, depending on the context and convenience, the inner product will replace the sum $\sum_{k=1}^{n}$ over $k$. The operator $L_n$ may also be rewritten as $L_n = \langle H, \rangle$, where $\langle H, \rangle$ is called Poisson bracket notation.

### 3.1 KINEMATIC OF PHASE SPACE VERSUS KINEMATIC OF CONTINUUM MECHANICS

Equations (29) and (30) clearly show that the convective rate of change of $U$ in the phase space, herein played by -$\hat{L_n}$, stems from the Hamiltonian function $H$ provided that $H$ is an integral of the system.

Consider now the material derivative operator $D\Psi/Dt$ applied to the extensive property $\Psi$ previously defined in Subsubsection (2.1.1):

$$\frac{D\Psi}{Dt} = \frac{\partial \Psi}{\partial t} + \mathbf{u} \cdot \nabla \Psi. \tag{31}$$

The comparison between the equations (29) and (31) calls for $L_n$ = - $\hat{\mathbf{u}} \cdot \nabla$. This comparison is attainable provided that $H$ is an integral of the system. In order to avoid confusion, the velocity field $\mathbf{u}$ is defined for a given actual physical space, whereas the velocity fields $\dot{\mathbf{q}} = (\dot{q_1}, ..., \dot{q_n})$ (generalized velocities) and $\hat{\mathbf{u}} = (\dot{q_1}, ..., \dot{q_n}, \dot{p_1}, ..., \dot{p_n})$ are defined for the correspondent configuration space and phase space, respectively. The operator $\nabla$ must be accordingly written:

$$\nabla = \left( \frac{\partial}{\partial q_1}, ..., \frac{\partial}{\partial q_n}, \frac{\partial}{\partial p_1}, ..., \frac{\partial}{\partial p_n} \right). \tag{32}$$

### 3.2 DERIVATION OF THE LIOUVILLE'S EQUATION THROUGH CONTINUUM CONCEPTS

The algebraic similarities between the kinematics of actual physical space and phase space helps us to identify the restrictions to be imposed on the construction of the integral function $H$ so as to render the kinetic and momentum operators that make frequent appearance in governing differential equations of statistical physics

Now let us foster the connection by deriving the so-called Liouville's equation through an approach which combines the transport equation (2) and conservation principle in phase space (this will require some abstraction). Consider a system point moving on the system trajectory $(q_1(t), ..., q_n(t), p_1(t), ..., p_n(t))$ in phase space, as time evolves. Now imagine a large number of mental copies of the same system, say $\eta$. This abstract collection of replicas ($\eta$ systems) is called an ensemble. In fluid mechanics streamlines of a flow never cross, and likewise in phase space system trajectories never cross. This follows from the fact that for a system with $n$ degrees of freedom the system trajectory (given by the equations (27) and (28)) is uniquely determined by $2n$ constants of motion $(\mathbf{q}(\mathbf{0}), \mathbf{p}(\mathbf{0})) = (q_1(0), ..., q_n(0), p_1(0), ..., p_n(0))$, that is, only one system trajectory passes through $(\mathbf{q}(\mathbf{0}), \mathbf{p}(\mathbf{0}))$. In fluid mechanics we apply the mass-conservation principle to a selected portion of fluid, and likewise in phase space, we can also apply a correspondent ensemble-conservation principle, which states that number of system points of a given ensemble remains constants as the motion unfolds in time. Each system comprises a system trajectory (a system point moving along it), whereas an ensemble comprises $\eta$ system trajectories (or $\eta$ system points moving along them).

Let us define the dynamical fuction $D(\mathbf{q}, \mathbf{p}, t)$, the number of system points per unit phase volume, written as follows:

$$D(\mathbf{q}, \mathbf{p}, t) = \frac{d\eta}{d\Omega}. \tag{33}$$

where $d\Omega$ denotes the phase volume element, written as:

$$d\Omega \equiv d\mathbf{q}d\mathbf{p} = \prod_{k=1}^{n} dq_k dp_k. \tag{34}$$

Thus, the product $D(\mathbf{q}, \mathbf{p}, t)d\mathbf{q}d\mathbf{p} \equiv D(\mathbf{q}, \mathbf{p}, t)d\Omega$ represents the number of system points in the phase volume element $d\Omega$ about the system point $(\mathbf{q}, \mathbf{p})$, at the time $t$

Since $D(\mathbf{q}, \mathbf{p}, t)$ represents the ensemble density function, it enjoys the property that, apart from a multiplicative constant $\xi$, it may be defined as a joint probability density function $f_n(\mathbf{q}, \mathbf{p}, t)$ as follows:

$$f_n(\mathbf{q}, \mathbf{p}, t) = \frac{D(\mathbf{q}, \mathbf{p}, t)}{\xi}, \quad \xi = \int_\Omega D(\mathbf{q}, \mathbf{p}, t)d\mathbf{q}d\mathbf{p}. \tag{35}$$

Whereas $D(\mathbf{q}, \mathbf{p}, t)$ is relevant to the entire ensemble, $f_n(\mathbf{q}, \mathbf{p}, t)$ addresses a single system of the ensemble. Here $f_n d\mathbf{q}d\mathbf{p}$ means the probability of finding a given system of the ensemble in the phase volume $d\mathbf{q}d\mathbf{p}$, about the state $(\mathbf{q}, \mathbf{p})$, at the instant $t$. Although $\eta$ and $\xi$ hold the same meaning, the latter has been adopted for the sake of normalizing. From the equation (35) is clear that $f_n(\mathbf{q}, \mathbf{p}, t)$ is the normalized joint probability density function:

$$\int_\Omega f_n(\mathbf{q}, \mathbf{p}, t)d\mathbf{q}d\mathbf{p} = 1. \tag{36}$$

For detailed explanation of statistical physics-related concepts, the reader is advised to look up textbooks like Balescu (1963), (Liboff), Harris (1971) and Salinas (1999). Now we have enough elements elements in phase space so as to derive the Liouville's equation through the ensemble-conservation principle combined with the transport equation (2) with assumptions and quantities appropriately adapted to the phase space:

**i)** $\eta$ is the extensive property in phase space ($\eta$ replaces $\Psi$),

**ii)** $f_n$ is specific property in phase space ($f_n$ replaces $\psi = \rho$ in this case),

**iii)** the Liouville's equation plays the role of continuity equation in phase space, and

**iv)** the intensive property is reduced to unity ($f_n = f_n\theta \quad \Rightarrow \quad \theta = 1$),

Thus, adapting the transport equation (2) to these quantities in phase space:

$$\frac{D\eta}{Dt} = \frac{D}{Dt}\int_\Omega f_n d\Omega = \int_\Omega \left[\frac{\partial f_n}{\partial t} + \nabla \cdot (f_n \hat{\mathbf{u}})\right] d\Omega = 0. \tag{37}$$

The equation (37) states that the number of system points of a given ensemble are neither created nor destroyed. By virtue of the arbitrariness of $\Omega$, the integrand of this equation is identically zero everywhere in the selected ensemble. Hence:

$$\frac{\partial f_n}{\partial t} + \nabla \cdot (f_n \hat{\mathbf{u}}) = 0.. \tag{38}$$

Algebraic manipulation of the operator $\nabla$ defined by equation (32) gives:

$$\nabla \cdot (f_n \hat{\mathbf{u}}) = f_n \nabla \cdot \hat{\mathbf{u}} + \hat{\mathbf{u}} \cdot \nabla f_n. \tag{39}$$

Now developing the term $\nabla \cdot \hat{\mathbf{u}}$ with the aid of the equations (27) and (28) gives:

$$\nabla \cdot \hat{\mathbf{u}} = \sum_{k=1}^{n} \left[ \frac{\partial \dot{q_k}}{\partial q_k} + \frac{\partial \dot{p_k}}{\partial p_k} \right] = \sum_{k=1}^{n} \left[ \frac{\partial}{\partial q_k} \left( \frac{\partial H}{\partial p_k} \right) + \frac{\partial}{\partial p_k} \left( \frac{\partial (-H)}{\partial q_k} \right) \right] = \sum_{k=1}^{n} \left[ \frac{\partial^2}{\partial q_k \partial p_k} - \frac{\partial^2}{\partial p_k \partial q_k} \right] H = 0. \tag{40}$$

Furthermore, with the aid of equations (29) and (30), the development of the term $\hat{\mathbf{u}} \cdot \nabla f_n$ leads to the operator $-L_n$ applied to $f_n$. Finally, by taking these results into account the so-called Liouville's equation may be written:

$$\frac{\partial f_n}{\partial t} - L_n f_n = \frac{\partial f_n}{\partial t} + \langle f_n, H \rangle = 0. \tag{41}$$

where $L_n = -\langle, \ H\rangle = \langle H, \ \rangle$ is also a very common notation in Statiscal physics called Poisson bracket form.
From equations (38), (39) and ( 40) the Liouville's equation may be written in terms of the material derivative operator:

$$\frac{Df_n}{Dt} = \frac{\partial f_n}{\partial t} + \hat{\mathbf{u}} \cdot \nabla f_n = 0. \tag{42}$$

The Equation (42) states that joint probability density $f_n$ remains constant along the systems trajectories. So we have obtained the Liouville's equation in the pure phase space by applying an approach of the continuum mechanics.

Within the scope of statistical physics this equation is usually obtained through concepts like canonical transformation (the motion of system points is itself canonical), canonical invariants like phase volume and the Liouville's theorem, which states that, for a system with $n$ degrees of freedom, the jacobian of a canonical transformation is unity. Another remarkable result that stems from the equation (40) is $\nabla \cdot \hat{\mathbf{u}} = 0$ (the ensemble is incompressible). Neglecting non-conservative forces in statistical physics renders incompressible ensemble, whereas neglecting viscous stress in fluid dynamics does not necessarily render an incompressible flow, i.e, the Euler's equation does not show explicitly whether the flow is compressible or incompressible.

### 3.3 DERIVATION OF THE KEY EQUATION THROUGH CONTINUUM CONCEPTS

As a motivation, kinetic equations of statistical physics plays the same role as that played by equations of motion of fluid dynamics (derived from equation (5)). In this Subsection we will derive the key equation (in the pure phase space) from which the master kinetic equation of statistical physics is obtainable through the ensemble-conservation principle combined with the transport equation (2) with assumptions and quantities appropriately adapted to the phase space.

Consider a $n$-degree of freedom system comprising $N$ particles. The kinetic stage of this system calls for the interaction between particles. Thus, reduced joint probability distribution $f_m$ ($m < n$) is relevant. Let us assume that a given subsystem comprises $m$ degrees of freedom with an agregate of $s$ particles. Then, this subsystem will be under the potential and kinetic effects of the complementary subsystem which comprises the remaining $(n - m)$ degrees of freedom, with the correspondent $(N - s)$ particles. If only translation mode is concerned, like in a gaseous enviroment, $n = 3N$. This yields a $2n$-degree of freedom phase space ($6N$-degree of freedom phase space).

The purpose is to obtain a differential equation for the reduced distribution function $f_m$. Let us label $Z$ a reasonable extensive property standing for the collision integral for the $(N - s)$-particle agregate, which stems from the Hamiltonian $H$.

**i)** $Z$ is the extensive property in phase space ($Z$ replaces $\Psi$), and

**ii)** $f_m$ is specific property in phase space ($f_m$ replaces $\psi$).

Let us define $\mathbf{u_m}$ as the velocity field associated with the given $m$ degrees of freedom subsystem and the correspondent $s$-particle agregate.

Adapting the transport equation (2) to these quantities in phase space:

$$\frac{DZ}{Dt} = \frac{D}{Dt} \int_{\bar{\Omega}} f_m d\bar{\Omega} = \int_{\bar{\Omega}} \left[ \frac{\partial f_m}{\partial t} + \nabla \cdot (f_m \mathbf{u_m}) \right] d\bar{\Omega}, \tag{43}$$

where $\bar{\Omega}$ denotes the phase volume element:

$$d\bar{\Omega} = \prod_{k=1}^{m} dq_k dp_k. \tag{44}$$

Algebraic manipulation of the operator $\nabla$ defined by equation (32) gives:

$$\nabla \cdot (f_m \mathbf{u_m}) = f_m \nabla \cdot \mathbf{u_m} + \mathbf{u_m} \cdot \nabla f_m. \tag{45}$$

Now developing the term $\nabla \cdot \mathbf{u_m}$ with the aid of the equations (27) and (28) and the summation limit redefined to $m$ gives:

$$\nabla \cdot \mathbf{u_m} = \sum_{k=1}^{m} \left[ \frac{\partial \dot{q_k}}{\partial q_k} + \frac{\partial \dot{p_k}}{\partial p_k} \right] = \sum_{k=1}^{m} \left[ \frac{\partial}{\partial q_k} \left( \frac{\partial H}{\partial p_k} \right) + \frac{\partial}{\partial p_k} \left( \frac{\partial (-H)}{\partial q_k} \right) \right] = \sum_{k=1}^{m} \left[ \frac{\partial^2}{\partial q_k \partial p_k} - \frac{\partial^2}{\partial p_k \partial q_k} \right] H = 0. \tag{46}$$

The $m$-degree of freedom subsystem remains incompressible ($\nabla \cdot \mathbf{u_m} = 0$). Thus the key equation may be rewritten:

$$\frac{DZ}{Dt} = \frac{D}{Dt} \int_{\bar{\Omega}} f_m d\bar{\Omega} = \int_{\bar{\Omega}} \left[ \frac{\partial f_m}{\partial t} + \mathbf{u_m} \cdot \nabla f_m \right] d\bar{\Omega}. \tag{47}$$

If we take the equations (29) and (30) with the sum limit renumbered to $m$, the development of the term $\mathbf{u_m} \cdot \nabla f_m$ leads to the operator $-L_m$ applied to $f_m$. By taking these results into account we obtain the general form of the key equation:

$$\frac{DZ}{Dt} = \frac{D}{Dt} \int_{\bar{\Omega}} f_m d\bar{\Omega} = \int_{\bar{\Omega}} \left[ \frac{\partial f_m}{\partial t} - L_m f_m \right] d\bar{\Omega}. \tag{48}$$

The most general equation of motion (Cauchy's equation) in fluid dynamics has been obtained with the aid of the continuity equation (4). Similarly, further development of the key equation (48), aimed at obtaining the extensive property $Z$ in terms of $H$ can be carried out with the aid of the Liouville's equation, here rewritten in its integral version:

$$\int_{\Omega} \left[ \frac{\partial f_n}{\partial t} - L_n f_n \right] d\Omega = \int_{\Omega} \left[ \frac{\partial f_n}{\partial t} \right] d\Omega - \int_{\Omega} L_n f_n d\Omega = \frac{\partial}{\partial t} \left[ \int_{\Omega} f_n d\Omega \right] - \int_{\Omega} L_n f_n d\Omega = 0. \tag{49}$$

The integration over $\Omega$ can be split over $\bar{\Omega}$ and $\bar{\bar{\Omega}}$. The operators $\partial/\partial t$ and $\int_{\bar{\Omega}}$ are interchangeable. Introducing these changes, the equation (49) may be rewritten as:

$$\int_{\bar{\Omega}} \left[ \frac{\partial}{\partial t} \left( \int_{\bar{\bar{\Omega}}} f_n d\bar{\bar{\Omega}} \right) - \int_{\bar{\bar{\Omega}}} L_n f_n d\bar{\bar{\Omega}} \right] d\bar{\Omega} = 0. \tag{50}$$

where $\bar{\Omega}$ has already been defined by (44), and $\bar{\bar{\Omega}}$ is defined as follows:

$$d\bar{\bar{\Omega}} = \prod_{k=m+1}^{n} dq_k dp_k. \tag{51}$$

Integrations over $\bar{\bar{\Omega}}$ can be further assessed by splitting the integral of the equation (36) over $\bar{\Omega}$ and $\bar{\bar{\Omega}}$:

$$\int_{\Omega} f_n d\Omega = \int_{\bar{\Omega}} \left[ \int_{\bar{\bar{\Omega}}} f_n d\bar{\bar{\Omega}} \right] d\bar{\Omega} = \int_{\bar{\Omega}} f_m d\bar{\Omega} = 1 \quad \text{and} \quad f_m = \int_{\bar{\bar{\Omega}}} f_n d\bar{\bar{\Omega}}. \tag{52}$$

The reduced joint probability density function $f_m$ remains normalized as shown by equation (52). The completion of this development requires the partition of the Liouville's operator $L_n = L_m + L_{m+1,n}$. The introduction of these changes into the equation (50) yieds:

$$\int_{\bar{\Omega}} \left[ \frac{\partial f_m}{\partial t} - \int_{\bar{\bar{\Omega}}} L_m f_n d\bar{\bar{\Omega}} - \int_{\bar{\bar{\Omega}}} (L_{m+1,n}) f_n d\bar{\bar{\Omega}} \right] d\bar{\Omega} = 0. \tag{53}$$

Since the second term on left hand side of equation (53) comprises integration over domain $\bar{\bar{\Omega}}$, whereas the reduced operator $L_m$ comprises partial differentiating with respect to domain $\bar{\Omega}$, it can be moved out from the integral. Furthermore, applying the equation (52) for $f_m$ and transposing the third term on the left hand side of the equation (53) we obtain:

$$\int_{\bar{\Omega}} \left[ \frac{\partial f_m}{\partial t} - L_m f_m \right] d\bar{\Omega} = \int_{\bar{\Omega}} \left[ \int_{\bar{\bar{\Omega}}} (L_{m+1,n}) f_n d\bar{\bar{\Omega}} \right] d\bar{\Omega}, \tag{54}$$

or

$$\int_{\bar{\Omega}} \left[ \frac{\partial f_m}{\partial t} - L_m f_m - \int_{\bar{\bar{\Omega}}} (L_{m+1,n}) f_n d\bar{\bar{\Omega}} \right] d\bar{\Omega} = 0. \tag{55}$$

Now by comparing the equations (47) and (54) we obtain:

$$\frac{DZ}{Dt} = \int_{\bar{\Omega}} \left[ \int_{\bar{\bar{\Omega}}} (L_{m+1,n}) f_n d\bar{\bar{\Omega}} \right] d\bar{\Omega} = \int_{\Omega} (L_{m+1,n}) f_n d\Omega. \tag{56}$$

Regarding the integrand of equation (55), it is worth remarking the arbitrariness of the quantity $d\bar{\Omega}$. It represents a phase volume element comprising a large number of virtual copies of a given subsystem trajectory so the integrand will vanish everywhere in the domain $\bar{\Omega}$. Hence:

$$\frac{\partial f_m}{\partial t} - L_m f_m = \int_{\bar{\bar{\Omega}}} (L_{m+1,n}) f_n d\bar{\bar{\Omega}}, \tag{57}$$

$$L_m = \sum_{k=1}^{m} \left[ \frac{\partial H}{\partial q_k} \frac{\partial}{\partial p_k} - \frac{\partial H}{\partial p_k} \frac{\partial}{\partial q_k} \right] \qquad \text{and} \qquad L_{m+1,n} = \sum_{k=m+1}^{n} \left[ \frac{\partial H}{\partial q_k} \frac{\partial}{\partial p_k} - \frac{\partial H}{\partial p_k} \frac{\partial}{\partial q_k} \right]. \tag{58}$$

where the equations (58) for $L_m$ and or $L_{m+1,n}$ have been rewritten for the sake of convenience.

Now proceeding to remarkable comments on equations (56) and (57). Regarding the equation (56), the material derivative operator $D/Dt$ apllied to $Z$ in phase space means the time rate of change following a subsystem trajectory, in the same manner as following the motion of the fluid in fluid mechanics. The material derivative of $Z$ in phase space seems subtle to be understood by the reader. Nevertheless, it is worth remarking that, from the equation (58), the operators $L_m$ and $L_{m+1,n}$ depend on $H$ which usually comprises two-body interaction potentials. The derivatives with respect to the generalized coordinates, applied to such potentials, and subsquently moved back to the actual physical space, will render a divergence operation quite similar to the that applied to stress tensor in fluid dynamics. Consider a $N$-particle system and the associated $NxN$ matrix, whose scalar components are 2-particle interaction potentials of the form $\Phi(i,j), i<j$. The application of the operator $L_{m+1,n}$ to this matrix yields a divergence operation similar to that already existent in fluid dynamics (Cauchy's equation).

Regarding the equation (57), it represents a kind of key equation in the pure phase space. To illustrate its usefulness, let us now derive the master kinetic equation of the the statistical physics by rewriting it in terms of the number of particles of a $N$-particle system, with a partition comprising $s$ particles. Assuming that only translation is relevant with no kinematic constraints with elastic collisions ($n = 3N$), and all particles having equal mass $m$, the Hamiltonian of the system may be written as:

$$H = \sum_{l=1}^{N} \frac{\mathbf{p_l} \cdot \mathbf{p_l}}{2m} + \left[ \sum_i \sum_j \Phi(i,j) \right]_{i<j} \qquad \text{and} \qquad \mathbf{p_l} = m\mathbf{v_l}. \tag{59}$$

where $\mathbf{v_l}$ is the velocity of the $l$-th particle of the system. The concerned operators $L_N$, $L_s$ and $L_{s+1,N}$ are rewritten as:

$$L_N = \sum_{l=1}^{N} \frac{\partial H}{\partial \mathbf{q_l}} \cdot \frac{\partial}{\partial \mathbf{p_l}} - \frac{\partial H}{\partial \mathbf{p_l}} \cdot \frac{\partial}{\partial \mathbf{q_l}}, \quad L_s = \sum_{l=1}^{s} \frac{\partial H}{\partial \mathbf{q_l}} \cdot \frac{\partial}{\partial \mathbf{p_l}} - \frac{\partial H}{\partial \mathbf{p_l}} \cdot \frac{\partial}{\partial \mathbf{q_l}} \text{ and } L_{s+1,N} = \sum_{l=s+1}^{N} \frac{\partial H}{\partial \mathbf{q_l}} \cdot \frac{\partial}{\partial \mathbf{p_l}} - \frac{\partial H}{\partial \mathbf{p_l}} \cdot \frac{\partial}{\partial \mathbf{q_l}}. \tag{60}$$

where the inner products comprise summation over cartesian coordinates $x_1, x_2, x_3$ of each particle. By virtue of the overwhelming algebraic manipulations, the development aimed at obtaining the kinetic equation will be left out. The work consists in substituting the given function $H$ into the operators $L_s$ and $L_{s+1,N}$, and subsequently inserting them into equation (57), here appropriately rewritten in terms of $N$, $s$, $i$ and $j$. Moreover, parts of the operator $L_{s+1,N}$ that contribute only surface terms in the domain $\bar{\bar{\Omega}}$ must be neglected. To so proceeding we obtain:

$$\left( \frac{\partial}{\partial t} - L_s \right) f_s = - \sum_{i=1}^{s} \frac{\partial}{\partial \mathbf{p_i}} \cdot \int_{\bar{\Omega}} \sum_{j=s+1}^{N} [\mathbf{G_{ij}} f_N] d(s+1)....dN. \tag{61}$$

where

$$\mathbf{G_{ij}} = - \frac{\partial \Phi(i,j)}{\partial \mathbf{x_i}}, \quad dl = d\mathbf{x_l} d\mathbf{p_l} \equiv \left[ \prod_{r=1}^{3} dx_r dp_r \right]_l, \quad l = s+1, ....N, \text{ and } r = 1,2,3. \tag{62}$$

$\mathbf{G_{ij}}$ is the force on $i$th particle due to the $j$th particle. Additional assumptions about symmetry permit further reductions in the equation (61). If we assume that particles are identical there is no reason to refuse that $f_s(1.,,,s)$ is symmetric, that is, $f_3(1,2,3) = f_3(1,3,2)$, where in the last case, particle 2 occupies state 3 and particle 3 occupies state 2. Therefore, the equivalence of the integrals under the $j$-sum in the equation (61) will lead to further simplification. The $s$th integral will give $(N-s)$ identical terms, the integration can be split over $d(s+1)$ and $d(s+2)d(s+3)...dN$, and we can assume $\mathbf{G_{ij}} = \mathbf{G_{is+1}}$. Thus, the equation (61) may be rewritten as:

$$\left(\frac{\partial}{\partial t} - L_s\right) f_s + (N-s)\sum_{i=1}^{s} \frac{\partial}{\partial \mathbf{p_i}} \cdot \int_{s+1} [\mathbf{G_{is+1}} f_{s+1}] d(s+1) = 0 \quad s = 1, ...., N. \tag{63}$$

The coupled $N$ equations given by the equation (63) are called the BBKGY equations or Hierarchy. This abbreviation stands for N.N **B** Bogoliubov, M. **B**. Born, **G**. Kirkwood, H.S. Green; and J. Yvon. The BBKGY equations are also identified by the shorthand notation $BY_s$, and they are root of the kinetic equations of statistical physics like the Vlazov equation and the Boltzmann equation.

## 4. CONCLUSIONS

This work performs a comparison between the approaches adopted in statistical mechanics and fluid mechanics with the purpose to strengthen the connection between both fields of knowledge, by interchanging mathematical tools and principles, like the use of transport equations of fluid mechanics, which allows the derivation of the key kinetic equations, in their bulky form, likewise the Cauchy's equation in fluid dynamics. The work also allowed the authors to foresee alternative strategies to implement a meshless numerical technique called Lattice Boltzmann Method which is initially intended to solve simple flows, and, at a further stage, to simulate two-phase flows with the attempt to answer open questions related to more complex flows, like a particulate immersed in a fluid under the action of a magnetic field. Some useful findings on integral functions defining algebraic structure of statistical physics have been found, like the possibility of introducing alternative integral functions other than the traditional ones adopted in the hamiltonian formalism. It would be worth trying to introduce a pseudo-potential like Rayleig function, a kind of *viscous damping potential* from which non-conservative forces can be furthely derived.

## 5. REFERENCES

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## 6. RESPONSABILITY NOTICE

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