Principles of kinetic theory for granular fluids*

Massimo Tessarotto

Department of Mathematics and Geosciences, University of Trieste, Via Valerio 12, 34127 Trieste, Italy and Institute of Physics, Faculty of Philosophy and Science, Silesian University in Opava, Bezučovo nám.13, CZ-74601 Opava, Czech Republic

Claudio Cremaschini

Institute of Physics, Faculty of Philosophy and Science, Silesian University in Opava, Bezučovo nám.13, CZ-74601 Opava, Czech Republic

(Dated: November 19, 2018)

Highlights are presented regarding recent developments of the kinetic theory of granular matter. These concern the discovery of an exact kinetic equation and a related exact H-theorem both holding for finite N-body systems formed by smooth hard-spheres systems.

PACS numbers: 03.50.De, 45.50.Dd, 45.50.Jj

INTRODUCTION

Although Ludwig Boltzmann’s discovery of his namesake equation and H-theorem dates back to more than a century [1], only a few papers have actually given a significant contribution to the advancement of kinetic theory itself. This refers in particular to the treatment of dense or granular systems, i.e., in which the finite size of constituent particles must be taken into account, starting from the phenomenological Enskog kinetic equation originally formulated by Enskog [2] for elastic smooth hard-spheres and its subsequent modified form [3]. In fact, in spite of the progress achieved in describing the kinetics and hydrodynamics of granular fluids, represented in particular by non-linear theories such as the Bogoliubov-Choh-Uhlenbeck theory [4] and the so-called ring kinetic theory [5], the solution of this problem has not changed significantly and has remained until recently “far from being complete” [6].

Concerning, instead, the treatment of dilute gases an exception is provided by Harold Grad’s seminal paper on the Principles of kinetic theory of gases and the related construction of Boltzmann kinetic equation [7][25]. Grad’s approach in fact represents a first attempt at an axiomatic formulation of the microscopic statistical description, i.e., based on classical statistical mechanics, for a classical N-body system $S_N$ in which all particles have, at least in principle, a finite-size. This is realized via the construction of the $N$-body probability density functions (PDF) $\rho^{(N)}(x,t)$ for a closed classical $N$-body system $S_N$, i.e., in which the number of particles $(N)$ remains constant. By assumption $S_N$ is immersed in a bounded and simply-connected subspace $\Omega$ of the Euclidean space $\mathbb{R}^3$ having rigid boundary $\delta\Omega$ and a finite canonical measure $L^3 = \mu(\Omega)$ (with $L$ being the corresponding configuration-space characteristic scale length). In particular, $S_N$ is identified, as in the case of Boltzmann kinetic theory, with the ensemble of $N$ like smooth hard spheres of diameter $\sigma$ and mass $m$, each one being labelled by its Newtonian state $x_j \equiv \{r_j, v_j\}$ (with $r_j$ and $v_j$, for all $j = 1, N$, denoting the particle center-of-mass position and velocity) and $x \equiv \{x_1, ..., x_N\}$ denoting the state of $S_N$ spanning the corresponding phase space $\Gamma^N \equiv (\Gamma_1)^N$. By assumption $x$ evolves in time from an arbitrary initial state $x(t_0) \equiv x_0$ due to instantaneous particle collisions occurring at discrete collision times $\{t_i\} \equiv \{t_i, i \in \mathbb{N}\}$. The collisions themselves are realized either by means of unary, binary or - in principle - arbitrary multiple elastic collisions occurring among the particles of $S_N$ and/or with its rigid boundary $\delta\Omega$, the latter being assumed stationary with respect to a suitable inertial frame (see Figure 1). Accordingly, for a collision event at time $t_i$ involving $k$ particles (for $k = 1, ..., N$) this means that the corresponding incoming and outgoing states (i.e., occurring immediately before and after collision), namely the lower and upper limits (for $j = 1, ..., k$) $\lim_{t_i^-} x_j(t) \equiv x_j^{(-)}(t_i) \equiv \{r_j(t_i), v_j^{(-)}(t_i)\}$ are related by the so-called elastic collision laws. Thus, for example, a binary collision event $(1, 2)$ between particles 1 and 2 occurs at time $t = t_i$ provided: 1) at the collision time $t_i$ the same particles are in instantaneous mutual contact so that $|r_2 - r_1| = \sigma$; 2) before collision the particles are approaching each other, in the sense that the relative incoming velocity $v_{12}^{(-)} \equiv v_1^{(-)} - v_2^{(-)}$ is such that $n_{12} \cdot v_{12}^{(-)} < 0$, with $n_{12}$ denoting the unit vector $n_{12} = \text{vers} \{r_1 - r_2\}$.

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* Based on a seminar presented at the Weizmann Institute of Science (Rehovot, Israel), May 4, 2015
The corresponding 2-particle elastic collision laws are then realized by the velocity transformations indicated in Figure 2. Similarly, the occurrence at time $t = t_i$ of a double binary collision event $(1, 2) \rightarrow (2, 3)$ requires simultaneously 1) that $|r_2 - r_1| = \sigma$ and $|r_2 - r_3| = \sigma$ with $|r_1 - r_3| > \sigma$, and in addition 2) that $n_{12} \cdot v_{12}^{(-)} < 0$ and $n_{23} \cdot v_{23}^{(-)} < 0$, namely that particles 1 and 2 as well as 2 and 3 are both approaching each other. Analogous collision laws can be established for arbitrary higher-order multiple collisions. As a consequence, the time-evolution of the $N$-body state $\mathbf{x}(t) \equiv \{x_1(t), ..., x_N(t)\}$ remains by construction uniquely prescribed for all $t \in I \equiv \mathbb{R}$.

Grad’s approach became popular in the subsequent literature being adopted by most authors (see for example Cercignani [18]). In particular, it was instrumental to overcome the notorious Loschmidt paradox [19], i.e., the claim that Boltzmann H-theorem might conflict with the time-reversal invariance of the Boltzmann-Sinai CDS. The subsequent response given by Boltzmann [20] was in itself manifestly self-contradictory since he conceded that “H-theorem could be violated in some cases” [27]. This circumstance might/should occur, according to Boltzmann, for suitable initial conditions of the 1-body PDF denoted as “high-entropy” states (see related discussion in Ref. [22]). Such a view, however, based on the proof given by Cercignani and Lampis in Ref. [23], appears incorrect. In fact, contrary to Loschmidt objection, the Boltzmann-H theorem preserves its full validity under time-reversal, being - in actual fact - time-reversal invariant. The property arises because, once the time-reversal transformation is performed,
the appropriate corresponding causal prescription must be adopted at the kinetic level for the time evolution of the 2-body PDF occurring across arbitrary binary collision events (see next section below). Such a prescription affects in turn the realization of the Boltzmann collision operator and of the Boltzmann kinetic equation too. As a consequence, in contrast to the aforementioned Boltzmann interpretation, the inequality characterizing the Boltzmann-H theorem remains necessarily unchanged under the action of the same transformation.

Despite this conclusion, the fundamental property of decay to kinetic equilibrium (DKE) (also usually referred to as Macroscopic irreversibility) which is implied by the Boltzmann H-theorem remains true. Accordingly, for suitably-smooth initial conditions the solution of the Boltzmann kinetic equation \( \rho_1(x_1, t) \) in the limit \( t \to +\infty \) should decay to a spatially-homogeneous Maxwellian PDF of the type

\[
\rho_M(v_1) = \frac{n_o}{\pi^{3/2}(2T_o/m)^{3/2}} \exp \left\{ -\frac{m(v_1 - V_o)^2}{2T_o} \right\},
\]

with \( \{n_o > 0, T_o > 0, V_o\} \) being suitable constant fluid fields. Such a result is highly non-trivial because it should rely on a global existence theorem for the Boltzmann kinetic equation. However, according to Villani [21], "... present-day mathematics is unable to prove (such a result) rigorously and in satisfactory generality," the obstacle being that it is not known "...whether solutions of the Boltzmann equation are smooth enough, except in certain particular cases." Until recently [10] the answer to this question, clearly of fundamental importance also for the practical applications of the Boltzmann equation, has remained elusive.

In addition, certain intrinsically physics-related aspects of Grad’s approach, as well as, incidentally, of the same one originally developed by Boltzmann, were similarly left unsolved, thus actually preventing its straightforward extension to the treatment of dense and/or granular fluids. In fact, both theories are actually specialized to the treatment of the so-called Boltzmann-Grad limit. For definiteness let us denote by \( \Delta \equiv \frac{kT_oN_o^2}{\pi^3} \) the global diluteness parameter. Then the prescription of the Boltzmann-Grad limit involves, besides suitable smoothness conditions (see discussion below), invoking in addition: A) first, the validity of the so-called dilute-gas asymptotic ordering for \( N, \sigma \) and \( L \), which is obtained by invoking the asymptotic condition \( N \equiv \frac{1}{\sigma} \gg 1 \), together with the requirements that \( \sigma \) and the scale length \( L \) be ordered respectively so that \( \sigma \sim O(\varepsilon^{1/2}) \) and \( L \sim O(\varepsilon^0) \). Then the second ordering implies in turn that \( \Delta \) must be considered of order \( \epsilon \) (\( \epsilon \equiv \frac{1}{N} \to 0^+ \)) Therefore, the issue arises of the proper extension of Boltzmann’s and Grad’s kinetic theories to the statistical treatment of: 1) granular systems, i.e., in which constituent particles have a finite-size [2]; 2) finite systems, i.e., statistical ensembles having a finite number \( N \) (of particles; 3) emphend or locally dense systems, i.e., for which the \( \Delta \sim O(1) \) or the characteristic scale length of 1-body PDF becomes comparable with the size of the particles \( \sigma \). A critical question in this connection is the physical basis of the involved microscopic statistical description [7][10] adopted by Grad. For this purpose it is useful to briefly analyze the basic assumptions laying at the basis of his approach.

**GRAD’S HERITAGE**

The axiomatic approach developed by Grad in his 1958 paper consists actually in two distinct steps. The first one is realized by the global unique prescription of the \( N \)-body probability density function (PDF) \( \rho^{(N)}(x,t) \), i.e., holding identically in the extended \( N \)-body phase space \( \Gamma^N \times I \). The second one, by the construction of the associated BBGKY hierarchy of equations obtained for all \( s = 1, \ldots, N-1 \) in terms of the reduced \( s \)-body PDF’s \( \rho_s^{(N)}(x_1, \ldots, x_s,t) \). Regarding the first step, once the initial condition \( \rho^{(N)}(x_1, \ldots, x_N, t) \) is set - with \( \rho_o^{(N)}(x) \) denoting an initial PDF belonging to a suitable functional class \( \{\rho_o^{(N)}(x)\} \) - the task involves fulfilling the following two basic requirements:

1) Physical prerequisite \#1: the first consists in the realization of the functional setting of \( \rho^{(N)}(x,t) \), namely of the functional class \( \{\rho^{(N)}(x,t)\} \) and hence also the corresponding one for the initial condition, namely \( \{\rho_o^{(N)}(x)\} \).

2) Physical prerequisite \#2: the second one is the prescription of the collision boundary condition (CBC), i.e., the relation between the incoming and outgoing \( N \)-body PDF’s holding at an arbitrary collision time \( t_i \in \{t_i\} \), namely \( \lim_{n \to t_i^\pm} \rho^{(N)}(x(t), t) \equiv \rho^{(N)(x)}(x^{(\pm)}(t_i), t_i) \), where in the case (−) the assumption of left-continuity is introduced requiring \( \rho^{(N)}(x^{(-)}(t_i), t_i) \equiv \rho^{(N)(-)}(x^{(-)}(t_i), t_i) \). Such a relationship must be prescribed in such a way as to permit one to represent uniquely either \( \rho^{(N)(+)}(x^{(+)}(t_i), t_i) \) in terms of \( \rho^{(N)(-)}(x^{(-)}(t_i), t_i) \) yielding in this way the causal CBC, or viceversa \( \rho^{(N)(-)}(x^{(-)}(t_i), t_i) \) in terms of \( \rho^{(N)(+)}(x^{(+)}(t_i), t_i) \) (anti-causal CBC). In both cases it is obvious that the appropriate prescriptions should be determined uniquely based on the axioms of classical statistical mechanics.
It is interesting, in this regard, to point out the choices adopted by Grad. Regarding the first one, \( \{ \rho^{(N)}(x,t) \} \) was identified with the class of stochastic PDF’s, i.e., represented by smooth ordinary functions. This allowed him to discover that the BBGKY hierarchy depends functionally on binary collisions only, because multiple collisions involve surface integrals on phase-space subset of lower dimension (see related discussion in Ref.[18]). However, the realization of the BBGKY hierarchy depends on the specific prescription adopted for the CBC. For this purpose he adopted the same choice originally introduced by Boltzmann [1] in his construction of the Boltzmann equation. This involves surface integrals on phase-space subset of lower dimension (see related discussion in Ref.[18]). However, the

It is interesting, in this regard, to point out the choices adopted by Grad. Regarding the first one, \( \rho^{(N)}(x,t) \) should remain constant across arbitrary collisions, i.e., requiring for arbitrary collision times \( t_i \) the so-called PDF-conserving CBC Lagrangian conservation law

\[
\rho^{(N)(+)}(x(+)(t_i), t_i) = \rho^{(N)(-)}(x(-)(t_i), t_i).
\]

(2)

Hence, validity of the causality principle requires suitably representing the surface integrals appearing in the BBGKY hierarchy so that \( \rho^{(N)(+)}(x(+)(t_i), t_i) \) should be represented in terms of \( \rho^{(N)}(x(-)(t_i), t_i) \) and not vice-versa [28]. The same equation (2) can formally be written also in the equivalent Eulerian form. This requires for arbitrary \( t \in I \) the equation

\[
\rho^{(N)(+)}(x(+), t) = \rho^{(N)(-)}(x(-), t)
\]

(3)

to hold, with \( x(-) \) and \( x(+) = x(+) (x(-)) \) denoting colliding states, respectively an arbitrary incoming and the corresponding outgoing one prescribed by means of the elastic collision laws. One can readily find out the key assumption underlying Grad’s choice (2). Indeed, in any collisionless time interval \( I_i \equiv [t_i, t_{i+1}] \) between two consecutive collision times \( t_i \) and \( t_{i+1} \), the same PDF must manifestly satisfy the integral Liouville equation

\[
\rho^{(N)}(x(t + \tau), t + \tau) = \rho^{(N)}(x(t), t),
\]

(4)

for all \( t + \tau \) and \( t \), belonging to a given collisionless time interval \( I_i \). It follows that Eq.(2) is therefore equivalent to the requirement that the \( N \)-body PDF should be globally conserved along an arbitrary Lagrangian trajectory \( \{ x(t) \} \).

THE NEW "AB INITIO" AXIOMATIC APPROACH

In a series of recent papers [10][10] a new solution has been adopted for Physical prerequisites #1 and 2, referred to as "ab initio" approach to the microscopic statistical description of \( S_N \). This is based on a careful rethinking of Grad 1958 axiomatic approach involving in place of his choices for the same prerequisites, respectively the introduction of suitable extended functional setting for the \( N \)-body PDF, i.e., an appropriate prescription of \( \{ \rho^{(N)}(x,t) \} \), and modified collision boundary condition (MCBC) to hold at arbitrary collision events. To start with one notices the peculiar non-local feature of the Lagrangian or Eulerian CBC indicated above (see Eqs.(2) and (3)), which relates the incoming and outgoing PDF’s evaluated at different phase-space states. The question which arises is whether a locality prescription for the appropriate collision boundary conditions should, instead, be adopted. More precisely, this means that CBC should be realized by means of a local relationship between \( \rho^{(N)(+)} \) and \( \rho^{(N)(-)} \) when both are evaluated at the same state. In other words, this requires prescribing the functional form of the outgoing PDF in terms of the same outgoing state only, i.e., after collision.

An additional feature emerges by inspection of Grad’s approach. In fact, although Eq.(2) can just be viewed as a restatement of the Liouville equation valid across collision times, the validity of Eq.(2) is actually non-mandatory. Indeed in order to satisfy the axiom of probability conservation it suffices that the integral Liouville equation holds only in the sense indicated above by Eq.(4), i.e., when \( t \) and \( t + \tau \) belong to the same collisionless time subset \( I_i \). In order to clarify this point let us notice in fact that, based on the axioms of classical statitical mechanics, the deterministic \( N \)-body PDF must be necessarily an admissible particular solution of the Liouville equation [11]. This means that the functional class \( \{ \rho^{(N)}(x,t) \} \) should include, besides ordinary functions, also distributions and in particular the deterministic Dirac delta \( N \)-body PDF \( \rho^{(N)}_H(x,t) \equiv \delta(x - x(t)) \). The physically-consistent characterization of the collision boundary conditions should therefore permit the treatment of such a case. However, by construction it follows that some PDF must satisfy the collision boundary condition requiring simultaneously that

\[
\begin{align*}
\rho_H^{(N)}(x, t_i) &\equiv \rho_H^{(N)(-)}(x, t_i) = \delta(x - x^{(-)}(t_i)), \\
\rho_H^{(N)(+)}(x, t_i) &\equiv \delta(x - x^{(+)}(t_i)).
\end{align*}
\]

(5)

On the other hand, an arbitrary stochastic PDF \( \rho^{(N)}(x(t), t) \) can always be represented in terms of the convolution integral \( \rho^{(N)}(x(t), t) = \int dx \rho^{(N)}(x, t) \delta(x - x(t)) \), which means that \( \rho^{(N)(+)}(x^{(+)}(t_i), t_i) = \int dx \rho^{(N)}(x, t_i) \delta(x - x^{(+)}(t_i)) \)
while \( \rho^{(-)(N)}(x^-(t), t, t) = \int d\mathbf{x}\rho^{(N)}(\mathbf{x}, t, t)\delta(\mathbf{x} - \mathbf{x}^-)(t, t) \) so that in particular \( \rho^{(-)(N)}(x^-(t), t, t) = \rho^{(N)}(x^-(t), t, t) \). Hence the correct realization of the CBC for stochastic PDF's is necessarily given by the causal relationship

\[
\rho^{(+))(N)}(x^+(t), t, t) = \rho^{(N)}(x^+(t), t, t),
\]

to be referred to as modified CBC (MCBC) in Lagrangian form. The corresponding Eulerian condition holding for arbitrary \( (x^+, t) \) is therefore provided by \( \rho^{(+))(N)}(x^+(t), t) = \rho^{(N)}(x^+(t), t) \). The physical interpretation of Eq. (6) is intuitive. It can be viewed, in fact, as the jump condition for the ensemble of tracers following the same deterministic trajectory and undergoing a collision event at time \( t \). For these particles the same \( N \)-body PDF \( \rho^{(N)}(x, t) \) must obviously be considered as prescribed and therefore it is manifest that its form cannot be affected by the said collision event occurring for the test particles. Notice, additionally, that the \( N \)-body Dirac delta itself can be considered as the limit of the sequence \( \{\rho^{(N)}(x, x(t)), i \in \mathbb{N}\} \) in which each function \( \rho^{(N)}(x, x(t)) \) is a PDF satisfying MCBC [1]. Hence Eq. (6) is a direct consequence of Eqs. (5) which holds in the case of arbitrary \( N \)-body PDF's different from the deterministic one. We notice that in Eq. (6) both the finite size of the particles and the elastic collision laws are explicitly taken into account. Such a choice can be shown to be of critical importance for the statistical treatment of granular or dense gases in which the finite size of the hard spheres becomes relevant [12]. In addition, one can show that MCBC warrants the conservation laws of the corresponding collision operators appearing in the BBGKY hierarchy [13] and the existence of the customary Boltzmann collision invariants [14].

Finally, it is obvious that MCBC must apply also to the Boltzmann equation. Nevertheless, as shown in Ref. [10] (see also Refs. [12, 16]), provided the 1-body PDF is sufficiently smooth the distinction between MCBC and PDF-conserving CBC becomes effectively irrelevant in such a case.

**PHYSICAL IMPLICATIONS**

The features outlined above imply a radical conceptual change of viewpoint in kinetic theory which sets it apart from the Boltzmann and Grad statistical theories as well as Enskog approach to finite-size hard-sphere systems [2] (see also related discussion in Ref. [12]). The consequences of the new Physical prerequisites are, in fact, far-reaching. Indeed, as shown in Ref. [12], the "ab initio" approach leads to the establishment of a kinetic equation, realized by the Master kinetic equation. The Master kinetic equation for the corresponding stochastic reduced 1-body PDF can be represented in terms of the integro-differential equation

\[
\left[ \frac{\partial}{\partial t} + \mathbf{v}_1 \cdot \frac{\partial}{\partial \mathbf{r}_1} \right] \rho^{(N)}(\mathbf{x}_1, t) = C_1 \left( \rho^{(N)}(\mathbf{x}_1, t) \right) ,
\]

where the operators \( C_1 \left( \rho^{(N)}(\mathbf{x}_1, t) \right) \) identifies the Master collision operator. Consistent with the causality principle, MCBC as well the existence of the customary Boltzmann collision invariants [14] this is found to be

\[
C_1 \left( \rho^{(N)}(\mathbf{x}_1, t) \right) = K_n \int d\mathbf{v}_2 \int_{\Sigma_{21}} d\Sigma_{21} \left| \mathbf{v}_2 \cdot \mathbf{n}_{21} \right| \Theta^*(\mathbf{x}_2) \left[ \rho^{(N)}(\mathbf{x}_1^+, \mathbf{x}_2^+, t) - \rho^{(N)}(\mathbf{x}_1, \mathbf{x}_2, t) \right] .
\]

Here the notation is given in accordance with Ref. [12]. Thus \( K_n = (N - 1)\sigma^2 \) is the Knudsen coefficient, \( U_1 \equiv \mathbb{R}^3 \) is the 1-body velocity space, \( \rho^{(N)}(\mathbf{x}_1, \mathbf{x}_2, t) \equiv \rho^{(N)}(\mathbf{r}_1, \mathbf{v}_1, t)\rho^{(N)}(\mathbf{r}_2, \mathbf{v}_2, t) \frac{k_1^{(N)}(\mathbf{r}_1, \mathbf{r}_2, t)}{k_1^{(N)}(\mathbf{r}_1, t)k_1^{(N)}(\mathbf{r}_2, t)} \) the 2-body PDF, the symbol \( \int_{\Sigma_{21}} d\Sigma_{21} \) denotes integration on the subset of the solid angle of incoming particles for which \( \mathbf{v}_1 \cdot \mathbf{n}_{21} < 0 \), while in the integrand \( \mathbf{r}_2 = \mathbf{r}_1 + \sigma\mathbf{n}_{21} \) labels the position of particle "2" which is colliding and hence is in contact with particle "1". Furthermore, the position-dependent functions \( k_1^{(N)}(\mathbf{r}_1, t) \) and \( k_1^{(N)}(\mathbf{r}_1, \mathbf{r}_2, t) \) identify so-called 1- and 2-body occupation coefficients. Remarkably, in difference with Enskog's kinetic equation [2], in the context of the "ab initio" approach they are uniquely prescribed [12]. From the physical point of view, these coefficients are related to the occupation domain of the hard spheres in the configuration space \( \Omega \) arising due to their finite size. Finally \( \Theta^*(\mathbf{x}_2) \) denotes the domain theta function \( \Theta(\mathbf{x}_2) = \left( \mathbf{r}_2 - \frac{\mathbf{R}}{2} \right)_+ \) with \( \mathbf{n}_2 \) denoting the inward normal unit vector to the boundary \( \partial\Omega \) and \( \Theta \) being the strong theta function. The really remarkable feature of Eq. (7) is that it
is exact, i.e., it holds for an $N$–body hard-sphere system having an arbitrary finite number of particles and for hard spheres having finite-size, namely with finite diameter $\sigma > 0$, and finite mass $m$ too. This follows as a consequence of both the extended functional setting indicated above and the MCBC adopted for the same $N$–body PDF.

Based on the construction of the Master kinetic equation, a host of new exciting developments in kinetic theory have opened up. In fact, in several respects the new "ab initio" approach differs significantly from previous literature. The main difference arises because of the non-asymptotic character of the new kinetic equation, i.e., the fact that it applies to arbitrary smooth hard sphere systems for which the finite number and size of the constituent particles is accounted for. Possible applications are ubiquitous (see Figure 3). These include examples such as: 1) Example #1: Environmental and material-science granular fluids (ambient atmosphere, sea-water and ocean dynamics, etc.); 2) Example #2: Biological granular fluids (bacterial motion in fluids, cell-blood dynamics in the human body, blood-vessels, capillaries, etc.); 3) Example #3: Industrial granular fluids (grain or pellet dynamics in metallurgical and chemical processes, air and water pollution dynamics, etc.); 4) Example #4: Geological fluids (slow dynamics of highly viscous granular fluids, inner Earth-core dynamics, etc.).

![Dense Granular Flows](image)

FIG. 3: Examples of dense granular flows

In most of the cases indicated above a self-consistent statistical description to be based on classical statistical mechanics, not mentioning a kinetic equation, was previously missing or largely unsatisfactory. The "ab initio" statistical approach provides such a missing link which is based on the Master kinetic equation established in Ref. [12].

Nevertheless in validity of the Boltzmann-Grad limit the Master equation reduces exactly to the Boltzmann kinetic equation [12] [16]. In fact, one notices that if such a limit is introduced the limit $(N - 1)\sigma^2 \to N\sigma^2$ applies and an arbitrary stochastic and 1–body PDF $\rho^{(N)}_1(x_1, t)$ can be replaced by its asymptotic approximation represented by the Boltzmann-Grad limit function $\rho_1(x_1, t)$. In the Master collision operator this occurs, however, only provided suitable smoothness assumptions hold for the 1–body PDF’s and the 1– and 2–body occupation coefficients $k^{(N)}_1(r_1, t)$ and $k^{(N)}_2(r_1, r_2, t)$. These require, more precisely that, when the diameter of the particles $\sigma$ becomes infinitesimal, it should be possible to replace a) the 1–body PDFs $\rho^{(N)}_1(r_2, v_2^{(+)}(t))$ and $\rho^{(N)}_1(r_2, v_2)(t)$ with their limits $\rho_1(r_1, v_2^{(+)}(t))$ and $\rho_1(r_1, v_2)(t)$ respectively; b) the 1– and 2–body occupation coefficients $k^{(N)}_1(r_1, t)$ and $k^{(N)}_2(r_1, r_2, t)$ with their limit functions, namely respectively $k_1(r_1, t) = k_2(r_1, r_2, t) = 1$ [12]. Moreover, for the same reasons indicated above, in the Master collision operator the integration on the sub-domain $v_{12} \cdot n_{12} < 0$ can be equivalently exchanged with $v_{12} \cdot n_{12} > 0$ while the domain theta function $\Theta (x_2)$ becomes $\Theta (x_2) \equiv \Theta (|r_2|)$ so that its contribution to the collision integral becomes ignorable in the case in which $\rho_1(r_2, v_2, t)$ is stochastic. Based on these premises, denoting $\rho_2(r_1, v_1, r_1, v_2, t) \equiv \rho_1(r_1, v_1, t)\rho_1(r_1, v_2, t)$ the 2–body PDF, it follows that in the Boltzmann-Grad limit the Master
collision operator becomes
\[ C_B (\rho_1 | \rho_1) \equiv N \sigma^2 \int_{V_1} d\mathbf{v}_2 \int^{(\ast)} d\Sigma_{12} |\mathbf{v}_{12} \cdot \mathbf{n}_{12}| \]
\[
\left[ \rho_2(\mathbf{r}_1, \mathbf{v}_1^{(-)}, \mathbf{r}_1, \mathbf{v}_2^{(-)}, t) - \rho_2(\mathbf{r}_1, \mathbf{v}_1, \mathbf{r}_1, \mathbf{v}_2, t) \right],
\]
which therefore coincides with the customary form of the Boltzmann collision operator \([12]\). As a consequence it is obvious that also the Boltzmann H-theorem pointed out originally by Boltzmann himself \([1]\).

\[
\rho_1(x_1, t).
\]

Despite such a conclusion, the Master kinetic equation has an entirely different physical character. In fact, as shown in Ref. \([15]\), in sharp contrast with the Boltzmann equation, its solution represented by the 1-body PDF admits an exact constant H-theorem in terms of Boltzmann-Shannon statistical entropy \(S(\rho_1(N)(t)) \equiv - \int_{\Gamma_1} d\mathbf{v}_1 \rho_1(N)(\mathbf{x}_1, t) \ln \rho_1(N)(\mathbf{x}_1, t)\), so that identically

\[
\frac{\partial}{\partial t} S(\rho_1(N)(t)) \equiv 0.
\]

A number of implications follow concerning the "ab initio" kinetic theory.

The first one is about the long-debated issue about the physical origin of the Boltzmann entropic inequality \([10]\) (see Refs. \([15, 17, 22]\)). This problem can be given a satisfactory answer within the new kinetic theory. In fact, as shown in Ref. \([15]\), if \(\rho_1(N)(x_1, t)\) is approximated in terms of its Boltzmann-Grad limit function \(\rho_1(x_1, t)\) the constant H-theorem \([11]\) is not at variance with the validity of the same inequality \([10]\). Indeed, once the replacement \(\rho_1(N)(x_1, t) \rightarrow \rho_1(x_1, t)\) is made in the corresponding 1-body Boltzmann-Shannon entropy \(S(\rho_1(t))\), this amounts to introduce a related information "error". Such an error unavoidably gives rise to an effective monotonic increase of the Boltzmann-Shannon entropy, so that the validity of Boltzmann H-theorem can actually be rigorously inferred \([15]\) for the same class of limit functions.

Second, the same conclusion proves the conjecture proposed originally by Grad on the physical origin of the Boltzmann entropic inequality. In fact, in his paper devoted to the principles of kinetic theory \([7]\) he suggested that, from the information-theory viewpoint, Boltzmann H-theorem should be understood in terms of "information loss" produced by the Boltzmann-Grad limit.

Third, the global existence problem for the Master kinetic equation has been recently addressed based on the corresponding N-body Liouville equation achieved in the context of the new "ab initio" approach \([16]\). In such a case, in fact, global existence and uniqueness for the 1-body PDF \(\rho_1(N)(x_1, t)\) can be established as a consequence of the global unique prescription of the corresponding N-body PDF \(\rho_1(N)(x, t)\) along arbitrary phase-space Lagrangian trajectories. Indeed, as shown in Ref. \([12]\), in validity of MCBC the same PDF can always be identified with a suitably-weighted factorizable solution in terms of the corresponding 1-body PDF \(\rho_1(N)(x_1, t)\). As a consequence the same 1-body PDF \(\rho_1(N)(x_1, t)\), to be identified in principle with an arbitrary stochastic PDF, is uniquely globally defined and, thanks again to MCBC, it necessarily satisfies the Master kinetic equation. These results are relevant also for the global existence problem posed by Villani \([24]\). In fact, analogous conclusions follow in principle also when the Boltzmann-Grad limit is considered and \(\rho_1(N)(x_1, t)\) is replaced with its limit function \(\rho_1(x_1, t)\). This requires, however, that the same smoothness conditions needed for the validity of the Boltzmann collision operator \([6]\) should hold globally in the extended 1-body phase space \(\Gamma_1 \times I\).

Fourth and last ("in cada stat venenum" paraphrasing Marziali’s famous statement) the question arises of the possible occurrence of the phenomenon of DKE for an arbitrary stochastic solution of the Master kinetic equation. The latter refers to the property whereby particular solutions of the same kinetic equation may decay to a local Maxwellian kinetic equilibrium of the type \([1]\). In the context of Boltzmann and Grad kinetic theories such a property is customarily associated with the entropic inequality \([10]\), implying in turn the occurrence of DKE for the same PDF’s. The question which arises, and remains still to be answered, is whether, despite the validity of the constant H-theorem \([11]\), the phenomenon of DKE may arise also for the Master kinetic equation, i.e., for suitably-smooth particular solutions of the same equation. The example-case recently pointed out \([17]\), corresponding to the statistical description of an incompressible Navier-Stokes granular fluid, suggests that this may be indeed the case. Further investigations in this direction are under way.
ACKNOWLEDGMENTS

Work developed in part within the research projects: A) the Albert Einstein Center for Gravitation and Astrophysics, Czech Science Foundation No. 14-37086G; B) the grant No. 02494/2013/RRC “kinetický přístup k proudění tekutin” (kinetic approach to fluid flow) in the framework of the “Research and Development Support in Moravian-Silesian Region”, Czech Republic; C) the research projects of the Czech Science Foundation GA ČR grant No. 14-07753P. One of the authors (M.T.) is grateful to the International Center for Theoretical Physics (Miramare, Trieste, Italy) for the hospitality during the preparation of the manuscript.

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[25] This was also the subject of his last public lecture before his death occurred on November 17, 1986. It was delivered as invited opening speech at the plenary session of the 15th RGD Symposium, held in Grado, Italy in July of the same year [8]. Unfortunately immediately after the presentation he suffered the symptoms of a heart attack from which he never fully recovered.
[26] this identifies the so-called *Boltzmann-Sinai classical dynamical system*.
[27] according to Drory [24] this might be the reason of the Boltzmann’s dramatic depression that led him to commit suicide on Sept.5, 1906 during his family Summer vacation in the castle of Duino, near Trieste, Italy.
[28] their exchange implies in fact, as pointed out in Ref. [24], a change of signature in the entropy production rate.