Weierstraß–Institut
für Angewandte Analysis und Stochastik

im Forschungsverbund Berlin e.V.

Preprint ISSN 0946 – 8633

Some new properties of the kinetic equation for the consistent Boltzmann algorithm

Alejandro L. Garcia[1], Wolfgang Wagner[2]

submitted: 9th July 2001

[1] Institute for Scientific Computing Research
Lawrence Livermore National Laboratory
Livermore, California 94550, USA
Permanent address: Physics Department
San Jose State University
San Jose, California 95192, USA
E-Mail: algarcia@algarcia.org

[2] Weierstrass Institute for
Applied Analysis and Stochastics
Mohrenstrasse 39
D-10117 Berlin, Germany
E-Mail: wagner@wias-berlin.de

Preprint No. 661
Berlin 2001

1991 Mathematics Subject Classification. 65C05, 76P05, 82C40.

Key words and phrases. Kinetic theory, direct simulation Monte Carlo, consistent Boltzmann algorithm, dense gases, H-theorem.

Edited by
Weierstraß–Institut für Angewandte Analysis und Stochastik (WIAS)
Mohrenstraße 39
D — 10117 Berlin
Germany

Fax: + 49 30 2044975
E-Mail (X.400): c=de;a=d400-gw;p=WIAS-BERLIN;s=preprint
E-Mail (Internet): preprint@wias-berlin.de
World Wide Web: http://www.wias-berlin.de/

Abstract

We study properties of the consistent Boltzmann algorithm for dense gases, using its limiting kinetic equation. First we derive an H-theorem for this equation. Then, following the classical derivation by Chapman and Cowling, we find approximations to the equations of continuity, momentum and energy. The first order correction terms with respect to the particle diameter turn out to be the same as for the Enskog equation. These results confirm previous derivations, based on the virial, of the corresponding equation of state.

Contents

1. Introduction **2**

2. H-theorem **4**

3. Equations of continuity, momentum and energy **6**

3.1. Left-hand side of the kinetic equation 6

3.2. Right-hand side of the kinetic equation 8

3.3. Comparison of both sides 10

Appendix: Moments of a Gaussian variable **12**

References **13**

1. Introduction

Direct Simulation Monte Carlo (DSMC) is presently the most widely used numerical algorithm in kinetic theory [4]. In this method, a system of simulation particles

$$\big(x_i(t), v_i(t)\big), \qquad i = 1, \ldots, N\,, \qquad t \geq 0\,,$$

is used to approximate the behaviour of the real gas. Independent motion (free flow) of the particles and their pairwise interactions (collisions) are separated using a splitting procedure. During the free flow step, particles are moved according to their velocities,

$$x_i(t + \Delta t) = x_i(t) + \int_t^{t+\Delta t} v_i(s)\, ds\,,$$

and boundary conditions are taken into account. During the collision step, particle pairs $(x, v), (y, w)$ are randomly chosen in small cells of the position space, according to the collision probability for the interparticle potential. The post-collision velocities

$$v^* = v + e\,(e, w - v)\,, \qquad w^* = w - e\,(e, w - v) \tag{1.1}$$

are determined by randomly selecting a direction vector e from the unit sphere $\mathcal{S}^2 \subset \mathcal{R}^3$. Here $(.,.)$ and $\|\,.\,\|$ denote the scalar product and the Euclidean norm in $\mathcal{R}^3$, respectively. The number of collisions at each time step Δt is computed from the local collision frequency.

Recently, the Consistent Boltzmann Algorithm (CBA) was introduced as a simple variant of DSMC for dense gases [2]. Besides the standard problems in kinetic theory, CBA has proved useful in the study of granular material [9] and nuclear physics [10]. Although CBA can be generalized to other potentials [1] here we will only consider the hard sphere gas with particle diameter σ. In CBA the collision process is as in DSMC with two modifications. First, when a pair collides each particle is displaced a distance σ into the direction e or $-e$, i.e. (cf. (1.1))

$$x^* = x + \sigma\,\frac{(v^* - w^*) - (v - w)}{\|(v^* - w^*) - (v - w)\|}\,, \qquad y^* = y - \sigma\,\frac{(v^* - w^*) - (v - w)}{\|(v^* - w^*) - (v - w)\|}\,. \tag{1.2}$$

Second, the dense hard sphere collision frequency is used.

The **limiting equation of CBA** (as $N \to \infty$) has been established in [8],

$$\frac{\partial}{\partial t}\, p(t, x, v) + (v, \nabla_x)\, p(t, x, v) = \int_{\mathcal{R}^3} dw \int_{\mathcal{S}^2} de\, B(v, w, e) \times \tag{1.3}$$
$$\Big[\chi(\varrho(t, x^*))\, p(t, x^*, v^*)\, p(t, x^*, w^*) - \chi(\varrho(t, x))\, p(t, x, v)\, p(t, x, w)\Big].$$

Here

$$B(v, w, e) = \text{const}\, |(e, w - v)| \tag{1.4}$$

is the hard sphere collision kernel, and

$$\varrho(t,x)=\int_{\mathcal{R}^3} p(t,x,v)\,dv$$

denotes the density. The function χ is equal to unity for a rarefied gas, and increases with increasing density, becoming infinity as the gas approaches the state of close-packing. With the notations

$$\mathcal{S}_+^2=\mathcal{S}_+^2(v,w)=\{e\,:\,(e,w-v)>0\}\,,\qquad \mathcal{S}_-^2=\{e\,:\,(e,w-v)<0\}\,, \tag{1.5}$$

equation (1.3) takes the form

$$\begin{aligned}\frac{\partial}{\partial t}p(t,x,v)+(v,\nabla_x)\,p(t,x,v)=2\int_{\mathcal{R}^3}dw\int_{\mathcal{S}_+^2}de\,B(v,w,e) \qquad\qquad (1.6)\\ \Big[\chi(\varrho(t,x+\sigma\,e))\,p(t,x+\sigma\,e,v^*)\,p(t,x+\sigma\,e,w^*)-\chi(\varrho(t,x))\,p(t,x,v)\,p(t,x,w)\Big].\end{aligned}$$

Compare this equation with the **Enskog equation** (cf. [7, Ch.16.3])

$$\begin{aligned}&\frac{\partial}{\partial t}p(t,x,v)+(v,\nabla_x)\,p(t,x,v)= \qquad\qquad (1.7)\\ &\quad 2\int_{\mathcal{R}^3}dw\int_{\mathcal{S}_+^2}de\,B(v,w,e)\Big[\chi(\varrho(t,x+\frac{1}{2}\sigma\,e))\,p(t,x,v^*)\,p(t,x+\sigma\,e,w^*)\\ &\qquad -\chi(\varrho(t,x-\frac{1}{2}\sigma\,e))\,p(t,x,v)\,p(t,x-\sigma\,e,w)\Big].\end{aligned}$$

Note that, in the case $\chi\equiv 1$, $\sigma=0$, both equations (1.6) and (1.7) reduce to the **Boltzmann equation**

$$\begin{aligned}&\frac{\partial}{\partial t}p(t,x,v)+(v,\nabla_x)\,p(t,x,v)=\\ &\quad\int_{\mathcal{R}^3}dw\int_{\mathcal{S}^2}de\,B(v,w,e)\,\Big[p(t,x,v^*)\,p(t,x,w^*)-p(t,x,v)\,p(t,x,w)\Big].\end{aligned}$$

Here we study some properties of equation (1.6). In Section 2 we derive an H-theorem. In Section 3, following the classical derivation by Chapman and Cowling [6], [7], we find approximations to the equations of continuity, momentum and energy. The first order correction terms with respect to the particle diameter turn out to be the same as for the Enskog equation. These results confirm previous derivations, based on the virial, of the corresponding equation of state [2].

2. H-theorem

According to (1.1), the displacements (1.2) take the form

$$x^* = x + \psi(v, w, e)\,, \qquad y^* = y - \psi(v, w, e)\,,$$

where the notation

$$\psi(v, w, e) = \sigma\, e\, \mathrm{sign}(e, w - v)$$

is used. Note that

$$\psi(v^*, w^*, e) = -\psi(v, w, e) = \psi(w, v, e) \tag{2.1}$$

and (cf. (1.4))

$$B(v, w, e) = B(v^*, w^*, e) = B(w, v, e) = B(v, w, -e)\,. \tag{2.2}$$

Using (2.1), (2.2), one obtains

$$\begin{aligned}
&\int_{\mathcal{R}^3} dx \int_{\mathcal{R}^3} dv \int_{\mathcal{R}^3} dw \int_{\mathcal{S}^2} de\, \varphi(x, v)\, B(v, w, e)\, \chi(\varrho(t, x^*))\, p(t, x^*, v^*)\, p(t, x^*, w^*) \\
&\quad = \int_{\mathcal{R}^3} dx \int_{\mathcal{R}^3} dv \int_{\mathcal{R}^3} dw \int_{\mathcal{S}^2} de\, \varphi(x - \psi(v, w, e), v)\, B(v, w, e)\, \chi(\varrho(t, x))\, p(t, x, v^*)\, p(t, x, w^*) \\
&\quad = \int_{\mathcal{R}^3} dx \int_{\mathcal{R}^3} dv \int_{\mathcal{R}^3} dw \int_{\mathcal{S}^2} de\, \varphi(x^*, v^*)\, B(v, w, e)\, \chi(\varrho(t, x))\, p(t, x, v)\, p(t, x, w)\,.
\end{aligned}$$

Thus, the weak form of equation (1.3) is

$$\begin{aligned}
&\frac{d}{dt} \int_{\mathcal{R}^3 \times \mathcal{R}^3} \varphi(x, v)\, p(t, x, v)\, dx\, dv = \int_{\mathcal{R}^3 \times \mathcal{R}^3} (v, (\nabla_x \varphi)(x, v))\, p(t, x, v)\, dx\, dv + \\
&\quad \int_{\mathcal{R}^3} \int_{\mathcal{R}^3} \int_{\mathcal{R}^3} \int_{\mathcal{S}^2} \chi(\varrho(t, x))\, B(v, w, e) \big[\varphi(x^*, v^*) - \varphi(x, v)\big] p(t, x, v)\, p(t, x, w)\, de\, dv\, dw\, dx\,,
\end{aligned}$$

or, equivalently,

$$\begin{aligned}
&\frac{d}{dt} \int_{\mathcal{R}^3 \times \mathcal{R}^3} \varphi(x, v)\, p(t, x, v)\, dx\, dv = \int_{\mathcal{R}^3 \times \mathcal{R}^3} (v, (\nabla_x \varphi)(x, v))\, p(t, x, v)\, dx\, dv + \\
&\quad \frac{1}{2} \int_{\mathcal{R}^3} dx \int_{\mathcal{R}^3} dv \int_{\mathcal{R}^3} dw \int_{\mathcal{S}^2} de\, \chi(\varrho(t, x))\, B(v, w, e) \times \\
&\quad \big[\varphi(x + \psi(v, w, e), v^*) + \varphi(x - \psi(v, w, e), w^*) - \varphi(x, v) - \varphi(x, w)\big] p(t, x, v)\, p(t, x, w)\,.
\end{aligned} \tag{2.3}$$

The form (2.3) is convenient for deriving an H-theorem. We consider

$$\varphi(x, v) = \log p(t, x, v)$$

and

$$H(t) = \int_{\mathcal{R}^3} \int_{\mathcal{R}^3} p(t, x, v)\, \log p(t, x, v)\, dv\, dx\,.$$

Note that

$$\int_{\mathcal{R}^3\times\mathcal{R}^3} (v, \nabla_x \log p(t,x,v))\, p(t,x,v)\, dx\, dv = \int_{\mathcal{R}^3\times\mathcal{R}^3} \frac{(v, \nabla_x p(t,x,v))}{p(t,x,v)}\, p(t,x,v)\, dx\, dv = 0\,.$$

Using the elementary inequality

$$a\,(\log b - \log a) \le b - a\,, \qquad a, b > 0\,,$$

one obtains

$$\begin{aligned}
\frac{d}{dt} H(t) &= \frac{1}{2}\int_{\mathcal{R}^3} dx \int_{\mathcal{R}^3} dv \int_{\mathcal{R}^3} dw \int_{\mathcal{S}^2} de\, \chi(\varrho(t,x))\, B(v,w,e) \times \\
&\quad \Big\{\log\Big[p(t, x+\psi(v,w,e), v^*)\, p(t, x-\psi(v,w,e), w^*)\Big] - \\
&\quad \log\Big[p(t,x,v)\, p(t,x,w)\Big]\Big\}\, p(t,x,v)\, p(t,x,w) \\
&\le \frac{1}{2}\int_{\mathcal{R}^3} dx \int_{\mathcal{R}^3} dv \int_{\mathcal{R}^3} dw \int_{\mathcal{S}^2} de\, \chi(\varrho(t,x))\, B(v,w,e) \\
&\quad \Big[p(t, x+\psi(v,w,e), v^*)\, p(t, x-\psi(v,w,e), w^*) - p(t,x,v)\, p(t,x,w)\Big] \\
&= \frac{1}{2}\int_{\mathcal{R}^3} dx \int_{\mathcal{R}^3} dv \int_{\mathcal{R}^3} dw \int_{\mathcal{S}^2} de\, \chi(\varrho(t,x))\, B(v,w,e) \times \\
&\quad \Big[p(t, x-\psi(v,w,e), v)\, p(t, x+\psi(v,w,e), w) - p(t,x,v)\, p(t,x,w)\Big] \\
&=: I(t)\,.
\end{aligned}$$

With the notations (1.5), the correction functional takes the form

$$\begin{aligned}
I(t) &= \int_{\mathcal{R}^3} dx \int_{\mathcal{R}^3} dv \int_{\mathcal{R}^3} dw \int_{\mathcal{S}^2_+(v,w)} de\, \chi(\varrho(t,x))\, B(v,w,e) \times \\
&\quad \Big[p(t, x-\psi(v,w,e), v)\, p(t, x+\psi(v,w,e), w) - p(t,x,v)\, p(t,x,w)\Big] \\
&= \int_{\mathcal{R}^3} dx \int_{\mathcal{R}^3} dv \int_{\mathcal{R}^3} dw \int_{\mathcal{S}^2_-(v,w)} de\, \chi(\varrho(t,x))\, B(v,w,e) \times \\
&\quad \Big[p(t, x-\psi(v,w,e), v)\, p(t, x+\psi(v,w,e), w) - p(t,x,v)\, p(t,x,w)\Big] \\
&= \int_{\mathcal{R}^3} dx \int_{\mathcal{R}^3} dv \int_{\mathcal{R}^3} dw \int_{\mathcal{S}^2_+(v,w)} de\, \chi(\varrho(t,x))\, B(v,w,e) \times \\
&\quad \Big[p(t, x-\sigma\, e, v)\, p(t, x+\sigma\, e, w) - p(t,x,v)\, p(t,x,w)\Big].
\end{aligned}$$

In analogy with [3], one may introduce the functional

$$\tilde{H}(t) = H(t) - \int_0^t I(s)\, ds\,,$$

for which

$$\frac{d}{dt}\tilde{H}(t) \le 0\,.$$

Note that, in the Boltzmann case $\sigma = 0$, one obtains $I(t) = 0$.

3. Equations of continuity, momentum and energy

We follow [7, Ch. 16] (cf. also [6, Ch. 16], [5, Ch. V.6]). Adapted to the notations of [7], equation (1.6) takes the form

$$\left[\frac{\partial}{\partial t} + c \cdot \frac{\partial}{\partial r}\right] f = \int\int dk\, dc_1\, \sigma^2\, (c_1 - c) \cdot k \Big[f'(r + \sigma\, k)\, f_1'(r + \sigma\, k) - f(r)\, f_1(r)\Big], \qquad (3.1)$$

where $f = n\,p$. Here n denotes the number density, and integration dk is over $\mathcal{S}_+^2(c, c_1)$ (cf. (1.5)). For simplicity we set $\chi \equiv 1$.

The uniform steady state is

$$f^{(0)} = n\, \left(\frac{m}{2\pi k\, T}\right)^{\frac{3}{2}} \exp\Big(- \frac{m\, \|c - c_0\|^2}{2k\, T}\Big). \qquad (3.2)$$

A first approximation to the solution of equation (3.1) is $f = f^{(0)}$, a second approximation is

$$f^{(1)} = f^{(0)}\, (1 + \Phi^{(1)})\,, \qquad (3.3)$$

where $\Phi^{(1)}$ is a linear function of the first derivatives of n, T and the mass velocity c_0. In the following derivations we neglect all products of derivatives and derivatives of higher order.

3.1. Left-hand side of the kinetic equation

Consider the left-hand side of equation (3.1):

$$\left[\frac{\partial}{\partial t} + c \cdot \frac{\partial}{\partial r}\right] f^{(1)} = \left[\frac{\partial}{\partial t} + c \cdot \frac{\partial}{\partial r}\right] f^{(0)} = f^{(0)} \left[\frac{\partial}{\partial t} + c \cdot \frac{\partial}{\partial r}\right] \log f^{(0)}\,.$$

Note that

$$\frac{\partial}{\partial t} \log f^{(0)} = \frac{1}{n}\frac{\partial}{\partial t} n - \frac{3}{2\,T}\frac{\partial}{\partial t} T + \frac{m}{2k\,T^2}\frac{\partial}{\partial t} T\, \|c - c_0\|^2 + \frac{m}{kT}\, (c - c_0) \cdot \frac{\partial}{\partial t}\, c_0$$

and

$$\frac{\partial}{\partial r} \log f^{(0)} = \frac{1}{n}\frac{\partial}{\partial r} n - \frac{3}{2\,T}\frac{\partial}{\partial r} T + \frac{m}{2k\,T^2}\frac{\partial}{\partial r} T\, \|c - c_0\|^2 + \frac{m}{kT} \left(\frac{\partial}{\partial r}\, c_0\right) (c - c_0)\,.$$

Multiplying with $\psi = 1$ and integrating with respect to c, one obtains

$$\int dc\, f^{(0)}\, \frac{\partial}{\partial t} \log f^{(0)} = \frac{\partial}{\partial t} n - \frac{3\,n}{2\,T}\frac{\partial}{\partial t} T + \frac{3\,n}{2\,T}\frac{\partial}{\partial t} T$$

and

$$\begin{aligned}\int dc\, f^{(0)}\, c \cdot \frac{\partial}{\partial r} \log f^{(0)} =& \\ & c_0 \cdot \frac{\partial}{\partial r} n - \frac{3n}{2\,T}\, c_0 \cdot \frac{\partial}{\partial r} T + \frac{m\,n}{2k\,T^2}\, c_0 \cdot \frac{\partial}{\partial r} T\, \frac{3kT}{m} + n\, \mathrm{div}(c_0) \\ =& \; c_0 \cdot \frac{\partial}{\partial r} n + n\, \mathrm{div}(c_0)\,.\end{aligned}$$

Finally,

$$\int dc\, f^{(0)} \left[\frac{\partial}{\partial t} + c \cdot \frac{\partial}{\partial r} \right] \log f^{(0)} = \frac{D}{Dt} n + n \,\mathrm{div}(c_0) \tag{3.4}$$

where

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + c_0 \cdot \frac{\partial}{\partial r} \,. \tag{3.5}$$

Multiplying with $\psi = c - c_0$ and integrating with respect to c, one obtains (cf. (A.2))

$$\int dc\, (c - c_0)\, f^{(0)} \frac{\partial}{\partial t} \log f^{(0)} = n \frac{\partial}{\partial t} c_0$$

and (cf. (A.2), (A.4), (A.3))

$$\begin{aligned}
&\int dc\, (c - c_0)\, f^{(0)}\, c \cdot \frac{\partial}{\partial r} \log f^{(0)} = \frac{kT}{m} \frac{\partial}{\partial r} n - \frac{3kn}{2m} \frac{\partial}{\partial r} T + \\
&\quad \frac{m}{2k\,T^2} \int dc\, (c - c_0)\, f^{(0)}\, (c - c_0) \cdot \frac{\partial}{\partial r} T\, \|c - c_0\|^2 + \\
&\quad \frac{m}{kT} \int dc\, (c - c_0)\, f^{(0)}\, (c - c_0) \cdot \left(\frac{\partial}{\partial r} c_0 \right) (c - c_0) + \frac{m}{kT} \int dc\, (c - c_0)\, f^{(0)}\, c_0 \left(\frac{\partial}{\partial r} c_0 \right) (c - c_0) \\
&= \frac{kT}{m} \frac{\partial}{\partial r} n - \frac{3kn}{2m} \frac{\partial}{\partial r} T + \frac{m}{2k\,T^2} 5n \left(\frac{kT}{m} \right)^2 \frac{\partial}{\partial r} T + \frac{m}{kT} \frac{kTn}{m}\, c_0 \left(\frac{\partial}{\partial r} c_0 \right) \\
&= \frac{kT}{m} \frac{\partial}{\partial r} n + \frac{nk}{m} \frac{\partial}{\partial r} T + n \left(c_0 \cdot \frac{\partial}{\partial r} \right) c_0 \,.
\end{aligned}$$

Note that $\frac{\partial}{\partial r} c_0$ is a matrix, $\left(\frac{\partial}{\partial r_i} c_{0,j} \right)_{i,j=1}^{3}$ and

$$\left[c_0 \left(\frac{\partial}{\partial r} c_0 \right) \right]_i = c_{0,1} \frac{\partial}{\partial r_1} c_{0,i} + c_{0,2} \frac{\partial}{\partial r_2} c_{0,i} + c_{0,3} \frac{\partial}{\partial r_3} c_{0,i} = \left(c_0 \cdot \frac{\partial}{\partial r} \right) c_0 \,.$$

Finally one obtains (cf. (3.5))

$$\begin{aligned}
&\int dc\, (c - c_0)\, f^{(0)} \left[\frac{\partial}{\partial t} + c \cdot \frac{\partial}{\partial r} \right] \log f^{(0)} = \\
&\quad n \frac{\partial}{\partial t} c_0 + n \left(c_0 \cdot \frac{\partial}{\partial r} \right) c_0 + \frac{kT}{m} \frac{\partial}{\partial r} n + \frac{nk}{m} \frac{\partial}{\partial r} T = n \frac{D}{Dt} c_0 + \frac{1}{m} \frac{\partial}{\partial r} (k\, n\, T) \,.
\end{aligned} \tag{3.6}$$

Multiplying with $\psi = \|c - c_0\|^2$ and integrating with respect to c, one obtains (cf. (A.5))

$$\begin{aligned}
\int dc\, \|c - c_0\|^2 f^{(0)} \frac{\partial}{\partial t} \log f^{(0)} &= \frac{\partial}{\partial t} n \frac{3kT}{m} - \frac{3}{2\,T} \frac{\partial}{\partial t} T\, n \frac{3kT}{m} + \frac{m}{2k\,T^2} \frac{\partial}{\partial t} T\, 15n \left(\frac{kT}{m} \right)^2 \\
&= \frac{3kT}{m} \frac{\partial}{\partial t} n - \frac{9kn}{2\,m} \frac{\partial}{\partial t} T + \frac{15kn}{2m} \frac{\partial}{\partial t} T = \frac{3kT}{m} \frac{\partial}{\partial t} n + \frac{3kn}{m} \frac{\partial}{\partial t} T
\end{aligned}$$

and (cf. (A.5), (A.6))

$$\int dc\, \|c-c_0\|^2\, f^{(0)}\, c\cdot \frac{\partial}{\partial r}\ \log f^{(0)} =$$
$$\frac{3kT}{m}\, c_0\cdot\frac{\partial}{\partial r}\,n - \frac{9kn}{2\,m}\,c_0\cdot\frac{\partial}{\partial r}\,T + \frac{m}{2k\,T^2}\,c_0\cdot\frac{\partial}{\partial r}\,T\,15n\,\left(\frac{kT}{m}\right)^2$$
$$+\frac{m}{kT}\int dc\,\|c-c_0\|^2\, f^{(0)}\,(c-c_0)\cdot\left(\frac{\partial}{\partial r}\,c_0\right)(c-c_0)$$
$$= \frac{3kT}{m}\, c_0\cdot\frac{\partial}{\partial r}\,n - \frac{9kn}{2\,m}\,c_0\cdot\frac{\partial}{\partial r}\,T + \frac{15nk}{2m}\,c_0\cdot\frac{\partial}{\partial r}\,T + \frac{m}{kT}\,5n\,\left(\frac{kT}{m}\right)^2\ \mathrm{div}(c_0)$$
$$= \frac{3kT}{m}\, c_0\cdot\frac{\partial}{\partial r}\,n + \frac{3kn}{m}\,c_0\cdot\frac{\partial}{\partial r}\,T + \frac{5nkT}{m}\,\mathrm{div}(c_0)\,.$$

Finally one obtains (cf. (3.5))

$$\int dc\,\|c-c_0\|^2\, f^{(0)}\left[\frac{\partial}{\partial t}\ + c\cdot\frac{\partial}{\partial r}\right]\log f^{(0)} = \frac{3kT}{m}\,\frac{D}{Dt}\,n + \frac{3kn}{m}\,\frac{D}{Dt}\,T + \frac{5nkT}{m}\,\mathrm{div}(c_0)\,. \tag{3.7}$$

3.2. Right-hand side of the kinetic equation

Consider the term in brackets at the right-hand side of equation (3.1). Expanding f_1 , f_1' by Taylor's theorem, and retaining only the first derivatives, gives

$$(f'\,f_1' - f\,f_1) + \sigma\,k\cdot\left(f'\,\frac{\partial}{\partial r}\,f_1' + f_1'\,\frac{\partial}{\partial r}\,f'\right). \tag{3.8}$$

Substituting from (3.3) into the **first term** on the right of (3.8) (neglecting terms as before) gives

$$f^{(0)}\,f_1^{(0)}\left(\Phi^{(1)'} + \Phi_1^{(1)'} - \Phi^{(1)} - \Phi_1^{(1)}\right), \tag{3.9}$$

since

$$f^{(0)'}\,f_1^{(0)'} = f^{(0)}\,f_1^{(0)}\,.$$

The **second term** on the right of (3.8) involves space-derivatives. Thus we may write $f^{(0)}$ in place of $f^{(1)}$ and obtain

$$f^{(0)'}\,f_1^{(0)'}\,\frac{\partial}{\partial r}\ \log f_1^{(0)'} + f_1^{(0)'}\,f^{(0)'}\,\frac{\partial}{\partial r}\ \log f^{(0)'} = f^{(0)}\,f_1^{(0)}\,\frac{\partial}{\partial r}\ \log\left[f_1^{(0)'}\,f^{(0)'}\right]$$

and

$$\frac{\partial}{\partial r}\ \log\left[f_1^{(0)'}\,f^{(0)'}\right] = \frac{2}{n}\,\frac{\partial}{\partial r}\,n - \frac{3}{T}\,\frac{\partial}{\partial r}\,T +$$
$$\frac{m}{2k\,T^2}\,\frac{\partial}{\partial r}\,T\left(\|c_1'-c_0\|^2 + \|c'-c_0\|^2\right) + \frac{m}{k\,T}\left(\frac{\partial}{\partial r}\,c_0\right)\left((c_1'-c_0)+(c'-c_0)\right)$$
$$= \ \ldots\ \ + \frac{m}{2k\,T^2}\,\frac{\partial}{\partial r}\,T\left(\|c_1-c_0\|^2 + \|c-c_0\|^2\right) + \frac{m}{k\,T}\left(\frac{\partial}{\partial r}\,c_0\right)\left((c_1-c_0)+(c-c_0)\right).$$

The integral on the right-hand side of the equation gives

$$
\begin{aligned}
I &= \int\int \sigma\, k \cdot \left(f^{(0)} f_1^{(0)} \frac{\partial}{\partial r} \log\left[f_1^{(0)\prime} f^{(0)\prime} \right] \right) \sigma^2 (c_1 - c) \cdot k\, dk\, dc_1 \\
&= \frac{2}{n} \sigma^3 f^{(0)} \int f_1^{(0)} \int k \cdot \frac{\partial}{\partial r} n\, (c_1 - c) \cdot k\, dk\, dc_1 \\
&\quad - \frac{3}{T} \sigma^3 f^{(0)} \int f_1^{(0)} \int k \cdot \frac{\partial}{\partial r} T\, (c_1 - c) \cdot k\, dk\, dc_1 \\
&\quad + \frac{m}{2k\,T^2} \sigma^3 f^{(0)} \int f_1^{(0)} \int k \cdot \frac{\partial}{\partial r} T \left(\|c_1 - c_0\|^2 + \|c - c_0\|^2 \right) (c_1 - c) \cdot k\, dk\, dc_1 \\
&\quad + \frac{m}{k\,T} \sigma^3 f^{(0)} \int f_1^{(0)} \int k \cdot \left(\frac{\partial}{\partial r} c_0 \right) \Big((c_1 - c_0) + (c - c_0) \Big) (c_1 - c) \cdot k\, dk\, dc_1 \qquad (3.10)
\end{aligned}
$$

According to [6, formula 16.8,2] we have

$$
\int k\, (c_1 - c) \cdot k\, dk = \frac{2\pi}{3} (c_1 - c)\,.
$$

Thus, (3.10) implies

$$
\begin{aligned}
I &= \frac{2\pi}{3} \frac{2}{n} \sigma^3 f^{(0)} \int f_1^{(0)} (c_1 - c) \cdot \frac{\partial}{\partial r} n\, dc_1 - \frac{2\pi}{3} \frac{3}{T} \sigma^3 f^{(0)} \int f_1^{(0)} (c_1 - c) \cdot \frac{\partial}{\partial r} T\, dc_1 \\
&\quad + \frac{2\pi}{3} \frac{m}{2k\,T^2} \sigma^3 f^{(0)} \int f_1^{(0)} (c_1 - c) \cdot \frac{\partial}{\partial r} T \left(\|c_1 - c_0\|^2 + \|c - c_0\|^2 \right) dc_1 \\
&\quad + \frac{2\pi}{3} \frac{m}{k\,T} \sigma^3 f^{(0)} \int f_1^{(0)} (c_1 - c) \cdot \left(\frac{\partial}{\partial r} c_0 \right) \Big((c_1 - c_0) + (c - c_0) \Big) dc_1\,. \qquad (3.11)
\end{aligned}
$$

Note that (cf. (3.2))

$$
\int f_1^{(0)} (c_1 - c_0) \cdot \frac{\partial}{\partial r} T \left(\|c_1 - c_0\|^2 + \|c - c_0\|^2 \right) dc_1 = 0\,,
$$

$$
\begin{aligned}
&\int f_1^{(0)} (c - c_0) \cdot \frac{\partial}{\partial r} T \left(\|c_1 - c_0\|^2 + \|c - c_0\|^2 \right) dc_1 \\
&\quad = (c - c_0) \cdot \frac{\partial}{\partial r} T\, n \left[\frac{3kT}{m} + \|c - c_0\|^2 \right],
\end{aligned}
$$

(cf. (A.1))

$$
\begin{aligned}
&\int f_1^{(0)} (c_1 - c_0) \cdot \left(\frac{\partial}{\partial r} c_0 \right) \Big((c_1 - c_0) + (c - c_0) \Big) dc_1 \\
&\quad = \int f_1^{(0)} (c_1 - c_0) \cdot \left(\frac{\partial}{\partial r} c_0 \right) (c_1 - c_0)\, dc_1 = n \frac{kT}{m} \operatorname{div}(c_0)
\end{aligned}
$$

and

$$
\int f_1^{(0)} (c - c_0) \cdot \left(\frac{\partial}{\partial r} c_0 \right) \Big((c_1 - c_0) + (c - c_0) \Big) dc_1 = n\, (c - c_0) \cdot \left(\frac{\partial}{\partial r} c_0 \right) (c - c_0)
$$

Thus, (3.11) implies

$$\begin{aligned}
I &= -\frac{2\pi}{3}\frac{2}{n}\sigma^3 f^{(0)} n\,(c-c_0)\cdot\frac{\partial}{\partial r}n + \frac{2\pi}{3}\frac{3}{T}\sigma^3 f^{(0)} n\,(c-c_0)\cdot\frac{\partial}{\partial r}T \\
&\quad -\frac{2\pi}{3}\frac{m}{2k\,T^2}\sigma^3 f^{(0)}(c-c_0)\cdot\frac{\partial}{\partial r}T\,n\left[\frac{3kT}{m}+\|c-c_0\|^2\right] \\
&\quad +\frac{2\pi}{3}\frac{m}{k\,T}\sigma^3 f^{(0)}\left[n\,\frac{kT}{m}\operatorname{div}(c_0) - n\,(c-c_0)\cdot\left(\frac{\partial}{\partial r}c_0\right)(c-c_0)\right] \\
&= -\frac{2\pi}{3}n\,\sigma^3 f^{(0)}\frac{2}{n}(c-c_0)\cdot\frac{\partial}{\partial r}n \\
&\quad -\frac{2\pi}{3}n\,\sigma^3 f^{(0)}(c-c_0)\cdot\frac{\partial}{\partial r}T\left[-\frac{3}{2\,T}+\frac{m}{2k\,T^2}\|c-c_0\|^2\right] \\
&\quad +\frac{2\pi}{3}n\,\sigma^3 f^{(0)}\left[\operatorname{div}(c_0)-\frac{m}{k\,T}(c-c_0)\cdot\left(\frac{\partial}{\partial r}c_0\right)(c-c_0)\right].
\end{aligned}$$

When multiplying with $\psi = 1\,,\ c-c_0\,,\ \|c-c_0\|^2$ and integrating with respect to c, many terms vanish. One obtains (cf. (A.1))

$$\int dc\,I = \frac{2\pi}{3}n\,\sigma^3\left[n\operatorname{div}(c_0) - \frac{m}{k\,T}\frac{k\,Tn}{m}\operatorname{div}(c_0)\right] = 0\,, \tag{3.12}$$

(cf. (A.2), (A.4), (A.3))

$$\begin{aligned}
\int dc\,(c-c_0)\,I &= -\frac{2\pi}{3}n\,\sigma^3\frac{2}{n}\frac{kTn}{m}\frac{\partial}{\partial r}n \\
&\quad +\frac{2\pi}{3}n\,\sigma^3\frac{3}{2\,T}\frac{kTn}{m}\frac{\partial}{\partial r}T - \frac{2\pi}{3}n\,\sigma^3\frac{m}{2k\,T^2}5n\left(\frac{kT}{m}\right)^2\frac{\partial}{\partial r}T \\
&= -\frac{2\pi}{3}n\,\sigma^3\frac{2kT}{m}\frac{\partial}{\partial r}n + \frac{2\pi}{3}n\,\sigma^3\frac{\partial}{\partial r}T\left[\frac{3kn}{2\,m}-\frac{5kn}{2\,m}\right] \\
&= -\frac{2\pi}{3}n\,\sigma^3\frac{2kT}{m}\frac{\partial}{\partial r}n - \frac{2\pi}{3}n\,\sigma^3\frac{kn}{m}\frac{\partial}{\partial r}T = -\frac{2\pi}{3m}\sigma^3\frac{\partial}{\partial r}(k\,n^2\,T)
\end{aligned} \tag{3.13}$$

and (cf. (A.6))

$$\begin{aligned}
\int dc\,\|c-c_0\|^2\,I &= \frac{2\pi}{3}n\,\sigma^3\operatorname{div}(c_0)\frac{3kTn}{m} - \frac{2\pi}{3}n\,\sigma^3\frac{m}{k\,T}5n\left(\frac{kT}{m}\right)^2\operatorname{div}(c_0) \\
&= \frac{2\pi}{3}n\,\sigma^3\operatorname{div}(c_0)\left[\frac{3kTn}{m}-\frac{5kTn}{m}\right] = -\frac{2\pi}{3}n\,\sigma^3\operatorname{div}(c_0)\frac{2kTn}{m}\,.
\end{aligned} \tag{3.14}$$

Note that the corresponding integrals of the term (3.9) are zero.

3.3. Comparison of both sides

From (3.4), (3.12) one obtains

$$\frac{D}{Dt}n + n\operatorname{div}(c_0) = 0\,. \tag{3.15}$$

This equation is identical with [7, (16.33,3)].

From (3.6), (3.13) one obtains

$$n \frac{D}{Dt} c_0 + \frac{1}{m} \frac{\partial}{\partial r} (k\, n\, T) + \frac{2\pi}{3m} \sigma^3 \frac{\partial}{\partial r} (k\, n^2\, T) = 0 \,,$$

or

$$n \frac{D}{Dt} c_0 + \frac{1}{m} \frac{\partial}{\partial r} \Big[k\, n\, T \Big[1 + \frac{2\pi}{3} \sigma^3 n \Big] \Big] = 0 \,. \tag{3.16}$$

Introducing (cf. [7, (16.33,2)])

$$p_0 = k\, n\, T \Big[1 + \frac{2\pi}{3} \sigma^3 n \Big] , \tag{3.17}$$

and up to some notations, equation (3.16) is identical with [7, formula 16.33,4]. This equation of state is in agreement with that obtained from the virial [2].

From (3.7), (3.14) one obtains

$$\frac{3kT}{m} \frac{D}{Dt} n + \frac{3kn}{m} \frac{D}{Dt} T + \frac{5nkT}{m} \operatorname{div}(c_0) + \frac{2\pi}{3} n\, \sigma^3 \operatorname{div}(c_0) \frac{2kTn}{m} = 0$$

or, using (3.15),

$$\frac{3kn}{m} \frac{D}{Dt} T + k\, T \operatorname{div}(c_0) \frac{2n}{m} \Big[1 + \frac{2\pi}{3} n\, \sigma^3 \Big] = 0 \,,$$

i.e.

$$\frac{D}{Dt} T + \frac{2}{3} T \operatorname{div}(c_0) \Big[1 + \frac{2\pi}{3} n\, \sigma^3 \Big] = 0 \,. \tag{3.18}$$

Taking into account (3.17), this equation is identical with [7, formula 16.33,5].

Equations (3.15), (3.16), (3.18) are the first order approximations to the equations of continuity, momentum and energy. These are the Euler equations with the hydrostatic pressure given by (3.17) and they are identical to those obtained for the Enskog equation (recall that for simplicity χ was taken as unity). For future work, the Chapman-Enskog analysis may be continued to evaluate the transport coefficients by computing the collisional transfer of momentum, energy, and for CBA, mass. We anticipate that, as with the Enskog equation, the resulting viscosity, thermal conductivity, and self-diffusion coefficient will be in good agreement with the results already obtained by Green-Kubo analysis (cf. [2] and [11]).

Acknowledgments. The authors want to thank B. Alder, F. Alexander, and M. Malek Mansour for useful discussions. This work was supported, in part, by a grant from the European Commision DG 12 (PSS*1045) and was performed, in part, at Lawrence Livermore National Laboratory under the auspices of the Department of Energy under Contract No. W-7405-Eng-48.

Appendix: Moments of a Gaussian variable

Let $\xi = c - c_0$. Then

$$\int dc\, f^{(0)}\, \xi \cdot A\, \xi = \int dc\, f^{(0)} \sum_{j,k} \xi_j\, a_{j,k}\, \xi_k = \frac{kTn}{m}\, [a_{1,1} + a_{2,2} + a_{3,3}]\,, \tag{A.1}$$

$$\int dc\, f^{(0)}\, \xi_i\, \xi \cdot b = \int dc\, f^{(0)} \xi_i^2\, b_i = \frac{kTn}{m}\, b_i\,, \tag{A.2}$$

$$\int dc\, f^{(0)}\, \xi_i\, \xi \cdot A\, \xi = \int dc\, f^{(0)}\, \xi_i \sum_{j,k} \xi_j\, a_{j,k}\, \xi_k = 0\,, \tag{A.3}$$

$$\int dc\, f^{(0)}\, \xi_i\, b \cdot A\, \xi = \int dc\, f^{(0)}\, \xi_i \sum_{j,k} b_j\, a_{j,k}\, \xi_k = 0 = \frac{kTn}{m} \sum_j b_j\, a_{j,i}\,,$$

$$\int dc\, f^{(0)}\, \xi_i\, \xi \cdot b\, \|\xi\|^2 = \int dc\, f^{(0)} \xi_i^2\, b_i\, \|\xi\|^2 = n\, b_i \left(\frac{kT}{m}\right)^2 [1 + 1 + 3]\,, \tag{A.4}$$

$$\int dc\, f^{(0)}\, \|\xi\|^4 = \int dc\, f^{(0)} (\xi_1^2 + \xi_2^2 + \xi_3^2)^2 = 15n \left(\frac{kT}{m}\right)^2 \tag{A.5}$$

and

$$\begin{aligned}
\int dc\, f^{(0)}\, \|\xi\|^2\, \xi \cdot A\, \xi &= \int dc\, f^{(0)}\, \|\xi\|^2 \sum_{j,k} \xi_j\, a_{j,k}\, \xi_k = \int dc\, f^{(0)} \sum_i \xi_i^2 \sum_j \xi_j^2\, a_{j,j} \\
&= n \left(\frac{kT}{m}\right)^2 [3\, a_{1,1} + a_{2,2} + a_{3,3} + a_{1,1} + 3\, a_{2,2} + a_{3,3} + a_{1,1} + a_{2,2} + 3\, a_{3,3}] \\
&= 5n \left(\frac{kT}{m}\right)^2 [a_{1,1} + a_{2,2} + a_{3,3}]\,. \qquad (A.6)
\end{aligned}$$

These formulas follow from elementary properties of one-dimensional Gaussian random variables, in particular, $E\eta^4 = 3\,(E\eta^2)^2$, i.e.

$$\frac{1}{n} \int dc\, f^{(0)}\, \|\xi_i\|^4 = 3 \left[\frac{1}{n} \int dc\, f^{(0)}\, \|\xi_i\|^2\right]^2 = 3 \left(\frac{kT}{m}\right)^2.$$

References

[1] F. J. Alexander and A. L. Garcia. The direct simulation Monte Carlo method. *Computers in Physics*, 11(6):588–593, 1997.

[2] F. J. Alexander, A. L. Garcia, and B. J. Alder. A consistent Boltzmann algorithm. *Phys. Rev. Lett.*, 74(26):5212–5215, 1995.

[3] N. Bellomo and M. Lachowicz. On the asymptotic theory of the Boltzmann and Enskog equations: a rigorous H-theorem for the Enskog equation. In *Mathematical aspects of fluid and plasma dynamics (Salice Terme, 1988)*, pages 15–30. Springer, Berlin, 1991.

[4] G. A. Bird. *Molecular Gas Dynamics and the Direct Simulation of Gas Flows.* Clarendon Press, Oxford, 1994.

[5] C. Cercignani. *The Boltzmann Equation and its Applications.* Springer, New York, 1988.

[6] S. Chapman and T. G. Cowling. *The Mathematical Theory of Non–Uniform Gases.* Cambridge Univ. Press, 1952.

[7] S. Chapman and T. G. Cowling. *The mathematical theory of non-uniform gases. An account of the kinetic theory of viscosity, thermal conduction and diffusion in gases.* Cambridge University Press, London, 1970.

[8] A. L. Garcia and W. Wagner. The limiting kinetic equation of the consistent Boltzmann algorithm for dense gases. *J. Statist. Phys.*, 101(5-6):1065–1086, 2000.

[9] H. J. Herrmann and S. Luding. Modeling granular media on the computer. *Contin. Mech. Thermodyn.*, 10(4):189–231, 1998.

[10] G. Kortemeyer, F. Daffin, and W. Bauer. Nuclear flow in consistent Boltzmann algorithm models. *Phys. Lett. B*, 374:25–30, 1996.

[11] T. E. Wainwright. Calculation of hard-sphere viscosity by means of correlation functions. *J. Chem. Phys.*, 40(10):2932–2937, 1964.