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Deviational particle Monte Carlo for the Boltzmann equation

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Abstract

The paper describes the deviational particle Monte Carlo method for the Boltzmann equation. The approach is an application of the general "control variates" variance reduction technique to the problem of solving a nonlinear equation. The deviation of the solution from a reference Maxwellian is approximated by a system of positive and negative particles. Previous results from the literature are modified and extended. New algorithms are proposed that cover the nonlinear Boltzmann equation (instead of a linearized version) with a general interaction model (instead of hard spheres). The algorithms are obtained as procedures for generating trajectories of Markov jump processes. This provides the framework for deriving the limiting equations, when the number of particles tends to infinity. These equations reflect the influence of various numerical approximation parameters. Detailed simulation schemes are provided for the variable hard sphere interaction model.

Contents

1 Introduction

Kinetic equations are crucial to an adequate description of many processes of scientific and industrial importance. In recent years there have been intensified research activities in the field of numerical algorithms for kinetic equations related to new areas of application. Typical gas flows in micro- and nano-machines are in the rarefied regime. Thus, the classical Boltzmann equation is often used to model such flows (cf. [14, 18, 6]).

We consider the Boltzmann equation

$$\frac{\partial}{\partial t} f(t,x,v) + (v,\nabla_x) f(t,x,v) = \int_{\mathcal{R}^3}\int_{\mathcal{S}^2} B(v,w,e)\Big[f(t,x,v')\,f(t,x,w') - f(t,x,v)\,f(t,x,w)\Big]de\,dw \tag{1.1}$$

with boundary condition

$$f(t,x,v)\,(v,n(x)) = \int_{\mathcal{R}^3_{\text{out}}(x)} q_{\text{ref}}(x,w;v)\,f(t,x,w)\,|(w,n(x))|\,dw + q_{\text{in}}(x,v)\,, \quad \forall\, x\in\partial D\,,\quad v\in\mathcal{R}^3_{\text{in}}(x)\,, \tag{1.2}$$

and initial condition

$$f(0,x,v) = f_0(x,v)\,, \qquad x\in D\,,\quad v\in\mathcal{R}^3\,. \tag{1.3}$$

The following notations are used: $\mathcal{R}^3$ - Euclidean space, $\mathcal{S}^2$ - unit sphere, D - domain in $\mathcal{R}^3$, ∂D - boundary of D, $(.,.)$ - scalar product, $\|.\|$ - Euclidean norm, $n(x)$ - unit inner normal vector at $x\in\partial D$, ∇_x - gradient, $\mathcal{R}^3_{\text{in}}(x)$ and $\mathcal{R}^3_{\text{out}}(x)$ - velocities leading a particle from $x\in\partial D$ inside (outside) the domain. The collision transformation

$$v' = v'(v,w,e) = \frac{v+w}{2} + e\,\frac{\|v-w\|}{2}\,, \qquad w' = w'(v,w,e) = \frac{v+w}{2} - e\,\frac{\|v-w\|}{2} \tag{1.4}$$

describes the relationship between post- and pre-collision velocities. The collision kernel has the form

$$B(v,w,e) = b(\|v-w\|,(e,u))\,, \qquad u = \frac{w-v}{\|w-v\|}\,, \tag{1.5}$$

for some non-negative function b. The non-negative functions q_{in} and q_{ref} are the inflow intensity and the reflection density. The initial density f_0 is any non-negative integrable function.

There are significant numerical challenges related to the new applications mentioned above. In classical aerospace problems the common numerical tool for handling the Boltzmann equation is the direct simulation Monte Carlo (DSMC) method (cf. [3, 10, 17]). DSMC is a general simulation method based on a stochastic particle system that imitates the behavior of a real gas. In the particular situation described by the Boltzmann equation (1.1) it approximates the solution f. However, in low Mach number (slow) rarefied flows, there is a small signal-to-noise ratio. Thus, due to statistical fluctuations, it is difficult to detect the macroscopic quantities (density, stream velocity, temperature) with sufficient accuracy. Variance reduction methods for DSMC are desperately needed.

Modifications of DSMC adapted to low speed rarefied gas flows were considered in [8, 20]. Some numerical schemes making use of local Maxwellians were introduced in [15]. A promising approach to the variance reduction problem has been studied in [1, 7, 13, 12, 2]. The authors consider systems of positive and negative particles that model the deviation of the solution to the Boltzmann equation from a given Maxwellian.

The purpose of this paper is to develop the deviational particle approach. New algorithms are proposed that cover the Boltzmann equation (1.1) with general collision kernels (1.5). They are derived as procedures for generating trajectories of Markov jump processes, thus fitting the framework of the convergence proof for DSMC in [21]. The limiting equations for the algorithms (when the particle number tends to infinity) reflect the influence of various numerical approximation parameters.

The paper is organized as follows. Section 2 describes the deviational particle approach. Reference Maxwellians are introduced and the modeling of initial and boundary conditions with deviational particles is discussed. Section 3 is concerned with the collision step for the linearized Boltzmann equation. Two different procedures are introduced - the collision process and the source-sink process. For each of them, detailed algorithms for generating their trajectories are given and the limiting equations are derived. Special cases of collision kernels are treated. Section 4 studies the collision step for the nonlinear Boltzmann equation. The collision process and the source-sink process are generalized to this situation. Detailed algorithms are given and special cases are considered. Section 5 contains comments concerning the results and directions for further studies. The Appendix provides some useful technical details related to collision kernels and to the Maxwellian distribution.

2 Deviational particle approach

In this section we describe the general setup of the deviational particle approach. The equations obtained from the standard DSMC splitting scheme are transformed in order to describe the deviation of the solution from a reference Maxwellian. Algorithms for the treatment of initial and boundary conditions with deviational particles are derived.

2.1 DSMC framework

discretization of state space

The standard DSMC method is based on a stochastic particle system

$$\Big(X_i^{(n)}(t), V_i^{(n)}(t)\Big), \qquad i = 1, \ldots, N^{(n)}(t)\,, \qquad t \geq 0\,. \tag{2.1}$$

This system approximates the solution of the Boltzmann equation (1.1) in the sense that

$$\int_D \int_{\mathcal{R}^3} \varphi(x,v)\, f(t,x,v)\, dv\, dx \quad \sim \quad g^{(n)} \sum_{i=1}^{N^{(n)}(t)} \varphi(X_i^{(n)}(t), V_i^{(n)}(t))\,, \tag{2.2}$$

where φ is any appropriate test function and $n = 1, 2, \ldots$ is a discretization parameter. If the initial system is not empty ($f_0 \neq 0$), then the particle weight is defined as

$$g^{(n)} = \frac{1}{n} \int_D \int_{\mathcal{R}^3} f_0(y,w)\, dw\, dy \tag{2.3}$$

so that n is the number of numerical particles at time zero. Otherwise, the particle weight is defined as

$$g^{(n)} = \frac{\tilde{t}}{n} \int_{\partial D} \int_{\mathcal{R}^3_{in}(x)} q_{\mathrm{in}}(x,v)\, dv\, \sigma(dx)\,, \tag{2.4}$$

where σ is the uniform surface measure and n represents the expected number of numerical particles entering the system during a typical time period $\tilde{t}$. According to (2.3) and (2.4), the weight $g^{(n)}$ is the number of real gas molecules represented by a numerical particle.

discretization of time

The two main components of the evolution of the particle system, spatial motion and collisions, are separated. In the free flow step, particles move independently of each other over a certain period of time. In the collision step, particles do not move over a certain period of time, but collide (change pairwise their velocities) according to some probabilistic rules that take into account their relative positions in space.

The splitting technique leads to a corresponding approximation of the limiting equation (1.1). The first equation, which corresponds to the free flow simulation step, has the form

$$\frac{\partial}{\partial t} f(t,x,v) + (v, \nabla_x) f(t,x,v) = 0\,, \tag{2.5}$$

with boundary condition (1.2). The second equation, which corresponds to the collision simulation step, has the form

$$\begin{aligned} \frac{\partial}{\partial t} f(t,x,v) = \\ \int_D \int_{\mathcal{R}^3} \int_{\mathcal{S}^2} h(x,y)\, B(v,w,e) \Big[f(t,x,v')\, f(t,y,w') - f(t,x,v)\, f(t,y,w) \Big] dedwdy \\ = \int_{\mathcal{R}^3} \int_{\mathcal{S}^2} B(v,w,e) \Big[f(t,x,v')\, \tilde{f}(t,x,w') - f(t,x,v)\, \tilde{f}(t,x,w) \Big] de\, dw\,, \end{aligned} \tag{2.6}$$

where

$$\tilde{f}(t,x,v) = \int_D h(x,y)\, f(t,y,v)\, dy\,. \tag{2.7}$$

The function h is a mollifying kernel influencing the collision intensity. It has the form

$$h(x,y) = \frac{1}{|D_l|} \sum_{l=1}^{l_c} \chi_{D_l}(x)\, \chi_{D_l}(y)\,, \tag{2.8}$$

where

$$D = \bigcup_{l=1}^{l_c} D_l \tag{2.9}$$

is a partition of the spatial domain into a finite number of disjoint cells, $|D_l|$ is the volume of the cell D_l and χ_{D_l} denotes the indicator function.

The free flow equation (2.5) and the collision equation (2.6) are coupled to each other via appropriate initial conditions. The coupling strategy determines the order of convergence with respect to the splitting parameter Δt . More details can be found in [17, p.68/69]. Here we do not introduce any additional notations for the solutions of equations (2.5), (2.6) and consider both equations with initial conditions at $t = 0$.

2.2 Reference Maxwellians

The solution is represented in the form

$$f(t,x,v) = M(x,v) + f_d(t,x,v)\,, \tag{2.10}$$

where

$$M(x,v) = \frac{n_M(x)}{\pi^{3/2}\, c_M(x)^3}\, \exp\left[-\frac{\|v-u_M(x)\|^2}{c_M(x)^2}\right] \tag{2.11}$$

with number density $n_M(x)$, bulk velocity $u_M(x)$, temperature $T_M(x)$ and "most probable speed"

$$c_M(x) = \sqrt{2kT_M(x)/m}\,. \tag{2.12}$$

Here k is Boltzmann's constant and m is the mass of a molecule. The Maxwellian (2.11) is assumed to be constant in each cell. The function f_d is the deviation of the solution f from the reference Maxwellian.

A system of positive and negative particles (cf. (2.1))

$$\Big(\varepsilon_i^{(n)}(t), X_i^{(n)}(t), V_i^{(n)}(t)\Big), \qquad i=1,\ldots,N^{(n)}(t)\,, \tag{2.13}$$

is introduced, with positions $X_i^{(n)}(t) \in D$, velocities $V_i^{(n)}(t) \in \mathcal{R}^3$ and signs $\varepsilon_i^{(n)}(t) = \pm 1$. The system (2.13) is constructed according to the modified equations satisfied by the deviation. It approximates the deviation in the sense that (cf. (2.2))

$$\int_D \int_{\mathcal{R}^3} \varphi(x,v)\, f_d(t,x,v)\, dv\, dx \quad \sim \quad g^{(n)} \sum_{i=1}^{N^{(n)}(t)} \varepsilon_i^{(n)}(t)\, \varphi(X_i^{(n)}(t), V_i^{(n)}(t))\,. \tag{2.14}$$

free flow equation

Consider equation (2.5) with boundary condition (1.2) and initial condition (1.3). Inside a cell, the deviation satisfies the same equation,

$$\frac{\partial}{\partial t} f_d(t,x,v) + (v, \nabla_x)\, f_d(t,x,v) = 0\,. \tag{2.15}$$

The initial condition takes the form

$$f_d(0,x,v) = f(0,x,v) - M(x,v)\,. \tag{2.16}$$

Boundary condition (1.2) transforms into

$$f_d(t,x,v)\,(v,n(x)) = \int_{\mathcal{R}^3_{\mathrm{out}}(x)} q_{\mathrm{ref}}(x,w;v)\, f_d(t,x,w)\, |(w,n(x))|\, dw + q_{\mathrm{in}}^M(x,v)\,,$$

where

$$q_{\mathrm{in}}^M(x,v) = \tag{2.17}$$
$$q_{\mathrm{in}}(x,v) + \int_{\mathcal{R}^3_{\mathrm{out}}(x)} q_{\mathrm{ref}}(x,w;v)\, M(x,w)\, |(w,n(x))|\, dw - M(x,v)\,(v,n(x))\,.$$

The deviational particles are reflected as usual according to q_{ref} . However, the inflow has to be generated according to the modified intensity (2.17).

There are also boundaries between neighboring cells. Let Γ be the boundary between cells 1 and 2. Denote by $f^{(i)}$ and $M^{(i)}$ the limits of the functions f and M at the boundary, taken from cell $i = 1, 2$, and by $n^{(i)}(x)$ the inner normal vector for cell i . The solution satisfies the boundary condition

$$f^{(1)}(t,x,v)\,(v,n^{(1)}(x)) = f^{(2)}(t,x,v)\,(v,n^{(1)}(x))\,, \qquad x \in \Gamma\,, \quad v \in \mathcal{R}^3\,. \tag{2.18}$$

The inflow in a cell is given by the outflow from the neighboring cell. Particles do not feel the cell boundary. The deviational approach (2.10) with

$$f^{(i)}(t,x,v) = M^{(i)}(v) + f_d^{(i)}(t,x,v)$$

transforms (2.18) into

$$\begin{aligned} & f_d^{(1)}(t,x,v)\,(v,n^{(1)}(x)) = \\ & \qquad f_d^{(2)}(t,x,v)\,(v,n^{(1)}(x)) + [M^{(2)}(v) - M^{(1)}(v)]\,(v,n^{(1)}(x))\,. \end{aligned} \tag{2.19}$$

If $M^{(1)} \neq M^{(2)}$, then the boundary condition (2.19) contains an inflow term. Thus, new particles are created at all boundaries between cells with non-identical Maxwellians.

collision equation

Consider equation (2.6) with initial condition (1.3). The weak form of equation (2.6) is

$$\begin{aligned} & \frac{d}{dt}\int_D \int_{\mathcal{R}^3} \varphi(x,v)\, f(t,x,v)\, dv\, dx = \\ & \quad \int_D \int_{\mathcal{R}^3} \int_D \int_{\mathcal{R}^3} \int_{\mathcal{S}^2} \varphi(x,v)\, h(x,y)\, B(v,w,e) \times \\ & \qquad \Big[f(t,x,v')\, f(t,y,w') - f(t,x,v)\, f(t,y,w)\Big] de\, dw\, dy\, dv\, dx \\ & = \int_D \int_{\mathcal{R}^3} \int_D \int_{\mathcal{R}^3} \int_{\mathcal{S}^2} \Big[\varphi(x,v') - \varphi(x,v)\Big] \times \\ & \qquad h(x,y)\, B(v,w,e)\, f(t,x,v)\, f(t,y,w)\, de\, dw\, dy\, dv\, dx \\ & = \int_D \int_{\mathcal{R}^3} \int_D \int_{\mathcal{R}^3} \int_{\mathcal{S}^2} \Big[\varphi(y,w') - \varphi(y,w)\Big] \times \\ & \qquad h(x,y)\, B(v,w,e)\, f(t,y,w)\, f(t,x,v)\, de\, dw\, dy\, dv\, dx \\ & = \frac{1}{2}\int_D \int_{\mathcal{R}^3} \int_D \int_{\mathcal{R}^3} \int_{\mathcal{S}^2} \Big[\varphi(x,v') + \varphi(y,w') - \varphi(x,v) - \varphi(y,w)\Big] \times \\ & \qquad h(x,y)\, B(v,w,e)\, f(t,x,v)\, f(t,y,w)\, de\, dw\, dy\, dv\, dx\,. \end{aligned} \tag{2.20}$$

The deviation satisfies the equation

$$\frac{\partial}{\partial t} f_d(t,x,v) =$$

$$\int_D \int_{\mathcal{R}^3} \int_{\mathcal{S}^2} h(x,y)\, B(v,w,e) \Big[f_d(t,x,v')\, f_d(t,y,w') -$$
$$f_d(t,x,v)\, f_d(t,y,w) \Big] de\, dw\, dy \, +$$
$$\int_D \int_{\mathcal{R}^3} \int_{\mathcal{S}^2} h(x,y)\, B(v,w,e) \Big[M(x,v')\, f_d(t,y,w') + M(y,w')\, f_d(t,x,v') -$$
$$M(x,v)\, f_d(t,y,w) - M(y,w)\, f_d(t,x,v) \Big] de\, dw\, dy$$
$$= \int_{\mathcal{R}^3} \int_{\mathcal{S}^2} B(v,w,e) \Big[f_d(t,x,v')\, \tilde{f}_d(t,x,w') - f_d(t,x,v)\, \tilde{f}_d(t,x,w) \Big] de\, dw \, +$$
$$\int_{\mathcal{R}^3} \int_{\mathcal{S}^2} B(v,w,e) \Big[M(x,v')\, \tilde{f}_d(t,x,w') + M(x,w')\, f_d(t,x,v') -$$
$$M(x,v)\, \tilde{f}_d(t,x,w) - M(x,w)\, f_d(t,x,v) \Big] de\, dw \,, \tag{2.21}$$

with initial condition (2.16), where (cf. (2.7), (2.8))

$$\tilde{f}_d(t,x,v) = \int_D h(x,y)\, f_d(t,y,v)\, dy \,. \tag{2.22}$$

The weak form of equation (2.21) is

$$\frac{d}{dt} \int_D \int_{\mathcal{R}^3} \varphi(x,v)\, f_d(t,x,v)\, dv\, dx = \tag{2.23}$$
$$\frac{1}{2} \int_D \int_{\mathcal{R}^3} \int_D \int_{\mathcal{R}^3} \int_{\mathcal{S}^2} \Big[\varphi(x,v') + \varphi(y,w') - \varphi(x,v) - \varphi(y,w) \Big] \times$$
$$h(x,y)\, B(v,w,e)\, f_d(t,x,v)\, f_d(t,y,w)\, de\, dw\, dy\, dv\, dx \, +$$
$$\int_D \int_{\mathcal{R}^3} \int_D \int_{\mathcal{R}^3} \int_{\mathcal{S}^2} \Big[\varphi(x,v') + \varphi(y,w') - \varphi(x,v) - \varphi(y,w) \Big] \times$$
$$h(x,y)\, B(v,w,e)\, M(x,v)\, f_d(t,y,w)\, de\, dw\, dy\, dv\, dx \,.$$

2.3 Initial conditions

initial state

The initial state of the system (2.13) is generated according to the function

$$f_0(x,v) - M(x,v) \,, \tag{2.24}$$

where M is a reference Maxwellian of the form (2.11). Then the system proceeds according to the free flow equation (2.15) and the collision equation (2.21).

change of the reference Maxwellian

The underlying Maxwellian can be changed either before the free flow step or before the collision step. This procedure is treated via the initial condition. The system of particles

$$\left(\varepsilon_i^{(n)}(0), X_i^{(n)}(0), V_i^{(n)}(0)\right) \tag{2.25}$$

approximates the function $f(0,x,v) - M(x,v)$. If, on the next step, the reference Maxwellian is supposed to be $\tilde{M}$, then the initial condition takes the form

$$\tilde{f}_d(0,x,v) = f(0,x,v) - \tilde{M}(x,v)\,. \tag{2.26}$$

Thus, one has to generate a system of particles

$$\left(\tilde{\varepsilon}_i^{(n)}(0), \tilde{X}_i^{(n)}(0), \tilde{V}_i^{(n)}(0)\right) \tag{2.27}$$

approximating the function

$$M(x,v) - \tilde{M}(x,v)\,. \tag{2.28}$$

The combined system (2.25), (2.27) corresponds to the initial condition (2.26).

Special cases are the transformations between the standard DSMC system and the deviational particle system. If $\tilde{M} = 0$, then the Maxwellian is replaced by particles. If $M = 0$, then only negative particles are added to the system, corresponding to the chosen Maxwellian.

implementation

Having in mind (2.24) and (2.28), we propose a procedure for generating particle systems approximating the difference $p_1 - p_2$ of two non-negative integrable functions on $\mathcal{R}^3$. Other constructions are possible.

Lemma 2.1 *Let* $\mathrm{Int}(x)$ *denote the integer part of a real number* x. *For (cf. (2.3), (2.4))*

$$i = 1,\dots,k^{(n)} \qquad \text{and} \qquad k^{(n)} = \mathrm{Int}\left(\frac{\int p_1(v)\,dv + \int p_2(v)\,dv}{g^{(n)}}\right)$$

construct a particle according to the following procedure:

- *generate a velocity* $v_i \in \mathcal{R}^3$ *according to*

$$\frac{p_1(v) + p_2(v)}{\int p_1(w)\,dw + \int p_2(w)\,dw}$$

- *with probability*

$$\frac{|p_1(v_i) - p_2(v_i)|}{p_1(v_i) + p_2(v_i)}\,,$$

  define weight

$$\varepsilon_i = \mathrm{sign}(p_1(v_i) - p_2(v_i))$$

- *otherwise, define weight* $\varepsilon_i = 0$

Then

$$\lim_{n\to\infty} \int_{\mathcal{R}^3} \varphi(v)\, \nu^{(n)}(dv) = \int_{\mathcal{R}^3} \varphi(v)\, [p_1(v) - p_2(v)]\, dv$$

for all bounded continuous function φ *, where*

$$\nu^{(n)}(dv) = g^{(n)} \sum_{i=1}^{k^{(n)}} \varepsilon_i\, \delta_{v_i}(dv)\,.$$

Proof. One obtains

$$\mathbb{E}\left[g^{(n)} \sum_{i=1}^{k^{(n)}} \varepsilon_i\, \varphi(v_i)\right] = g^{(n)} \sum_{i=1}^{k^{(n)}} \int_{\mathcal{R}^3} \frac{|p_1(v) - p_2(v)|}{p_1(v) + p_2(v)} \times$$

$$\mathrm{sign}(p_1(v) - p_2(v))\, \varphi(v)\, \frac{p_1(v) + p_2(v)}{\int p_1(w)\, dw + \int p_2(w)\, dw}\, dv$$

$$= \frac{k^{(n)}\, g^{(n)}}{\int p_1 + \int p_2} \int_{\mathcal{R}^3} [p_1(v) - p_2(v)]\, \varphi(v)\, dv \quad \to \quad \int_{\mathcal{R}^3} [p_1(v) - p_2(v)]\, \varphi(v)\, dv$$

and, since $\mathrm{Var}(\varepsilon_i\, \varphi(v_i)) < \infty$,

$$\mathrm{Var}\left[g^{(n)} \sum_{i=1}^{k^{(n)}} \varepsilon_i\, \varphi(v_i)\right] =$$

$$(g^{(n)})^2 \sum_{i=1}^{k^{(n)}} \mathrm{Var}(\varepsilon_i\, \varphi(v_i)) = (g^{(n)})^2\, k^{(n)}\, \mathrm{Var}(\varepsilon_1\, \varphi(v_1)) \quad \to \quad 0$$

as $n \to \infty$. This completes the proof (cf. [17, Section A.4]). ■

Remark 2.2 *The simplest way is to generate* $k_1^{(n)} = \frac{\int p_1}{g^{(n)}}$ *positive particles according to* p_1 *, and* $k_2^{(n)} = \frac{\int p_2}{g^{(n)}}$ *negative particles according to* p_2 *. Note that* $k_1^{(n)} = k_2^{(n)} = n$ *, if* $\int p_1 = \int p_2 = \int f_0$ *. Thus, these particles would be very many, even if* p_1 *and* p_2 *were close to each other. This would not be efficient. However, the procedure from Lemma 2.1 does not produce any particles, when* $p_1 = p_2$ *.*

2.4 Boundary conditions

The relationship between stochastic particle systems and boundary conditions is discussed in [17, Section 3.2]. The generalization to sign-changing inflow intensities is straightforward.

inflow boundaries

At an inflow boundary $\Gamma_{in} \subset \partial D$ one typically assumes $q_{\mathrm{ref}} = 0$ (absorption) and

$$q_{in}(x,v) = M_{in}(x,v)\,\big(v,n(x)\big)\,,$$

where M_{in} is an inflow Maxwellian. The modified inflow term (2.17) takes the form

$$q_{in}^M(x,v) = [M_{in}(x,v) - M(x,v)]\,\big(v,n(x)\big)\,. \tag{2.29}$$

If

$$M_{in}(x,v) = M(x,v)\,, \tag{2.30}$$

then the modified inflow term is zero. In the case of **pure absorption** ($q_{\mathrm{in}} = 0$) one obtains

$$q_{in}^M(x,v) = -M(x,v)\,\big(v,n(x)\big)\,.$$

boundaries between cells

The inflow term in (2.19) takes the form

$$\tilde{q}_{\mathrm{in}}^{(1)}(x,v) = [M^{(2)}(v) - M^{(1)}(v)]\,\big(v,n^{(1)}(x)\big)\,, \qquad \big(v,n^{(1)}(x)\big) \ge 0\,, \tag{2.31}$$

for cell 1, and

$$\tilde{q}_{\mathrm{in}}^{(2)}(x,v) = [M^{(1)}(v) - M^{(2)}(v)]\,\big(v,n^{(2)}(x)\big)\,, \qquad \big(v,n^{(2)}(x)\big) \ge 0\,, \tag{2.32}$$

for cell 2.

reflective boundaries

At a reflective boundary one typically assumes $q_{\mathrm{in}} = 0$ (no inflow) and the Maxwell boundary condition

$$q_{\mathrm{ref}}(x,w;v) = \\ (1-\alpha)\,\delta(v - w + 2\,n(x)\,\big(n(x),w\big)) + \frac{\alpha}{F_{\mathrm{b}}(x)}\,M_{\mathrm{b}}(x,v)\,\big(v,n(x)\big)\,, \tag{2.33}$$

for some $\alpha \in [0,1]$, where M_{b} is a boundary Maxwellian and

$$F_{\mathrm{b}}(x) = \int_{\mathcal{R}^3_{in}(x)} M_{\mathrm{b}}(x,v)\,\big(v,n(x)\big)\,dv\,. \tag{2.34}$$

The modified inflow term (2.17) takes the form

$$\begin{aligned} q_{\mathrm{in}}^M(x,v) \;\; = \;\; & \Big[(1-\alpha)\,M(x, v - 2\,n(x)\,\big(n(x),v\big)) + \\ & \frac{\alpha}{F_{\mathrm{b}}(x)}\,F_{\mathrm{out}}^M(x)\,M_{\mathrm{b}}(x,v) - M(x,v)\Big]\big(v,n(x)\big)\,, \end{aligned}$$

where

$$F_{\rm out}^M(x) = \int_{\mathcal{R}^3_{\rm out}(x)} M(x,w)\, |(w,n(x))|\, dw$$

is the out-going flux of the Maxwellian M .

In the case of **specular reflection** ($\alpha = 0$) one obtains

$$q_{\rm in}^M(x,v) = \Big[M(x, v - 2\, n(x)\, (n(x),v)) - M(x,v)\Big]\, (v,n(x))\,. \tag{2.35}$$

If (cf. (2.11))

$$(u_M(x), n(x)) = 0\,, \tag{2.36}$$

then the modified inflow term (2.35) is zero.

In the case of **diffuse reflection** ($\alpha = 1$) one obtains

$$q_{\rm in}^M(x,v) = \left[\frac{F_{\rm out}^M(x)}{F_{\rm b}(x)}\, M_{\rm b}(x,v) - M(x,v)\right]\, (v,n(x))\,. \tag{2.37}$$

If

$$M_{\rm b}(x,v) = M(x,v)\,,$$

then the modified inflow term (2.37) takes the form

$$q_{\rm in}^M(x,v) = \left[\frac{F_{\rm out}^M(x)}{F_{\rm in}^M(x)} - 1\right]\, M(x,v)\, (v,n(x))\,, \tag{2.38}$$

where (cf. (2.34))

$$F_{\rm in}^M(x) = \int_{\mathcal{R}^3_{\rm in}(x)} M(x,w)\, (w,n(x))\, dw\,.$$

The term (2.38) is zero provided that

$$F_{\rm out}^M(x) = F_{\rm in}^M(x)\,. \tag{2.39}$$

This is fulfilled if (2.36) holds.

Reflection of deviational particles is performed as usual. It remains to implement the creation terms.

implementation

To increase efficiency, we introduce fictitious inflow events. Assume that the inflow intensity (2.17) satisfies

$$|q_{\rm in}^M(x,v)| \le \hat{q}_{\rm in}^M(x,v)\,,$$

for some majorant function $\hat{q}_{\rm in}^M$. The general procedure is as follows:

Algorithm 2.3

1. *Make a time step with parameter*

$$\hat{\lambda}_{\text{in}}^{M} = \frac{1}{g^{(n)}} \int_{\partial D} \int_{\mathcal{R}^3_{\text{in}}(x)} \hat{q}_{\text{in}}^{M}(x,v)\, dv\, \sigma(dx)\,.$$

Stop, when the final time is exceeded.

2. *Generate a position* $x \in \partial D$ *and a velocity* $v \in \mathcal{R}^3_{\text{in}}(x)$ *according to the density*

$$\frac{1}{\hat{\lambda}_{\text{in}}^{M}\, g^{(n)}}\, \hat{q}_{\text{in}}^{M}(x,v)\,.$$

3. *With probability*

$$1 - \frac{|q_{\text{in}}^{M}(x,v)|}{\hat{q}_{\text{in}}^{M}(x,v)}\,,$$

reject the inflow event and go to **1.**

4. *Add a particle with position* x , *velocity* v *and sign*

$$\text{sign}\; q_{\text{in}}^{M}(x,v)$$

to the system and go to **1.**

Assume that $\Gamma \subset \partial D$ is some plane part of the boundary so that

$$n(x) = e\,, \quad \forall\, x \in \Gamma\,, \qquad \text{for some } e \in \mathcal{S}^2\,.$$

Consider an inflow intensity of the form (cf. (2.29), (2.31), (2.32), (2.37))

$$q_{in}^{M}(x,v) = \chi_\Gamma(x)\Big(M^{(2)}(v) - M^{(1)}(v)\Big)(v,e)$$

and the majorant

$$\hat{q}_{in}^{M}(x,v) = \chi_\Gamma(x)\Big(M^{(2)}(v) + M^{(1)}(v)\Big)(v,e)\,, \tag{2.40}$$

where χ_Γ denotes the indicator function. Define

$$F_{\text{in}}^{(i)} = \int_{(w,e)\geq 0} M^{(i)}(v)\,(v,e)\, dv\,, \qquad i = 1,2\,.$$

Algorithm 2.3 takes the form:

Algorithm 2.4

1. *Make a time step with parameter*

$$\hat{\lambda}_{\text{in}}^{M} = \frac{|\Gamma|}{g^{(n)}} \Big[F_{\text{in}}^{(2)} + F_{\text{in}}^{(1)} \Big],$$

where $|\Gamma|$ *is the surface area. Stop, when the final time is exceeded.*

2. *Choose an index* $i = 1, 2$ *with probabilities*

$$\frac{F_{\text{in}}^{(i)}}{F_{\text{in}}^{(2)} + F_{\text{in}}^{(1)}} .$$

3. *For given* i *, generate a velocity* v *according to the density*

$$\frac{1}{F_{\text{in}}^{(i)}} \; M^{(i)}(v) \, (v, e) \, . \tag{2.41}$$

4. *With probability*

$$1 - \frac{|M^{(2)}(v) - M^{(1)}(v))|}{M^{(2)}(v) + M^{(1)}(v))} \, ,$$

reject the inflow event. Go to **1.**

5. *Generate a position* $x \in \Gamma$ *uniformly.*

6. *Add a particle with position* x *, velocity* v *and sign*

$$\operatorname{sign}\Big(M^{(2)}(v) - M^{(1)}(v) \Big)$$

to the system. Go to **1.**

The generation of a Maxwellian inflow (2.41) was studied in the literature (cf. [17, Section B.5], [11]).

3 Collision step for the linearized BE

In this section we study the evolution of the particle system (2.13) during the collision step, when only the linear part on the right-hand side of equation (2.21) or (in the weak form) (2.23) is taken into account. The transition to the limiting equations is performed using the empirical measures (cf. (2.14))

$$\mu^{(n)}(t,dx,dv) = g^{(n)} \sum_{i=1}^{N^{(n)}(t)} \varepsilon_i^{(n)}(t)\, \delta_{X_i^{(n)}(t)}(dx)\, \delta_{V_i^{(n)}(t)}(dv)\,. \tag{3.1}$$

We introduce two different processes leading to similar limiting equations, thus providing more degrees of freedom for the approach. Detailed algorithms are constructed for the general collision kernel (1.5) and then specified for the variable hard sphere model

$$B(v,w,e) = C_\beta \, \|v-w\|^\beta\,, \qquad \beta \ge 0\,, \qquad C_\beta \ge 0\,. \tag{3.2}$$

The special cases of hard spheres and pseudo-Maxwell molecules are obtained for $\beta = 1$ and $\beta = 0$, respectively.

3.1 Collision process

Here particles jump independently and each jump creates two additional particles.

3.1.1 Generator and limiting equation

Consider states of the form

$$z = (\varepsilon_1, x_1, v_1; \ldots; \varepsilon_N, x_N, v_N)\,. \tag{3.3}$$

Introduce the generator

$$\mathcal{A}\Phi(z) = \tag{3.4}$$
$$\sum_{i=1}^{N} \int_D \int_{\mathcal{R}^3} \int_{\mathcal{S}^2} [\Phi(J(z,i,y,w,e)) - \Phi(z)]\, h(x_i,y)\, B(v_i,w,e)\, M(y,w)\, de\, dw\, dy\,,$$

where J replaces $(\varepsilon_i, x_i, v_i)$ by $(\varepsilon_i, x_i, v'(v_i,w,e))$ and adds $(\varepsilon_i, y, w'(v_i,w,e))$ and $(-\varepsilon_i, y, w)$. Using test functions

$$\Phi(z) = g^{(n)} \sum_{i=1}^{N} \varepsilon_i\, \varphi(x_i, v_i)\,, \tag{3.5}$$

one obtains

$$\mathcal{A}\Phi(Z(t)) = g^{(n)} \sum_{i=1}^{N^{(n)}(t)} \int_D \int_{\mathcal{R}^3} \int_{\mathcal{S}^2} \Big[\varepsilon_i^{(n)}(t)\, \varphi(X_i^{(n)}(t), v'(V_i^{(n)}(t),w,e)) +$$

$$
\varepsilon_i^{(n)}(t)\,\varphi(y,w'(V_i^{(n)}(t),w,e)) - \varepsilon_i^{(n)}(t)\,\varphi(X_i^{(n)}(t),V_i^{(n)}(t)) - \varepsilon_i^{(n)}(t)\,\varphi(y,w)\Big] \times
$$
$$
h(X_i^{(n)}(t),y)\,B(V_i^{(n)}(t),w,e)\,M(y,w)\,de\,dw\,dy
$$
$$
= \int_D\int_{\mathcal{R}^3}\int_D\int_{\mathcal{R}^3}\int_{\mathcal{S}^2}\Big[\varphi(x,v'(v,w,e)) + \varphi(y,w'(v,w,e)) - \varphi(x,v) - \varphi(y,w)\Big] \times
$$
$$
h(x,y)\,B(v,w,e)\,M(y,w)\,de\,dw\,dy\,\mu^{(n)}(t,dx,dv)
$$

leading (as $n \to \infty$) to the limiting equations (cf. (2.23))

$$
\frac{d}{dt}\int_D\int_{\mathcal{R}^3}\varphi(x,v)\,f_d(t,x,v)\,dv\,dx = \tag{3.6}
$$
$$
\int_D\int_{\mathcal{R}^3}\int_D\int_{\mathcal{R}^3}\int_{\mathcal{S}^2}\Big[\varphi(x,v'(v,w,e)) + \varphi(y,w'(v,w,e)) - \varphi(x,v) - \varphi(y,w)\Big] \times
$$
$$
h(x,y)\,B(v,w,e)\,M(y,w)\,f_d(t,x,v)\,de\,dw\,dy\,dv\,dx
$$

or (cf. (2.21), (2.22))

$$
\frac{\partial}{\partial t}f_d(t,x,v) =
$$
$$
\int_D\int_{\mathcal{R}^3}\int_{\mathcal{S}^2} h(x,y)\,B(v,w,e)\Big[M(x,v')\,f_d(t,y,w') + M(y,w')\,f_d(t,x,v') -
$$
$$
M(x,v)\,f_d(t,y,w) - M(y,w)\,f_d(t,x,v)\Big]\,de\,dw\,dy
$$
$$
= \int_{\mathcal{R}^3}\int_{\mathcal{S}^2} B(v,w,e)\Big[M(x,v')\,\tilde{f}_d(t,x,w') + M(x,w')\,f_d(t,x,v') - \tag{3.7}
$$
$$
M(x,v)\,\tilde{f}_d(t,x,w) - M(x,w)\,f_d(t,x,v)\Big]\,de\,dw\,.
$$

3.1.2 General simulation procedure

Assume that the collision kernel (1.5) satisfies

$$
B(v,w,e) \le B_{\max}(v,w,e) := b_{\max}(\|v-w\|,(e,u))\,, \qquad u = \frac{w-v}{\|w-v\|}\,, \tag{3.8}
$$

for all arguments and some function $b_{\max}$. Rewrite the generator (3.4) in the form

$$
\mathcal{A}\Phi(z) = \sum_{i=1}^{N}\int_D\int_{\mathcal{R}^3}\int_{\mathcal{S}^2}\int[\Phi(\tilde z) - \Phi(z)]\,\lambda(z,i,y,w,e,d\tilde z) \times \tag{3.9}
$$
$$
h(x_i,y)\,B_{\max}(v_i,w,e)\,M(y,w)\,de\,dw\,dy\,,
$$

where

$$
\lambda(z,i,y,w,e,d\tilde z) =
$$
$$
\delta_{J(z,i,y,w,e)}(d\tilde z)\,\frac{B(v_i,w,e)}{B_{\max}(v_i,w,e)} + \delta_z(d\tilde z)\,\frac{B_{\max}(v_i,w,e) - B(v_i,w,e)}{B_{\max}(v_i,w,e)}\,.
$$

Define the functions

$$\begin{aligned} E(x,v) &= \int_D \int_{\mathcal{R}^3} \int_{\mathcal{S}^2} h(x,y)\, B(v,w,e)\, M(y,w)\, de\, dw\, dy \\ &= \int_{\mathcal{R}^3} \int_{\mathcal{S}^2} B(v,w,e)\, M(x,w)\, de\, dw \end{aligned} \tag{3.10}$$

and

$$E_{\max}(x,v) = \int_{\mathcal{R}^3} \int_{\mathcal{S}^2} B_{\max}(v,w,e)\, M(x,w)\, de\, dw\,. \tag{3.11}$$

The representation (3.9) suggests the following algorithm:

1. Make a time step with parameter

$$\sum_{i=1}^{N} E_{\max}(x_i, v_i)\,. \tag{3.12}$$

Stop, when the final time is exceeded.

2. Choose an index $i = 1, \ldots, N$ according to the probabilities

$$\frac{E_{\max}(x_i, v_i)}{\sum_{j=1}^{N} E_{\max}(x_j, v_j)}\,. \tag{3.13}$$

3. For given i, generate $w \in \mathcal{R}^3$ according to the density

$$\frac{1}{E_{\max}(x_i, v_i)} \left(\int_{\mathcal{S}^2} B_{\max}(v_i, w, e)\, de \right) M(x_i, w)\,. \tag{3.14}$$

4. For given i and w, generate $e \in \mathcal{S}^2$ according to the density

$$\frac{B_{\max}(v_i, w, e)}{\int_{\mathcal{S}^2} B_{\max}(v_i, w, u)\, du}\,. \tag{3.15}$$

5. With probability

$$1 - \frac{B(v_i, w, e)}{B_{\max}(v_i, w, e)}\,,$$

reject the parameters i, w, e and go to **2.**

6. Choose y uniformly in the cell to which x_i belongs.

7. Replace $(\varepsilon_i, x_i, v_i)$ by

$$(\varepsilon_i, x_i, v'(v_i, w, e))\,, \qquad (\varepsilon_i, y, w'(v_i, w, e))\,, \qquad (-\varepsilon_i, y, w) \tag{3.16}$$

and go to **1.**

In the variable hard sphere model (3.2) we choose (cf. (3.8))

$$B_{\max}(v,w,e) = c_0 + c_1\,\|v-w\| \tag{3.17}$$

so that

$$b_{\max}(\xi,\zeta) = c_0 + c_1\,\xi\,. \tag{3.18}$$

One obtains (cf. (3.11), (2.11))

$$E_{\max}(x,v) = 4\,\pi\left(c_0\,n_M(x) + c_1\int_{\mathcal{R}^3}\|v-w\|\,M(x,w)\,dw\right), \tag{3.19}$$

The general simulation procedure takes a particularly simple form in the case of pseudo-Maxwell molecules ($\beta = 0$ with $c_0 = C_0$ and $c_1 = 0$):

Algorithm 3.1 (Pseudo-Maxwell molecules)

1. *Make a time step with parameter*

$$4\,\pi\,C_0\sum_{i=1}^{N} n_M(x_i)\,.$$

Stop, when the final time is exceeded.

2. *Choose an index* $i = 1,\ldots,N$ *according to the probabilities*

$$\frac{n_M(x_i)}{\sum_{j=1}^{N} n_M(x_j)}\,. \tag{3.20}$$

3. *For given* i *, generate* $w \in \mathcal{R}^3$ *according to the Maxwellian* $M(x_i,w)$ *.*

4. *For given* i *and* w *, generate* $e \in \mathcal{S}^2$ *uniformly.*

5. *Choose* y *uniformly in the cell to which* x_i *belongs.*

6. *Replace particle* $(\varepsilon_i, x_i, v_i)$ *by three particles (3.16) and go to* **1.**

Finally, we specify the general simulation procedure for the hard sphere model ($\beta = 1$ with $c_0 = 0$ and $c_1 = C_1$):

Algorithm 3.2 (Hard sphere model)

1. *Make a time step with parameter*

$$4\,\pi\,C_1\sum_{i=1}^{N}\int_{\mathcal{R}^3}\|v_i-w\|\,M(x_i,w)\,dw\,. \tag{3.21}$$

Stop, when the final time is exceeded.

2. *Choose an index* $i = 1, \ldots, N$ *according to the probabilities*

$$\frac{1}{\sum_{j=1}^{N} \int_{\mathcal{R}^3} \|v_j - w\| \, M(x_j, w) \, dw} \int_{\mathcal{R}^3} \|v_i - w\| \, M(x_i, w) \, dw \,. \tag{3.22}$$

3. *For given* i , *generate* $w \in \mathcal{R}^3$ *according to the density*

$$\frac{1}{\int_{\mathcal{R}^3} \|v_i - u\| \, M(x_i, u) \, du} \, \|v_i - w\| \, M(x_i, w) \,. \tag{3.23}$$

4. *For given* i *and* w , *generate* $e \in \mathcal{S}^2$ *uniformly.*

5. *Choose* y *uniformly in the cell to which* x_i *belongs.*

6. *Replace particle* $(\varepsilon_i, x_i, v_i)$ *by three particles (3.16) and go to* **1.**

3.2 Source-sink process

Here the jumps of particles are replaced by creation and deletion events. The main idea is to avoid the blow-up of the system by introducing appropriate source terms that lead to cancellation of positive and negative particles.

3.2.1 Generator and limiting equation

Introduce

$$K^{(1)}(x, v; y, w) = \tag{3.24}$$
$$\frac{4\, h(x, y)}{\|w - v\|} \int_{\Gamma(w-v)} \frac{b\left(\|w - v + u\|, \frac{2\,\|w-v\|^2}{\|w-v+u\|^2} - 1\right)}{\|w - v + u\|} \, M(x, v + u) \, du \,,$$

$$K^{(2)}(x, v; y, w) = \tag{3.25}$$
$$\frac{4\, h(x, y)}{\|w - v\|} \int_{\Gamma(w-v)} \frac{b\left(\|w - v + u\|, 1 - \frac{2\,\|w-v\|^2}{\|w-v+u\|^2}\right)}{\|w - v + u\|} \, M(x, v + u) \, du$$

and

$$K^{(3)}(x, v; y, w) = -h(x, y) \, M(x, v) \int_{\mathcal{S}^2} B(v, w, e) \, de \,, \tag{3.26}$$

where $\Gamma(v)$ denotes the plane through the origin orthogonal to v . It follows from Lemma 6.3 and Corollary 6.4 (with $\gamma(v) = M(x, v)$) that

$$\int_D \int_{\mathcal{R}^3} \varphi(x, v) \, K^{(k)}(x, v; y, w) \, dv \, dx = \int_D \int_{\mathcal{R}^3} \varphi(x, v) \, \nu^{(k)}(y, w; dx, dv) \,, \qquad k = 1, 2 \,, \tag{3.27}$$

where

$$\nu^{(1)}(y,w;dx,dv) = h(y,x)\,dx \int_{\mathcal{R}^3}\int_{\mathcal{S}^2} \delta_{v'(w,u,e)}(dv)\,B(w,u,e)\,M(x,u)\,de\,du\,, \quad (3.28)$$

$$\nu^{(2)}(y,w;dx,dv) = h(y,x)\,dx \int_{\mathcal{R}^3}\int_{\mathcal{S}^2} \delta_{w'(w,u,e)}(dv)\,B(w,u,e)\,M(x,u)\,de\,du \quad (3.29)$$

and φ is any appropriate test function. Note that (cf. (3.10), (6.8))

$$E(y,w) = \int_{\mathcal{R}^3}\int_{\mathcal{S}^2} B(v,w,e)\,M(y,v)\,de\,dv\,. \quad (3.30)$$

It is a consequence of (3.27) (with $\varphi = 1$) and (3.30) that

$$\int_D \int_{\mathcal{R}^3} |K^{(k)}(x,v;y,w)|\,dv\,dx = E(y,w)\,, \qquad k = 1,2,3\,. \quad (3.31)$$

Consider an auxiliary parameter $\theta \in \Theta$, where Θ is a measurable space. Introduce functions $s^{(k)}$ and probability measures A such that (cf. (3.24)–(3.26))

$$\int_\Theta s^{(k)}(z,i,x,v,\theta)\,A(z,x,v,d\theta) = K^{(k)}(x,v;x_i,v_i)\,, \quad (3.32)$$

for all $k = 1,2,3$, $v \in \mathcal{R}^3$, z (cf. (3.3)) and $i = 1,\ldots,N$. Let

$$\{I_l(z)\}\,, \qquad l = 1,\ldots,L(z)\,, \quad (3.33)$$

be a partition of the index set $\{1,\ldots,N\}$ and

$$S_l(z,x,v,\theta) = \sum_{i\in I_l(z)} \varepsilon_i \Big[s^{(1)}(z,i,x,v,\theta) + s^{(2)}(z,i,x,v,\theta) + s^{(3)}(z,i,x,v,\theta)\Big]. \quad (3.34)$$

Consider the **generator**

$$\mathcal{A}\Phi(z) = \sum_{l=1}^{L(z)} \int_D \int_{\mathcal{R}^3} \int_\Theta \Big[\Phi(J_{0,l}(z,x,v,\theta)) - \Phi(z)\Big]\,|S_l(z,x,v,\theta)|\,A(z,x,v,d\theta)\,dv\,dx\,+$$
$$\sum_{i=1}^{N} \Big[\Phi(J_1(z,i)) - \Phi(z)\Big] E(x_i,v_i) =: \mathcal{A}_S\Phi(z) + \mathcal{A}_E\Phi(z)\,, \quad (3.35)$$

where $J_{0,l}(z,x,v,\theta)$ adds a particle $(\operatorname{sign} S_l(z,x,v,\theta),x,v)$ to the system, and $J_1(z,i)$ removes particle (ε_i,v_i) from the system.

Using test functions (3.5), one obtains (cf. (3.27))

$$
\begin{aligned}
&\mathcal{A}_S\Phi(Z(t)) = \\
&\quad \sum_{l=1}^{L(Z(t))} \int_D \int_{\mathcal{R}^3} \int_\Theta \Big[g^{(n)} \operatorname{sign} S_l(Z(t),x,v,\theta) \Big] \varphi(x,v)\, |S_l(Z(t),x,v,\theta)| \times \\
&\qquad\qquad A(Z(t),x,v,d\theta)\, dv\, dx \\
&= g^{(n)} \sum_{i=1}^N \varepsilon_i(t) \int_D \int_{\mathcal{R}^3} \varphi(x,v) \left[\sum_{k=1}^3 \int_\Theta s^{(k)}(Z(t),i,x,v,\theta)\, A(Z(t),x,v,d\theta) \right] dv\, dx \\
&= g^{(n)} \sum_{i=1}^N \varepsilon_i(t) \sum_{k=1}^3 \left[\int_D \int_{\mathcal{R}^3} \varphi(x,v)\, K^{(k)}(x,v;X_i(t),V_i(t))\, dv\, dx \right] \\
&= g^{(n)} \sum_{i=1}^N \varepsilon_i(t) \Big[\int_D \int_{\mathcal{R}^3} \int_{\mathcal{S}^2} \Big[\varphi(x,v'(V_i(t),u,e)) + \varphi(x,w'(V_i(t),u,e)) - \\
&\qquad\qquad \varphi(x,u) \Big] h(X_i(t),x)\, B(V_i(t),u,e)\, M(x,u)\, de\, du\, dx \Big] \\
&= \int_D \int_{\mathcal{R}^3} \int_D \int_{\mathcal{R}^3} \int_{\mathcal{S}^2} \Big[\varphi(x,v'(w,u,e)) + \varphi(x,w'(w,u,e)) - \varphi(x,u) \Big] \times \\
&\qquad\qquad h(y,x)\, B(w,u,e)\, M(x,u)\, de\, du\, dx\, \mu^{(n)}(t,dy,dw)
\end{aligned}
$$

and

$$
\begin{aligned}
\mathcal{A}_E\Phi(Z(t)) &= -g^{(n)} \sum_{i=1}^N \varepsilon_i(t)\, \varphi(X_i(t),V_i(t))\, E(X_i(t),V_i(t)) \\
&= -\int_D \int_{\mathcal{R}^3} \varphi(x,v)\, E(x,v)\, \mu^{(n)}(t,dx,dv)\,,
\end{aligned}
$$

leading (as $n \to \infty$) to the **limiting equation**

$$
\begin{aligned}
&\frac{d}{dt} \int_D \int_{\mathcal{R}^3} \varphi(x,v)\, f_d(t,x,v)\, dv\, dx = \\
&\quad \int_D \int_{\mathcal{R}^3} \int_D \int_{\mathcal{R}^3} \int_{\mathcal{S}^2} \Big[\varphi(x,v') + \varphi(x,w') - \varphi(x,v) - \varphi(y,w) \Big] \times \\
&\qquad\qquad h(x,y)\, B(v,w,e)\, M(x,v)\, f_d(t,y,w)\, de\, dw\, dy\, dv\, dx
\end{aligned} \tag{3.36}
$$

or (cf. Lemma 6.2 and (2.22))

$$
\begin{aligned}
&\frac{\partial}{\partial t} f_d(t,x,v) = \\
&\quad \int_D \int_{\mathcal{R}^3} \int_{\mathcal{S}^2} h(x,y)\, B(v,w,e) \Big[M(x,v')\, f_d(t,y,w') + M(y,w')\, f_d(t,y,v') - \\
&\qquad\qquad M(x,v)\, f_d(t,y,w) - M(y,w)\, f_d(t,x,v) \Big] de\, dw\, dy \\
&= \int_{\mathcal{R}^3} \int_{\mathcal{S}^2} B(v,w,e) \Big[M(x,v')\, \tilde{f}_d(t,x,w') + M(x,w')\, \tilde{f}_d(t,x,v') - \\
&\qquad\qquad M(x,v)\, \tilde{f}_d(t,x,w) - M(x,w)\, f_d(t,x,v) \Big] de\, dw\,.
\end{aligned} \tag{3.37}
$$

3.2.2 General simulation procedure

Define (cf. (3.8), (3.24)–(3.26))

$$K^{(1)}_{\max}(x,v;y,w) = \tag{3.38}$$
$$\frac{4\,h(x,y)}{\|w-v\|}\int_{\Gamma(w-v)} \frac{b_{\max}\Big(\|w-v+u\|,\frac{2\,\|w-v\|^2}{\|w-v+u\|^2}-1\Big)}{\|w-v+u\|}\;M(x,v+u)\,du\,,$$

$$K^{(2)}_{\max}(x,v;y,w) = \tag{3.39}$$
$$\frac{4\,h(x,y)}{\|w-v\|}\int_{\Gamma(w-v)} \frac{b_{\max}\Big(\|w-v+u\|,1-\frac{2\,\|w-v\|^2}{\|w-v+u\|^2}\Big)}{\|w-v+u\|}\;M(x,v+u)\,du\,,$$

$$K^{(3)}_{\max}(x,v;y,w) = M(x,v)\,h(x,y)\int_{\mathcal{S}^2} B_{\max}(v,w,e)\,de\,. \tag{3.40}$$

The functions $K^{(k)}_{\max}$ are obtained in analogy with $K^{(k)}$ when replacing B by $B_{\max}$ and taking the absolute value ($k=3$). Note that (cf. (3.31))

$$E_{\max}(y,w) = \int_D\int_{\mathcal{R}^3} K^{(k)}_{\max}(x,v;y,w)\,dv\,dx\,,\qquad k=1,2,3\,.$$

Consider functions $s^{(k)}_{\max}$ such that (cf. (3.32))

$$|s^{(k)}| \le s^{(k)}_{\max}\,. \tag{3.41}$$

Assume

$$\int_\Theta |s^{(k)}(z,i,x,v,\theta)|\,A(z,x,v,d\theta) = |K^{(k)}(x,v;x_i,v_i)| \tag{3.42}$$

and

$$\int_\Theta s^{(k)}_{\max}(z,i,x,v,\theta)\,A(z,x,v,d\theta) = K^{(k)}_{\max}(x,v;x_i,v_i)\,, \tag{3.43}$$

for all $k=1,2,3$, $v\in\mathcal{R}^3$, z (cf. (3.3)) and $i=1,\ldots,N$. Introduce functions (cf. (3.34))

$$g_l(z,x,v,\theta) = \tag{3.44}$$
$$\sum_{i\in I_l(z)}\Big[s^{(1)}_{\max}(z,i,x,v,\theta)+s^{(2)}_{\max}(z,i,x,v,\theta)+s^{(3)}_{\max}(z,i,x,v,\theta)\Big],$$

satisfying (cf. (3.41))

$$|S_l(z,x,v,\theta)| \;\le\; g_l(z,x,v,\theta)\,,$$

and measures

$$\lambda_{0,l}(z,x,v,\theta,d\tilde{z}) = \qquad (3.45)$$
$$\delta_{J_{0,l}(z,x,v,\theta)}(d\tilde{z})\,\frac{|S_l(z,x,v,\theta)|}{g_l(z,x,v,\theta)} + \delta_z(d\tilde{z})\,\frac{g_l(z,x,v,\theta)-|S_l(z,x,v,\theta)|}{g_l(z,x,v,\theta)}\,.$$

Note that (cf. (3.35))

$$\sum_{l=1}^{L(z)}\int_D\int_{\mathcal{R}^3}\int_\Theta \Big[\Phi(J_{0,l}(z,x,v,\theta))-\Phi(z)\Big]\,|S_l(z,x,v,\theta)|\,A(z,x,v,d\theta)\,dv\,dx =$$
$$\sum_{l=1}^{L(z)}\int_D\int_{\mathcal{R}^3}\int_\Theta\Big(\int\Big[\Phi(\tilde{z})-\Phi(z)\Big]\,\lambda_{0,l}(z,x,v,\theta,d\tilde{z})\Big)\,g_l(z,x,v,\theta)\,\times$$
$$A(z,x,v,d\theta)\,dv\,dx$$
$$= \sum_{l=1}^{L(z)}\sum_{i\in I_l(z)}\sum_{k=1}^{3}\int_D\int_{\mathcal{R}^3}\int_\Theta\Big(\int\Big[\Phi(\tilde{z})-\Phi(z)\Big]\,\lambda_{0,l}(z,x,v,\theta,d\tilde{z})\Big)\,\times$$
$$s_{\max}^{(k)}(z,i,x,v,\theta)\,A(z,x,v,d\theta)\,dv\,dx$$
$$= \sum_{i=1}^{N}E_{\max}(x_i,v_i)\sum_{k=1}^{3}\int_D\int_{\mathcal{R}^3}\Big\{\int_\Theta\Big(\int\Big[\Phi(\tilde{z})-\Phi(z)\Big]\,\lambda_{0,l(i)}(z,x,v,\theta,d\tilde{z})\Big)\,\times$$
$$\frac{s_{\max}^{(k)}(z,i,x,v,\theta)}{K_{\max}^{(k)}(x,v;x_i,v_i)}\,A(z,x,v,d\theta)\Big\}\,\frac{K_{\max}^{(k)}(x,v;x_i,v_i)}{E_{\max}(x_i,v_i)}\,dv\,dx\,, \qquad (3.46)$$

where $l(i)$ is the index of the cluster to which i belongs. Consider functions $\hat{s}$ such that (cf. (3.30))

$$\int_{\mathcal{R}^3}\hat{s}(z,i,v)\,M(x_i,v)\,dv = E(x_i,v_i)\,. \qquad (3.47)$$

Introduce the measures

$$\lambda_1(z,i,v,d\tilde{z}) = \delta_{J_1(z,i)}(d\tilde{z})\,\frac{\hat{s}(z,i,v)}{\hat{s}_{\max}(z,i,v)} + \delta_z(d\tilde{z})\,\frac{\hat{s}_{\max}(z,i,v)-\hat{s}(z,i,v)}{\hat{s}_{\max}(z,i,v)}\,.$$

Note that (cf. (3.35))

$$\sum_{i=1}^{N}\Big[\Phi(J_1(z,i))-\Phi(z)\Big]E(x_i,v_i) = \qquad (3.48)$$
$$\sum_{i=1}^{N}E_{\max}(x_i,v_i)\int_{\mathcal{R}^3}\Big(\int\Big[\Phi(\tilde{z})-\Phi(z)\Big]\lambda_1(z,i,v,d\tilde{z})\Big)\,\frac{\hat{s}_{\max}(z,i,v)}{E_{\max}(x_i,v_i)}\,M(x_i,v)\,dv\,.$$

Using (3.46) and (3.48), rewrite the generator (3.35) in the form

$$\mathcal{A}\Phi(z) = \qquad (3.49)$$

$$\sum_{i=1}^{N} E_{\max}(x_i,v_i) \sum_{k=1}^{3} \int_D \int_{\mathcal{R}^3} \left\{ \int_\Theta \left(\int \left[\Phi(\tilde z) - \Phi(z)\right] \lambda_{0,l(i)}(z,x,v,\theta,d\tilde z) \right) \times \right.$$
$$\left. \frac{s^{(k)}_{\max}(z,i,x,v,\theta)}{K^{(k)}_{\max}(x,v;x_i,v_i)}\, A(z,x,v,d\theta) \right\} \frac{K^{(k)}_{\max}(x,v;x_i,v_i)}{E_{\max}(x_i,v_i)}\, dv\, dx \,+$$
$$\sum_{i=1}^{N} E_{\max}(x_i,v_i) \int_{\mathcal{R}^3} \left(\int \left[\Phi(\tilde z) - \Phi(z)\right] \lambda_1(z,i,v,d\tilde z) \right) \frac{\hat s_{\max}(z,i,v)}{E_{\max}(x_i,v_i)}\, M(x_i,v)\, dv\,.$$

The representation (3.49) suggests the following algorithm:

1. Make a time step with parameter (cf. (3.12))

$$\sigma_{\max}(z) = 4 \sum_{i=1}^{N} E_{\max}(x_i,v_i)\,. \tag{3.50}$$

Stop, when the final time is exceeded.

2. Choose an index $i = 1,\ldots,N$ according to the probabilities (cf. (3.13))

$$\frac{4}{\sigma_{\max}(z)}\, E_{\max}(x_i,v_i)\,. \tag{3.51}$$

3. With probabilities $1/4$, choose between creation ($k = 1,2,3$) and deletion (go to **5.1.**).

4.1. For given i and k, choose $x \in D$ and $v \in \mathcal{R}^3$ according to the density

$$\frac{1}{E_{\max}(x_i,v_i)}\, K^{(k)}_{\max}(x,v;x_i,v_i)\,. \tag{3.52}$$

4.2. For given i, k, x and v, choose θ according to the distribution

$$\frac{1}{K^{(k)}_{\max}(x,v;x_i,v_i)}\, s^{(k)}_{\max}(z,i,x,v,\theta)\, A(z,x,v,d\theta)\,. \tag{3.53}$$

4.3. With probability

$$1 - \frac{\left|\sum_{j\in I_{l(i)}(z)} \varepsilon_j \left[s^{(1)}(z,j,x,v,\theta) + s^{(2)}(z,j,x,v,\theta) + s^{(3)}(z,j,x,v,\theta)\right]\right|}{\sum_{j\in I_{l(i)}(z)} \left[s^{(1)}_{\max}(z,j,x,v,\theta) + s^{(2)}_{\max}(z,j,x,v,\theta) + s^{(3)}_{\max}(z,j,x,v,\theta)\right]}\,,$$

reject the creation event and go to **1.**

4.4. Add the particle with position x, velocity v and sign

$$\operatorname{sign}\left(\sum_{j\in I_{l(i)}(z)} \varepsilon_j \left[s^{(1)}(z,j,x,v,\theta) + s^{(2)}(z,j,x,v,\theta) + s^{(3)}(z,j,x,v,\theta)\right] \right)$$

to the system and go to **1.**

5.1. For given i , choose $v \in \mathcal{R}^3$ according to the density

$$\frac{1}{E_{\max}(x_i, v_i)} \, \hat{s}_{\max}(z, i, v) \, M(x_i, v) \, .$$

5.2. With probability

$$1 - \frac{\hat{s}(z, i, v)}{\hat{s}_{\max}(z, i, v)} \, ,$$

reject the deletion event and go to **1.**

5.3. Remove the particle $(\varepsilon_i, x_i, v_i)$ from the system and go to **1.**

3.2.3 The implicit method

Here we consider specific choices of the functions $s^{(k)}$, $s^{(k)}_{\max}$ and the probability measures A satisfying conditions (3.32) and (3.41)–(3.43).

Lemma 3.3 *Consider the parameter set*

$$\Theta = \Big\{ \theta = (\theta_1, \ldots, \theta_N) \, , \quad \theta_i \in \Gamma(v - v_i) \, , \quad i = 1, \ldots, N \Big\} \tag{3.54}$$

and the measures (cf. (2.11))

$$A(z, x, v, d\theta) = \frac{1}{n_M(x)} \int_{\mathcal{R}^3} \left[\prod_{i=1}^{N} \delta_{\pi_{v_i - v}(w)}(d\theta_i) \right] M(x, v + w) \, dw \, , \tag{3.55}$$

where (cf. Remark 6.7)

$$\pi_{v_i - v}(w) \in \Gamma(v_i - v)$$

is the projection of the velocity w . Consider functions $q^{(k)}$ and $q^{(k)}_{\max}$ such that

$$|q^{(k)}| \le q^{(k)}_{\max} \, , \tag{3.56}$$

$$\frac{1}{n_M(x)} \int_{\mathcal{R}^3} q^{(k)}(x, v, y, w, \pi_{w-v}(c)) \, M(x, v + c) \, dc = K^{(k)}(x, v; y, w) \tag{3.57}$$

$$\frac{1}{n_M(x)} \int_{\mathcal{R}^3} |q^{(k)}(x, v, y, w, \pi_{w-v}(c))| \, M(x, v + c) \, dc = |K^{(k)}(x, v; y, w)| \tag{3.58}$$

and

$$\frac{1}{n_M(x)} \int_{\mathcal{R}^3} q^{(k)}_{\max}(x, v, y, w, \pi_{w-v}(c)) \, M(x, v + c) \, dc = K^{(k)}_{\max}(x, v; y, w) \, . \tag{3.59}$$

Then the functions

$$s^{(k)}(z,i,x,v,\theta) = q^{(k)}(x,v,x_i,v_i,\theta_i)$$

and

$$s^{(k)}_{\max}(z,i,x,v,\theta) = q^{(k)}_{\max}(x,v,x_i,v_i,\theta_i)$$

satisfy conditions (3.32) and (3.41)–(3.43).

Proof. The definitions imply, e.g.,

$$\begin{aligned}\int_\Theta s^{(k)}(z,i,x,v,\theta)\,A(z,x,v,d\theta) = \\ &\int_\Theta q^{(k)}(x,v,x_i,v_i,\theta_i)\,A(z,x,v,d\theta) \\ = &\frac{1}{n_M(x)}\int_{\mathcal{R}^3} q^{(k)}(x,v,x_i,v_i,\pi_{v_i-v}(w))\,M(x,v+w)\,dw\end{aligned}$$

so that the assertion follows from assumptions (3.56)–(3.59). ■

Lemma 3.4 *The functions*

$$q^{(1)}(x,v,y,w,u) = \\ \frac{4\,h(x,y)}{\|w-v\|}\left[\int_{\Gamma(w-v)} M(x,v+c)\,dc\right]\frac{b\left(\|w-v+u\|,\frac{2\,\|w-v\|^2}{\|w-v+u\|^2}-1\right)}{\|w-v+u\|}, \tag{3.60}$$

$$q^{(1)}_{\max}(x,v,y,w,u) = \\ \frac{4\,h(x,y)}{\|w-v\|}\left[\int_{\Gamma(w-v)} M(x,v+c)\,dc\right]\frac{b_{\max}\left(\|w-v+u\|,\frac{2\,\|w-v\|^2}{\|w-v+u\|^2}-1\right)}{\|w-v+u\|}, \tag{3.61}$$

$$q^{(2)}(x,v,y,w,u) = \\ \frac{4\,h(x,y)}{\|w-v\|}\left[\int_{\Gamma(w-v)} M(x,v+c)\,dc\right]\frac{b\left(\|w-v+u\|,1-\frac{2\,\|w-v\|^2}{\|w-v+u\|^2}\right)}{\|w-v+u\|}, \tag{3.62}$$

and

$$q^{(2)}_{\max}(x,v,y,w,u) = \\ \frac{4\,h(x,y)}{\|w-v\|}\left[\int_{\Gamma(w-v)} M(x,v+c)\,dc\right]\frac{b_{\max}\left(\|w-v+u\|,1-\frac{2\,\|w-v\|^2}{\|w-v+u\|^2}\right)}{\|w-v+u\|} \tag{3.63}$$

satisfy conditions (3.56)–(3.59).

Proof. Condition (3.56) is obviously fulfilled. Applying Lemma 6.8 with

$$\varphi(u) = 1\,, \qquad \psi(v,a) = \frac{b\left(a, \frac{2\,\|v\|^2}{a^2} - 1\right)}{a}\,,$$

one obtains

$$\int_{\Gamma(v)} \frac{b\left(\|v+u\|, \frac{2\,\|v\|^2}{\|v+u\|^2} - 1\right)}{\|v+u\|}\, M_{V,T}(u)\, du = \tag{3.64}$$
$$\left[\int_{\Gamma(v)} M_{V,T}(c)\, dc\right] \int_{\mathcal{R}^3} \frac{b\left(\|v+\pi_v(w)\|, \frac{2\,\|v\|^2}{\|v+\pi_v(w)\|^2} - 1\right)}{\|v+\pi_v(w)\|}\, M_{V,T}(w)\, dw\,.$$

When replacing $v \to w - v$ and $V \to u_M - v$, equation (3.64) implies (cf. (3.24))

$$K^{(1)}(x,v;y,w) = \frac{4\,h(x,y)}{n_M(x)\,\|w-v\|} \left[\int_{\Gamma(w-v)} M(x,v+c)\, dc\right] \times$$
$$\int_{\mathcal{R}^3} \frac{b\left(\|w-v+\pi_{w-v}(w)\|, \frac{2\,\|w-v\|^2}{\|w-v+\pi_{w-v}(w)\|^2} - 1\right)}{\|w-v+\pi_{w-v}(w)\|}\, M(x,v+w)\, dw\,.$$

Thus, conditions (3.57) and (3.58) are fulfilled for $k = 1$. Condition (3.59) follows when b is replaced by $b_{\max}$. The case $k = 2$ is treated analogously. ■

Remark 3.5 *The functions*

$$s^{(k)}(z,i,x,v,\theta) = K^{(k)}(x,v;x_i,v_i)\,, \qquad s^{(k)}_{\max}(z,i,x,v,\theta) = K^{(k)}_{\max}(x,v;x_i,v_i)$$

satisfy conditions (3.32) and (3.41)–(3.43) for any choice of the probability measures A *.*

Remark 3.6 *A position* x *and a velocity* v *with density (3.52) are obtained according to (3.27). The position is generated uniformly in the cell to which* x_i *belongs. The velocity is generated according to (3.14) in the case* $k = 3$ *and as*

$$v = v'(v_i,w,e) \quad (k=1) \qquad \text{or} \qquad v = w'(v_i,w,e) \quad (k=2)\,,$$

where w, e *are chosen according to (3.14), (3.15).*

Remark 3.7 *For* $k = 1, 2$ *, the distribution (3.53) of the auxiliary parameter* θ *takes the form*

$$\frac{1}{K^{(k)}_{\max}(x,v;x_i,v_i)}\, q^{(k)}_{\max}(x,v,x_i,v_i,\theta_i) \int_{\mathcal{R}^3} \left[\prod_{j=1}^{N} \delta_{\pi_{v_j-v}(w)}(d\theta_j)\right] \frac{M(x,v+w)}{n_M(x)}\, dw =$$
$$\frac{1}{K^{(k)}_{\max}(x,v;x_i,v_i)} \int_{\mathcal{R}^3} q^{(k)}_{\max}(x,v,x_i,v_i,\pi_{v_i-v}(w)) \times$$
$$\left[\frac{q^{(k)}_{\max}(x,v,x_i,v_i,\theta_i)}{q^{(k)}_{\max}(x,v,x_i,v_i,\pi_{v_i-v}(w))} \prod_{j=1}^{N} \delta_{\pi_{v_j-v}(w)}(d\theta_j)\right] \frac{M(x,v+w)}{n_M(x)}\, dw\,.$$

We choose A, $s^{(k)}$ and $s^{(k)}_{\max}$ according to Lemmas 3.3, 3.4 ($k=1,2$) and Remark 3.5 ($k=3$), and (cf. (3.47), (3.10))

$$\hat{s}(z,i,v)=\int_{\mathcal{S}^2} B(v,v_i,e)\,de\,,\qquad \hat{s}_{\max}(z,i,v)=\int_{\mathcal{S}^2} B_{\max}(v,v_i,e)\,de\,. \tag{3.65}$$

The following algorithm is obtained:

Algorithm 3.8 (Implicit method)

1. *Make a time step with parameter (3.50). Stop, when the final time is exceeded.*

2. *Choose an index* $i=1,\ldots,N$ *according to the probabilities (3.51).*

3. *With probabilities* $1/4$, *choose between creation* ($k=1,2,3$) *and deletion (go to* **5.1.**).

4.1. *For given* i, *construct a position* $x\in D$ *and a velocity* $v\in\mathcal{R}^3$.

4.1.1. *Generate* x *uniformly in the cell to which* x_i *belongs.*

4.1.2. *Generate* $w\in\mathcal{R}^3$ *according to the density (cf. Remark 3.6)*

$$\frac{1}{E_{\max}(x_i,v_i)}\left(\int_{\mathcal{S}^2} B_{\max}(v_i,w,e)\,de\right)M(x_i,w)\,. \tag{3.66}$$

4.1.3. *If* $k=3$, *then choose* $v=w$ *and go to* **4.2.1.**

4.1.4. *For given* w, *generate* e *according to the density (cf. Remark 3.6)*

$$\frac{B_{\max}(v_i,w,e)}{\int_{\mathcal{S}^2} B_{\max}(v_i,w,u)\,du}\,. \tag{3.67}$$

4.1.5. *If* $k=1$, *then calculate* $v=v'(v_i,w,e)$ *and go to* **4.2.2.**

4.1.6. *Calculate* $v=w'(v_i,w,e)$ *and go to* **4.2.2.**

4.2. *For given* i, x *and* v, *construct an auxiliary parameter* θ.

4.2.1. *Generate* $\tilde{w}\in\mathcal{R}^3$ *according to the density*

$$\frac{1}{n_M(x)}\,M(x,v+\tilde{w}) \tag{3.68}$$

and go to **4.2.3.**

4.2.2. *Generate* $\tilde{w}\in\mathcal{R}^3$ *according to the density (cf. Remark 3.7)*

$$\frac{1}{K^{(k)}_{\max}(x,v;x_i,v_i)}\,q^{(k)}_{\max}(x,v,x_i,v_i,\pi_{v_i-v}(\tilde{w}))\,\frac{M(x,v+\tilde{w})}{n_M(x)}\,. \tag{3.69}$$

4.2.3. *Compute*

$$\theta_j = \pi_{v_j - v}(\tilde{w}) \,, \qquad j \in I_{l(i)}(z) \,.$$

4.3. *With probability*

$$1 - \frac{\left| \sum_{j \in I_{l(i)}(z)} \varepsilon_j \left[q^{(1)}(x,v,x_j,v_j,\theta_j) + q^{(2)}(x,v,x_j,v_j,\theta_j) + K^{(3)}(x,v;x_j,v_j) \right] \right|}{\sum_{j \in I_{l(i)}(z)} \left[q^{(1)}_{\max}(x,v,x_j,v_j,\theta_j) + q^{(2)}_{\max}(x,v,x_j,v_j,\theta_j) + K^{(3)}_{\max}(x,v;x_j,v_j) \right]} \,, \tag{3.70}$$

reject the creation event and go to **1.**

4.4. *Add the particle with position* x , *velocity* v *and sign*

$$\mathrm{sign} \left(\sum_{j \in I_{l(i)}(z)} \varepsilon_j \left[q^{(1)}(x,v,x_j,v_j,\theta_j) + q^{(2)}(x,v,x_j,v_j,\theta_j) + K^{(3)}(x,v;x_j,v_j) \right] \right) \tag{3.71}$$

to the system and go to **1.**

5.1. *For given* i , *choose* $v \in \mathcal{R}^3$ *according to the density (3.66).*

5.2. *With probability*

$$1 - \frac{\int_{\mathcal{S}^2} B(v_i,v,e)\, de}{\int_{\mathcal{S}^2} B_{\max}(v_i,v,e)\, de} \,,$$

reject the deletion event and go to **1.**

5.3. *Remove the particle* $(\varepsilon_i, x_i, v_i)$ *from the system and go to* **1.**

3.2.4 Variable hard sphere model

In the case (3.2) one obtains from (3.26), (3.60), (3.62)

$$K^{(3)}(x,v;y,w) = -4\,\pi\, C_\beta\, h(x,y)\, M(x,v)\, \|v-w\|^\beta \,, \tag{3.72}$$

$$q^{(k)}(x,v,y,w,u) = \frac{4\, C_\beta\, h(x,y)}{\|w-v\|} \left(\int_{\Gamma(w-v)} M(x,v+c)\, dc \right) \|w-v+u\|^{\beta-1} \tag{3.73}$$

and from (3.38)-(3.40), (3.61), (3.63) (with (3.17))

$$K^{(k)}_{\max}(x,v;y,w) = \frac{4\, h(x,y)}{\|w-v\|} \times \tag{3.74}$$
$$\left(c_0 \int_{\Gamma(w-v)} \frac{1}{\|w-v+u\|}\; M(x,v+u)\, du + c_1 \int_{\Gamma(w-v)} M(x,v+u)\, du \right),$$

$$K^{(3)}_{\max}(x,v;y,w) = 4\,\pi\,h(x,y)\,M(x,v)\Big(c_0 + c_1\,\|v-w\|\Big)\,, \tag{3.75}$$

$$q^{(k)}_{\max}(x,v,y,w,u) = \tag{3.76}$$
$$\frac{4\,h(x,y)}{\|w-v\|}\left(\int_{\Gamma(w-v)} M(x,v+c)\,dc\right)\left(\frac{c_0}{\|w-v+u\|}+c_1\right),$$

for $k=1,2$.

Remark 3.9 *Due to (3.74) (cf. (3.28), (3.29)), step 4.1 of Algorithm 3.8 simplifies.*

Remark 3.10 *The density (3.69) takes the form (cf. (3.74), (3.76))*

$$\frac{\left(\int_{\Gamma(v_i-v)} M(x,v+u)\,du\right)\left(\frac{c_0}{\|v_i-v+\pi_{v_i-v}(\tilde w)\|}+c_1\right)\frac{1}{n_M(x)}\,M(x,v+\tilde w)}{c_0\int_{\Gamma(v_i-v)}\frac{1}{\|v_i-v+u\|}\,M(x,v+u)\,du + c_1\int_{\Gamma(v_i-v)} M(x,v+u)\,du}\,. \tag{3.77}$$

If $u\perp v_i-v$, then $\|v_i-v+u\|\ge\|v_i-v\|$ and

$$\frac{1}{\|v_i-v+u\|}\le\frac{1}{\|v_i-v\|}\,. \tag{3.78}$$

In accordance with (3.78), the density (3.77) can be generated using the acceptance-rejection technique with the majorant function

$$\frac{\left(\int_{\Gamma(v_i-v)} M(x,v+u)\,du\right)\left(\frac{c_0}{\|v_i-v\|}+c_1\right)\frac{1}{n_M(x)}\,M(x,v+\tilde w)}{c_0\int_{\Gamma(v_i-v)}\frac{1}{\|v_i-v+u\|}\,M(x,v+u)\,du + c_1\int_{\Gamma(v_i-v)} M(x,v+u)\,du}\,.$$

The implicit method (Algorithm 3.8) takes the form:

Algorithm 3.11 (Variable hard sphere model)

1. *Make a time step with parameter (cf. (3.19))*

$$\sigma_{\max}(z) = 16\,\pi\left(c_0\sum_{i=1}^N n_M(x_i) + c_1\sum_{i=1}^N\int_{\mathcal{R}^3}\|v_i-w\|\,M(x_i,w)\,dw\right).$$

Stop, when the final time is exceeded.

2. *Choose an index $i=1,\dots,N$ according to the probabilities*

$$\frac{16\,\pi}{\sigma_{\max}(z)}\left(c_0\,n_M(x_i) + c_1\int_{\mathcal{R}^3}\|v_i-w\|\,M(x_i,w)\,dw\right).$$

3. *With probabilities $1/4$, choose between creation ($k=1,2,3$) and deletion (go to* **5.1.***).*

4.1. *For given i, construct a position $x \in D$ and a velocity $v \in \mathcal{R}^3$.*

4.1.1. *Generate x uniformly in the cell to which x_i belongs.*

4.1.2. *Generate $w \in \mathcal{R}^3$ according to the density (cf. (3.17))*

$$\frac{4\,\pi}{E_{\max}(x_i,v_i)}\Big(c_0 + c_1\,\|v_i - w\|\Big)M(x_i,w)\,. \tag{3.79}$$

4.1.3. *If $k = 3$, then choose $v = w$ and go to* **4.2.1.**

4.1.4. *Generate $e \in \mathcal{S}^2$ uniformly, calculate $v = v'(v_i, w, e)$ and go to* **4.2.2.**

4.2. *For given i, x and v, construct an auxiliary parameter θ.*

4.2.1. *Generate $\tilde{w} \in \mathcal{R}^3$ according to the density $M(x_i, v+\tilde{w})/n_M(x_i)$ and go to* **4.2.4.**

4.2.2. *Generate $\tilde{w} \in \mathcal{R}^3$ according to the density $M(x_i, v+\tilde{w})/n_M(x_i)$.*

4.2.3. *With probability (cf. Remark 3.10)*

$$1 - \frac{\frac{c_0}{\|v_i - v + \pi_{v_i - v}(\tilde{w})\|} + c_1}{\frac{c_0}{\|v_i - v\|} + c_1}\,,$$

go to **4.2.2.**

4.2.4. *Compute $\theta_j = \pi_{v_j - v}(\tilde{w})$, $j \in I_{l(i)}(z)$.*

4.3. *With probability (3.70), reject the creation event and go to* **1.**

4.4. *Add the particle with position x, velocity v and sign (3.71) to the system and go to* **1.**

5.1. *For given i, choose $w \in \mathcal{R}^3$ according to the density (3.79).*

5.2. *With probability*

$$1 - \frac{C_\beta\,\|v_i - w\|^\beta}{c_0 + c_1\,\|v_i - w\|}\,,$$

reject the deletion event and go to **1.**

5.3. *Remove the particle $(\varepsilon_i, x_i, v_i)$ from the system and go to* **1.**

In the case $\beta = 0$ (with $c_0 = C_0$ and $c_1 = 0$), Algorithm 3.11 takes the form:

Algorithm 3.12 (Pseudo-Maxwell molecules)

1. *Make a time step with parameter*

$$16\,\pi\,C_0\sum_{i=1}^{N} n_M(x_i)\,.$$

Stop, when the final time is exceeded.

2. *Choose an index* $i=1,\dots,N$ *according to the probabilities (3.20).*

3. *With probabilities* $1/4$ *, choose between creation (*$k=1,2,3$*) and deletion (go to* **5.***).*

4.1. *For given* i *, construct a position* $x\in D$ *and a velocity* $v\in\mathcal{R}^3$ *.*

4.1.1. *Generate* x *uniformly in the cell to which* x_i *belongs.*

4.1.2. *Generate* $w\in\mathcal{R}^3$ *according to the density* $M(x_i,w)/n_M(x_i)$ *.*

4.1.3. *If* $k=3$ *, then choose* $v=w$ *and go to* **4.2.1.**

4.1.4. *Generate* $e\in\mathcal{S}^2$ *uniformly, calculate* $v=v'(v_i,w,e)$ *and go to* **4.2.2.**

4.2. *For given* $i\,,x$ *and* v *, construct an auxiliary parameter* θ *.*

4.2.1. *Generate* $\tilde{w}\in\mathcal{R}^3$ *according to the density* $M(x_i,v+\tilde{w})/n_M(x_i)$ *and go to* **4.2.4.**

4.2.2. *Generate* $\tilde{w}\in\mathcal{R}^3$ *according to the density* $M(x_i,v+\tilde{w})/n_M(x_i)$ *.*

4.2.3. *With probability*

$$1-\frac{\|v_i-v\|}{\|v_i-v+\pi_{v_i-v}(\tilde{w})\|}\,,$$

go to **4.2.2.**

4.2.4. *Compute* $\theta_j=\pi_{v_j-v}(\tilde{w})\,,\;j\in I_{l(i)}(z)$ *.*

4.3. *With probability (cf. (3.72), (3.73), (3.75), (3.76))*

$$1-\frac{\left|\sum_{j\in I_{l(i)}(z)}\varepsilon_j\,h(x,x_j)\left[\frac{2}{\|v_j-v\|\,\|v_j-v+\theta_j\|}\left(\int_{\Gamma(v_j-v)}M(x,v+u)\,du\right)-\pi\,M(x,v)\right]\right|}{\sum_{j\in I_{l(i)}(z)}h(x,x_j)\left[\frac{2}{\|v_j-v\|\,\|v_j-v+\theta_j\|}\left(\int_{\Gamma(v_j-v)}M(x,v+u)\,du\right)+\pi\,M(x,v)\right]}\,, \tag{3.80}$$

reject the creation event and go to **1.**

4.4. *Add the particle with position* x , *velocity* v *and sign*

$$\mathrm{sign}\left(\sum_{j\in I_{l(i)}(z)} \varepsilon_j\, h(x,x_j)\times \right. \tag{3.81}$$

$$\left. \left[\frac{2}{\|v_j-v\|\,\|v_j-v+\theta_j\|}\left(\int_{\Gamma(v_j-v)} M(x,v+u)\,du\right)-\pi\,M(x,v)\right]\right)$$

to the system and go to **1.**

5. *Remove the particle* $(\varepsilon_i, x_i, v_i)$ *from the system and go to* **1.**

In the case $\beta = 1$ (with $c_0 = 0$ and $c_1 = C_1$), Algorithm 3.11 takes the form:

Algorithm 3.13 (Hard sphere model)

1. *Make a time step with parameter*

$$16\,\pi\,C_1 \sum_{i=1}^{N} \int_{\mathcal{R}^3} \|v_i - w\|\, M(x_i,w)\,dw\,. \tag{3.82}$$

Stop, when the final time is exceeded.

2. *Choose an index* $i = 1,\ldots,N$ *according to the probabilities*

$$\frac{1}{\sum_{j=1}^{N}\int_{\mathcal{R}^3}\|v_j-w\|\,M(x_j,w)\,dw}\int_{\mathcal{R}^3}\|v_i-w\|\,M(x_i,w)\,dw\,. \tag{3.83}$$

3. *With probabilities* $1/4$, *choose between creation (*$k = 1,2,3$*) and deletion (go to* **5.***).*

4.1. *For given* i , *construct a position* $x \in D$ *and a velocity* $v \in \mathcal{R}^3$.

4.1.1. *Generate* x *uniformly in the cell to which* x_i *belongs.*

4.1.2. *Generate* $w \in \mathcal{R}^3$ *according to the density*

$$\frac{1}{\int_{\mathcal{R}^3}\|v_i-u\|\,M(x_i,u)\,du}\,\|v_i-w\|\,M(x_i,w)\,. \tag{3.84}$$

4.1.3. *If* $k = 3$, *then choose* $v = w$ *and go to* **4.3.**

4.1.4. *Generate* $e \in \mathcal{S}^2$ *uniformly and calculate* $v = v'(v_i,w,e)$.

4.2. *This step is redundant.*

4.3. *With probability (cf. (3.72), (3.73), (3.75), (3.76))*

$$1-\frac{\left|\sum_{j\in I_{l(i)}(z)}\varepsilon_j\,h(x,x_j)\left[\frac{2}{\|v_j-v\|}\left(\int_{\Gamma(v_j-v)}M(x,v+u)\,du\right)-\pi\,M(x,v)\,\|v-v_j\|\right]\right|}{\sum_{j\in I_{l(i)}(z)}h(x,x_j)\left[\frac{2}{\|v_j-v\|}\left(\int_{\Gamma(v_j-v)}M(x,v+u)\,du\right)+\pi\,M(x,v)\,\|v-v_j\|\right]}\,, \tag{3.85}$$

reject the creation event and go to **1.**

4.4. *Add the particle with position x, velocity v and sign*

$$\operatorname{sign}\left(\sum_{j\in I_{l(i)}(z)}\varepsilon_j\,h(x,x_j)\times \left[\frac{2}{\|v_j-v\|}\left(\int_{\Gamma(v_j-v)}M(x,v+u)\,du\right)-\pi\,M(x,v)\,\|v-v_j\|\right]\right) \tag{3.86}$$

to the system and go to **1.**

5. *Remove the particle (ε_i,x_i,v_i) from the system and go to* **1.**

3.3 Implementation issues

3.3.1 Generating distributions

waiting time parameter

The integrals in (3.21) and (3.82) are explicitly known so that the sums can easily be updated after each jump. Indeed, Lemma 6.6 with (cf. (2.11), (2.12))

$$V=V(x,v)=u_M(x)-v\,,\qquad T=T(x)=\frac{k\,T_M(x)}{m} \tag{3.87}$$

implies

$$\int_{\mathcal{R}^3}\|w-v\|\,M(x,w)\,dw= n_M(x)\sqrt{\frac{2\,T(x)}{\pi}}\left[\exp\left(-U^2\right)+\left(\frac{1}{U}+2\,U\right)\frac{\sqrt{\pi}}{2}\,\mathrm{erf}(U)\right], \tag{3.88}$$

where

$$U=U(x,v)=\frac{\|u_M(x)-v\|}{\sqrt{2\,T(x)}}$$

and

$$\mathrm{erf}(s)=\frac{2}{\sqrt{\pi}}\int_0^s\exp\left(-r^2\right)dr\,,\qquad s\ge 0\,. \tag{3.89}$$

index distribution

The generation of the probabilities (3.22) and (3.83) is performed using the acceptance-rejection technique. Since

$$\|w - v\|\, M(x,w) \le \|w - u_M(x)\|\, M(x,w) + \|u_M(x) - v\|\, M(x,w) \tag{3.90}$$

and (cf. (2.11) and (3.88))

$$\int_{\mathcal{R}^3} \Big[\|w - u_M(x)\|\, M(x,w) + \|u_M(x) - v\|\, M(x,w)\Big] dw = \\ n_M(x)\left[2\sqrt{2\,T(x)/\pi} + \|u_M(x) - v\|\right], \tag{3.91}$$

one obtains

$$\int_{\mathcal{R}^3} \|w - v_i\|\, M(x_i,w)\, dw \;\le\; n_M(x_i)\left[c_{\mathrm{rel}}(z,m(i)) + 2\sqrt{2\,T(x_i)/\pi}\right], \tag{3.92}$$

where $m(i)$ is the index of the cell to which particle i belongs, and

$$c_{\mathrm{rel}}(z,m) = \max_{i:\, x_i\in D_m} \|v_i - u_M(x_i)\|\,, \qquad m = 1,\ldots,l_c\,. \tag{3.93}$$

Thus, a cell index is generated according to the probabilities

$$\frac{\sum_{i:\, x_i\in D_m} n_M(x_i)\left[c_{\mathrm{rel}}(z,m(i)) + 2\sqrt{2\,T(x_i)/\pi}\right]}{\sum_{i=1}^{N} n_M(x_i)\left[c_{\mathrm{rel}}(z,m(i)) + 2\sqrt{2\,T(x_i)/\pi}\right]}\,, \qquad m = 1,\ldots,l_c\,.$$

Inside the cell, the index i is chosen uniformly and accepted with probability (cf. (3.88))

$$\frac{\sqrt{2\,T(x_i)/\pi}\left[\exp\left(-U(x_i,v_i)^2\right) + \left(\frac{1}{U(x_i,v_i)} + 2\,U(x_i,v_i)\right)\frac{\sqrt{\pi}}{2}\,\mathrm{erf}(U(x_i,v_i))\right]}{c_{\mathrm{rel}}(z,m(i)) + 2\sqrt{2\,T(x_i)/\pi}}\,.$$

Remark 3.14 *There are many alternatives, when applying the acceptance-rejection technique. Instead of the right-hand side of (3.92), one may use a uniform majorant over all cells. Instead of (3.93), one may also use shells in the velocity space (cf. [16]) in order to obtain a more precise majorant.*

velocity distribution

The generation of the densities (3.23) and (3.84) is performed using the acceptance-rejection technique with the majorant (3.90). The velocity w is generated according to the density

$$\frac{\|w - u_M(x_i)\|\, M(x_i,w)}{2\,n_M(x_i)\,\sqrt{2\,T(x_i)/\pi}}\,, \tag{3.94}$$

with probability (cf. (3.91))

$$\frac{2}{2+\sqrt{\pi}\,U(x_i,v_i)}\,,$$

and according to the density $M(x_i,w)/n_M(x_i)$, with the remaining probability. It is accepted with probability (cf. (3.90))

$$\frac{\|w-v_i\|}{\|w-u_M(x_i)\|+\|u_M(x_i)-v_i\|}\,.$$

Remark 3.15 *The acceptance rate in dependence on x_i, v_i takes the form (cf. (3.88), (3.91))*

$$\frac{\left[2\,U(x_i,v_i)+\frac{1}{U(x_i,v_i)}\right]\frac{\sqrt{\pi}}{2}\,\mathrm{erf}\,(U(x_i,v_i))+\exp\,(-U(x_i,v_i)^2)}{2+\sqrt{\pi}\,U(x_i,v_i)}\,. \tag{3.95}$$

Expression (3.95) equals 1 at $U=0$ and $U\to\infty$. It has a minimum of about 0.7 for U between 1 and 2. Thus, (3.90) seems to provide a rather efficient majorant.

rejection probability and sign

The expressions (3.80), (3.81), (3.85), (3.86) are explicitly known, due to the formula

$$\int_{\Gamma(w-v)} M(x,v+y)\,dy=\frac{n_M(x)}{\sqrt{\pi}\,c_M(x)}\,\exp\left(-\frac{(u_M(x)-v,w-v)^2}{c_M(x)^2\,\|w-v\|^2}\right), \tag{3.96}$$

which follows from Lemma 6.8.

3.3.2 Comments on the implicit method

The implicit method (Algorithm 3.8) is ready for implementation provided that the collision kernel B and its majorant kernel $B_{\max}$ are such that the integrals (cf. (3.65))

$$\int_{\mathcal{S}^2} B(v,w,e)\,de \qquad \text{and} \qquad \int_{\mathcal{S}^2} B_{\max}(v,w,e)\,de \tag{3.97}$$

as well as the quantity $E_{\max}$ (cf. (3.11)) are explicitly known (and finite). All necessary distributions (3.51), (3.66)–(3.69) can be generated directly or by appropriate acceptance-rejection techniques. There are some specific parameters involved in the method. Namely, rather general functions $B_{\max}$, $q^{(k)}$ and $q^{(k)}_{\max}$ are used instead of the simple choices

$$B_{\max}=B\,,\qquad q^{(k)}=K^{(k)}\,,\qquad q^{(k)}_{\max}=|K^{(k)}|\,. \tag{3.98}$$

The following comments are to illustrate the utility of these parameters.

When choosing the parameters as in (3.98), explicit knowledge of the quantity E is necessary for performing Steps 1 (waiting time) and 2 (choice of the index) of the implicit method. Explicit knowledge of $K^{(k)}$ is needed for calculating both the acceptance probability (3.70) and the signs (3.71) of the new particles (Steps 4.3 and 4.4).

The implicit method does not assume that the integrals in the representations (3.24), (3.25) of the functions $K^{(k)}$ can be calculated analytically. Neither it assumes explicit knowledge of the quantity E defined in (3.10). This becomes essential even in the study of the variable hard sphere model. In this special case one obtains

$$K^{(k)}(x,v;y,w) = \frac{4\,C_\beta\,h(x,y)}{\|w-v\|}\int_{\Gamma(w-v)} \|w-v+u\|^{\beta-1}\; M(x,v+u)\,du\,, \quad k=1,2\,,$$

and

$$E(x,v) = 4\,\pi\,C_\beta \int_{\mathcal{R}^3} \|v-w\|^{\beta}\, M(x,w)\,dw\,.$$

These expressions do not seem to be analytically tractable in general, when $\beta \in (0,1)$.

If the function E is explicitly known, then one can choose $B_{\max} = B$. It follows that

$$E_{\max} = E\,, \qquad K^{(k)}_{\max} = |K^{(k)}|\,, \qquad q^{(k)}_{\max}(x,v,y,w,u) = |q^{(k)}(x,v,y,w,u)|\,,$$

and several steps of the algorithm simplify. We call the corresponding algorithm the "semi-implicit method". An example is Algorithm 3.12 for pseudo-Maxwell molecules.

If the functions $K^{(k)}$ as well as the quantity E are explicitly known, then one can make the choice (3.98). The behavior of the process does not depend on θ so that the generation of θ becomes redundant. We call the corresponding algorithm the "explicit method". An example is Algorithm 3.13 for the hard-sphere model.

Remark 3.16 *If the first integral in (3.97) is not explicitly known, then one can introduce an additional parameter $e \in \mathcal{S}^2$ and consider*

$$A(z,x,v,d\theta) = \frac{1}{n_M(x)}\int_{\mathcal{R}^3}\left[\prod_{i=1}^{N} \delta_{\pi_{v_i-v(w)}}(d\theta_i) \times p(e)\,de\right] M(x,v+w)\,dw\,,$$

where p is a strictly positive probability density on $\mathcal{S}^2$, and (cf. (3.26))

$$s^{(3)}(z,i,x,v,\theta) = -M(x,v)\,\frac{B(v,v_i,e)}{p(e)}\,.$$

3.3.3 Clustering and cancellation effect

Here we discuss the choice of the partition $\{I_l(z)\}$ (cf. (3.33)). These index clusters are involved in Steps 4.3 and 4.4 of the implicit method (Algorithm 3.8). On the one hand, they influence the cancellation effect via the rejection probability (3.70). The acceptance rate for handling the source term (creating particles) is (cf. (3.46))

$$\frac{\sum_{l=1}^{L(z)} \int_D \int_{\mathcal{R}^3} \int_\Theta |S_l(z,x,v,\theta)|\, A(z,x,v,d\theta)\, dv\, dx}{\sum_{l=1}^{L(z)} \int_D \int_{\mathcal{R}^3} \int_\Theta g_l(z,x,v,\theta)\, A(z,x,v,d\theta)\, dv\, dx}\,, \tag{3.99}$$

where (cf. (3.34))

$$S_l(z,x,v,\theta) = \sum_{i \in I_l(z)} \varepsilon_i \left[q^{(1)}(x,v,x_i,v_i,\theta_i) + q^{(2)}(x,v,x_i,v_i,\theta_i) + K^{(3)}(x,v;x_i,v_i) \right] \tag{3.100}$$

and (cf. (3.44))

$$g_l(z,x,v,\theta) = \sum_{i \in I_l(z)} \left[q^{(1)}_{\max}(x,v,x_i,v_i,\theta_i) + q^{(2)}_{\max}(x,v,x_i,v_i,\theta_i) + K^{(3)}_{\max}(x,v;x_i,v_i) \right]. \tag{3.101}$$

Note that the denominator in formula (3.99) does not depend on the choice of the clusters, since

$$\sum_{l=1}^{L(z)} \int_D \int_{\mathcal{R}^3} \int_\Theta g_l(z,x,v,\theta)\, A(z,x,v,d\theta)\, dv\, dx = \sum_{i=1}^{N} \int_D \int_{\mathcal{R}^3} \int_\Theta \left[q^{(1)}_{\max}(x,v,x_i,v_i,\theta_i) + q^{(2)}_{\max}(x,v,x_i,v_i,\theta_i) + K^{(3)}_{\max}(x,v;x_i,v_i) \right].$$

When positive and negative terms in expression (3.100) cancel each other, the probability of rejection becomes bigger so that less particles are created. On the other hand, big clusters reduce the efficiency of the method, due to the summations involved in formulas (3.100) and (3.101). Thus, it is important to avoid frequent summations over big subsystems.

The following two extremal choices illustrate the problem.

Example 3.17 (one cluster) *If there is only one cluster*

$$I_1(z) = \{1, \ldots, N\}\,,$$

then the nominator in formula (3.99) takes the form

$$\int_D \int_{\mathcal{R}^3} \int_\Theta \left| \sum_{i=1}^{N} \varepsilon_i \left[q^{(1)}(x,v,x_i,v_i,\theta_i) + q^{(2)}(x,v,x_i,v_i,\theta_i) + K^{(3)}(x,v;x_i,v_i) \right] \right| \times A(z,x,v,d\theta)\, dv\, dx\,.$$

This expression is the smallest over all choices of cluster systems. Thus, the cancellation effect is the strongest (less particles are created), but the effort for each particle significantly increases.

Example 3.18 (single particle clusters) *In the case of single particle clusters,*

$$I_l(z) = \{l\}\,, \qquad l = 1, \ldots, L(z) = N\,,$$

the nominator in formula (3.99) takes the form

$$\sum_{i=1}^{N} \int_D \int_{\mathcal{R}^3} \int_\Theta \left| q^{(1)}(x,v,x_i,v_i,\theta_i) + q^{(2)}(x,v,x_i,v_i,\theta_i) + K^{(3)}(x,v;x_i,v_i) \right| \times \\ A(z,x,v,d\theta)\, dv\, dx\,.$$

This expression is the biggest over all choices of cluster systems. Still there is some cancellation due to sign change of $q^{(1)}, q^{(2)}$ (positive) and $K^{(3)}$ (negative).

There is considerable freedom in choosing the clusters. It is possible that they depend on the state of the process, or on the Maxwellian. The clusters can be changed at the beginning of each collision time step.

In order to obtain sufficient cancellation, the clusters should combine positive and negative particles with similar velocities. The last example provides a choice that seems to be quite reasonable.

Example 3.19 (clustering with velocity cells) *Let $\{C_l\}_{l=1,\ldots,L}$ be a finite partition of the velocity space $\mathcal{R}^3$ and*

$$I_l(z) = \Big\{ i = 1, \ldots, N \,:\, v_i \in C_l \Big\}\,, \qquad l = 1, \ldots, L\,.$$

If there is a big cloud of particles with different signs but similar velocities, then these particles are actually redundant and will be canceled rather efficiently by the algorithm.

4 Collision step for the nonlinear BE

In this section we first study the evolution of the particle system (2.13) during the collision step, when only the nonlinear part on the right-hand side of equation (2.21) or (in the weak form) (2.23) is taken into account. We generalize the collision process and the source-sink process from the previous section to the nonlinear case. Finally, the algorithms for the linear and the nonlinear parts are combined to cover the full Boltzmann equation.

Consider states z of the form (3.3). In the algorithms, the sub-processes in different spatial cells (cf. (2.9)) are generated independently. Let

$$N_m(z) = \#\{i = 1, \ldots, N \; : \; x_i \in D_m\}, \qquad m = 1, \ldots, l_c, \tag{4.1}$$

denote the number of particles in the cell D_m.

4.1 Collision process

4.1.1 Generator and limiting equation

Introduce the generator

$$\mathcal{A}\Phi(z) = \frac{g^{(n)}}{2} \sum_{i,j=1}^{N} \int_{\mathcal{S}^2} [\Phi(J(z,i,j,e)) - \Phi(z)] \, h(x_i, x_j) \, B(v_i, v_j, e) \, de \tag{4.2}$$

where J replaces $(\varepsilon_i, x_i, v_i)$ and $(\varepsilon_j, x_j, v_j)$ by

- if $\varepsilon_i = \varepsilon_j = 1$, then

$$(\varepsilon_i, x_i, v'(v_i, v_j, e)) \quad \text{and} \quad (\varepsilon_j, x_j, w'(v_i, v_j, e)) \tag{4.3}$$

- if $\varepsilon_i = 1$ and $\varepsilon_j = -1$, then

$$(-\varepsilon_i, x_i, v'(v_i, v_j, e)), \quad (\varepsilon_j, x_j, w'(v_i, v_j, e)) \quad \text{and} \quad (\varepsilon_i, x_i, v_i), \quad (\varepsilon_i, x_i, v_i) \tag{4.4}$$

- if $\varepsilon_i = -1$ and $\varepsilon_j = 1$, then

$$(\varepsilon_i, x_i, v'(v_i, v_j, e)), \quad (-\varepsilon_j, x_j, w'(v_i, v_j, e)) \quad \text{and} \quad (\varepsilon_j, x_j, v_j), \quad (\varepsilon_j, x_j, v_j) \tag{4.5}$$

- if $\varepsilon_i = \varepsilon_j = -1$, then

$$\begin{aligned} &(-\varepsilon_i, x_i, v'(v_i, v_j, e)), \quad (-\varepsilon_j, x_j, w'(v_i, v_j, e)) \quad \text{and} \\ &\qquad (\varepsilon_i, x_i, v_i), \quad (\varepsilon_i, x_i, v_i), \quad (\varepsilon_j, x_j, v_j), \quad (\varepsilon_j, x_j, v_j). \end{aligned} \tag{4.6}$$

According to (4.4), (4.5), a "+/−"-collision creates two negative particles and doubles the old positive particle. According to (4.6), a "−/−"-collision creates two positive particles and doubles both old particles.

Introduce I^+ and I^- as the sets of indices corresponding to positive and negative signs, respectively. Then one obtains

$$\sum_{i,j\in I^+} h(x_i,x_j)\,B(v_i,v_j,e)\times$$
$$\Big[\varepsilon_i\,\varphi(x_i,v'(v_i,v_j,e))+\varepsilon_j\,\varphi(x_j,w'(v_i,v_j,e))-\varepsilon_i\,\varphi(x_i,v_i)-\varepsilon_j\,\varphi(x_j,v_j)\Big]=$$
$$\sum_{i,j\in I^+} h(x_i,x_j)\,B(v_i,v_j,e)\times \tag{4.7}$$
$$\Big[\varphi(x_i,v'(v_i,v_j,e))+\varphi(x_j,w'(v_i,v_j,e))-\varphi(x_i,v_i)-\varphi(x_j,v_j)\Big]\varepsilon_i\,\varepsilon_j\,,$$

$$\sum_{i\in I^+,\,j\in I^-} h(x_i,x_j)\,B(v_i,v_j,e)\Big[-\varepsilon_i\,\varphi(x_i,v'(v_i,v_j,e))+$$
$$\varepsilon_j\,\varphi(x_j,w'(v_i,v_j,e))+2\,\varepsilon_i\,\varphi(x_i,v_i)-\varepsilon_i\,\varphi(x_i,v_i)-\varepsilon_j\,\varphi(x_j,v_j)\Big]=$$
$$\sum_{i\in I^+,\,j\in I^-} h(x_i,x_j)\,B(v_i,v_j,e)\times \tag{4.8}$$
$$\Big[\varphi(x_i,v'(v_i,v_j,e))+\varphi(x_j,w'(v_i,v_j,e))-\varphi(x_i,v_i)-\varphi(x_j,v_j)\Big]\varepsilon_i\,\varepsilon_j$$

and

$$\sum_{i,j\in I^-} h(x_i,x_j)\,B(v_i,v_j,e)\Big[-\varepsilon_i\,\varphi(x_i,v'(v_i,v_j,e))-\varepsilon_j\,\varphi(x_j,w'(v_i,v_j,e))+$$
$$2\,\varepsilon_i\,\varphi(x_i,v_i)+2\,\varepsilon_j\,\varphi(x_j,v_j)-\varepsilon_i\,\varphi(x_i,v_i)-\varepsilon_j\,\varphi(x_j,v_j)\Big]=$$
$$\sum_{i,j\in I^-} h(x_i,x_j)\,B(v_i,v_j,e)\times \tag{4.9}$$
$$\Big[\varphi(x_i,v'(v_i,v_j,e))+\varphi(x_j,w'(v_i,v_j,e))-\varphi(x_i,v_i)-\varphi(x_j,v_j)\Big]\varepsilon_i\,\varepsilon_j\,.$$

Using the test functions (3.5) and (4.7)-(4.9), one obtains

$$\mathcal{A}\Phi(Z(t))=\frac{(g^{(n)})^2}{2}\sum_{i,j=1}^{N^{(n)}(t)}\varepsilon_i^{(n)}(t)\,\varepsilon_j^{(n)}(t)\,h(X_i^{(n)}(t),X_j^{(n)}(t))\times$$
$$\int_{\mathcal{S}^2}B(V_i^{(n)}(t),V_j^{(n)}(t),e)\Big[\varphi(X_i^{(n)}(t),v'(V_i^{(n)}(t),V_j^{(n)}(t),e))+$$
$$\varphi(X_j^{(n)}(t),w'(V_i^{(n)}(t),V_j^{(n)}(t),e))-\varphi(X_i^{(n)}(t),V_i^{(n)}(t))-\varphi(X_j^{(n)}(t),V_j^{(n)}(t))\Big]de$$
$$=\ \frac{1}{2}\int_D\int_{\mathcal{R}^3}\int_D\int_{\mathcal{R}^3}\int_{\mathcal{S}^2}\Big[\varphi(x,v'(v,w,e))+\varphi(y,w'(v,w,e))-\varphi(x,v)-\varphi(y,w)\Big]\times$$
$$h(x,y)\,B(v,w,e)\,de\,\mu^{(n)}(t,dy,dw)\,\mu^{(n)}(t,dx,dv)$$

leading (as $n \to \infty$) to the limiting equations

$$
\begin{aligned}
&\frac{d}{dt}\int_D\int_{\mathcal{R}^3}\varphi(x,v)\,f_d(t,x,v)\,dv\,dx = \qquad (4.10)\\
&\quad\frac{1}{2}\int_D\int_{\mathcal{R}^3}\int_D\int_{\mathcal{R}^3}\int_{\mathcal{S}^2}\Big[\varphi(x,v'(v,w,e))+\varphi(y,w'(v,w,e))-\varphi(x,v)-\varphi(y,w)\Big]\times\\
&\qquad\qquad h(x,y)\,B(v,w,e)\,f_d(t,y,w)\,f_d(t,x,v)\,de\,dw\,dy\,dv\,dx
\end{aligned}
$$

or

$$
\begin{aligned}
\frac{\partial}{\partial t}f_d(t,x,v) &= \int_D\int_{\mathcal{R}^3}\int_{\mathcal{S}^2}h(x,y)\,B(v,w,e)\times\\
&\qquad \Big[f_d(t,x,v')\,f_d(t,y,w')-f_d(t,x,v)\,f_d(t,y,w)\Big]de\,dw\,dy\,.
\end{aligned}
$$

4.1.2 General simulation procedure

Rewrite the generator (4.2) in the form

$$\mathcal{A}\Phi(z) = \int[\Phi(\tilde{z})-\Phi(z)]\,\lambda(z,d\tilde{z})\,, \qquad (4.11)$$

where

$$
\begin{aligned}
&\lambda(z,d\tilde{z}) = \frac{g^{(n)}}{2}\sum_{i,j=1}^{N}h(x_i,x_j)\times\\
&\quad\left\{\int_{\mathcal{S}^2}\delta_{J(z,i,j,e)}(d\tilde{z})\,B(v_i,v_j,e)\,de+\delta_z(d\tilde{z})\left[\tilde{E}_0(z,m(i))-\int_{\mathcal{S}^2}B(v_i,v_j,e)\,de\right]\right\}
\end{aligned}
$$

and

$$\tilde{E}_0(z,m) \geq \int_{\mathcal{S}^2}B(v_i,v_j,e)\,de\,, \qquad \forall\, i,j\ :\ x_i,x_j\in D_m\,. \qquad (4.12)$$

The representation (4.11) suggests the following algorithm:

1. Make a time step with parameter (cf. (4.1))

$$\frac{1}{2\,|D_m|}\,g^{(n)}\,N_m(z)^2\,\tilde{E}_0(z,m)\,. \qquad (4.13)$$

Stop, when the final time is exceeded.

2. Choose indices $i,j\ :\ x_i,x_j\in D_m$ uniformly.

3. With probability

$$1-\frac{\int_{\mathcal{S}^2}B(v_i,v_j,e)\,de}{\tilde{E}_0(z,m)}\,,$$

reject the indices i,j and go to **1.**

4. For given i, j , generate $e \in \mathcal{S}^2$ according to the density

$$\frac{B(v_i, v_j, e)}{\int_{\mathcal{S}^2} B(v_i, v_j, u)\, du} .$$

5. Replace $(\varepsilon_i, x_i, v_i)$ and $(\varepsilon_j, x_j, v_j)$ according to (4.3)–(4.6) and go to **1.**

In the variable hard sphere model (3.2) we choose (cf. (4.12))

$$\tilde{E}_0(z, m) = 4\,\pi\, C_\beta\, V_{\mathrm{rel}}(z, m)^\beta ,$$

where

$$V_{\mathrm{rel}}(z, m) \geq \|v_i - v_j\| , \qquad \forall\, i, j \,:\, x_i, x_j \in D_m . \tag{4.14}$$

The general simulation procedure takes the form:

Algorithm 4.1 (Variable hard sphere model)

1. *Make a time step with parameter*

$$\frac{2\,\pi\, C_\beta}{|D_m|}\, g^{(n)}\, N_m(z)^2\, V_{\mathrm{rel}}(z, m)^\beta .$$

Stop, when the final time is exceeded.

2. *Choose indices* $i, j \,:\, x_i, x_j \in D_m$ *uniformly.*

3. *With probability*

$$1 - \frac{\|v_i - v_j\|^\beta}{V_{\mathrm{rel}}(z, m)^\beta} ,$$

reject the indices i, j *and go to* **1.**

4. *For given* i, j *, generate* $e \in \mathcal{S}^2$ *uniformly.*

5. *Replace* $(\varepsilon_i, x_i, v_i)$ *and* $(\varepsilon_j, x_j, v_j)$ *according to (4.3)–(4.6) and go to* **1.**

4.2 Source-sink process

4.2.1 Generator and limiting equation

source term

Introduce

$$K_\delta^{(1)}(x, v; y_1, w_1, y_2, w_2) = \tag{4.15}$$

$$\frac{4\, h(x, y_1)\, h(x, y_2)}{\|w_2 - v\|} \int_{\Gamma(w_2 - v)} \frac{b\left(\|w_2 - v + u\|, \frac{2\,\|w_2 - v\|^2}{\|w_2 - v + u\|^2} - 1\right)}{\|w_2 - v + u\|}\; h_\delta(v - w_1 + u)\, du ,$$

$$K_\delta^{(2)}(x,v;y_1,w_1,y_2,w_2) = \tag{4.16}$$
$$\frac{4\,h(x,y_1)\,h(x,y_2)}{\|w_2-v\|}\int_{\Gamma(w_2-v)} \frac{b\left(\|w_2-v+u\|, 1-\frac{2\,\|w_2-v\|^2}{\|w_2-v+u\|^2}\right)}{\|w_2-v+u\|}\;h_\delta(v-w_1+u)\,du$$

and

$$K_\delta^{(3)}(x,v;y_1,w_1,y_2,w_2) = -h(x,y_1)\,h(x,y_2)\,h_\delta(v-w_1)\int_{\mathcal{S}^2} B(v,w_2,e)\,de\,, \tag{4.17}$$

where h_δ, $\delta > 0$, is a rotationally symmetric smoothing kernel on $\mathcal{R}^3$. It follows from Lemma 6.3 and Corollary 6.4 (with $\gamma(v) = h_\delta(v-w_1)$) that

$$\int_D \int_{\mathcal{R}^3} \varphi(x,v)\,K_\delta^{(k)}(x,v;y_1,w_1,y_2,w_2)\,dv\,dx = \tag{4.18}$$
$$\int_D \int_{\mathcal{R}^3} \varphi(x,v)\,\nu_\delta^{(k)}(y_1,w_1,y_2,w_2;dx,dv)\,, \qquad k=1,2\,,$$

where

$$\nu_\delta^{(1)}(y_1,w_1,y_2,w_2;dx,dv) = \tag{4.19}$$
$$h(x,y_1)\,h(x,y_2)\,dx\int_{\mathcal{R}^3}\int_{\mathcal{S}^2} \delta_{v'(w_2,u,e)}(dv)\,B(w_2,u,e)\,h_\delta(u-w_1)\,de\,du$$

and

$$\nu_\delta^{(2)}(y_1,w_1,y_2,w_2;dx,dv) = \tag{4.20}$$
$$h(x,y_1)\,h(x,y_2)\,dx\int_{\mathcal{R}^3}\int_{\mathcal{S}^2} \delta_{w'(w_2,u,e)}(dv)\,B(w_2,u,e)\,h_\delta(u-w_1)\,de\,du\,.$$

Define

$$E_\delta(w_1,w_2) \;=\; \int_{\mathcal{R}^3}\int_{\mathcal{S}^2} B(w_2,u,e)\,h_\delta(u-w_1)\,de\,du \tag{4.21}$$

and note that

$$\int_D h(x,y_1)\,h(x,y_2)\,dx = h(y_1,y_2)\,.$$

It follows from (4.17)–(4.20) that (cf. (6.8))

$$\int_D \int_{\mathcal{R}^3} |K_\delta^{(k)}(x,v;y_1,w_1,y_2,w_2)|\,dv\,dx = h(y_1,y_2)\,E_\delta(w_1,w_2)\,.$$

Consider probability measures A_δ and functions $s_\delta^{(k)}$ such that (cf. (3.32))

$$\int_\Theta s_\delta^{(k)}(z,i,j,x,v,\theta)\,A_\delta(z,i,x,v,d\theta) = K_\delta^{(k)}(x,v;x_i,v_i,x_j,v_j)\,. \tag{4.22}$$

Introduce the terms (cf. (3.33))

$$S_{\delta,l}(z,i,x,v,\theta) = g^{(n)} \sum_{j\in I_l(z)} \varepsilon_i\,\varepsilon_j \sum_{k=1}^{3} s_\delta^{(k)}(z,i,j,x,v,\theta)\,. \tag{4.23}$$

Consider the generator

$$\begin{aligned} \mathcal{A}_S\Phi(z) \;&=\; \sum_{i=1}^{N}\sum_{l=1}^{L(z)} \int_D\int_{\mathcal{R}^3}\int_\Theta \Big[\Phi(J_{\delta,0,l}(z,i,x,v,\theta)) - \Phi(z)\Big] \times \\ &\qquad |S_{\delta,l}(z,i,x,v,\theta)|\, A_\delta(z,i,x,v,d\theta)\,dv\,dx\,, \end{aligned} \tag{4.24}$$

where $J_{\delta,0,l}(z,i,x,v,\theta)$ adds a particle

$$(\operatorname{sign} S_{\delta,l}(z,i,x,v,\theta), x, v)$$

to the system. Using test functions (3.5), one obtains (cf. (4.18)–(4.20))

$$\begin{aligned} &\mathcal{A}_S\Phi(Z(t)) = g^{(n)} \sum_{i=1}^{N}\sum_{l=1}^{L(Z(t))} \int_D\int_{\mathcal{R}^3}\int_\Theta \varphi(x,v)\, S_{\delta,l}(Z(t),i,x,v,\theta)\, A_\delta(z,i,x,v,d\theta)\,dv\,dx \\ &= (g^{(n)})^2 \sum_{i,j=1}^{N} \varepsilon_i(t)\,\varepsilon_j(t) \sum_{k=1}^{3} \int_D\int_{\mathcal{R}^3} \varphi(x,v)\, K_\delta^{(k)}(x,v;X_i(t),V_i(t),X_j(t),V_j(t))\,dv\,dx \\ &= (g^{(n)})^2 \sum_{i,j=1}^{N} \varepsilon_i(t)\,\varepsilon_j(t) \int_D\int_{\mathcal{R}^3}\int_{\mathcal{S}^2} \Big[\varphi(x,v'(V_j(t),u,e)) + \varphi(x,w'(V_j(t),u,e))\Big] \times \\ &\qquad h(x,X_i(t))\,h(x,X_j(t))\,B(V_j(t),u,e)\,h_\delta(u-V_i(t))\,de\,du\,dx - \\ &\quad (g^{(n)})^2 \sum_{i,j=1}^{N} \varepsilon_i(t)\,\varepsilon_j(t) \int_D\int_{\mathcal{R}^3}\int_{\mathcal{S}^2} \varphi(x,v) \times \\ &\qquad h(x,X_i(t))\,h(x,X_j(t))\,B(v,V_j(t),e)\,h_\delta(v-V_i(t))\,de\,dv\,dx \\ &= \int_D\int_{\mathcal{R}^3}\int_D\int_{\mathcal{R}^3}\int_D\int_{\mathcal{R}^3}\int_{\mathcal{S}^2} \Big[\varphi(x,v'(w_2,u,e)) + \varphi(x,w'(w_2,u,e))\Big] \times \\ &\quad h(x,y_1)\,h(x,y_2)\,B(w_2,u,e)\,h_\delta(u-w_1)\,de\,du\,dx\,\mu^{(n)}(t,dy_1,dw_1)\,\mu^{(n)}(t,dy_2,dw_2) - \\ &\quad \int_D\int_{\mathcal{R}^3}\int_D\int_{\mathcal{R}^3}\int_D\int_{\mathcal{R}^3}\int_{\mathcal{S}^2} \varphi(x,v) \times \\ &\quad h(x,y_1)\,h(x,y_2)\,B(v,w_2,e)\,h_\delta(v-w_1)\,de\,dv\,dx\,\mu^{(n)}(t,dy_1,dw_1)\,\mu^{(n)}(t,dy_2,dw_2) \end{aligned}$$

leading (as $n\to\infty$) to the expression

$$\begin{aligned} &\int_D\int_{\mathcal{R}^3}\int_D\int_{\mathcal{R}^3}\int_D\int_{\mathcal{R}^3}\int_{\mathcal{S}^2} \Big[\varphi(x,v'(w_2,u,e)) + \varphi(x,w'(w_2,u,e))\Big] h(x,y_1)\,h(x,y_2) \times \\ &\qquad B(w_2,u,e)\,h_\delta(u-w_1)\,de\,du\,dx\,f_d(t,y_1,w_1)\,f_d(t,y_2,w_2)\,dw_1\,dy_1\,dw_2\,dy_2 - \\ &\quad \int_D\int_{\mathcal{R}^3}\int_D\int_{\mathcal{R}^3}\int_D\int_{\mathcal{R}^3}\int_{\mathcal{S}^2} \varphi(x,v)\,h(x,y_1)\,h(x,y_2) \times \end{aligned}$$

$$
\begin{aligned}
&\qquad B(v,w_2,e)\,h_\delta(v-w_1)\,de\,dv\,dx\;\; f_d(t,y_1,w_1)\,f_d(t,y_2,w_2)\,dw_1\,dy_1\,dw_2\,dy_2 \\
&= \int_D\int_{\mathcal{R}^3}\int_D\int_{\mathcal{R}^3}\int_{\mathcal{S}^2}\Big[\varphi(x,v'(w_2,u,e))+\varphi(x,w'(w_2,u,e))\Big]\times \\
&\qquad h(x,y_2)\,B(w_2,u,e)\,\tilde f_d^{(\delta)}(t,x,u)\,f_d(t,y_2,w_2)\,de\,du\,dx\,dw_2\,dy_2 - \\
&\quad \int_D\int_{\mathcal{R}^3}\int_D\int_{\mathcal{R}^3}\int_{\mathcal{S}^2}\varphi(x,v)\times \\
&\qquad h(x,y_2)\,B(v,w_2,e)\,\tilde f_d^{(\delta)}(t,x,v)\,f_d(t,y_2,w_2)\,de\,dv\,dx\,dw_2\,dy_2 \\
&= \int_D\int_{\mathcal{R}^3}\int_D\int_{\mathcal{R}^3}\int_{\mathcal{S}^2}\Big[\varphi(x,v'(v,w,e))+\varphi(x,w'(v,w,e))\Big]\times \\
&\qquad h(x,y)\,B(v,w,e)\,\tilde f_d^{(\delta)}(t,x,w)\,f_d(t,y,v)\,de\,dw\,dx\,dv\,dy - \\
&\quad \int_D\int_{\mathcal{R}^3}\int_D\int_{\mathcal{R}^3}\int_{\mathcal{S}^2}\varphi(x,w)\times \qquad\qquad (4.25)\\
&\qquad h(x,y)\,B(v,w,e)\,\tilde f_d^{(\delta)}(t,x,w)\,f_d(t,y,v)\,de\,dw\,dx\,dv\,dy\,,
\end{aligned}
$$

where

$$
f_d^{(\delta)}(t,x,v)=\int_{\mathcal{R}^3} h_\delta(v-u)\,f_d(t,x,u)\,du \tag{4.26}
$$

and (cf. (2.7), (2.22))

$$
\tilde f_d^{(\delta)}(t,x,v)=\int_D h(x,y)\,f_d^{(\delta)}(t,y,v)\,dy\,. \tag{4.27}
$$

sink term

Consider functions $\hat s_\delta$ such that (cf. (4.21))

$$
\int_{\mathcal{R}^3}\hat s_\delta(z,j,i,v)\,h_\delta(v)\,dv = h(x_i,x_j)\,E_\delta(v_j,v_i)\,. \tag{4.28}
$$

Introduce the terms

$$
\hat S_{\delta,l}(z,i,v) \quad = \quad g^{(n)}\sum_{j\in I_l(z)}\varepsilon_j\,\hat s_\delta(z,j,i,v)\,, \tag{4.29}
$$

$$
\hat S^+_{\delta,l}(z,i,v)=\begin{cases}\hat S_{\delta,l}(z,i,v)\,, & \text{if}\quad \hat S_{\delta,l}(z,i,v)\ge 0\,,\\ 0\,, & \text{otherwise}\,,\end{cases}
$$

and

$$
\hat S^-_{\delta,l}(z,i,v)=\begin{cases}-\hat S_{\delta,l}(z,i,v)\,, & \text{if}\quad \hat S_{\delta,l}(z,i,v)< 0\,,\\ 0\,, & \text{otherwise}\,.\end{cases}
$$

Consider the generator

$$\mathcal{A}_E\Phi(z) = \sum_{i=1}^{N}\sum_{l=1}^{L(z)}\int_{\mathcal{R}^3}\Big\{\Big[\Phi(\hat{J}_0(z,i))-\Phi(z)\Big]\hat{S}^-_{\delta,l}(z,i,v)+ \Big[\Phi(\hat{J}_1(z,i))-\Phi(z)\Big]\hat{S}^+_{\delta,l}(z,i,v)\Big\}\,h_\delta(v)\,dv\,, \tag{4.30}$$

where $\hat{J}_0(z,i)$ adds a particle (ε_i,x_i,v_i) to the system and $\hat{J}_1(z,i)$ removes particle (ε_i,x_i,v_i) from the system.

Using test functions (3.5), one obtains

$$\begin{aligned}
&\mathcal{A}_E\Phi(Z(t)) = \\
&\quad g^{(n)}\sum_{i=1}^{N}\sum_{l=1}^{L(z)}\int_{\mathcal{R}^3}\varepsilon_i(t)\,\varphi(X_i(t),V_i(t))\Big[\hat{S}^-_{\delta,l}(Z(t),i,v)-\hat{S}^+_{\delta,l}(Z(t),i,v)\Big]h_\delta(v)\,dv\\
&= -g^{(n)}\sum_{i=1}^{N}\sum_{l=1}^{L(z)}\int_{\mathcal{R}^3}\varepsilon_i(t)\,\varphi(X_i(t),V_i(t))\,\hat{S}_{\delta,l}(Z(t),i,v)\,h_\delta(v)\,dv\\
&= -(g^{(n)})^2\sum_{i,j=1}^{N}\int_{\mathcal{R}^3}\varepsilon_i(t)\,\varepsilon_j(t)\,\varphi(X_i(t),V_i(t))\,\hat{s}_\delta(Z(t),j,i,v)\,h_\delta(v)\,dv\\
&= -(g^{(n)})^2\sum_{i,j=1}^{N}\varepsilon_i(t)\,\varepsilon_j(t)\,\varphi(X_i(t),V_i(t))\,h(X_i(t),X_j(t))\,E_\delta(V_j(t),V_i(t))\\
&= -\int_D\int_{\mathcal{R}^3}\int_D\int_{\mathcal{R}^3}\int_{\mathcal{R}^3}\int_{\mathcal{S}^2}\varphi(x,v)\,\times\\
&\qquad h(x,y)\,B(v,u,e)\,h_\delta(u-w)\,de\,du\,\mu_n(t,dy,dw)\,\mu_n(t,dx,dv)
\end{aligned}$$

leading (as $n\to\infty$) to the term (cf. (4.26), (4.27))

$$\begin{aligned}
&-\int_D\int_{\mathcal{R}^3}\int_D\int_{\mathcal{R}^3}\int_{\mathcal{R}^3}\int_{\mathcal{S}^2}\varphi(x,v)\times\\
&\qquad h(x,y)\,B(v,u,e)\,h_\delta(u-w)\,de\,du\,f_d(t,y,w)\,f_d(t,x,v)\,dy\,dw\,dx\,dv\\
&= -\int_D\int_{\mathcal{R}^3}\int_{\mathcal{R}^3}\int_{\mathcal{S}^2}\varphi(x,v)\,B(v,u,e)\,\tilde{f}_d^{(\delta)}(t,x,u)\,f_d(t,x,v)\,de\,du\,dx\,dv \qquad (4.31)\\
&= -\int_D\int_{\mathcal{R}^3}\int_D\int_{\mathcal{R}^3}\int_{\mathcal{S}^2}\varphi(x,v)\,h(x,y)\,B(v,w,e)\,\tilde{f}_d^{(\delta)}(t,x,w)\,f_d(t,x,v)\,de\,dy\,dw\,dx\,dv\\
&= -\int_D\int_{\mathcal{R}^3}\int_D\int_{\mathcal{R}^3}\int_{\mathcal{S}^2}\varphi(y,v)\,h(x,y)\,B(v,w,e)\,\tilde{f}_d^{(\delta)}(t,x,w)\,f_d(t,y,v)\,de\,dy\,dw\,dx\,dv\,.
\end{aligned}$$

Note that $\tilde{f}_d^{(\delta)}$ is constant in the cells.

limiting equation

According to (4.25) and (4.31), the process with the generator

$$\frac{1}{2}\Big(\mathcal{A}_S+\mathcal{A}_E\Big)$$

corresponds to the limiting equation (cf. (2.20))

$$\frac{d}{dt}\int_D \int_{\mathcal{R}^3} \varphi(x,v)\, f_d(t,x,v)\, dv\, dx = \tag{4.32}$$
$$\frac{1}{2}\int_D \int_{\mathcal{R}^3} \int_D \int_{\mathcal{R}^3} \int_{\mathcal{S}^2} \Big[\varphi(x,v'(v,w,e)) + \varphi(x,w'(v,w,e)) - \varphi(x,w) - \varphi(y,v)\Big] \times$$
$$h(x,y)\, B(v,w,e)\, \tilde{f}_d^{(\delta)}(t,x,w)\, f_d(t,y,v)\, de\, dw\, dy\, dv\, dx\,.$$

Removing the test function one obtains the equation

$$\frac{\partial}{\partial t} f_d(t,x,v) = \frac{1}{2}\int_D \int_{\mathcal{R}^3} \int_{\mathcal{S}^2} h(x,y)\, B(v,w,e) \Big[\tilde{f}_d^{(\delta)}(t,x,w')\, f_d(t,y,v') +$$
$$\tilde{f}_d^{(\delta)}(t,x,v')\, f_d(t,y,w') - \tilde{f}_d^{(\delta)}(t,x,v)\, f_d(t,y,w) - \tilde{f}_d^{(\delta)}(t,y,w)\, f_d(t,x,v)\Big] de\, dw$$
$$= \frac{1}{2}\int_{\mathcal{R}^3} \int_{\mathcal{S}^2} B(v,w,e) \Big[\tilde{f}_d^{(\delta)}(t,x,w')\, \tilde{f}_d(t,x,v') +$$
$$\tilde{f}_d^{(\delta)}(t,x,v')\, \tilde{f}_d(t,x,w') - \tilde{f}_d^{(\delta)}(t,x,v)\, \tilde{f}_d(t,x,w) - \tilde{f}_d^{(\delta)}(t,x,w)\, f_d(t,x,v)\Big] de\, dw\,.$$

Note the analogy with (3.36) and (3.37).

4.2.2 The implicit method

source term

Lemma 4.2 *Let the smoothing kernel h_δ be a Maxwellian, i.e.*

$$h_\delta(v) = \frac{1}{(2\pi\,\delta)^{3/2}} \exp\left(-\frac{\|v\|^2}{2\,\delta}\right), \qquad \delta > 0\,. \tag{4.33}$$

Consider the parameter set (3.54) and the probability measures (cf. (3.55))

$$A_\delta(z,i,x,v,d\theta) = \int_{\mathcal{R}^3} \left[\prod_{j=1}^N \delta_{\pi_{v_j - v}(w)}(d\theta_j)\right] h_\delta(v - v_i + w)\, dw\,.$$

Consider functions

$$q_\delta^{(1)}(x,v;y_1,w_1,y_2,w_2,u) = \frac{4\,h(x,y_1)\,h(x,y_2)}{\|w_2 - v\|}\times \tag{4.34}$$
$$\left[\int_{\Gamma(w_2-v)} h_\delta(v - w_1 + c)\, dc\right] \frac{b\left(\|w_2 - v + u\|, \frac{2\,\|w_2-v\|^2}{\|w_2-v+u\|^2} - 1\right)}{\|w_2 - v + u\|}\,,$$

$$q_\delta^{(2)}(x,v;y_1,w_1,y_2,w_2,u) = \frac{4\,h(x,y_1)\,h(x,y_2)}{\|w_2 - v\|}\times \tag{4.35}$$
$$\left[\int_{\Gamma(w_2-v)} h_\delta(v - w_1 + c)\, dc\right] \frac{b\left(\|w_2 - v + u\|, 1 - \frac{2\,\|w_2-v\|^2}{\|w_2-v+u\|^2}\right)}{\|w_2 - v + u\|}$$

and

$$q_\delta^{(3)}(x,v;y_1,w_1,y_2,w_2,u) = K_\delta^{(3)}(x,v;y_1,w_1,y_2,w_2)\,. \tag{4.36}$$

Then the functions

$$s_\delta^{(k)}(z,i,j,x,v,\theta) = q_\delta^{(k)}(x,v,x_i,v_i,x_j,v_j,\theta_j)\,, \qquad k=1,2,3\,, \tag{4.37}$$

satisfy assumption (4.22).

Proof. One obtains

$$\int_\Theta s_\delta^{(1)}(z,i,j,x,v,\theta)\,A_\delta(z,i,x,v,d\theta) =$$
$$\int_{\mathcal{R}^3} q_\delta^{(1)}(x,v,x_i,v_i,x_j,v_j,\pi_{v_j-v}(w))\,h_\delta(v-v_i+w)\,dw$$
$$= \frac{4\,h(x,x_i)\,h(x,x_j)}{\|v_j-v\|}\left[\int_{\Gamma(v_j-v)} h_\delta(v-v_i+c)\,dc\right]\times$$
$$\int_{\mathcal{R}^3} \frac{b\left(\|v_j-v+\pi_{v_j-v}(w)\|,\frac{2\,\|v_j-v\|^2}{\|v_j-v+\pi_{v_j-v}(w)\|^2}-1\right)}{\|v_j-v+\pi_{v_j-v}(w)\|}\,h_\delta(v-v_i+w)\,dw$$

so that (4.22) (with $k=1$) is a consequence of Lemma 6.8 (cf. (3.64)) and (4.33). The case $k=2$ is treated analogously, and the case $k=3$ is obvious. ■

Define $K_{\delta,\max}^{(k)}$, $E_{\delta,\max}$, $q_{\delta,\max}^{(k)}$ and $s_{\delta,\max}^{(k)}$ in analogy with (4.15)–(4.17), (4.21) and (4.34)–(4.37), respectively, with b replaced by $b_{\max}$, and taking the absolute value (in case $k=3$). Introduce an upper bound

$$\tilde{E}_{\delta,\max}(z,m) \ge E_{\delta,\max}(v_i,v_j)\,, \qquad \forall\, i,j\;:\; x_i,x_j\in D_m\,. \tag{4.38}$$

Consider functions (cf. (4.23))

$$g_{\delta,l}(z,i,x,v,\theta) = g^{(n)} \sum_{j\in I_l(z)} \sum_{k=1}^{3} s_{\delta,\max}^{(k)}(z,i,j,x,v,\theta)$$

and measures (cf. (3.45), (4.24))

$$\lambda_{\delta,0,l}(z,i,x,v,\theta,d\tilde{z}) =$$
$$\delta_{J_{\delta,0,l}(z,i,x,v,\theta)}(d\tilde{z})\,\frac{|S_{\delta,l}(z,i,x,v,\theta)|}{g_{\delta,l}(z,i,x,v,\theta)} + \delta_z(d\tilde{z})\,\frac{g_{\delta,l}(z,i,x,v,\theta)-|S_{\delta,l}(z,i,x,v,\theta)|}{g_{\delta,l}(z,i,x,v,\theta)}\,.$$

The generator (4.24) takes the form

$$\mathcal{A}_S\Phi(z) = \sum_{i=1}^{N}\sum_{l=1}^{L(z)} \int_D \int_{\mathcal{R}^3} \int_\Theta \left(\int \Big[\Phi(\tilde{z})-\Phi(z)\Big]\,\lambda_{\delta,0,l}(z,i,x,v,\theta,d\tilde{z})\right)\times$$
$$g_{\delta,l}(z,i,x,v,\theta)\,A_\delta(z,i,x,v,d\theta)\,dv\,dx$$

$$
\begin{aligned}
&= g^{(n)} \sum_{i,j=1}^{N} \sum_{k=1}^{3} \int_D \int_{\mathcal{R}^3} \int_\Theta \Big(\int \Big[\Phi(\tilde z) - \Phi(z)\Big]\, \lambda_{\delta,0,l(j)}(z,i,x,v,\theta,d\tilde z) \Big) \times \\
&\qquad\qquad s^{(k)}_{\delta,\max}(z,i,j,x,v,\theta)\, A_\delta(z,i,x,v,d\theta)\, dv\, dx \\
&= g^{(n)} \sum_{i,j=1}^{N} h(x_i,x_j)\, E_{\delta,\max}(v_i,v_j) \times \\
&\quad \sum_{k=1}^{3} \int_D \int_{\mathcal{R}^3} \Big\{ \int_\Theta \Big(\int \Big[\Phi(\tilde z) - \Phi(z)\Big]\, \lambda_{\delta,0,l(j)}(z,i,x,v,\theta,d\tilde z) \Big) \times \\
&\quad \frac{s^{(k)}_{\delta,\max}(z,i,j,x,v,\theta)}{K^{(k)}_{\delta,\max}(x,v;x_i,v_i,x_j,v_j)}\, A_\delta(z,i,x,v,d\theta) \Big\} \frac{K^{(k)}_{\delta,\max}(x,v;x_i,v_i,x_j,v_j)}{h(x_i,x_j)\, E_{\delta,\max}(v_i,v_j)}\, dv\, dx\, + \\
&\quad 3\, g^{(n)} \sum_{i,j=1}^{N} h(x_i,x_j) \Big(\tilde E_{\delta,\max}(z,m(i)) - E_{\delta,\max}(v_i,v_j) \Big) \int \Big[\Phi(\tilde z) - \Phi(z)\Big]\, \delta_z(d\tilde z)\,,
\end{aligned}
\tag{4.39}
$$

where $l(j)$ is the index of the cluster to which the particle j belongs and $m(i)$ is the index of the cell to which particle i belongs.

sink term

Consider the function

$$
\hat s_\delta(z,j,i,v) = h(x_i,x_j) \int_{\mathcal{S}^2} B(v_i, v_j - v, e)\, de\,, \tag{4.40}
$$

which satisfies assumption (4.28). If E_δ is explicitly known, then one can choose (cf. (4.21))

$$
\hat s_\delta(z,j,i,v) = h(x_i,x_j)\, E_\delta(v_j,v_i)\,. \tag{4.41}
$$

Define $\hat s_{\delta,\max}$ in analogy with (4.40) and (4.41), respectively, where B is replaced by $B_{\max}$. Consider functions (cf. (4.29))

$$
\hat g_{\delta,l}(z,i,v) = g^{(n)} \sum_{j \in I_l(z)} \hat s_{\delta,\max}(z,j,i,v)
$$

and measures

$$
\begin{aligned}
&\hat\lambda_{1,l}(z,i,v,d\tilde z) = \\
&\quad \delta_{\hat J_0(z,i)}(d\tilde z)\, \frac{\hat S^-_{\delta,l}(z,i,v)}{\hat g_{\delta,l}(z,i,v)} + \delta_{\hat J_1(z,i)}(d\tilde z)\, \frac{\hat S^+_{\delta,l}(z,i,v)}{\hat g_{\delta,l}(z,i,v)} + \delta_z(d\tilde z)\, \frac{\hat g_{\delta,l}(z,i,v) - |\hat S_{\delta,l}(z,i,v)|}{\hat g_{\delta,l}(z,i,v)}\,.
\end{aligned}
$$

The generator (4.30) takes the form

$$
\mathcal{A}_E \Phi(z) = \sum_{i=1}^{N} \sum_{l=1}^{L(z)} \int_{\mathcal{R}^3} \Big(\int \Big[\Phi(\tilde z) - \Phi(z)\Big] \hat\lambda_{1,l}(z,i,v,d\tilde z) \Big)\, \hat g_{\delta,l}(z,i,v)\, h_\delta(v)\, dv
$$

$$= \; g^{(n)} \sum_{i,j=1}^{N} \int_{\mathcal{R}^3} \left(\int \Big[\Phi(\tilde z) - \Phi(z)\Big] \hat\lambda_{1,l(j)}(z,i,v,d\tilde z) \right) \hat s_{\delta,\max}(z,j,i,v)\, h_\delta(v)\, dv$$

$$= \; g^{(n)} \sum_{i,j=1}^{N} \int_{\mathcal{R}^3} \left(\int \Big[\Phi(\tilde z) - \Phi(z)\Big] \hat\lambda_{1,l(i)}(z,j,v,d\tilde z) \right) \hat s_{\delta,\max}(z,i,j,v)\, h_\delta(v)\, dv$$

$$\begin{aligned} = \; & g^{(n)} \sum_{i,j=1}^{N} h(x_i,x_j)\, E_{\delta,\max}(v_i,v_j) \times \qquad (4.42) \\ & \int_{\mathcal{R}^3} \left(\int \Big[\Phi(\tilde z) - \Phi(z)\Big] \hat\lambda_{1,l(i)}(z,j,v,d\tilde z) \right) \frac{\hat s_{\delta,\max}(z,i,j,v)}{h(x_i,x_j)\, E_{\delta,\max}(v_i,v_j)}\, h_\delta(v)\, dv + \\ & g^{(n)} \sum_{i,j=1}^{N} h(x_i,x_j) \Big(\tilde E_{\delta,\max}(z,m(i)) - E_{\delta,\max}(v_i,v_j) \Big) \int \Big[\Phi(\tilde z) - \Phi(z)\Big]\, \delta_z(d\tilde z)\,. \end{aligned}$$

pathwise behavior

The representations (4.39) and (4.42) suggest the following algorithm:

Algorithm 4.3 (Implicit method)

1. *Make a time step with parameter (cf. (4.1))*

$$\frac{2}{|D_m|}\, g^{(n)}\, N_m(z)^2\, \tilde E_{\delta,\max}(z,m)\,. \qquad (4.43)$$

Stop, when the final time is exceeded.

2. *Choose indices* $i,j\;:\;x_i,x_j \in D_m$ *uniformly.*

3. *With probability (cf. (6.19))*

$$1 - \frac{\int_{\mathcal{R}^3} \int_{\mathcal{S}^2} B_{\max}(v_j,u,e)\, M_{v_i,\delta}(u)\, de\, du}{\tilde E_{\delta,\max}(z,m)}\,, \qquad (4.44)$$

go to **1.**

4. *With probabilities* $1/4$, *choose* $k = 1,2,3$ *or go to* **6.**

5. *Perform a jump according to the source term with index* k .

5.1. *For given* i,j , *generate* $x \in D$ *and* $v \in \mathcal{R}^3$ *according to the density (cf. (4.17)–(4.20))*

$$\frac{1}{h(x_i,x_j)\, E_{\delta,\max}(v_i,v_j)}\; K^{(k)}_{\delta,\max}(x,v;x_i,v_i,x_j,v_j)\,.$$

5.1.1. *Generate* x *uniformly in the cell* D_m .

5.1.2. *Generate $w \in \mathcal{R}^3$ according to the density*

$$\frac{1}{E_{\delta,\max}(v_i,v_j)} \left(\int_{\mathcal{S}^2} B_{\max}(v_j,w,e)\, de \right) M_{v_i,\delta}(w)\,.$$

5.1.3. *If $k=3$, then choose $v=w$ and go to* **5.2.**

5.1.4. *For given w, generate $e \in \mathcal{S}^2$ according to the density*

$$\frac{B_{\max}(v_j,w,e)}{\int_{\mathcal{S}^2} B_{\max}(v_j,w,u)\, du}\,.$$

5.1.5. *If $k=1$, then calculate $v = v'(v_j,w,e)$ and go to* **5.2.**

5.1.6. *Calculate $v = w'(v_j,w,e)$.*

5.2. *For given i,j,x and v, generate the auxiliary parameter θ according to the distribution (cf. Remark 3.7)*

$$\frac{1}{K^{(k)}_{\delta,\max}(x,v;x_i,v_i,x_j,v_j)}\, s^{(k)}_{\delta,\max}(z,i,j,x,v,\theta)\, A_\delta(z,i,x,v,d\theta)\,.$$

5.2.1. *Generate $\tilde{w} \in \mathcal{R}^3$ according to the density*

$$\frac{1}{K^{(k)}_{\delta,\max}(x,v;x_i,v_i,x_j,v_j)}\, q^{(k)}_{\delta,\max}(x,v,x_i,v_i,x_j,v_j,\pi_{v_j-v}(\tilde{w}))\, M_{v_i,\delta}(v+\tilde{w})\,. \tag{4.45}$$

5.2.2. *Compute*

$$\theta_\alpha = \pi_{v_\alpha - v}(\tilde{w})\,, \qquad \alpha \in I_{l(j)}(z)\,.$$

5.3. *With probability*

$$1 - \frac{|S_{\delta,l(j)}(z,i,x,v,\theta)|}{g_{\delta,l(j)}(z,i,x,v,\theta)} = \tag{4.46}$$
$$1 - \frac{\left| \sum_{\alpha \in I_{l(j)}(z)} \sum_{k=1}^3 \varepsilon_i\, \varepsilon_\alpha\, q^{(k)}_\delta(x,v,x_i,v_i,x_\alpha,v_\alpha,\theta_\alpha) \right|}{\sum_{\alpha \in I_{l(j)}(z)} \sum_{k=1}^3 q^{(k)}_{\delta,\max}(x,v,x_i,v_i,x_\alpha,v_\alpha,\theta_\alpha)}\,,$$

go to **1.**

5.4. *Add the particle with position x, velocity v and sign*

$$\operatorname{sign} S_{\delta,l(j)}(z,i,x,v,\theta) = \tag{4.47}$$
$$\operatorname{sign} \left(\sum_{\alpha \in I_{l(j)}(z)} \sum_{k=1}^3 \varepsilon_i\, \varepsilon_\alpha\, q^{(k)}_\delta(x,v,x_i,v_i,x_\alpha,v_\alpha,\theta_\alpha) \right)$$

to the system and go to **1.**

6. *Perform a jump according to the sink term.*

6.1. *For given* i, j, *generate* $v \in \mathcal{R}^3$ *according to the density*

$$\frac{|D_m|}{E_{\delta,\max}(v_i, v_j)} \; \hat{s}_{\delta,\max}(z, i, j, v)\, M_{0,\delta}(v)\,.$$

6.2. *With probability*

$$1 - \frac{|\hat{S}_{\delta,l(i)}(z, j, v)|}{\hat{g}_{\delta,l(i)}(z, j, v)} = 1 - \frac{\left|\sum_{\alpha\in I_{l(i)}(z)} \varepsilon_\alpha\, \hat{s}_\delta(z, \alpha, j, v)\right|}{\sum_{\alpha\in I_{l(i)}(z)} \hat{s}_{\delta,\max}(z, \alpha, j, v)}\,,$$

go to **1.**

6.3. *If*

$$\sum_{\alpha\in I_{l(i)}(z)} \varepsilon_\alpha\, \hat{s}_\delta(z, \alpha, j, v) \quad > \quad 0\,,$$

then delete particle i *and go to* **1.**

6.4. *Double particle* i *and go to* **1.**

4.2.3 Variable hard sphere model

In the case (3.2) one obtains from (4.15), (4.16), (4.21), (4.34)-(4.36)) (with (4.33))

$$K_\delta^{(k)}(x, v; y_1, w_1, y_2, w_2) = \tag{4.48}$$
$$\frac{4\, C_\beta\, h(x, y_1)\, h(x, y_2)}{\|w_2 - v\|} \int_{\Gamma(w_2 - v)} \|w_2 - v + u\|^{\beta-1}\, M_{w_1,\delta}(v + u)\, du\,,$$

$$E_\delta(w_1, w_2) = 4\pi\, C_\beta \int_{\mathcal{R}^3} \|w_2 - u\|^\beta\, M_{w_1,\delta}(u)\, du\,,$$

$$q_\delta^{(k)}(x, v; y_1, w_1, y_2, w_2, u) =$$
$$\frac{4\, C_\beta\, h(x, y_1)\, h(x, y_2)}{\|w_2 - v\|} \left(\int_{\Gamma(w_2 - v)} M_{w_1,\delta}(v + c)\, dc\right) \|w_2 - v + u\|^{\beta-1}\,,$$

$$q_\delta^{(3)}(x, v; y_1, w_1, y_2, w_2, u) =$$
$$K_\delta^{(3)}(x, v; y_1, w_1, y_2, w_2) = -4\pi\, C_\beta\, h(x, y_1)\, h(x, y_2)\, M_{w_1,\delta}(v)\|v - w_2\|^\beta\,,$$

and (with (3.17))

$$K_{\delta,\max}^{(k)}(x, v; y_1, w_1, y_2, w_2) = \frac{4\, h(x, y_1)\, h(x, y_2)}{\|w_2 - v\|} \times$$
$$\left[c_0 \int_{\Gamma(w_2 - v)} \frac{1}{\|w_2 - v + u\|}\, M_{w_1,\delta}(v + u)\, du + c_1 \int_{\Gamma(w_2 - v)} M_{w_1,\delta}(v + u)\, du\right],$$

$$E_{\delta,\max}(w_1,w_2) = 4\pi \left[c_0 + c_1 \int_{\mathcal{R}^3} \|w_2 - u\| \, M_{w_1,\delta}(u)\, du\right], \tag{4.49}$$

$$q^{(k)}_{\delta,\max}(x,v;y_1,w_1,y_2,w_2,u) =$$
$$\frac{4\,h(x,y_1)\,h(x,y_2)}{\|w_2 - v\|} \left(\int_{\Gamma(w_2-v)} M_{w_1,\delta}(v+c)\,dc\right) \left[\frac{c_0}{\|w_2 - v + u\|} + c_1\right],$$

$$q^{(3)}_{\delta,\max}(x,v;y_1,w_1,y_2,w_2,u) =$$
$$K^{(3)}_{\delta,\max}(x,v;y_1,w_1,y_2,w_2) = 4\pi\, h(x,y_1)\,h(x,y_2)\,M_{w_1,\delta}(v)\left[c_0 + c_1\,\|v - w_2\|\right],$$

for $k = 1,2$. Lemma 6.6 implies (cf. (3.89))

$$\int_{\mathcal{R}^3} \|w_2 - u\|\, M_{w_1,\delta}(u)\,du = \sqrt{\frac{2\,\delta}{\pi}} \times$$
$$\left\{\left[2\,\frac{\|w_1 - w_2\|}{\sqrt{2\,\delta}} + \frac{\sqrt{2\,\delta}}{\|w_1 - w_2\|}\right] \frac{\sqrt{\pi}}{2}\,\mathrm{erf}\left(\frac{\|w_1 - w_2\|}{\sqrt{2\,\delta}}\right) + \exp\left(-\frac{\|w_1 - w_2\|^2}{2\,\delta}\right)\right\}$$
$$\le \quad \|w_1 - w_2\| + 2\sqrt{\frac{2\,\delta}{\pi}}\,. \tag{4.50}$$

According to (4.38), we choose (cf. (4.49), (4.50), (4.14))

$$\tilde{E}_{\delta,\max}(z,m) = 4\pi\left[c_0 + c_1\left(V_{\mathrm{rel}}(z,m) + 2\sqrt{\frac{2\,\delta}{\pi}}\right)\right].$$

According to the choice (4.40), one obtains

$$\hat{s}_\delta(z,j,i,v) = 4\pi\, C_\beta\, h(x_i,x_j)\,\|v_i - v_j + v\|^\beta$$

and

$$\hat{s}_{\delta,\max}(z,j,i,v) = 4\pi\, h(x_i,x_j)\left[c_0 + c_1\,\|v_i - v_j + v\|\right].$$

Density (4.45) is generated by an acceptance-rejection technique (cf. Remark 3.10).

The implicit method (Algorithm 4.3) takes the form:

Algorithm 4.4 (Variable hard sphere model)

1. *Make a time step with parameter*

$$\frac{8\pi\, g^{(n)}\, N_m(z)^2}{|D_m|}\left[c_0 + c_1\left(V_{\mathrm{rel}}(z,m) + 2\sqrt{\frac{2\,\delta}{\pi}}\right)\right].$$

Stop, when the final time is exceeded.

2. *Choose indices* $i, j \, : \, x_i, x_j \in D_m$ *uniformly.*

3. *With probability*

$$1 - \frac{c_0 + c_1 \int_{\mathcal{R}^3} \|v_j - u\| \, M_{v_i,\delta}(u) \, du}{c_0 + c_1 \Big(V_{\mathrm{rel}}(z,m) + 2\, \sqrt{2\,\delta/\pi} \Big)} \,, \tag{4.51}$$

go to **1.**

4. *With probabilities* $1/4$, *choose* $k = 1, 2, 3$ *or go to* **6.**

5. *Perform a jump according to the source term.*

5.1. *For given* i, j, *generate* $x \in D$ *and* $v \in \mathcal{R}^3$.

5.1.1. *Generate* x *uniformly in the cell* D_m.

5.1.2. *Generate* $w \in \mathcal{R}^3$ *according to the density*

$$\frac{[c_0 + c_1 \, \|v_j - w\|] \, M_{v_i,\delta}(w)}{\int_{\mathcal{R}^3} [c_0 + c_1 \, \|v_j - u\|] \, M_{v_i,\delta}(u) \, du} \,. \tag{4.52}$$

5.1.3. *If* $k = 3$, *then choose* $v = w$ *and go to* **5.2.1.**

5.1.4. *Generate* $e \in \mathcal{S}^2$ *uniformly, calculate* $v = v'(v_j, w, e)$ *and go to* **5.2.2.**

5.2. *For given* i, j, x *and* v, *generate the auxiliary parameter* θ.

5.2.1. *Generate* $\tilde{w} \in \mathcal{R}^3$ *according to the density* $M_{v_i,\delta}(v + \tilde{w})$ *and go to* **5.2.4.**

5.2.2. *Generate* $\tilde{w} \in \mathcal{R}^3$ *according to the density* $M_{v_i,\delta}(v + \tilde{w})$.

5.2.3. *With probability*

$$1 - \frac{\frac{c_0}{\|v_j - v + \pi_{v_j - v}(\tilde{w})\|} + c_1}{\frac{c_0}{\|v_j - v\|} + c_1} \,,$$

go to **5.2.2.**

5.2.4. *Compute* $\theta_\alpha = \pi_{v_\alpha - v}(\tilde{w})$, $\alpha \in I_{l(j)}(z)$.

5.3. *With probability*

$$1 - \frac{\Big| \sum_{\alpha \in I_{l(j)}(z)} \sum_{k=1}^{3} \varepsilon_i \, \varepsilon_\alpha \, q_\delta^{(k)}(x, v, x_i, v_i, x_\alpha, v_\alpha, \theta_\alpha) \Big|}{\sum_{\alpha \in I_{l(j)}(z)} \sum_{k=1}^{3} q_{\delta,\max}^{(k)}(x, v, x_i, v_i, x_\alpha, v_\alpha, \theta_\alpha)} \,,$$

go to **1.**

5.4. *Add the particle with position x, velocity v and sign*

$$\text{sign}\left(\sum_{\alpha\in I_{l(j)}(z)}\sum_{k=1}^{3}\varepsilon_i\,\varepsilon_\alpha\,q_\delta^{(k)}(x,v,x_i,v_i,x_\alpha,v_\alpha,\theta_\alpha)\right)$$

to the system and go to **1.**

6. *Perform a jump according to the sink term.*

6.1. *For given i,j, generate $v\in\mathcal{R}^3$ according to the density*

$$\frac{[c_0+c_1\,\|v_j-v_i+v\|]\,M_{0,\delta}(v)}{\int_{\mathcal{R}^3}[c_0+c_1\,\|v_j-v_i+u\|]\,M_{0,\delta}(u)\,du}\,. \tag{4.53}$$

6.2. *With probability*

$$1-\frac{\left|\sum_{\alpha\in I_{l(i)}(z)\,:\,x_\alpha\in D_m}\varepsilon_\alpha\,C_\beta\,\|v_j-v_\alpha+v\|^\beta\right|}{\sum_{\alpha\in I_{l(i)}(z)\,:\,x_\alpha\in D_m}\left[c_0+c_1\,\|v_j-v_\alpha+v\|\right]}\,,$$

go to **1.**

6.3. *If*

$$\sum_{\alpha\in I_{l(i)}(z)\,:\,x_\alpha\in D_m}\varepsilon_\alpha\,\|v_j-v_\alpha+v\|^\beta \;>\; 0\,,$$

then delete particle i and go to **1.**

6.4. *Double particle i and go to* **1.**

In the case $\beta=0$ (with $c_0=C_0$ and $c_1=0$), Algorithm 4.4 takes the form:

Algorithm 4.5 (Pseudo-Maxwell molecules)

1. *Make a time step with parameter*

$$\frac{8\pi\,C_0\,g^{(n)}\,N_m(z)^2}{|D_m|}\,.$$

Stop, when the final time is exceeded.

2. *Choose indices $i,j\,:\,x_i,x_j\in D_m$ uniformly.*

3. *This step is redundant.*

4. *With probabilities $1/4$, choose $k=1,2,3$ or go to* **6.**

5. *Perform a jump according to the source term.*

5.1. *For given* i, j , *generate* $x \in D$ *and* $v \in \mathcal{R}^3$.

5.1.1. *Generate* x *uniformly in the cell* D_m .

5.1.2. *Generate* $w \in \mathcal{R}^3$ *according to the density* $M_{v_i,\delta}(w)$.

5.1.3. *If* $k = 3$, *then choose* $v = w$ *and go to* **5.2.1.**

5.1.4. *Generate* $e \in \mathcal{S}^2$ *uniformly, calculate* $v = v'(v_j, w, e)$ *and go to* **5.2.2.**

5.2. *For given* i, j, x *and* v , *generate the auxiliary parameter* θ .

5.2.1. *Generate* $\tilde{w} \in \mathcal{R}^3$ *according to the density* $M_{v_i,\delta}(v + \tilde{w})$ *and go to* **5.2.4.**

5.2.2. *Generate* $\tilde{w} \in \mathcal{R}^3$ *according to the density* $M_{v_i,\delta}(v + \tilde{w})$.

5.2.3. *With probability*

$$1 - \frac{\|v_j - v\|}{\|v_j - v + \pi_{v_j - v}(\tilde{w})\|} ,$$

go to **5.2.2.**

5.2.4. *Compute* $\theta_\alpha = \pi_{v_\alpha - v}(\tilde{w})$, $\alpha \in I_{l(j)}(z)$.

5.3. *With probability*

$$1 - \frac{\left|\sum_{\alpha \in I_{l(j)}(z)\,:\,x_\alpha \in D_m} \varepsilon_\alpha \left[\frac{2}{\|v_\alpha - v\|\,\|v_\alpha - v + \theta_\alpha\|}\left(\int_{\Gamma(v_\alpha - v)} M_{v_i,\delta}(v + c)\,dc\right) - \pi\, M_{v_i,\delta}(v)\right]\right|}{\sum_{\alpha \in I_{l(j)}(z)\,:\,x_\alpha \in D_m} \left[\frac{2}{\|v_\alpha - v\|\,\|v_\alpha - v + \theta_\alpha\|}\left(\int_{\Gamma(v_\alpha - v)} M_{v_i,\delta}(v + c)\,dc\right) + \pi\, M_{v_i,\delta}(v)\right]} , \tag{4.54}$$

go to **1.**

5.4. *Add the particle with position* x , *velocity* v *and sign*

$$\operatorname{sign}\left(\varepsilon_i \sum_{\alpha \in I_{l(j)}(z)\,:\,x_\alpha \in D_m} \varepsilon_\alpha \times \left[\frac{2}{\|v_\alpha - v\|\,\|v_\alpha - v + \theta_\alpha\|}\left(\int_{\Gamma(v_\alpha - v)} M_{v_i,\delta}(v + c)\,dc\right) - \pi\, M_{v_i,\delta}(v)\right]\right) \tag{4.55}$$

to the system and go to **1.**

6. *Perform a jump according to the sink term.*

6.1. *This step is redundant.*

6.2. *With probability*

$$1 - \frac{\left|\sum_{\alpha \in I_{l(i)}(z)\,:\,x_\alpha \in D_m} \varepsilon_\alpha\right|}{\sum_{\alpha \in I_{l(i)}(z)\,:\,x_\alpha \in D_m} 1},$$

go to **1.**

6.3. *If*

$$\sum_{\alpha \in I_{l(i)}(z)\,:\,x_\alpha \in D_m} \varepsilon_\alpha \;>\; 0\,,$$

then delete particle i *and go to* **1.**

6.4. *Double particle* i *and go to* **1.**

In the case $\beta = 1$ (with $c_0 = 0$ and $c_1 = C_1$), we make the choice (4.41) instead of (4.40). One obtains

$$\hat{s}_\delta(z, j, i, v) = \hat{s}_{\delta,\max}(z, j, i, v) = 4\pi\, C_1\, h(x_i, x_j) \int_{\mathcal{R}^3} \|v_i - u\|\, M_{v_j,\delta}(u)\, du\,.$$

Algorithm 4.4 (with step 6 from Algorithm 4.3) takes the form:

Algorithm 4.6 (Hard sphere model)

1. *Make a time step with parameter*

$$\frac{8\pi\, C_1\, g^{(n)}\, N_k^2}{|D_k|} \left(V_{\mathrm{rel}}(z, m) + \sqrt{\frac{2\,\delta}{\pi}} \right).$$

Stop, when the final time is exceeded.

2. *Choose indices* $i, j \,:\, x_i, x_j \in D_m$ *uniformly.*

3. *With probability*

$$1 - \frac{\int_{\mathcal{R}^3} \|v_j - u\|\, M_{v_i,\delta}(u)\, du}{V_{\mathrm{rel}}(z, m) + 2\sqrt{\frac{2\,\delta}{\pi}}}\,, \tag{4.56}$$

go to **1.**

4. *With probabilities* $1/4$, *choose* $k = 1, 2, 3$ *or go to* **6.**

5. *Perform a jump according to the source term.*

5.1. *For given* i, j, *generate* $x \in D$ *and* $v \in \mathcal{R}^3$.

5.1.1. *Generate* x *uniformly in the cell* D_m.

5.1.2. *Generate $w \in \mathcal{R}^3$ according to the density*

$$\frac{\|v_j - w\| \, M_{v_i,\delta}(w)}{\int_{\mathcal{R}^3} \|v_j - u\| \, M_{v_i,\delta}(u) \, du} \,. \tag{4.57}$$

5.1.3. *If $k = 3$, then choose $v = w$ and go to* **5.3.**

5.1.4. *Generate $e \in \mathcal{S}^2$ uniformly and calculate $v = v'(v_j, w, e)$.*

5.2. *This step is redundant.*

5.3. *With probability*

$$1 - \frac{\left|\sum_{\alpha \in I_{l(j)}(z)\,:\,x_\alpha \in D_m} \varepsilon_\alpha \left[\frac{2}{\|v_\alpha - v\|} \left(\int_{\Gamma(v_\alpha - v)} M_{v_i,\delta}(v+c)\, dc\right) - \pi \, M_{v_i,\delta}(v) \, \|v - v_\alpha\|\right]\right|}{\sum_{\alpha \in I_{l(j)}(z)\,:\,x_\alpha \in D_m} \left[\frac{2}{\|v_\alpha - v\|} \left(\int_{\Gamma(v_\alpha - v)} M_{v_i,\delta}(v+c)\, dc\right) + \pi \, M_{v_i,\delta}(v) \, \|v - v_\alpha\|\right]} \,, \tag{4.58}$$

go to **1.**

5.4. *Add the particle with position x, velocity v and sign*

$$\operatorname{sign}\left(\varepsilon_i \sum_{\alpha \in I_{l(j)}(z)\,:\,x_\alpha \in D_m} \varepsilon_\alpha \times \left[\frac{2}{\|v_\alpha - v\|} \left(\int_{\Gamma(v_\alpha - v)} M_{v_i,\delta}(v+c)\, dc\right) - \pi \, M_{v_i,\delta}(v) \, \|v - v_\alpha\|\right]\right) \tag{4.59}$$

to the system and go to **1.**

6. *Perform a jump according to the sink term.*

6.1. *This step is redundant.*

6.2. *With probability*

$$1 - \frac{\left|\sum_{\alpha \in I_{l(i)}(z)\,:\,x_\alpha \in D_m} \varepsilon_\alpha \int_{\mathcal{R}^3} \|v_j - u\| \, M_{v_\alpha,\delta}(u) \, du\right|}{\sum_{\alpha \in I_{l(i)}(z)\,:\,x_\alpha \in D_m} \int_{\mathcal{R}^3} \|v_j - u\| \, M_{v_\alpha,\delta}(u) \, du} \,, \tag{4.60}$$

go to **1.**

6.3. *If*

$$\sum_{\alpha \in I_{l(i)}(z)\,:\,x_\alpha \in D_m} \varepsilon_\alpha \int_{\mathcal{R}^3} \|v_j - u\| \, M_{v_\alpha,\delta}(u) \, du \quad > \quad 0 \,, \tag{4.61}$$

then delete particle i and go to **1.**

6.4. *Double particle i and go to* **1.**

4.2.4 Comments

The algorithms described above are ready for implementation. The integrals in (4.51), (4.56), (4.60), (4.61) are explicitly known (cf. (4.50)). Densities (4.52) and (4.53) and (4.57) are generated in analogy with (3.94). The integrals in (4.54), (4.55), (4.58), (4.59) are obtained from Lemma 6.8 as

$$\int_{\Gamma(v_\alpha - v)} M_{v_i,\delta}(v+c)\,dc = \frac{1}{\sqrt{2\pi\,\delta}}\,\exp\left(-\frac{(v_i - v, v_\alpha - v)^2}{2\,\delta\,\|v_\alpha - v\|^2}\right).$$

The main new component of the source-sink algorithms for the nonlinear equation is the smoothing kernel $M_{0,\delta}$. This parameter allowed us to apply all the techniques developed for the linearized equation. Cancellation is achieved when positive and negative particles are close to each other, so that the corresponding functions q_δ in the acceptance probabilities (4.46) have similar absolute values. When δ is chosen too small, then these functions become more and more singular (cf. (4.58)) so that the cancellation effect is drastically reduced.

As in the linearized case, the introduction of the clusters avoids the inefficient calculation of the rejection probabilities (4.46) and the signs (4.47) of the new particles. The clusters can depend on the spatial cells, since the corresponding processes are independent. If there are only few particles in a cell, then clusters do not seem to make sense. However, the clusters from Example 3.19 would work. If there was only one particle in a cluster, then there would be no cancellation. But if the few particles in the cell had velocities far from each other, they would not create a cancellation effect anyway.

A new component of the algorithms in the nonlinear case, which is also related to the efficiency issue, is the function $\tilde{E}_{\delta,\max}(z,m)$. This parameter avoids calculating the waiting time parameter

$$g^{(n)} \sum_{i,j=1}^{N} E_{\delta,\max}(x_i, v_i, x_j, v_j)$$

instead of (4.43), and generating the indices according to the probabilities

$$\frac{E_{\delta,\max}(x_i, v_i, x_j, v_j)}{\sum_{k,l=1}^{N} E_{\delta,\max}(x_k, v_k, x_l, v_l)}$$

instead of the uniform distribution, both related to N^2-effort.

4.3 The combined algorithm

Finally, the linear and the nonlinear parts are combined to get an algorithm for the full Boltzmann equation. For example, the combined collision process in a cell D_m is obtained by using the waiting time parameter (cf. (3.12), (4.13))

$$\sum_{i:\, x_i \in D_m} E_{\max}(x_i, v_i) + \frac{1}{2\,|D_m|}\, g^{(n)}\, N_m(z)^2\, \tilde{E}_0(z,m)\,. \qquad (4.62)$$

Then the linear algorithm is applied with probability

$$\frac{\sum_{i:\, x_i \in D_m} E_{\max}(x_i, v_i)}{\sum_{i:\, x_i \in D_m} E_{\max}(x_i, v_i) + \frac{1}{2\,|D_m|}\, g^{(n)}\, N_m(z)^2\, \tilde{E}_0(z,m)}\,,$$

and the nonlinear algorithm is used with the remaining probability. Analogously, the combined source-sink process in a cell D_m is obtained by using the waiting time parameter (cf. (3.50), (4.43))

$$4 \sum_{i:\, x_i \in D_m} E_{\max}(x_i, v_i) + \frac{2}{|D_m|}\, g^{(n)}\, N_m(z)^2\, \tilde{E}_{\delta,\max}(z,m)\,. \tag{4.63}$$

The factor 4 in the expression (4.63) (compared to (4.62)) provides an instructive illustration of the relationship between the collision process and the source-sink process. The jump events of the collision process consist of transformations of one particle into three (linear part) or of two particles into six (nonlinear part). In the source-sink process these events are splitted into either deletion or (three types of) creation of particles. Therefore, the number of jump attempts increases by a factor 4 .

limiting equations

The limiting equations for the combined algorithm are obtained by combining the corresponding equations for the linear and nonlinear parts, respectively. For example, equations (3.6) and (4.10) provide equation (2.23) for the combined collision process.

The limiting equation for the combined source-sink process is obtained from (3.36) and (4.32) as

$$\begin{aligned}
&\frac{d}{dt} \int_D \int_{\mathcal{R}^3} \varphi(x,v)\, f_d(t,x,v)\, dv\, dx = \\
&\quad \int_D \int_{\mathcal{R}^3} \int_D \int_{\mathcal{R}^3} \int_{\mathcal{S}^2} \Big[\varphi(x,v'(v,w,e)) + \varphi(x,w'(v,w,e)) - \varphi(x,v) - \varphi(y,w)\Big] \times \\
&\qquad\qquad h(x,y)\, B(v,w,e)\, M(x,v)\, f_d(t,y,w)\, de\, dw\, dy\, dv\, dx \;+ \\
&\quad \frac{1}{2} \int_D \int_{\mathcal{R}^3} \int_D \int_{\mathcal{R}^3} \int_{\mathcal{S}^2} \Big[\varphi(x,v'(v,w,e)) + \varphi(x,w'(v,w,e)) - \varphi(x,w) - \varphi(y,v)\Big] \times \\
&\qquad\qquad h(x,y)\, B(v,w,e)\, \tilde{f}_d^{(\delta)}(t,x,w)\, f_d(t,y,v)\, de\, dw\, dy\, dv\, dx\,.
\end{aligned}$$

The collision process and the source-sink process have (slightly) different limiting equations. Roughly speaking, more smoothing is involved in the equation for the source-sink process. Thus, there is a deviation from the DSMC limiting equation (dependent on cell size parameter Δx and the velocity smoothing parameter δ).

There is some deviation even in the linearized case, since equation (3.37) is different from equation (3.7) (cf. the second part of (2.21)). This difference is due to the fact that the position of the new particles are generated uniformly. The generation of uniform positions for the new particles in the source-sink approach is quite natural. The existing particles do not have an identical influence on the velocity of the new particle, so that there is no reason to use some of the positions of the old particles for the new particle, instead of the uniform.

conservation properties

The combined collision process satisfies conservation properties during each jump, since (cf. (3.4)

$$\varphi(v_i) = \varphi(v'(v_i, w, e)) + \varphi(w'(v_i, w, e)) - \varphi(w)$$

and (cf. (4.3)-(4.6))

$$\begin{aligned} \varphi(v_i) - \varphi(v_j) &= -\varphi(v'(v_i, v_j, e)) - \varphi(w'(v_i, v_j, e)) + 2\,\varphi(v_i)\,, \\ \varphi(v_i) + \varphi(v_j) &= -\varphi(v'(v_i, v_j, e)) - \varphi(w'(v_i, v_j, e)) + 2\,\varphi(v_i) + 2\,\varphi(v_j)\,. \end{aligned}$$

This is not the case for the source-sink process. However, the weak form of the limiting equations implies that asymptotic conservation properties hold. Moreover, considering the pre-limit expressions for the empirical measures (3.1), one can establish that the expected values of momentum and energy are conserved.

mixed approach

The generality in the construction of the algorithms allows one to introduce various combinations of the different ingredients. The collision process has better conservation properties and a more accurate limiting equation, but leads to a blow-up of the system. The source-sink process does not have very desirable properties, but it provides a way to reduce/avoid the blow-up. It would be possible to model the linear term with the source-sink process and the nonlinear term with the collision process. The limiting equation depends on the way of combination.

Alternatively, one might try using the collision process, when there are only few particles in a spatial cell, and the source-sink process otherwise.

5 Conclusions and outlook

The deviational particle approach to the numerical treatment of the Boltzmann equation goes back to [1]. A similar idea was published in [7]. More details about the collision processes and the modeling of boundary conditions are given in [2], where also methods of particle removal at the boundary and via a cancellation radius are considered. The source-sink idea was described in [13] as an alternative "which removes the necessity for a cancellation step". An extended version was given in [12]. The treatment of the source-sink method was restricted to the hard-sphere model and the linearized Boltzmann equation.

The deviational particle approach is a special case of the general variance reduction method known as "control variates" (cf., e.g., [9]). In contrast to the well-known "importance sampling" technique, where approximate knowledge about the solution is used to improve the probabilistic sampling procedure, this method uses the knowledge as a deterministic approximation to the solution and leaves the stochastic simulation part for an appropriately transformed problem describing the deviation from that approximation. I am not aware of any previous applications of the control variates technique to the solution of nonlinear equations. The main question is whether the transformed problem can be solved in a sufficiently efficient way so that there remains a net variance reduction effect. However, in my opinion this general variance reduction technique has the potential to give significant improvements in the context of low Mach number rarefied gas flows.

The original motivation for this paper was to understand the deviational particle approach from the point of view of Markov jump processes and to provide the basis for a theoretical convergence study in the spirit of [21]. This task was easy for the collision process, but turned out to be rather involved as far as the source-sink process was concerned. In particular, the generalization to the nonlinear equation was not so straightforward as one might have expected. Moreover, the extension to interaction models beyond the hard-sphere case was a real challenge. Some new ideas were needed in order to treat even the case of pseudo-Maxwell molecules. This model is not really important in the context of engineering applications. However, it is a very useful tool for validating numerical algorithms (in particular, new collision routines), since complete analytical solutions are available in the spatially homogeneous case.

There are further modifications in the source-sink process, as compared to the papers cited above. The change of the reference Maxwellian is treated in a different way. The collision step is performed in the continuous time setup, as in the Bird scheme in contrary to Nanbu's scheme. The single particle majorant makes the generation of particles according to the source term more directly related to usual collisions. The introduction of clusters replaces the method of summing up only a small randomly chosen number of terms.

The main purpose of the paper is the detailed description of the deviational particle Monte Carlo method for the nonlinear Boltzmann equation with a general collision kernel. The limiting equations are derived in a heuristic way and provide a justification for the method. A rigorous proof can be obtained following the lines for standard DSMC, but doing this would have made the paper even longer. The algorithm presented in this paper contains many degrees of freedom. These parameters are subject to certain restrictions, but otherwise they can be chosen arbitrarily. The restrictions guarantee that the algorithm converges to the limiting equations described in the paper. Intensive numerical experiments will be necessary in order to find out the best choices of the parameters (velocity clusters, smoothing parameter).

The main challenge for future research is the study of the stationary behavior of the processes. Even in the case of standard DSMC only partial results are available (see [4]). The first question is whether the cancellation effect achieved by the source-sink modeling is strong enough to keep the number of particles bounded. Otherwise, alternative reduction methods have to be developed. The second problem concerns the conservation of momentum and energy in the source-sink process. Conservation on average is a rather weak property. The behavior of the fluctuations around the mean value for large times should be studied, as well as corresponding properties of the steady state.

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6 Appendix

6.1 Collision transformations and collision kernels

Here we introduce the collision transformation

$$v^* = v^*(v, w, e) = v + e\,(e, w - v)\,, \qquad w^* = w^*(v, w, e) = w - e\,(e, w - v)\,. \quad (6.1)$$

While (1.4) is commonly used in the context of numerics, (6.1) is more convenient for theoretical derivations (cf. [5] or [19]). Both transformations are equivalent in the following sense.

Lemma 6.1 *Let γ and ψ be any functions such that the integrals exist. Then*

$$\int_{\mathcal{S}^2} B(v, w, e)\, \gamma(v')\, \psi(w')\, de = \int_{\mathcal{S}^2} B^*(v, w, e)\, \gamma(v^*)\, \psi(w^*)\, de\,, \quad (6.2)$$

where

$$B^*(v, w, e) = 2\,|(e, u)|\, B(v, w, 2\,e\,(e, u) - u)\,, \quad (6.3)$$

$$B(v, w, e) = \frac{1}{\sqrt{2\,(1 + (e, u))}}\, B^*\Big(v, w, \frac{e + u}{\sqrt{2\,(1 + (e, u))}}\Big) \quad (6.4)$$

and

$$u = u(v, w) = \frac{w - v}{\|w - v\|}\,. \quad (6.5)$$

Proof. According to [17, Section 1.2] one obtains

$$\begin{aligned}
&\int_{\mathcal{S}^2} B(v, w, e)\, \gamma(v')\, \psi(w')\, de = \int_{\mathcal{S}^2} \Phi(e + u)\, de = 2 \int_{\mathcal{S}^2} |(e, u)|\, \Phi(2\,e\,(e, u))\, de \\
&= \int_{\mathcal{S}^2} |(e, u)|\, B(v, w, 2\,e\,(e, u) - u) \times \\
&\qquad \gamma\Big(v + \frac{\|v - w\|}{2}\, 2\,e\,(e, u)\Big)\, \psi\Big(w - \frac{\|v - w\|}{2}\, 2\,e\,(e, u)\Big) de \\
&= 2 \int_{\mathcal{S}^2} |(e, u)|\, B(v, w, 2\,e\,(e, u) - u)\, \gamma(v + e\,(e, w - v))\, \psi(w - e\,(e, w - v))\, de \\
&= \int_{\mathcal{S}^2} B^*(v, w, e)\, \gamma(v^*)\, \psi(w^*)\, de\,,
\end{aligned}$$

and the proof is completed. ■

According to Lemma 6.1 one obtains equivalence of the equations with different collision transformations. In particular, (6.2) implies

$$\int_{\mathcal{S}^2} B(v, w, e)\, de = \int_{\mathcal{S}^2} B^*(v, w, e)\, de\,.$$

Collision kernels of the form

$$B^*(v,w,e) = b^*(\|v-w\|, |(e,u)|) \tag{6.6}$$

correspond to (cf. (6.4))

$$\begin{aligned} B(v,w,e) &= \frac{1}{\sqrt{2\,(1+(e,u))}}\, b^*\left(\|v-w\|, \left|\frac{(e,u)+1}{\sqrt{2\,(1+(e,u))}}\right|\right) \\ &= \frac{1}{\sqrt{2\,(1+(e,u))}}\, b^*\left(\|v-w\|, \sqrt{\frac{1+(e,u)}{2}}\right). \end{aligned}$$

Thus, the kernels B have the form (1.5) with

$$b(x,y) = \frac{1}{\sqrt{2\,(1+y)}}\, b^*\left(x, \sqrt{\frac{1+y}{2}}\right), \qquad x \ge 0\,, \quad y \in [-1,1]\,.$$

On the other hand, given a kernel B of the form (1.5), one obtains (cf. (6.3))

$$\begin{aligned} B^*(v,w,e) &= 2\,|(e,u)|\, b(\|v-w\|, (2\,e\,(e,u)-u,u)) \\ &= 2\,|(e,u)|\, b(\|v-w\|, 2\,(e,u)^2-1)\,. \end{aligned}$$

Thus, the corresponding kernel B^* has the form (6.6) with

$$b^*(x,y) = 2\,y\, b(x, 2\,y^2-1)\,, \qquad x \ge 0\,, \quad y \in [0,1]\,. \tag{6.7}$$

Note that

$$B(v,w,-e) = B(w,v,e)\,. \tag{6.8}$$

For the **variable hard sphere model** (3.2), kernel (6.3) takes the form

$$B^*(v,w,e) = 2\,C_\beta\, |(e,u)|\, \|v-w\|^\beta = 2\,C_\beta\, |(e,v-w)|\, \|v-w\|^{\beta-1}\,. \tag{6.9}$$

For the **hard sphere model** ($\beta = 1$ with $C_1 = d^2/4$, where d is the diameter) one obtains

$$B(v,w,e) = \frac{d^2}{4}\, \|w-v\| \tag{6.10}$$

and

$$B^*(v,w,e) = \frac{d^2}{2}\, |(e,w-v)|\,. \tag{6.11}$$

In the case of **pseudo-Maxwell molecules** ($\beta = 0$), kernel (6.9) takes the form (cf. (6.5))

$$B^*(v,w,e) = 2\,C_0\, |(e,u)|\,.$$

Lemma 6.2 *Consider collision kernels of the form (1.5). Let* γ *and* ψ *be any functions such that the integrals exist. Then*

$$\int_{\mathcal{R}^3}\int_{\mathcal{R}^3}\int_{\mathcal{S}^2} \varphi(v)\, B(v,w,e)\, \gamma(w')\, \psi(v')\, de\, dw\, dv = \int_{\mathcal{R}^3}\int_{\mathcal{R}^3}\int_{\mathcal{S}^2} \varphi(v')\, B(v,w,e)\, \gamma(w)\, \psi(v)\, de\, dw\, dv\,. \tag{6.12}$$

Property (6.12) holds when replacing B, v', w' *by* B^*, v^*, w^* .

Proof. The assertion follows from [17, Lemma 1.10]. For kernels of the form (6.6) one obtains

$$\begin{aligned}
\int_{\mathcal{R}^3}\int_{\mathcal{R}^3}\int_{\mathcal{S}^2} \varphi(v)\, B^*(v,w,e)\, \gamma(w^*)\, \psi(v^*)\, de\, dw\, dv = \\
\int_{\mathcal{R}^3}\int_{\mathcal{R}^3}\int_{\mathcal{S}^2} \varphi(v)\, B(v,w,e)\, \gamma(w')\, \psi(v')\, de\, dw\, dv \\
= \int_{\mathcal{R}^3}\int_{\mathcal{R}^3}\int_{\mathcal{S}^2} \varphi(v')\, B(v,w,e)\, \gamma(w)\, \psi(v)\, de\, dw\, dv \\
= \int_{\mathcal{R}^3}\int_{\mathcal{R}^3}\int_{\mathcal{S}^2} \varphi(v^*)\, B^*(v,w,e)\, \gamma(w)\, \psi(v)\, de\, dw\, dv\,,
\end{aligned}$$

according to Lemma 6.1. ■

Lemma 6.3 *Consider collision kernels of the form (1.5). Let* γ *and* ψ *be any functions such that the integrals exist. Then*

$$\int_{\mathcal{R}^3}\int_{\mathcal{S}^2} B(v,w,e)\, \gamma(w')\, \psi(v')\, de\, dw = \int_{\mathcal{R}^3} \kappa(v,w)\, \psi(w)\, dw\,, \tag{6.13}$$

where

$$\kappa(v,w) = \frac{4}{\|w-v\|} \int_{\Gamma(w-v)} \frac{b\left(\|w-v+u\|, \frac{2\,\|w-v\|^2}{\|w-v+u\|^2} - 1\right)}{\|w-v+u\|}\, \gamma(v+u)\, du \tag{6.14}$$

and $\Gamma(v)$ *denotes the plane through the origin orthogonal to* v *. Moreover,*

$$\int_{\mathcal{R}^3} \varphi(v)\, \kappa(v,w)\, dv \;=\; \int_{\mathcal{R}^3} \varphi(v)\, \nu(w,dv)\,, \tag{6.15}$$

where

$$\nu(w,dv) = \int_{\mathcal{R}^3}\int_{\mathcal{S}^2} \delta_{v'(w,u,e)}(dv)\, B(w,u,e)\, \gamma(u)\, de\, du$$

and φ *is any appropriate test function.*

Proof. Using Lemma 6.1 and the substitution $w - v \to \tilde{w} \to w$, one obtains

$$\int_{\mathcal{R}^3}\int_{\mathcal{S}^2} B(v,w,e)\,\gamma(w')\,\psi(v')\,de\,dw = \int_{\mathcal{R}^3}\int_{\mathcal{S}^2} B^*(v,w,e)\,\gamma(w^*)\,\psi(v^*)\,de\,dw =$$
$$\int_{\mathcal{R}^3}\int_{\mathcal{S}^2} b^*(\|v-w\|,|(e,u)|)\,\gamma(w^*)\,\psi(v^*)\,de\,dw = \tag{6.16}$$
$$\int_{\mathcal{R}^3}\int_{\mathcal{S}^2} b^*(\|w\|,|(e,w)|/\|w\|)\,\gamma(v+w-e\,(e,w))\,\psi(v+e\,(e,w))\,de\,dw\,.$$

Changing the order of integration and introducing a rotation $Q(e)w \to \tilde{w} \to w$ such that the first coordinate axis is parallel to e, (6.16) takes the form

$$\int_{\mathcal{S}^2}\int_{\mathcal{R}^3} b^*(\|w\|,|w_1|/\|w\|)\,\gamma(v+Q(e)'w-e\,w_1)\,\psi(v+e\,w_1)\,dw\,de \tag{6.17}$$
$$= \int_{\mathcal{S}^2}\int_{\mathcal{R}}\left[\int_{\Gamma(e)} b^*(\|e\,x+y\|,\|e\,x\|/\|e\,x+y\|)\,\gamma(v+y)\,dy\right]\psi(v+e\,x)\,dx\,de\,.$$

Considering x and e as spherical coordinates, i.e. $x^2\,dx\,de = dw$, one obtains from (6.17)

$$2\int_{\mathcal{R}^3}\|w\|^{-2}\left[\int_{\Gamma(w)} b^*(\|w+y\|,\|w\|/\|w+y\|)\,\gamma(v+y)\,dy\right]\psi(v+w)\,dw\,.$$

The factor 2 occurs due to symmetry with respect to x and $-x$. The substitution $v + w \to \tilde{w} \to w$ gives

$$2\int_{\mathcal{R}^3}\|w-v\|^{-2}\left[\int_{\Gamma(w-v)} b^*(\|w-v+y\|,\|w-v\|/\|w-v+y\|)\,\gamma(v+y)\,dy\right]\psi(w)\,dw\,.$$

Thus, assertion (6.13) follows from (6.7). Lemma 6.2 and (6.13) imply

$$\int_{\mathcal{R}^3}\varphi(v)\int_{\mathcal{R}^3}\kappa(v,w)\,\psi(w)\,dw\,dv = \int_{\mathcal{R}^3}\varphi(v)\int_{\mathcal{R}^3}\int_{\mathcal{S}^2} B(v,w,e)\,\gamma(w')\,\psi(v')\,de\,dw\,dv$$
$$= \int_{\mathcal{R}^3}\int_{\mathcal{R}^3}\int_{\mathcal{S}^2}\varphi(v')\,B(v,w,e)\,\gamma(w)\,\psi(v)\,de\,dw\,dv\,,$$

and assertion (6.15) follows for $\psi = \delta_w$. ■

Corollary 6.4 *Let the assumptions of Lemma 6.3 be fulfilled. Then*

$$\int_{\mathcal{R}^3}\int_{\mathcal{S}^2} B(v,w,e)\,\gamma(v')\,\psi(w')\,de\,dw = \int_{\mathcal{R}^3}\tilde{\kappa}(v,w)\,\psi(w)\,dw\,,$$

where

$$\tilde{\kappa}(v,w) = \frac{4}{\|w-v\|}\int_{\Gamma(w-v)}\frac{b\left(\|w-v+u\|,1-\frac{2\,\|w-v\|^2}{\|w-v+u\|^2}\right)}{\|w-v+u\|}\,\gamma(v+u)\,du\,. \tag{6.18}$$

Moreover,

$$\int_{\mathcal{R}^3} \varphi(v)\, \tilde{\kappa}(v,w)\, dv \;=\; \int_{\mathcal{R}^3} \varphi(v)\, \tilde{\nu}(w,dv)\,,$$

where

$$\tilde{\nu}(w,dv) = \int_{\mathcal{R}^3} \int_{\mathcal{S}^2} \delta_{w'(w,u,e)}(dv)\, B(w,u,e)\, \gamma(u)\, de\, du$$

and φ is any appropriate test function.

Proof. Note that (cf. (1.4))

$$\begin{aligned}\int_{\mathcal{S}^2} B(v,w,e)\,\gamma(v')\,\psi(w')\,de &= \int_{\mathcal{S}^2} B(v,w,-e)\,\gamma(v'(v,w,-e))\,\psi(w'(v,w,-e))\,de \\ &= \int_{\mathcal{S}^2} B(v,w,-e)\,\gamma(w')\,\psi(v')\,de\,.\end{aligned}$$

Since the kernel $\tilde{B}(v,w,e) = B(v,w,-e)$ has the form (1.5) with $\tilde{b}(x,y) = b(x,-y)$, the assertions follow from Lemma 6.3. ■

Remark 6.5 *In the variable hard sphere case (3.2), both functions (6.14) and (6.18) take the form*

$$\kappa_\beta(v,w) = 4\, C_\beta\, \|w-v\|^{-1} \int_{\Gamma(w-v)} \|w-v+y\|^{\beta-1}\, \gamma(v+y)\, dy\,.$$

In the hard sphere case (6.10), one obtains

$$\kappa_1(v,w) = \frac{d^2}{\|w-v\|} \int_{\Gamma(w-v)} \gamma(v+y)\, dy\,.$$

6.2 Properties of the Maxwellian

Lemma 6.6 (non-central moment) *The Maxwellian*

$$M_{V,T}(w) = \frac{1}{(2\pi\, T)^{3/2}}\, \exp\left(-\frac{\|w-V\|^2}{2\,T}\right) \tag{6.19}$$

satisfies

$$\int_{\mathcal{R}^3} \|w\|\, M_{V,T}(w)\, dw = \tag{6.20}$$

$$\sqrt{\frac{2\,T}{\pi}} \left\{ \exp\left(-\|u\|^2\right) + \left(\frac{1}{\|u\|} + 2\,\|u\|\right) \int_0^{\|u\|} \exp\left(-r^2\right) dr \right\},$$

where

$$u = \frac{V}{\sqrt{2\,T}}\,.$$

Proof. The substitution

$$w = \sqrt{2\,T}\,\tilde{w}\,, \qquad dw = (2\,T)^{3/2}\,d\tilde{w}$$

implies

$$\begin{aligned}\int_{\mathcal{R}^3} \|w\|\, M_{V,T}(w)\, dw &= \sqrt{\frac{2\,T}{\pi^3}} \int_{\mathcal{R}^3} \|\tilde{w}\|\, \exp\left(-\frac{\|\sqrt{2\,T}\,\tilde{w} - V\|^2}{2\,T}\right) d\tilde{w} \\ &= \frac{1}{\pi}\sqrt{\frac{2\,T}{\pi}} \int_{\mathcal{R}^3} \|w\|\, \exp\left(-\|w-u\|^2\right) dw\,. \end{aligned} \tag{6.21}$$

Expressing w in spherical coordinates

$$w = r\,e\,, \quad e = (\cos\varphi_1, \sin\varphi_1\, \cos\varphi_2, \sin\varphi_1\, \sin\varphi_2)\,, \qquad dw = r^2\, dr\, \sin\varphi_1\, d\varphi_1\, d\varphi_2\,,$$

where the first axis is parallel to u, one obtains

$$\int_{\mathcal{R}^3} \|w\|\, \exp\left(-\|w-u\|^2\right) dw = \tag{6.22}$$

$$\int_0^\infty r^2\, dr \int_0^{2\pi} d\varphi_2 \int_0^\pi \sin\varphi_1\, d\varphi_1\, r\, \exp\left(-\left[r^2 - 2\,r\,\|u\|\, \cos\varphi_1 + \|u\|^2\right]\right)$$

$$= \; 2\,\pi\, \exp\left(-\|u\|^2\right) \int_0^\infty r^3\, \exp\left(-r^2\right) dr \int_0^\pi \sin\varphi_1\, d\varphi_1\, \exp\left(2\,r\,\|u\|\, \cos\varphi_1\right).$$

Note that

$$\int_0^\pi \exp\left(\alpha\, \cos x\right) \sin x\, dx = \int_{-1}^1 \exp(\alpha\, y)\, dy = \frac{1}{\alpha}\left[e^\alpha - e^{-\alpha}\right].$$

Thus, (6.22) implies

$$\int_{\mathcal{R}^3} \|w\|\, \exp\left(-\|w-u\|^2\right) dw = \tag{6.23}$$

$$\frac{\pi}{\|u\|}\, \exp\left(-\|u\|^2\right) \int_0^\infty r^2\, \exp\left(-r^2\right) \Big[\exp\left(2\,r\,\|u\|\right) - \exp\left(-2\,r\,\|u\|\right)\Big] dr$$

$$\begin{aligned} &= \frac{\pi}{\|u\|} \int_0^\infty r^2 \Big[\exp\left(-(r-\|u\|)^2\right) - \exp\left(-(r+\|u\|)^2\right)\Big] dr \\ &= \frac{\pi}{\|u\|}\left\{\int_{-\|u\|}^\infty (r+\|u\|)^2\, \exp\left(-r^2\right) dr - \int_{\|u\|}^\infty (r-\|u\|)^2\, \exp\left(-r^2\right)\Big] dr\right\} \\ &= \frac{\pi}{\|u\|}\left\{\int_{-\|u\|}^{\|u\|} \left(r^2 + \|u\|^2\right) \exp\left(-r^2\right) dr + \int_{\|u\|}^\infty 4\,r\,\|u\|\, \exp\left(-r^2\right)\Big] dr\right\}. \end{aligned}$$

Since

$$\int_0^x r^2\, \exp\left(-r^2\right) dr = -\frac{x}{2}\, \exp\left(-x^2\right) + \frac{1}{2}\int_0^x \exp\left(-r^2\right) dr$$

and

$$\int_x^\infty 2\,r\,\exp\left(-r^2\right)dr = \exp\left(-x^2\right),$$

one obtains from (6.23)

$$\int_{\mathcal{R}^3} \|w\|\,\exp\left(-\|w-u\|^2\right)dw =$$
$$\frac{\pi}{\|u\|}\left\{-\|u\|\,\exp\left(-\|u\|^2\right)+\int_0^{\|u\|}\exp\left(-r^2\right)dr+\right.$$
$$\left.2\,\|u\|^2\int_0^{\|u\|}\exp\left(-r^2\right)dr+2\,\|u\|\,\exp\left(-\|u\|^2\right)\right\}$$
$$= \frac{\pi}{\|u\|}\left\{\|u\|\,\exp\left(-\|u\|^2\right)+(1+2\,\|u\|^2)\int_0^{\|u\|}\exp\left(-r^2\right)dr\right\}. \qquad (6.24)$$

Finally, (6.21) and (6.24) imply (6.20) and the proof is completed. ∎

Remark 6.7 *Let $\Gamma(v)$ denote the plane through the origin orthogonal to v. The projection of a vector x onto $\Gamma(v)$ is obtained as*

$$\pi_v(x) = x - \frac{(x,v)}{\|v\|^2}\,v\,.$$

Note that

$$\begin{aligned}\pi_v(Qx) &= Qx - \frac{(Qx,v)}{\|v\|^2}\,v = Qx - \frac{(x,Q'v)}{\|Q'v\|^2}\,Q\,Q'v\\ &= Q\left[x - \frac{(x,Q'v)}{\|Q'v\|^2}\,Q'v\right] = Q\,\pi_{Q'v}(x)\,,\end{aligned}$$

where Q is any rotation.

Lemma 6.8 *The Maxwellian (6.19) satisfies*

$$\int_{\Gamma(v)} M_{V,T}(y)\,dy = \frac{1}{\sqrt{2\pi\,T}}\exp\left(-\frac{(V,v)^2}{2\,T\,\|v\|^2}\right) \qquad (6.25)$$

and

$$\int_{\Gamma(v)} \varphi(y)\,\psi(v,\|v+y\|)\,M_{V,T}(y)\,dy =$$
$$\left[\int_{\Gamma(v)} M_{V,T}(x)\,dx\right]\int_{\mathcal{R}^3}\varphi(\pi_v(w))\,\psi(v,\|v+\pi_v(w)\|)\,M_{V,T}(w)\,dw\,,$$

for any functions φ and ψ such that the integrals exist.

Proof. Consider a random variable ξ with density

$$p_\xi(y) = \frac{1}{\int_{\Gamma(v)} M_{V,T}(x)\,dx}\, M_{V,T}(y)\,\chi_{\Gamma(v)}(y)$$

and $\eta = Q'\xi$, where Q is any rotation. Note that $Qy \perp v$ iff $y \perp Q'(v)$. Since $\|Qv - V\| = \|v - Q'V\|$, it follows that

$$M_{V,T}(Qv) = M_{Q'V,T}(v)\,. \tag{6.26}$$

Thus, one obtains

$$\begin{aligned} p_\eta(y) &= p_\xi(Qy) = \frac{1}{\int_{\Gamma(v)} M_{V,T}(x)\,dx}\, M_{V,T}(Qy)\,\chi_{\Gamma(v)}(Qy) \\ &= \frac{1}{\int_{\Gamma(v)} M_{V,T}(x)\,dx}\, M_{Q'V,T}(y)\,\chi_{\Gamma(Q'(v))}(y)\,. \end{aligned} \tag{6.27}$$

In particular, (6.27) implies

$$\int_{\Gamma(v)} M_{V,T}(x)\,dx = \int_{\Gamma(Q'(v))} M_{Q'V,T}(y)\,dy\,. \tag{6.28}$$

Let Q be such that

$$Q'(v) = (0,0,c)\,. \tag{6.29}$$

One obtains from (6.28)

$$\int_{\Gamma(v)} M_{V,T}(x)\,dx = \frac{1}{\sqrt{2\pi\,T}} \exp\left(-\frac{(Q'V)_3^2}{2T}\right). \tag{6.30}$$

The third component of $Q'V$ corresponds to the distance between the center of the Maxwellian and the plane $\Gamma(v)$, which is $|(V,w)|/\|w\|$, so that (6.25) holds.

Remark 6.7 and (6.26) imply

$$\begin{aligned} &\int_{\mathcal{R}^3} \varphi(\pi_v(w))\,\psi(v,\|v+\pi_v(w)\|)\,M_{V,T}(w)\,dw \\ =& \int_{\mathcal{R}^3} \varphi(\pi_v(Qw))\,\psi(v,\|v+\pi_v(Qw)\|)\,M_{V,T}(Qw)\,dw \\ =& \int_{\mathcal{R}^3} \varphi(Q\,\pi_{Q'v}(w))\,\psi(v,\|v+Q\pi_{Q'v}(w)\|)\,M_{Q'V,T}(w)\,dw \\ =& \int_{\mathcal{R}^3} \varphi(Q\,\pi_{Q'v}(w))\,\psi(v,\|Q'v+\pi_{Q'v}(w)\|)\,M_{Q'V,T}(w)\,dw \end{aligned} \tag{6.31}$$

and

$$\int_{\Gamma(v)} \varphi(y)\,\psi(v,\|v+y\|)\,M_{V,T}(y)\,dy =$$

$$\begin{aligned}
& \int \chi_{\Gamma(v)}(Qy)\, \varphi(Qy)\, \psi(v, \|v+Qy\|)\, M_{V,T}(Qy)\, dy \\
= & \int_{\Gamma(Q'v)} \varphi(Qy)\, \psi(v, \|v+Qy\|)\, M_{V,T}(Qy)\, dy \\
= & \int_{\Gamma(Q'v)} \varphi(Qy)\, \psi(v, \|Q'v+y\|)\, M_{Q'V,T}(y)\, dy\,, \qquad (6.32)
\end{aligned}$$

for any rotation Q. If the rotation (6.29) is used, then (6.31) takes the form

$$\int_{\mathcal{R}^3} \varphi(Q(w_1,w_2,0))\, \psi\left(v, \sqrt{c^2+w_1^2+w_2^2}\right) M_{Q'V,T}(w)\, dw \qquad (6.33)$$

and (6.32) gives

$$\int\int \varphi(Q(y_1,y_2,0))\, \psi\left(v, \sqrt{c^2+y_1^2+y_2^2}\right) M_{Q'V,T}(y_1,y_2,0)\, dy_1\, dy_2\,. \qquad (6.34)$$

Note that

$$M_{V,T}(w_1,w_2,w_3) = \prod_{i=1}^{3} \frac{1}{\sqrt{2\pi\, T}} \exp\left(-\frac{(w_i-V_i)^2}{2T}\right).$$

Thus, (6.33) takes the form

$$\begin{aligned}
& \int\int \varphi(Q(w_1,w_2,0)) \times \qquad (6.35) \\
& \psi\left(v, \sqrt{c^2+w_1^2+w_2^2}\right) \left[\prod_{i=1}^{2} \frac{1}{\sqrt{2\pi\, T}} \exp\left(-\frac{(w_i-(Q'V)_i)^2}{2T}\right)\right] dw_1\, dw_2
\end{aligned}$$

and (6.34) gives

$$\begin{aligned}
& \int\int \varphi(Q(y_1,y_2,0))\, \psi\left(v, \sqrt{c^2+y_1^2+y_2^2}\right) \times \qquad (6.36) \\
& \left[\prod_{i=1}^{2} \frac{1}{\sqrt{2\pi\, T}} \exp\left(-\frac{(y_i-(Q'V)_i)^2}{2T}\right)\right] dy_1\, dy_2 \times \frac{1}{\sqrt{2\pi\, T}} \exp\left(-\frac{(Q'V)_3^2}{2T}\right).
\end{aligned}$$

Comparing (6.35) and (6.36) and taking into account (6.30) completes the proof. ■

References

[1] L. L. Baker and N. G. Hadjiconstantinou, *Variance reduction for Monte Carlo solutions of the Boltzmann equation*, Phys. Fluids, 17 (2005), pp. 051703(1–4).

[2] ——, *Variance-reduced particle methods for solving the Boltzmann equation*, Journal of Theoretical and Computational Nanoscience, 5 (2008), pp. 165–174.

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

[4] S. Caprino, M. Pulvirenti, and W. Wagner, *Stationary particle systems approximating stationary solutions to the Boltzmann equation*, SIAM J. Math. Anal., 29 (1998), pp. 913–934.

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

[6] ——, *Slow rarefied flows.Theory and application to micro-electro-mechanical systems*, Birkhäuser, Basel, 2006.

[7] J. Chun and D. L. Koch, *A direct simulation Monte Carlo method for rarefied gas flows in the limit of small Mach number*, Phys. Fluids, 17 (2005), pp. 107107(1–14).

[8] J. Fan and C. Shen, *Statistical simulation of low-speed rarefied gas flows*, J. Comput. Phys., 167 (2001), pp. 393–412.

[9] G. S. Fishman, *Monte Carlo: Concepts, Algorithms, and Applications*, Springer, New York, 1996.

[10] A. L. Garcia, *Numerical Methods for Physics.*, Prentice Hall, 2000. Second edition.

[11] A. L. Garcia and W. Wagner, *Generation of the Maxwellian inflow distribution*, J. Comput. Phys., 217 (2006), pp. 693–708.

[12] T. M. M. Homolle and N. G. Hadjiconstantinou, *A low-variance deviational simulation Monte Carlo for the Boltzmann equation*, J. Comput. Phys., 226 (2007), pp. 2341–2358.

[13] ——, *Low-variance deviational simulation Monte Carlo*, Phys. Fluids, 19 (2007), pp. 041701(1–4).

[14] G. Karniadakis, A. Beskok, and N. Aluru, *Microflows and nanoflows. Fundamentals and simulation*, Springer, New York, 2005.

[15] L. Pareschi and G. Russo, *Time relaxed Monte Carlo methods for the Boltzmann equation*, SIAM J. Sci. Comput., 23 (2001), pp. 1253–1273.

[16] S. Rjasanow and W. Wagner, *On time counting procedures in the DSMC method for rarefied gases*, Math. Comput. Simulation, 48 (1998), pp. 151–176.

[17] ——, *Stochastic Numerics for the Boltzmann Equation*, Springer, Berlin, 2005.

[18] C. Shen, *Rarefied Gas Dynamics. Fundamentals, Simulations and Microflows*, Springer, New York, 2005.

[19] Y. Sone, *Molecular Gas Dynamics. Theory, Techniques, and Applications*, Birkhäuser, Boston, 2007.

[20] Q. Sun and I. Boyd, *A direct simulation method for subsonic, microscale gas flows*, J. Comput. Phys., 179 (2002), pp. 400–425.

[21] W. Wagner, *A convergence proof for Bird's direct simulation Monte Carlo method for the Boltzmann equation*, J. Statist. Phys., 66 (1992), pp. 1011–1044.