An Analysis of Baganoff's Shuffle Algorithm

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Abstract

The paper presents the shuffle algorithm proposed by Baganoff, which can be implemented in simulation methods for the Boltzmann equation to simplify the binary collision process. It is shown that the shuffle algorithm is a discrete approximation of an isotropic collision law. The transition probability as well as the scattering cross section of the shuffle algorithm are opposed to the corresponding quantites of a hard-sphere model. The discrepancy between measures on a sphere is introduced in order to quantify the approximation error by using the shuffle algorithm.

Keywords: Rarefied gas flows; Boltzmann equation; particle methods; binary collisions; scattering cross sections; variable hard–shere model; discrepancy on the sphere.

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1 Baganoff's Shuffle Algorithm

Numerical methods for the Boltzmann equation, which are available for realistic problems like the reentry of a space vehicle, are first of all particle methods. The numerical effort of these particle methods, as for example the Bird algorithm [?] or the Finite–Pointset–Method [?], [?], grows rapidly with each step approximating reality. The most extensive part of the simulation process for the Boltzmann equation is, however, the collision process.

The shuffle algorithm proposed by Baganoff [?] provides a method of approximating the probability distribution of the collision parameters in order to achieve a very simple numerical scheme.

To explain the idea of the algorithm we first give a brief description of the collision process in a particle method for the Boltzmann equation. The collision of two particles is based, as in nature, on the conservation of momentum and energy. Having detected a colliding pair of particles with equal mass and velocities v and w, the post–collision velocities v' and w' are given by

$$v' = G + \frac{1}{2} g n' \tag{1}$$

$$w' = G - \frac{1}{2} g n' \tag{2}$$

where $G = (v+w)/2$ defines the center–of–mass velocity and $g = |v-w|$ the magnitude of the relative velocity. The collision parameter $n' \in S^2$ (the sphere in $\mathbb{R}^3$) is a random variable with a density distribution dependent on the scattering cross section. Normally the collision law can be assumed to be isotropic (see for example the variable hard–sphere model), i.e. the collision parameter n' is uniformly distributed on the sphere S^2. Choosing a collision parameter n' simply means to rotate the relative velocity vector.

Another way of changing the direction of the relative velocity which is very simple from a computational point of view is an arbitrary permutation of the three components of the vector n (n denoting the direction of the relative velocity, i.e. $n = (v-w)/|v-w|$). Furthermore, a different sign in front of one component leads to a new direction $n' \in S^2$ too.

Example of a possible transformation:

$$n = (n_1, n_2, n_3) \quad \xRightarrow{Collision} \quad n' = (n_2, -n_1, n_3)$$

The set of all possible transformations, i.e. permutations of the components and changing the sign of one component, is a finite subgroup $\mathcal{Q}$ in the orthogonal group $\mathcal{O}(3)$ in $\mathbb{R}^3$. Baganoff's shuffle algorithm chooses a uniformly distributed transformation $T \in \mathcal{Q}$ (instead of $T \in \mathcal{O}$) and performs the rotation of the relative velocity to obtain $n' = Tn$. It is obvious that the shuffle algorithm represents a discrete approximation of an isotropic collision law.

From a numerical point of view it is reasonable to apply such a 'Baganoff' transformation directly to the vector $v - w$, the vector of the relative velocity, because it makes then the calculation of the magnitude of $v - w$ unnecessary.
Using the shuffle algorithm instead of an isotropic collision law also means to change the differential cross section in the Boltzmann equation.
In order to obtain the scattering kernel belonging to the Baganoff model we will first consider the transition probability of the relative velocity directions during a collision. For an isotropic collision law this transition probability is given by

$$W_H(n \to n')d\omega(n') = d\omega(n') \tag{3}$$

where ω denotes the normalized surface measure on S^2.
The following transition propability can be directly related to Baganoff's shuffle model:

$$W_B(n \to n')d\omega(n') = \frac{1}{|\mathcal{Q}|} \sum_{T \in \mathcal{Q}} \delta(Tn) \tag{4}$$

The differential cross section for the variable hard–sphere model (VHS–model) is given by

$$\sigma_{VHS}(|v - w|, n')d\omega(n') = \sigma_{tot}(|v - w|)W_H(n \to n')d\omega(n')$$

with a total cross section $\sigma_{tot}(|v-w|)$ prescibing the collision frequency of the model. Hence

$$\sigma_{VHS}(|v - w|, n') = \sigma_{tot}(|v - w|) \tag{5}$$

Analogous to the VHS–model a variable Baganoff scattering cross section can be defined with the same total scattering cross section.

$$\sigma_{VBS}(|v - w|, n')d\omega(n') = \sigma_{tot}(|v - w|)W_B(n \to n')d\omega(n')$$

Now we can write the differential cross section for the variable Baganoff model:

$$\sigma_{VBS}(|v - w|, n') = \sigma_{tot}(|v - w|)\frac{1}{|\mathcal{Q}|} \sum_{T \in \mathcal{Q}} \delta(Tn) \tag{6}$$

Here and in the following we also use the notation of densities for discrete measures.

The subject of this paper is an analysis of the shuffle algorithm with the use of the mathematical description given above. For a theoretical investigation of the approximation error it is necessary to introduce a distance between measures on the sphere, which will be described in the following section. The comparison of the variable Baganoff model and the variable hard–sphere model with same total cross sections is subdivided into three parts. In section 3 we derive the distribution of the deflection angle and compare the result with numerical investigations performed by Feiereisen [?]. Section 4 studies the error obtained by the Baganoff model for a given velocity distribution. Finally we calculate the residuum of the Boltzmann equation for the two models.

2 The discrepancy on a sphere

The discrepancy is a usual distance in particle simulation methods. In the sequel we show that an analogous definition on the sphere S^2 is helpful for comparing different scattering cross sections. Before introducing the spherical discrepancy we review the notation of discrepancy on a closed interval [**?**].

Definition 1: *Let μ and ν be normalized measures on $[a, b]$. Then we define for all $\rho \in [a, b]$ the* local discrepancy *$R_\rho(\mu, \nu)$ by*

$$R_\rho(\mu, \nu) := \mu([-1, \rho)) - \nu([-1, \rho))$$
$$D_{[a,b]}(\mu, \nu) := \sup_{\rho \in [a,b]} |R_\rho(\mu, \nu)|$$

$D_{[a,b]}(\mu, \nu)$ is called the (extreme) discrepancy *of μ and ν.*

The following theorem (proved for example in [**?**]) shows that the discrepancy is a meanigful distance.

Theorem 2: *Let $(\mu_n)_{n \in N}$ be a sequence of normalized measures and ν an absolut continuous normalized measure on $[a, b]$. Then (μ_n) converges weakly to ν if and only if*

$$\lim_{n \to \infty} D_{[a,b]}(\mu_n, \nu) = 0$$

Now we introduce the discrepancy on the sphere S^2 using sherical caps. A set $C(p, \rho) = \{x \in S^2 | < p, x > \in \ (\rho, 1]\}$ is called a (spherical) cap with center $p \in S^2$ and height $1 - \rho$, $\rho \in [-1, 1]$.

Definition 3: *Let μ and ν be normalized measures on S^2. Then we define for all $p \in S^2$ and all $\rho \in [-1, 1]$ the* local discrepancy *$R_{(p,\rho)}(\mu, \nu)$* on *S^2 by*

$$R_{(p,\rho)}(\mu, \nu) := \mu(C(p, \rho)) - \nu(C(p, \rho))$$
$$D_{S^2}(\mu, \nu) := \sup_{p \in S^2, \rho \in [-1,1]} |R_{(p,\rho)}|$$

$D_{S^2}(\mu, \nu)$ is called (extreme) discrepancy on *S^2 of μ and ν.*

With the measurable mapping $P_p : S^2 \to [-1, 1]$ defined for all $p \in S^2$ by

$$P_p(x) =< p, x >$$

the discrepancy reads

$$D_{S^2}(\mu, \nu) = \sup_{p \in S^2} D_{[-1,1]}(P_p[\mu], P_p[\nu]) \tag{7}$$

where $P_p[\mu]$ is the image of μ under the mapping P_p.
Many properties of the discrepancy on S^2 result directly from the one–dimensional discrepancy on $[-1, 1]$ with equation (**??**). To prove the next theorem, which is the analogon of Theorem **??**, we additionally need the following lemma proved by Gerl [**?**].

Lemma 4: *Every polynomial $g(x_1, x_2, x_3)$ over S^2 can be represented as a linear combination of functions $< p^i, x >^{k(i)}, k(i) \in I\!N$ with a suitable sequence $(p^i)_{i \in N}$ on S^2.*

Theorem 5: *Let $(\mu_n)_{n \in N}$ be a sequence of normalized measures and ν an absolut continuous normalized measure on S^2. (μ_n) converges weakly to ν if and only if*

$$\lim_{n \to \infty} D_{S^2}(\mu_n, \nu) = 0$$

Proof: First we assume

$$\lim_{n \to \infty} D_{S^2}(\mu_n, \nu) = 0$$

or equivalent

$$\lim_{n \to \infty} D_{[-1,1]}(P_p[\mu_n], P_p[\nu]) = 0 \qquad \text{for all } p \in S^2$$

Then, as a consequence of Theorem **??**,

$$P_p[\mu_n] \xrightarrow{w} P_p[\nu] \qquad \text{for all } p \in S^2$$

where w denotes the weak convergence of measures [**?**]. This means, by definition, that for all continuous, bounded $\phi : [-1, 1] \to I\!R$ the following equation holds

$$\lim_{n \to \infty} \int_{-1}^{1} \phi dP_p[\mu_n] = \int_{-1}^{1} \phi dP_p[\nu]$$

With the use of the transformation rule, we obtain for all p and all ϕ

$$\lim_{n \to \infty} \int_{S^2} \phi(< p, x >) d\mu_n(x) = \int_{S^2} \phi(< p, x >) d\nu(x)$$

Application of Lemma **??** yields to

$$\lim_{n \to \infty} \int_{S^2} g(x) d\mu_n(x) = \int_{S^2} g(x) d\nu(x)$$

for all polynomials $g(x_1, x_2, x_3)$ on S^2. Since the polynomials are dense in the set of the continuous functions, we obtain by definition of the weak convergence

$$\mu_n \xrightarrow{w} \nu$$

The conversion is trivial. ■

Remark 6: It is obvious that we can also generalize the definition of the spherical discrepancy to the n–dimensional case. All statements above are true replacing S^2 by S^n.
In this paper we only need the discrepancy in the case where ν is the normalized Borel–Lebesgue measure. To simplify the notation we omit the second argument in R and D and write for example

$$D_{S^2}(\mu) = D_{S^2}(\mu, \omega)$$

Finally we note a lemma which is necessary to prove Theorem **??** in section 4.

Lemma 7: *Let* $(x_i)_{i=1\ldots n}$ *a finite sequence on the sphere* S^2. *Then the local discrepancy* $R_{(p,\rho)}(\frac{1}{n}\sum\delta(x_i))$ *takes all intermediate values in the open interval* (m, M) *with*

$$m = \inf_{p\in S^2,\rho\in[-1,1]} R_{(p,\rho)}(\frac{1}{n}\sum\delta(x_i))$$

$$M = \sup_{p\in S^2,\rho\in[-1,1]} R_{(p,\rho)}(\frac{1}{n}\sum\delta(x_i))$$

The proof follows immediately considering the function $R_{(p,\rho)}(\frac{1}{n}\sum\delta(x_i))$ for fixed $p \in S^2$.

3 The deflection angle

First we compare functionals of the velocities before and after collision. In the center–of–mass system there can only be a difference in the direction of the relative velocity, because momentum and energy are conserved in a collision. A physically meaningful functional is the angle between the direction of the relative velocity $n \in S^2$ before and $n' \in S^2$ after collision. This angle is called deflection angle and is defined by

$$\cos\phi := \ < n, n' >$$

with $\phi \in [0, \pi]$. With the knowledge of the transition probability (**??**) respectively (**??**), it is possible to compare the probability densities of the deflection angles in both cases.

Theorem 8: *The density* Φ_H *of the deflection angle* ϕ *in the hard–sphere model is given by*

$$\Phi_H(\phi) = \frac{1}{2}\sin\phi$$

for all $\phi \in [0, \pi]$. *Therefore the cosine of the deflection angle denoted by* $\gamma :=< n, n' >$ *is uniformly distributed on* $[-1, 1]$.

Proof: n' is uniformly distributed on S^2. Let n be the polar axis of a spherical coordinate system (χ, ϵ). Then we have

$$d\omega(n') = \frac{1}{4\pi}\sin\chi d\chi d\epsilon$$

and

$$\cos\phi = \ < n, n' > \ = \cos\chi$$

Hence $\phi = \chi$ and integration with respect to ϵ finishs the proof. ∎

Feiereisen [?] approximates the distribution of the deflection angle for Baganoff's model by using a numerical simulation. He stated that remarkable differences to the hard–sphere model were observable in five discrete points, $\phi = 0, \frac{\pi}{3}, \frac{\pi}{2}, \frac{2\pi}{3}, \pi$. The following theorem verifies this experiment analytically.

Theorem 9: *In the Baganoff model the density* Φ_B *of* ϕ *is*

$$\begin{aligned}\Phi_B(\phi)d\phi = \quad & \frac{1}{48}(\delta(0)+\delta(\pi)) \\ + \quad & \frac{3}{32\sqrt{2}}\left(\frac{1}{\sqrt{1+\cos\phi}}+\frac{1}{\sqrt{1-\cos\phi}}\right)\sin\phi d\phi \\ + \quad & \frac{1}{6\sqrt{3}}\left(\frac{1}{\sqrt{1+2\cos\phi}}+\frac{1}{\sqrt{1-2\cos\phi}}\right)\sin\phi d\phi \\ + \quad & \frac{1}{16}\frac{1}{\sqrt{|\cos\phi|}}\sin\phi d\phi\end{aligned}$$

with the abbreviation $\frac{1}{\sqrt{-a}} = 0$ *for* $a \geq 0$.

Proof: For fixed $n \in S^2$ n' is prescribed by the measure

$$\frac{1}{|\mathcal{Q}|}\sum_{T\in\mathcal{Q}}\delta(Tn)$$

Then $\gamma = \; < n, n' >$ is for fixed n distributed as

$$\frac{1}{|\mathcal{Q}|}\sum_{T\in\mathcal{Q}}\delta(< n, Tn >)$$

For the density Γ_B of γ we obtain by integration over all n:

$$\Gamma_B(\gamma)d\gamma = \frac{1}{|\mathcal{Q}|}\sum_{T\in\mathcal{Q}}\int_{S^2}\delta(< n, Tn >)d\omega(n)$$

The integrals

$$\int_{S^2}\delta(< n, Tn >)d\omega(n)$$

can be easily computed for every $T \in \mathcal{Q}$.
In summary

$$\begin{aligned}\Gamma_B(\gamma)d\gamma = \quad & \frac{1}{48}(\delta(1)+\delta(-1)) \\ + \quad & \frac{3}{32\sqrt{2}}\left(\frac{d\gamma}{\sqrt{1+\gamma}}+\frac{d\gamma}{\sqrt{1-\gamma}}\right) \\ + \quad & \frac{1}{6\sqrt{3}}\left(\frac{d\gamma}{\sqrt{1+2\gamma}}+\frac{d\gamma}{\sqrt{1-2\gamma}}\right) \\ + \quad & \frac{1}{16}\left(\frac{d\gamma}{\sqrt{\gamma}}+\frac{d\gamma}{\sqrt{-\gamma}}\right)\end{aligned}$$

with the abbreviation $\frac{1}{\sqrt{-a}} = 0$ for $a \geq 0$.
The substitution $\gamma = \cos\phi$ completes the proof. ■

Figure 1: Continuous part of $\Gamma_B(\gamma)$ and $\Gamma_H(\gamma)$

Figure 1 shows the continuous part of $\Gamma_B(\gamma)d\gamma$ and $\Gamma_H(\gamma)d\gamma$. In contrary to the statement of Feiereisen important differences can be observed not only at the five values $\gamma = 0, \pm\frac{1}{2}, \pm 1$. With the aid of the discrepancy it is possible to describe this error qualitatively (see figure 2).

Lemma 10:

(i) For $\rho \in [-1,1]$:

$$R_\rho(\Gamma_B(\gamma)d\gamma) = \frac{1}{2}\rho + \frac{1}{6\sqrt{3}}(\sqrt{1-2\rho} - \sqrt{1+2\rho}) + \frac{3}{16\sqrt{2}}(\sqrt{1-\rho} - \sqrt{1+\rho}) - \frac{1}{8}\mathrm{sign}(\rho)\sqrt{|\rho|}$$

with the abbreviation $\sqrt{-a} = 0$ for $a > 0$.

(ii) The extreme discrepancy of Γ_B is given by

$$D_{[-1,1]}(\Gamma_B(\gamma)d\gamma) = R_{\pm\frac{1}{2}}(\Gamma_B(\gamma)d\gamma) \approx 0.0431$$

Figure 2: Local discrepancy of $R_\rho(\Gamma_B(\gamma)d\gamma)$

4 The distribution of the direction of the relative velocity

Now we consider the consequences of the collision process in both models for a given velocity distrbution. Let $f(v)$ be the velocity distribution of a particle system with the normalization

$$\int_{R^3} f(v)dv = 1 \tag{8}$$

With the same argument as in the last chapter it is sufficient to consider the distribution of the direction of the relative velocity

$$F(n) = \int_0^\infty \int_{R^3} 4\pi g^2 f(G + \frac{g}{2}n) f(G - \frac{g}{2}n) dG dg \tag{9}$$

We obtain the post–collision distribution F' for the relative velocity direction dependent on the corresponding transition probability $W(n \to n')$ by

$$F'(n') = \int_{S^2} F(n) W(n \to n') d\omega(n) \tag{10}$$

With the usual notations we get

$$F'_H(n') = 1 \tag{11}$$

and

$$F'_B(n') = \frac{1}{|\mathcal{Q}|}\sum_{T\in\mathcal{Q}} F(Tn') \tag{12}$$

To prove the second equation, we consider for all $\Omega \subset S^2$ the following term and make use of the group property of $\mathcal{Q}$.

$$\begin{aligned}
\int_\Omega F'_B(n')d\omega(n') &= \frac{1}{|\mathcal{Q}|}\sum_{T\in\mathcal{Q}}\int_{S^2}\mathcal{X}_\Omega(Tn)F(n)d\omega(n) \\
&= \int_{S^2}\frac{1}{|\mathcal{Q}|}\sum_{T\in\mathcal{Q}}\mathcal{X}_\Omega(n)F(T^{-1}n)d\omega(n) \\
&= \int_\Omega \frac{1}{|\mathcal{Q}|}\sum_{T\in\mathcal{Q}} F(Tn')d\omega(n')
\end{aligned}$$

Hence

$$F'_B(n') = \frac{1}{|\mathcal{Q}|}\sum_{T\in\mathcal{Q}} F(Tn')$$

For any velocity distribution we can define the error between the two models with the discrepancy on S^2, because $F'_H = 1$ by (**??**).

Definition 11:

$$B_{err}(f) := D_{S^2}(F'_B d\omega)$$

is called the Baganoff error *according to the relative velocity distribution.*

An estimation of the Baganoff error, i.e. the deviation from F'_B to the uniform distribution, is given by

$$B_{err}(f) \leq D_{S^2}(F d\omega) \tag{13}$$

because

$$\begin{aligned}
B_{err}(f) &= \sup_{p\in S^2, \rho\in[-1,1]}\left|\int_{C(p,\rho)}\left(\frac{1}{|\mathcal{Q}|}\sum_{T\in\mathcal{Q}}F(Tn)-1\right)d\omega(n)\right| \\
&\leq \frac{1}{|\mathcal{Q}|}\sum_{T\in\mathcal{Q}}\left(\sup_{p\in S^2,\rho\in[-1,1]}\left|\int_{C(T^{-1}p,\rho)}(F(n)-1)d\omega(n)\right|\right) \\
&= D_{S^2}(F d\omega)
\end{aligned}$$

Example 12: The distribution $F^{(M)}(n)$ of a Maxwellian

$$f^{(M)}(v) = \frac{1}{(2\pi)^{\frac{3}{2}}} \exp\left(-\frac{|v|^2}{2}\right)$$

is uniformly distributed on S^2. This property is invariant under collisions such that

$$F_B^{(M)'}(n') = 1 = F_H^{(M)'}(n')$$

We note here an alternative interpretation of the discrepancy $D_{S^2}(Fd\omega)$. $D_{S^2}(Fd\omega)$ can be regarded as a measure for the deviation of a distribution F from the Maxwell distribution. Accordingly the meaning of equation (**??**) is, that in the Baganoff case the deviation after a collision is bounded by the deviation before.
An upper bound for all velocity distributions is a consequence of the following estimation. As in the proof of equation (**??**), we obtain

$$\begin{aligned} B_{err}(f) &= \sup_{p\in S^2, \rho\in[-1,1]} \left| \int_{S^2} F(n) \left(\frac{1}{|\mathcal{Q}|} \sum_{T\in\mathcal{Q}} \mathcal{X}_{C(p,\rho)}(Tn) - \int\limits_{C(p,\rho)} d\omega(n') \right) d\omega(n) \right| \\ &\le \sup_{p\in S^2, \rho\in[-1,1]} \int_{S^2} F(n) \left| R_{(p,\rho)}((Tn)_{T\in\mathcal{Q}}) \right| d\omega(n) \\ &\le \int_{S^2} F(n) D_{S^2}((Tn)_{T\in\mathcal{Q}}) d\omega(n) \\ &\le \sup_{n\in S^2} D_{S^2}((Tn)_{T\in\mathcal{Q}}) \end{aligned}$$

With the fact, that

$$|R_{(p,\rho)}((Tn)_{T\in\mathcal{Q}})| \le |R_{(p_0,0)}((Tp_0)_{T\in\mathcal{Q}})| = \frac{1}{3}$$

with $p_0 = (0,0,1)$, we obtain the inequality

$$0 \le B_{err}(f) \le \frac{1}{3}$$

5 The residuum in the Boltzmann equation

In this part we compare the Boltzmann equation with the two different collision cross sections for the hard–sphere and the shuffle model. This leads to a quantity similar to the Baganoff error.
For simplicity we only consider the homogeneous Boltzmann equation

$$\frac{\partial f}{\partial t}(t,v) = J(f,f)(t,v)$$

with

$$J(f,f)(v) = \int_{R^3}\int_{S^2} |v-w|\sigma(|v-w|,n')\left(f(v')f(w') - f(v)f(w)\right) d\omega(n')dw$$

where v' and w' are given by relation (1) and (2). The inhomogeneous case can be treated in the same way.
The two Boltzmann equations with σ_{VBS} and σ_{VHS} only differ in the first term of the collision operator:

$$\int_{R^3}\int_{S^2} |v-w|\sigma(|v-w|,n')f(v')f(w')d\omega(n')dw$$

From a weak formulation of the Boltzmann equation we obtain naturally a meaningful error restricting the class of test functions. Here we use characteristic functions on open balls.

Definition 13: *Let $B_r(q) := \{x \in \mathbb{R}^3 |\ |x-q| < r\}$ the open ball with center $q \in \mathbb{R}^3$ and radius $r > 0$. Then we define*

$$B_{res}(f) := \sup_{q\in R^3, r>0} \left| \int_{R^3}\int_{R^3}\int_{S^2} \left(|v-w|\sigma_{VBS}(|v-w|,n') - \sigma_{VHS}(|v-w|,n')\right) \right.$$
$$\left. \times \quad \mathcal{X}_{B_r(q)}(v) f(v')f(w')d\omega(n')dwdv \right|$$

the Baganoff residuum *with respect to the Boltzmann equation.*

The analogy to the Baganoff error is shown in the next theorem.

Theorem 14:

$$B_{res}(f) = \sup_{p\in S^2, \rho\in[-1,1]} \left| \int_{C(p,\rho)} \left(\frac{1}{|\mathcal{Q}|}\sum_{T\in\mathcal{Q}} F_\sigma(Tn) - \int_{S^2} F_\sigma(n')d\omega(n')\right) d\omega(n) \right|$$

with

$$F_\sigma(n) := \int_0^\infty \int_{R^3} 4\pi g^3 \sigma_{tot}(g) f(G + \frac{g}{2}n) f(G - \frac{g}{2}n) dGdg$$

for all $n \in S^2$.

Proof: The substitution

$$G = v + w, \qquad g = \frac{1}{2}|v-w|, \qquad n = \frac{v-w}{|v-w|}$$

yields to the equation

$$B_{res}(f) \;=\; \sup_{q\in R^3, r>0} \left| \int_0^\infty \int_{R^3}\int_{S^2}\int_{S^2} 4\pi g^3 \mathcal{X}_{B_r(q)}(G + \frac{g}{2}n) f(G + \frac{g}{2}n') \right.$$
$$\left. \times f(G - \frac{g}{2}n')\left(\sigma_{VBS}(g,n') - \sigma_{VHS}(g,n')\right) d\omega(n')d\omega(n)dGdg \right|$$

For any function $h(g, G, n)$ we have obviously

$$\int_{S^2} \mathcal{X}_{B_r(q)}(G + \frac{g}{2}n) h(g, G, n) d\omega(n) = \int_{S^2} \mathcal{X}_{C(p,\rho)}(n) h(g, G, n) d\omega(n)$$

with the center and the height of the cap $C(p, \rho)$ given by

$$p = \frac{q - G}{|q - G|}$$

and

$$1 - \rho = \begin{cases} 0 & \text{for} \quad 2|q - G| > 2r + g \\ \frac{4|q-G|^2 + g^2 - 4r^2}{4g|q-G|} & \text{for} \quad 2r - g \leq 2|q - G| \leq 2r + g \\ 2 & \text{for} \quad 2|q - G| < 2r - g \end{cases}$$

In summary we can write

$$\begin{aligned} B_{res}(f) &= \sup_{q \in R^3, r > 0} \left| \int_{S^2} \int_0^\infty \int_{R^3} 4\pi g^3 \sigma_{tot}(g) f(G + \frac{g}{2}n) f(G - \frac{g}{2}n) \right. \\ &\quad \times \left. \left(\frac{1}{|\mathcal{Q}|} \sum_{T \in \mathcal{Q}} \mathcal{X}_{C(p,\rho)}(Tn) - \int\limits_{C(p,\rho)} d\omega(n') \right) dG dg d\omega(n) \right| \end{aligned}$$

By definition of F_σ and the local discrepancy $R_{(p,\rho)}$, we obtain with a mean value theorem for integrals

$$B_{res}(f) = \sup_{q \in R^3, r > 0} \left| \int_{S^2} F_\sigma(n) \mu(n, q, r) d\omega(n) \right|$$

where $\mu(n, q, r)$ denotes a suitable intermediate value of $R_{(p,\rho)}((Tn)_{T \in \mathcal{Q}})$.
The application of Lemma **??** causes the existence of $G^* \in \mathbb{R}^3$ and $g^* > 0$, such that with $p^*(q, G^*)$ and $\rho^*(q, r, G^*, g^*)$ holds

$$\begin{aligned} B_{res}(f) &= \sup_{q \in R^3, r > 0} \left| \int\limits_{S^2} F_\sigma(n) R_{(p^*,\rho^*)}((Tn)_{T \in \mathcal{Q}}) d\omega(n) \right| \\ &= \sup_{q \in R^3, r > 0} \left| \frac{1}{|\mathcal{Q}|} \sum_{T \in \mathcal{Q}} \int\limits_{S^2} F_\sigma(n) \mathcal{X}_{C(p^*,\rho^*)}(Tn) d\omega(n) - \int\limits_{S^2} F_\sigma(n') d\omega(n') \int\limits_{C(p^*,\rho^*)} d\omega(n) \right| \\ &= \sup_{q \in R^3, r > 0} \left| \int\limits_{C(p^*,\rho^*)} \left(\frac{1}{|\mathcal{Q}|} \sum_{T \in \mathcal{Q}} F_\sigma(Tn) - \int\limits_{S^2} F_\sigma(n') d\omega(n') \right) d\omega(n) \right| \end{aligned}$$

Substitution of the supremum with respect to q and r by the supremum over p and ρ completes the proof. ∎

Remark 15: In general, the integral $\int_{S^2} F_\sigma(n')d\omega(n')$ is not equal to one. If we take another normalization condition, namely $\int\int |v-w|\sigma_{tot}(|v-w|)f(v)f(w)dwdv = 1$ instead of the normalization $\int f(v)dv = 1$, we get

$$\int_{S^2} \tilde{F}_\sigma(n')d\omega(n') = 1$$

and hence a modified Baganoff residuum

$$\begin{aligned} B_{mod}(f) \quad &:= \quad \sup_{p,\rho} \left| \int\limits_{C(p,\rho)} \Big(\frac{1}{|\mathcal{Q}|}\sum_{T\in\mathcal{Q}} \tilde{F}_\sigma(n) - 1\Big)d\omega(n)\right| \\ &= \quad D_{S^2}\left(\frac{1}{|\mathcal{Q}|}\sum_{T\in\mathcal{Q}} \tilde{F}_\sigma(Tn)d\omega(n)\right) \end{aligned}$$

So the similarity to the Baganoff error is obvious. The modified Baganoff residuum and the Baganoff error only differ in the function F_σ respectively F. In the case of Maxwell molecules, i.e. $\sigma_{tot}(g) = g^{-1}$, the two quantities B_{res} and B_{err} agree. Therefore the statements and estimations discussed in the last section are also true for the Baganoff residuum with any σ_{tot}, which can be directly seen by substituting F by F_σ.

Example 16: Let again $f^{(M)}$ be a Maxwellian, then it is easy to see, that for every σ_{tot} we have

$$B_{res}(f^{(M)}) = B_{mod}(f^{(M)}) = 0$$

Numerical calculations with the Finite–Pointset–Method [?] show that using the shuffle algorithm the reduction in the computational time is relatively small. One reason for this is that the choice of collision partners and the calculation of the collision probabilities is much more time–consuming and has to be done for every particle in every time step, whereas the shuffle algorithm is only executed if a collision occurs. Moreover it is necessary to compute the magnitude of the relative velocity to get the collision probability. Therefore there is no gain to rotate $v-w$ instead of $(v-w)/|v-w|$.

The computational results coincide with the statements of the previous and this section. There are differences in the velocity distributions for the Baganoff and the hard–sphere model which decrease approaching the equilibrium state (for a detailed description see [?]). On the other hand, no relevant errors can be detected for the low moments of the velocity distribution being alone important for the applications.

Conclusion

Baganoff's shuffle algorithm has been compared with the variable hard–sphere model under different aspects. The comparison represents the analytical confirmation of the numerical results obtained by Feiereisen, but by using an analytic solution technique a more detailed analysis of the differences is possible.
The application of the discrepancy on the sphere leads to an explicit error for the differences between the Baganoff and the hard–sphere model as a function of the relative velocity distribution. The residuum of the Boltzmann equation with the scattering cross sections for both models is reduced to the Baganoff error. Baganoff error and residuum vanish for a Maxwell distribution.
The theoretical investigation proposed in this paper provides a tool, which can be directly extended to a more general analysis of any scattering cross section.

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