A generalized collision mechanism for stochastic particle schemes approximating Boltzmann type equations

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Abstract. A generalized collision mechanism for Boltzmann type stochastic particle schemes is developed. This mechanism is based on the idea of random weight transfer originating from random discrete velocity models. The problem of applying the new degrees of freedom for the purpose of variance reduction is studied. Some results of numerical experiments are given.

Contents

1. Introduction

We study stochastic particle schemes of the form

$$Z^{(n)}(t) = \left\{ \left(w_i^{(n)}(t) \,,\, g_i^{(n)}(t) \right) \,, \quad i = 1, \ldots, m^{(n)}(t) \right\} \,, \quad t \geq 0 \,. \tag{1.1}$$

Each particle has a state $w_i^{(n)}(t)$ from a locally compact separable metric space $\mathcal{W}$ (e.g., $\mathcal{W} = \mathcal{X} \times \mathcal{V}$, where $\mathcal{X}$ is the position space and $\mathcal{V}$ is the velocity space) and a weight $g_i^{(n)}(t) \in [0,1]$. The variable $m^{(n)}(t)$ denotes the number of particles in the system. Finally, the index n indicates the parameter with respect to which convergence is considered.

The system of particles (1.1) is defined as a Markov process with the infinitesimal generator

$$\mathcal{A}(\Phi)(z) = \tag{1.2}$$
$$\sum_{1 \leq i \neq j \leq m} \int_{\mathcal{W}} \int_{\mathcal{W}} \Big[\Phi(J(z,i,j,\tilde{w}_1,\tilde{w}_2)) - \Phi(z) \Big] \, Q(z,i,j,d\tilde{w}_1,d\tilde{w}_2) \,,$$

where Φ is an appropriate function on the state space

$$\mathcal{Z} = \left\{ z = ((w_1,g_1),\ldots,(w_m,g_m)) \in \cup_{k=1}^{\infty} \left(\mathcal{W} \times [0,1] \right)^k \;:\; \sum_{i=1}^{m} g_i \leq 1 \right\} . \tag{1.3}$$

The transformation $J(z,i,j,\tilde{w}_1,\tilde{w}_2) \,:\, \mathcal{Z} \to \mathcal{Z}$ is defined as

$$[J(z,i,j,\tilde{w}_1,\tilde{w}_2)]_k = \begin{cases} (w_k, g_k) & \text{, if} \quad k \leq m \,,\; k \neq i,j \,, \\ (\tilde{w}_1, G(z,i,j,\tilde{w}_1,\tilde{w}_2)) & \text{, if} \quad k = i \,, \\ (\tilde{w}_2, G(z,i,j,\tilde{w}_1,\tilde{w}_2)) & \text{, if} \quad k = j \,, \\ (w_i, g_i - G(z,i,j,\tilde{w}_1,\tilde{w}_2)) & \text{, if} \quad k = m+1 \,, \\ (w_j, g_j - G(z,i,j,\tilde{w}_1,\tilde{w}_2)) & \text{, if} \quad k = m+2 \,. \end{cases} \tag{1.4}$$

The behaviour of the system (1.1) is characterized by a jump mechanism. During each jump, two particles at the states w_i and w_j create two new particles at the states $\tilde{w}_1$ and $\tilde{w}_2$ giving them a certain amount of weight.

The **jump kernel** Q determines the intensity of jumps (interpreted as collisions between particles) and the distribution of the jump targets $(\tilde{w}_1, \tilde{w}_2)$. It is assumed to satisfy

$$Q(z,i,j,\mathcal{W},\mathcal{W}) \leq C_{Q,max} \, \max(g_i, g_j) \,. \tag{1.5}$$

The intensity of jumps is estimated according to (1.5) (cf. also (1.3)),

$$\pi(z) = \sum_{1 \leq i \neq j \leq m} Q(z,i,j,\mathcal{W},\mathcal{W}) \leq$$
$$\leq C_{Q,max} \sum_{1 \leq i \neq j \leq m} (g_i + g_j) \leq 2\, C_{Q,max} \, (m-1) \,, \quad \forall z \in \mathcal{Z} \,. \tag{1.6}$$

Though the right–hand side of (1.6) is unbounded, existence of the process can be established (cf. [5, Ch. 4, Problem 5]).

The **weight transfer function** G describes the amount of weight given to the particles in the post–collision states. Concerning the function G we assume

$$0 < G(z, i, j, \tilde{w}_1, \tilde{w}_2) \le \min(g_i, g_j) \tag{1.7}$$

so that the weight components of the process remain positive (particles with weight zero are removed from the system).

The deterministic equation, which is to be solved numerically by means of an exact or approximate simulation of the particle system (1.1), has the form

$$\frac{d}{dt}\int_{\mathcal{W}} \varphi(w)\,\lambda(t, dw) = \int_{\mathcal{W}}\int_{\mathcal{W}}\int_{\mathcal{W}}\int_{\mathcal{W}} \tag{1.8}$$
$$[\varphi(\tilde{w}_1) + \varphi(\tilde{w}_2) - \varphi(w_1) - \varphi(w_2)]\,\beta(w_1, w_2, d\tilde{w}_1, d\tilde{w}_2)\,\lambda(t, dw_1)\,\lambda(t, dw_2)\,,$$

$$\int_{\mathcal{W}} \varphi(w)\,\lambda(0, dw) = \int_{\mathcal{W}} \varphi(w)\,\lambda_0(dw)\,, \tag{1.9}$$

where φ is an arbitrary bounded measurable test function, β is an appropriate kernel, and λ_0 is a given initial value. Eq. (1.8) describes the time evolution of a measure–valued function λ.

The parameters Q and G of the particle system (1.1), (1.2) are related to the kernel β appearing in Eq. (1.8) via the **basic relationship**

$$G(z, i, j, \tilde{w}_1, \tilde{w}_2)\,Q(z, i, j, d\tilde{w}_1, d\tilde{w}_2) = g_i\,g_j\,\beta(w_i, w_j, d\tilde{w}_1, d\tilde{w}_2)\,, \tag{1.10}$$

where $z = ((w_1, g_1), \ldots, (w_m, g_m))$.

Remark 1.1 *The (spatially homogeneous) Boltzmann equation is obtained in the special case* $\mathcal{W} = \mathcal{V} = \mathcal{R}^3$,

$$\beta(v_1, v_2, d\tilde{v}_1, d\tilde{v}_2) = \frac{1}{2}\int_{\mathcal{S}^2} \delta_{v_1^*}(d\tilde{v}_1)\,\delta_{v_2^*}(d\tilde{v}_2)\,B(v_1, v_2, e)\,de\,,$$

where B is the collision kernel and $\mathcal{S}^2$ denotes the unit sphere in the Euclidean space $\mathcal{R}^3$. The post–collision velocities v_1^* and v_2^* are determined as

$$v_1^* = v_1 + e\,(e, v_2 - v_1)\,, \quad v_2^* = v_2 + e\,(e, v_1 - v_2)\,, \tag{1.11}$$

where $(.,.)$ denotes the scalar product.

Consider the empirical measures corresponding to the system (1.1)

$$\mu^{(n)}(t,dw) = \sum_{i=1}^{m^{(n)}(t)} g_i^{(n)}(t)\, \delta_{w_i^{(n)}(t)}(dw)\,, \tag{1.12}$$

where δ denotes the Dirac measure. Functionals of the solution of Eq. (1.8) are estimated by the corresponding functionals of the empirical measures (1.12), i.e.

$$\int_{\mathcal{W}} \varphi(w)\, \lambda(t,dw) \approx \sum_{i=1}^{m^{(n)}(t)} g_i^{(n)}(t)\, \varphi(w_i^{(n)}(t))\,. \tag{1.13}$$

It is assumed that the initial state $Z^{(n)}(0)$ of the system (1.1) is such that $\mu^{(n)}(0)$ converges to the initial value λ_0 of Eq. (1.8), (1.9). This is the origin of the dependence of the particle system on the index n. Thus, it is natural to assume

$$m^{(n)}(0) = n\,. \tag{1.14}$$

The problem of convergence of the empirical measures (1.12) to the solution of Eq. (1.8) is considered in Section 2. The pathwise behaviour of the Markov process (1.1) is described in Section 3. The generator (1.2) depends on the two parameters Q and G. They are related to the kernel β of the limiting equation (1.8) via equation (1.10) and are subject to the conditions (1.5), (1.7). The considerable freedom one still has in choosing them is discussed in Section 4. In Section 5 we show how this choice may be adapted to the special problem to be solved, in order to achieve a reduction of the statistical fluctuations of the estimator at the right–hand side of (1.13). Results of numerical experiments are given in Section 6.

We refer to [1], [3], [4, Ch. 10], [6], [12], [13], [15], [16] concerning particle simulation schemes for the Boltzmann equation and to [7], [8] concerning random discrete velocity models.

2. Convergence of the empirical measures

The convergence result will be stated in terms of the bounded Lipschitz metric, which is equivalent to weak convergence of probability measures (cf. [5, p. 150]),

$$\varrho(\nu_1,\nu_2) = \sup_{\|\varphi\|_L \le 1} \Big| \int_{\mathcal{W}} \varphi(w)\, \nu_1(dw) - \int_{\mathcal{W}} \varphi(w)\, \nu_2(dw) \Big|\,,$$

where

$$\|\varphi\|_L = \max\left(\sup_{w\in\mathcal{W}}|\varphi(w)|\,,\quad \sup_{w_1,w_2\in\mathcal{W}\,,\,w_1\neq w_2}\frac{|\varphi(w_1)-\varphi(w_2)|}{r(w_1,w_2)}\right)\,,$$

and r is the metric in $\mathcal{W}$.

Let the parameters Q and G of the particle system (1.1) and the kernel β of Eq. (1.8) satisfy (1.5), (1.7), (1.10),

$$\beta(w_1,w_2,\mathcal{W},\mathcal{W}) \le C_{\beta,max} \tag{2.1}$$

and

$$\begin{aligned} &|\int_{\mathcal{W}}\int_{\mathcal{W}}[\varphi(\tilde w_1)+\varphi(\tilde w_2)]\,\beta(w_1,w_2,d\tilde w_1,d\tilde w_2)- \\ &\qquad\int_{\mathcal{W}}\int_{\mathcal{W}}[\varphi(\tilde w_1)+\varphi(\tilde w_2)]\,\beta(\hat w_1,\hat w_2,d\tilde w_1,d\tilde w_2)| \le \\ &\qquad \le C_{\beta,L}\,\|\varphi\|_L\,[r(w_1,\hat w_1)+r(w_2,\hat w_2)]\,. \end{aligned} \tag{2.2}$$

In the case $\mathcal{W}\subset\mathcal{R}^d$, we assume that

$$\sup_n \mathcal{E}\sup_{t\in[0,T]}\int_{\mathcal{W}}\|w\|^2\,\mu^{(n)}(t,dw)<\infty\,,\quad \forall T>0\,, \tag{2.3}$$

where $\mathcal{E}$ denotes mathematical expectation, and

$$\sup_{t\in[0,T]}\int_{\mathcal{W}}\|w\|^2\,\lambda(t,dw)<\infty\,,\quad \forall T>0\,. \tag{2.4}$$

Conditions (2.3), (2.4) are not needed when $\mathcal{W}$ is compact. In the special case mentioned in Remark 1.1, they reduce to the conditions

$$\sup_n \mathcal{E}\int_{\mathcal{W}}\|w\|^2\,\mu^{(n)}(0,dw)<\infty \quad\text{and}\quad \int_{\mathcal{W}}\|w\|^2\,\lambda_0(dw)<\infty\,,$$

because of the conservation properties of the collision transformation (1.11).

Under the above mentioned assumptions, the following theorem holds.

Theorem 2.1 *If*

$$\lim_{n\to\infty}\mathcal{E}\varrho(\mu^{(n)}(0),\lambda_0)=0 \quad\textit{and}\quad \lim_{n\to\infty}\mathcal{E}\max_{i=1,\dots,n}g_i^{(n)}(0)=0\,,$$

then

$$\lim_{n\to\infty}\mathcal{E}\sup_{t\in[0,T]}\varrho(\mu^{(n)}(t),\lambda(t))=0\,,\quad \forall T>0\,. \tag{2.5}$$

Theorem 2.1 generalizes Theorem 3.1 in [17], where the special case of the spatially homogeneous Boltzmann equation was considered. Also, the restriction on the length T of the time interval in (2.5) has been removed. Since the proof of the theorem is similar to that in [17], we only sketch the main ideas and provide the basic estimates.

Consider a function

$$\Phi(z) = \sum_{i=1}^{m} g_i \, \varphi(w_i) \,, \quad z = ((w_1, g_1), \ldots, (w_m, g_m)) \,,$$

where φ is a measurable bounded function on $\mathcal{W}$. Notice that

$$\Phi(Z^{(n)}(t)) = \int_{\mathcal{W}} \varphi(w) \, \mu^{(n)}(t, dw) \,, \tag{2.6}$$

where $Z^{(n)}$ is the Markov process (1.1), and $\mu^{(n)}$ is the empirical measure defined in (1.12). Using (1.4), we find

$$\begin{aligned}\Phi(J(z, i, j, \tilde{w}_1, \tilde{w}_2)) = \\ \Phi(z) + G(z, i, j, \tilde{w}_1, \tilde{w}_2) \, [\varphi(\tilde{w}_1) + \varphi(\tilde{w}_2) - \varphi(w_i) - \varphi(w_j)] \,,\end{aligned}$$

and, according to (1.2) and (1.10),

$$\begin{aligned}&\mathcal{A}(\Phi)(z) = \\ &\sum_{1 \le i \ne j \le m} g_i \, g_j \int_{\mathcal{W}} \int_{\mathcal{W}} [\varphi(\tilde{w}_1) + \varphi(\tilde{w}_2) - \varphi(w_i) - \varphi(w_j)] \, \beta(w_i, w_j, d\tilde{w}_1, d\tilde{w}_2) \,.\end{aligned} \tag{2.7}$$

Analogously, one finds

$$\begin{aligned}\mathcal{A}(\Phi^2)(z) = 2 \, \Phi(z) \, \mathcal{A}(\Phi)(z) + \sum_{1 \le i \ne j \le m} g_i \, g_j \int_{\mathcal{W}} \int_{\mathcal{W}} \\ [\varphi(\tilde{w}_1) + \varphi(\tilde{w}_2) - \varphi(w_i) - \varphi(w_j)]^2 \, G(z, i, j, \tilde{w}_1, \tilde{w}_2) \, \beta(w_i, w_j, d\tilde{w}_1, d\tilde{w}_2) \,.\end{aligned} \tag{2.8}$$

Note that

$$|\Phi(z)| \le \|\varphi\| \sum_{i=1}^{m} g_i \le \|\varphi\| \,, \tag{2.9}$$

where $\|.\|$ denotes the sup–norm. Using (2.1), one obtains from (2.7) that

$$|\mathcal{A}(\Phi)(z)| \le 4 \, \|\varphi\| \, C_{\beta,max} \tag{2.10}$$

and, from (2.8), (2.9) and (2.10), that

$$|\mathcal{A}(\Phi^2)(z)| \le 24 \, \|\varphi\|^2 \, C_{\beta,max} \,.$$

Consequently, the functions Φ and Φ^2 belong to the domain of the generator (1.2) (cf. [5, Ch. 4, Problem 15]). Therefore, the following representation holds,

$$\Phi(Z^{(n)}(t)) = \Phi(Z^{(n)}(0)) + \int_0^t \mathcal{A}(\Phi)(Z^{(n)}(s))\, ds + M^{(n)}(t)\,, \tag{2.11}$$

where $M^{(n)}(t)$ is a martingale, and

$$\mathcal{E}\left[M^{(n)}(t)\right]^2 = \mathcal{E}\int_0^t \left[\mathcal{A}(\Phi^2) - 2\,\Phi\,\mathcal{A}(\Phi)\right](Z^{(n)}(s))\, ds\,. \tag{2.12}$$

Using (2.11), (2.6) and (2.7), one obtains

$$\begin{aligned} \int_{\mathcal{W}} \varphi(w)\mu^{(n)}(t,dw) = \int_{\mathcal{W}} \varphi(w)\mu^{(n)}(0,dw) + \int_0^t \int_{\mathcal{W}}\int_{\mathcal{W}} \\ \left\{\int_{\mathcal{W}}\int_{\mathcal{W}} \left[\varphi(\tilde{w}_1)+\varphi(\tilde{w}_2)-\varphi(w_1)-\varphi(w_2)\right]\beta(w_1,w_2,d\tilde{w}_1,d\tilde{w}_2)\right\} \\ \mu^{(n)}(s,dw_1)\,\mu^{(n)}(s,dw_2)\,ds - R^{(n)}(t) + M^{(n)}(t)\,, \end{aligned} \tag{2.13}$$

where

$$\begin{aligned} R^{(n)}(t) = \int_0^t \sum_{i=1}^{m^{(n)}(s)} \left[g_i^{(n)}(s)\right]^2 \times \\ \left\{\int_{\mathcal{W}}\int_{\mathcal{W}} \left[\varphi(\tilde{w}_1)+\varphi(\tilde{w}_2)-2\,\varphi(w_i^{(n)}(s))\right]\beta(w_i^{(n)}(s),w_i^{(n)}(s),d\tilde{w}_1,d\tilde{w}_2)\right\} ds\,. \end{aligned} \tag{2.14}$$

Representation (2.13) shows the origin of Eq. (1.8). Note that

$$\max_{i=1,\ldots,m^{(n)}(s)} g_i^{(n)}(s) \le \max_{i=1,\ldots,n} g_i^{(n)}(0)\,, \tag{2.15}$$

because of (1.4) and (1.14). Thus, the term $R^{(n)}(t)$ defined in (2.14) is easily estimated,

$$|R^{(n)}(t)| \le 4\,\|\varphi\|\,C_{\beta,max}\,t \max_{i=1,\ldots,n} g_i^{(n)}(0)\,. \tag{2.16}$$

Using (2.8), (2.15), and the obvious estimate (cf. (1.7))

$$G(Z^{(n)}(s),i,j,\tilde{w}_1,\tilde{w}_2) \le \max_{i=1,\ldots,m^{(n)}(s)} g_i^{(n)}(s)\,,$$

one obtains from (2.12) that

$$\mathcal{E}\left[M^{(n)}(t)\right]^2 \le 16\,\|\varphi\|^2\,C_{\beta,max}\,t \max_{i=1,\ldots,n} g_i^{(n)}(0)\,. \tag{2.17}$$

Using the representation (2.13) as well as the estimates (2.16), (2.17), and assumption (2.2), the proof can be completed in analogy with [17].

3. Pathwise behaviour of the stochastic process

Once the parameters G and Q are fixed, the generator (1.2) and therefore the stochastic evolution of the process (1.1) are determined. But there are different ways of generating trajectories of the process.

The process is a jump process with a generator of the form

$$\mathcal{A}(\Phi)(z) = \int_{\mathcal{Z}} \Big[\Phi(\tilde{z}) - \Phi(z)\Big]\, q(z, d\tilde{z})\,, \tag{3.1}$$

where

$$q(z, d\tilde{z}) = \sum_{1\le i\ne j\le m} \int_{\mathcal{W}} \int_{\mathcal{W}} \delta_{J(z,i,j,\tilde{w}_1,\tilde{w}_2)}(d\tilde{z})\, Q(z,i,j,d\tilde{w}_1,d\tilde{w}_2)\,.$$

The generator (3.1) does not change if one replaces q by

$$\begin{aligned} \hat{q}(z, d\tilde{z}) \;=\; \sum_{1\le i\ne j\le m} \Big\{ & \int_{\mathcal{W}} \int_{\mathcal{W}} \delta_{J(z,i,j,\tilde{w}_1,\tilde{w}_2)}(d\tilde{z})\, Q(z,i,j,d\tilde{w}_1,d\tilde{w}_2) \\ & + [\hat{Q}_{max}(z,i,j) - Q(z,i,j,\mathcal{W},\mathcal{W})]\, \delta_z(d\tilde{z}) \Big\}\,, \end{aligned} \tag{3.2}$$

where $\hat{Q}_{max}$ is a function such that

$$Q(z,i,j,\mathcal{W},\mathcal{W}) \le \hat{Q}_{max}(z,i,j)\,. \tag{3.3}$$

Thus, the behaviour of the Markov process (1.1) can be described as follows.

Coming to a state $z = ((w_1, g_1), \ldots, (w_m, g_m))$, the process stays there for a **random waiting time** $\hat{\tau}(z)$, which has an exponential distribution with the parameter

$$\hat{\pi}(z) = \hat{q}(z, \mathcal{Z}) = \sum_{1\le i\ne j\le m} \hat{Q}_{max}(z,i,j)\,, \tag{3.4}$$

i.e.

$$\text{Prob}\,\{\hat{\tau}(z) \ge t\} = \exp(-\hat{\pi}(z)\,t)\,.$$

Then, the process jumps into a state $\tilde{z}$, which is distributed according to the **jump distribution**

$$\hat{\pi}(z)^{-1}\,\hat{q}(z, d\tilde{z})\,.$$

According to (3.2), the **distribution of the parameters** i **and** j is determined by the probabilities

$$\frac{\hat{Q}_{max}(z,i,j)}{\sum_{1\le i\ne j\le m}\hat{Q}_{max}(z,i,j)}\,. \tag{3.5}$$

Given i and j, there is a certain **probability that a jump is fictitious**. Namely, the new state is $\tilde{z}=z$ with probability

$$1-\frac{Q(z,i,j,\mathcal{W},\mathcal{W})}{\hat{Q}_{max}(z,i,j)}\,. \tag{3.6}$$

Otherwise, the **distribution of the parameters** $\tilde{w}_1$ **and** $\tilde{w}_2$ is

$$\frac{Q(z,i,j,d\tilde{w}_1,d\tilde{w}_2)}{Q(z,i,j,\mathcal{W},\mathcal{W})}\,, \tag{3.7}$$

and the new state is $\tilde{z}=J(z,i,j,\tilde{w}_1,\tilde{w}_2)$.

A trivial choice of the function $\hat{Q}_{max}$ is (cf. (3.3))

$$\hat{Q}_{max}(z,i,j)=Q(z,i,j,\mathcal{W},\mathcal{W})\,. \tag{3.8}$$

In this case, there will be no fictitious jumps (cf. (3.6)). However, in general one has quadratic (with respect to the number of particles m) effort in the calculation of the waiting time parameter (3.4) or the probabilities (3.5). An appropriate choice of the function $\hat{Q}_{max}$ may lead to a substantial simplification of the modelling of the process. Note that the distribution of the process remains the same.

We give an example, where the parameter $\hat{\pi}(z)$ of the waiting time distribution is known analytically. Because of (1.5), one may choose

$$\hat{Q}_{max}(z,i,j)=C_{Q,max}\,(g_i+g_j)\,. \tag{3.9}$$

Note that $z=((w_1,g_1),\ldots,(w_m,g_m))$. According to (3.4), one obtains

$$\hat{\pi}(z)=2\,C_{Q,max}\,(m-1)\sum_{i=1}^{m}g_i\,. \tag{3.10}$$

The probabilities (3.5) take the form

$$\frac{g_i+g_j}{2\,(m-1)\,\bar{g}(z)}\,,\quad \text{where}\quad \bar{g}(z)=\sum_{i=1}^{m}g_i\,. \tag{3.11}$$

Consequently, first the index i is to be chosen according to the probabilities

$$\frac{(m-2)\,g_i+\bar{g}(z)}{2\,(m-1)\,\bar{g}(z)}\,, \tag{3.12}$$

and then, given i, the index j is to be chosen according to the probabilities

$$\frac{g_i + g_j}{(m-2)\, g_i + \bar{g}(z)} \,. \tag{3.13}$$

Both distributions (3.12) and (3.13) are of the form

$$\frac{d + g_i}{c}\,, \quad i = 1, \ldots, l\,.$$

They may be modelled by the acceptance-rejection technique in the following way: choose i uniformly and check the condition

$$\eta \le \frac{d + g_i}{d + g_{max}}\,,$$

where η is uniformly on $[0,1]$ and $g_{max} \ge \max_{i=1,\ldots,l} g_i$.

The idea of the introduction of fictitious jumps is to obtain an equivalent stochastic mechanism of modelling trajectories, which is numerically more efficient. One generates more jumps by a much simplified stochastic mechanism and plays an additional game of chance (leading to fictitious jumps) to reduce the number of jumps to the right one. This idea is present in many of the algorithms known in the literature ([2], [9], [10], [11]).

4. Free parameters of the collision mechanism

The parameters G and Q satisfying (1.7) and (1.10) can be represented in the form

$$\begin{aligned} G(z,i,j,\tilde{w}_1,\tilde{w}_2) &= [1+\gamma(z,i,j,\tilde{w}_1,\tilde{w}_2)]^{-1} \min(g_i,g_j)\,, \\ Q(z,i,j,d\tilde{w}_1,d\tilde{w}_2) &= [1+\gamma(z,i,j,\tilde{w}_1,\tilde{w}_2)] \max(g_i,g_j)\, \beta(w_i,w_j,d\tilde{w}_1,d\tilde{w}_2)\,. \end{aligned} \tag{4.1}$$

The function γ is supposed to be such that

$$0 \le \gamma(z,i,j,\tilde{w}_1,\tilde{w}_2)] \le C_{\gamma,max}\,. \tag{4.2}$$

Condition (1.5) is fulfilled with

$$C_{Q,max} = (1 + C_{\gamma,max})\, C_{\beta,max} \tag{4.3}$$

provided that β satisfies (2.1).

Example 4.1 *The trivial choice of the function* γ *is*

$$\gamma(z,i,j,\tilde{w}_1,\tilde{w}_2) = 0\,,$$

for which one obtains

$$\begin{aligned} G(z,i,j,\tilde{w}_1,\tilde{w}_2) &= \min(g_i,g_j) \\ Q(z,i,j,d\tilde{w}_1,d\tilde{w}_2) &= \max(g_i,g_j)\,\beta(w_i,w_j,d\tilde{w}_1,d\tilde{w}_2)\,. \end{aligned}$$

If, in addition, there are identical initial weights, then the function G *reduces to a constant. Thus, there is a complete weight transfer during each collision (cf. (1.4)), and one obtains the standard DSMC method.*

Example 4.2 *Consider a subset* W_1 *of the space* $\mathcal{W}\times\mathcal{W}$, *and define*

$$\gamma(z,i,j,\tilde{w}_1,\tilde{w}_2) = \gamma_1(w_i,w_j) = \begin{cases} \kappa_1 \ge 0\,, & \textit{if} \quad (w_i,w_j)\in W_1\,, \\ 0 \quad , & \textit{otherwise.} \end{cases} \tag{4.4}$$

In this case, particles with states described by the set W_1 *will remain in the system, simply loosing a part of their weight during each collision.*

Example 4.3 *Consider subsets* W_2 *and* $\tilde{W}_2$ *of the space* $\mathcal{W}\times\mathcal{W}$, *and define*

$$\gamma(z,i,j,\tilde{w}_1,\tilde{w}_2) = \gamma_2(w_i,w_j,\tilde{w}_1,\tilde{w}_2) = \tag{4.5}$$
$$\begin{cases} \kappa_2 \ge 0\,, & \textit{if} \quad (w_i,w_j)\in W_2 \quad \textit{and} \quad (\tilde{w}_1,\tilde{w}_2)\in \tilde{W}_2\,, \\ 0 \quad , & \textit{otherwise.} \end{cases}$$

In this case, the distribution of the parameters $\tilde{w}_1,\tilde{w}_2$ *changes (cf. (3.7)) in such a way that particles jump with larger probability from states described by the set* W_2 *into states described by the set* $\tilde{W}_2$.

Note that, unlike the introduction of fictitious jumps in Section 3, different choices of the function γ lead to different stochastic particle schemes (1.1). What these schemes have in common, is the limit of their empirical measures (1.12) given by Theorem 2.1. However, the approach to this limit depends on the choice of γ.

If $\gamma=0$, then there is the largest possible weight transfer function G and the lowest possible jump kernel Q (cf. (4.1)). Consequently, there is the slowest possible increase of the number of particles in the system. In particular, maximal one new particle may occur during a collision.

If $\gamma>0$, then only a part of the weights of the particles in the pre–collision states is transferred to the particles in the post–collision states during the collision (cf. (4.1), (1.4)). This effect is compensated by a corresponding increase of the kernel Q leading to smaller time intervals between collisions (cf. (3.4) with the choice (3.8)) and, possibly, a change of the distribution of the parameters $i, j, \tilde{w}_1, \tilde{w}_2$ (cf. (3.5) with the choice (3.8), and (3.7)). Another effect of an increased kernel Q is a faster growth of the number of particles in the system.

On the other hand, the distribution of the post–collision states $\tilde{w}_1, \tilde{w}_2$ may be changed according to different purposes via an appropriate choice of the function γ (cf. (4.1), (3.7)). The effect of an increased jump kernel Q is then compensated by a decrease of the weight transfer function G. Thus, if an artificially favoured post–collision state comes out, only a correspondingly smaller part of the weight is transferred.

5. A model kinetic equation

Consider the special case with the space $\mathcal{W} = [0,1]$, where the points 0 and 1 are identified, and the kernel

$$\beta(w_1, w_2, d\tilde{w}_1, d\tilde{w}_2) = \delta_{\psi(w_1+w_2)}(d\tilde{w}_1)\, \delta_{w_2}(d\tilde{w}_2)\,, \tag{5.1}$$

where the function ψ is defined as

$$\psi(x) = x - n\,, \quad x \in [n, n+1)\,,\ n = -1, 0, 1\,.$$

Then Eq. (1.8) takes the form

$$\begin{aligned} \frac{d}{dt} \int_0^1 \varphi(v)\, f(t,v)\, dv \;&=\; \int_0^1 \int_0^1 \varphi(\psi(v_1+v_2))\, f(t,v_1)\, f(t,v_2)\, dv_1\, dv_2 \\ &\quad - \int_0^1 \int_0^1 \varphi(v_1)\, f(t,v_1)\, f(t,v_2)\, dv_1\, dv_2\,. \end{aligned} \tag{5.2}$$

The first term on the right side of (5.2) is transformed by an appropriate substitution of the integration variables,

$$\begin{aligned} &\int_0^1 \int_0^1 \varphi(\psi(v_1+v_2))\, f(t,v_1)\, f(t,v_2)\, dv_1\, dv_2 = \\ &\qquad = \int_0^1 \int_0^1 \varphi(u)\, f(t,v_1)\, f(t,\psi(u-v_1))\, du\, dv_1\,. \end{aligned} \tag{5.3}$$

Removing the test functions one obtains from (5.2) and (5.3) the equation

$$\frac{\partial}{\partial t} f(t,v) = \int_0^1 dw\, [f(t,\psi(v-w))\, f(t,w) - f(t,v)\, f(t,w)]\,. \tag{5.4}$$

Remark 5.1 *The limiting equation (5.4) is also obtained for*

$$\beta(w_1, w_2, d\tilde{w}_1, d\tilde{w}_2) = \frac{1}{2}\,\delta_{\psi(w_1+w_2)}(d\tilde{w}_1)\,\delta_{\psi(w_1+w_2)}(d\tilde{w}_2)\,, \tag{5.5}$$

instead of (5.1). The kernel (5.5) is preferable since it leads to a lower intensity function and thus to a slower growth of the number of particles in the system.

We want to illustrate the new opportunities achieved by the introduction of the generalized collision mechanism, where the parameters G and Q are considered as degrees of freedom of the numerical algorithm. To this end, we consider the problem of calculating small probabilities, i.e. functionals of the solution of Eq. (5.4) of the form

$$p_\varepsilon(t) = \int_{1-\varepsilon}^{1} f(t,w)\,dw\,, \quad \varepsilon > 0\,. \tag{5.6}$$

For small ε, only very few particles reach the integration set $[1-\varepsilon, 1]$. The standard statistical estimator (cf. (1.13) and Example 4.1) of the functional (5.6) has large fluctuations.

We consider two strategies of tackling this problem using special choices of the function γ in (4.1). The first strategy is to avoid that particles disappear once they have reached the region $[1-\varepsilon, 1]$. The second strategy is to encourage particles to enter the desired region, i.e. to give a preference to certain outcomes of collisions by an appropriate choice of the corresponding probability distribution.

We introduce the function

$$\gamma(z,i,j,\tilde{w}_1,\tilde{w}_2) = \gamma_1(w_i,w_j) + \gamma_2(w_i,w_j,\tilde{w}_1,\tilde{w}_2)\,,$$

where the functions γ_1 and γ_2 are defined in (4.4) and (4.5), respectively, with the corresponding sets

$$\begin{aligned} W_1 &= \{(w_1,w_2) : \quad w_1 \in [1-\varepsilon,1] \quad \text{or} \quad w_2 \in [1-\varepsilon,1]\}\,, \\ W_2 &= \{(w_1,w_2) : \quad w_1\,,\, w_2 \notin [1-\varepsilon,1]\}\,, \\ \tilde{W}_2 &= \{(w_1,w_2) : \quad \tilde{w}_1\,,\, \tilde{w}_2 \in [1-\varepsilon,1]\}\,. \end{aligned}$$

Note that $\tilde{w}_1 = \tilde{w}_2$ with probability one, according to (5.5). The function γ takes the form

$$\gamma(z,i,j,\tilde{w}_1,\tilde{w}_2) = \begin{cases} \kappa_1\,, & \text{if} \quad w_i \in [1-\varepsilon,1] \quad \text{or} \quad w_j \in [1-\varepsilon,1]\,, \\ \kappa_2\,, & \text{if} \quad w_i, w_j \notin [1-\varepsilon,1] \quad \text{and} \quad \tilde{w}_1,\tilde{w}_2 \in [1-\varepsilon,1]\,, \\ 0\,, & \text{otherwise.} \end{cases} \tag{5.7}$$

Consider $\hat{Q}_{max}$ in the form (cf. (3.9), (4.3), (4.2), (5.5))

$$\hat{Q}_{max}(z,i,j) = \frac{1+\max(\kappa_1,\kappa_2)}{2}\,(g_i+g_j)\,. \tag{5.8}$$

According to (3.10) with $C_{Q,max} = \frac{1+\max(\kappa_1,\kappa_2)}{2}$, the parameter of the waiting time distribution is

$$\hat{\pi}(z) = (1+\max(\kappa_1,\kappa_2))\,(m-1)\sum_{i=1}^{m} g_i\,. \tag{5.9}$$

The indices i,j are distributed according to (3.11), i.e. independently of κ_1 and κ_2 .

The jump is fictitious with probability (cf. (3.6), (4.1), (5.5), (5.8))

$$1-\frac{1+\gamma(z,i,j,\psi(w_i+w_j),\psi(w_i+w_j))}{1+\max(\kappa_1,\kappa_2)}\,\frac{\max(g_i,g_j)}{(g_i+g_j)}\,. \tag{5.10}$$

The parameters $\tilde{w}_1,\tilde{w}_2$ are determined as (cf. (3.7), (4.1), (5.5))

$$\tilde{w}_1 = \tilde{w}_2 = \psi(w_i+w_j)\,.$$

Consider, for example, the case $\kappa_1 = 1$, $\kappa_2 \ge \kappa_1$. The jump is fictitious with probability

$$1-\frac{2}{1+\kappa_2}\,\frac{\max(g_i,g_j)}{(g_i+g_j)}\,,$$

if $w_i \in [1-\varepsilon,1]$ or $w_j \in [1-\varepsilon,1]$. In the case $w_i,w_j \notin [1-\varepsilon,1]$, the jump is fictitious with probability

$$1-\frac{\max(g_i,g_j)}{(g_i+g_j)}\,,\quad \text{if}\quad \tilde{w}_1,\tilde{w}_2 \in [1-\varepsilon,1]\,,$$

and

$$1-\frac{1}{1+\kappa_2}\,\frac{\max(g_i,g_j)}{(g_i+g_j)}\,,\quad \text{if}\quad \tilde{w}_1,\tilde{w}_2 \notin [1-\varepsilon,1]\,.$$

This means that for large κ_2 jumps to a state inside the set $[1-\varepsilon,1]$ are significantly favoured. However, during each such jump only the amount of weight $[1+\kappa_2]^{-1}\,\min(g_i,g_j)$ is transferred.

6. Numerical experiments

We consider the model equation (5.4) and calculate the functional (5.6), which has the form

$$\int_{\mathcal{W}} \varphi(w)\, f(t,w)\, dw \quad \text{with} \quad \varphi(w) = \P_{[1-\varepsilon,1]}(w)\,, \tag{6.1}$$

where ¶ denotes the indicator function. The functional (6.1) is approximated by the random variables (cf. (1.13))

$$\xi^{(n)}(t) = \sum_{i=1}^{m^{(n)}(t)} g_i^{(n)}(t)\, \varphi(w_i^{(n)}(t))\,. \tag{6.2}$$

In order to estimate the fluctuations of the random variables (6.2), a number N of independent ensembles of particles is generated. The corresponding values of the random variables are denoted by $\xi_1^{(n)}(t), \ldots, \xi_N^{(n)}(t)$. Then the empirical mean

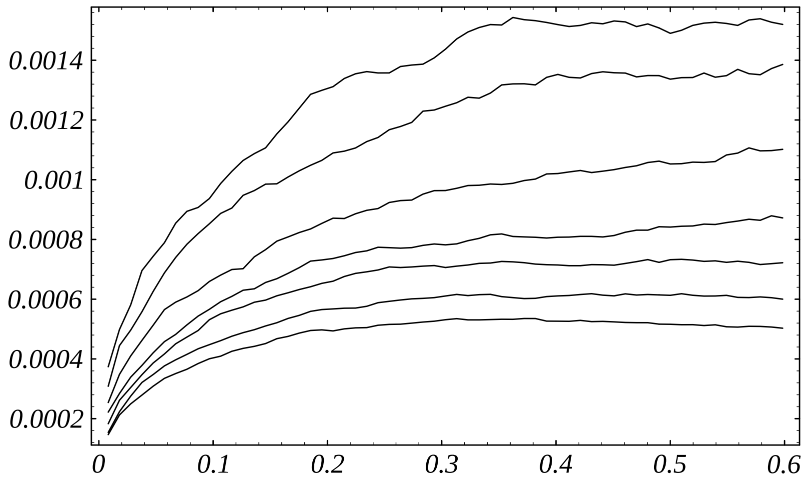
$$\frac{1}{N} \sum_{j=1}^{N} \xi_j^{(n)}(t) \tag{6.3}$$

converges as $N \to \infty$ to the expectation of the random variable (6.2). The statistical fluctuations around this deterministic limit are characterized by the quantity $\sqrt{\frac{\mathcal{D}^{(n)}(t)}{N}}$, where $\mathcal{D}^{(n)}(t)$ denotes the mean square deviation of the random variable (6.2) from its expectation. The order of convergence of the fluctuations is $\frac{1}{\sqrt{N}}$. However, the actual size of the fluctuations depends strongly on the value of $\mathcal{D}^{(n)}(t)$.

We want to compare the stochastic particle scheme based on the function γ defined in (5.7), with the standard algorithm, which corresponds to $\gamma \equiv 0$, or $\kappa_1 = \kappa_2 = 0$ (cf. Example 4.1).

First we illustrate the effect of the parameter κ_2 on the variance of the estimators (6.2). We choose $\varepsilon = 0.01$ and the parameters $\kappa_1 = 1$, $n = 100$, $N = 1000$. Figure 1 shows the curves for the quantities $\sqrt{\frac{\mathcal{D}^{(n)}(t)}{N}}$ on the time interval $[0, 0.6]$, for various values of κ_2. The curves are ordered from above according to the increasing values of κ_2.

Figure 1



Fluctuations for kappa2=0.5,1,2.5,5,10,20,50

Note that the fluctuations are very small at time zero, since we are able to approximate the initial distribution by particle systems with variable weights.

Variance reduction is obtained for increasing values of κ_2. But another effect has to be taken into account. When κ_2 is large, the number of collisions increases rapidly (cf. (5.9)), although many of them are fictitious (cf. (5.10)). The algorithm becomes much more time–consuming. Table 1 shows this effect at $t = 0.6$. In the fourth column, the products of the variance and the CPU–time (in appropriate units) are displayed. These products give a rough estimate of the effort needed with different schemes to reach a given statistical accuracy.

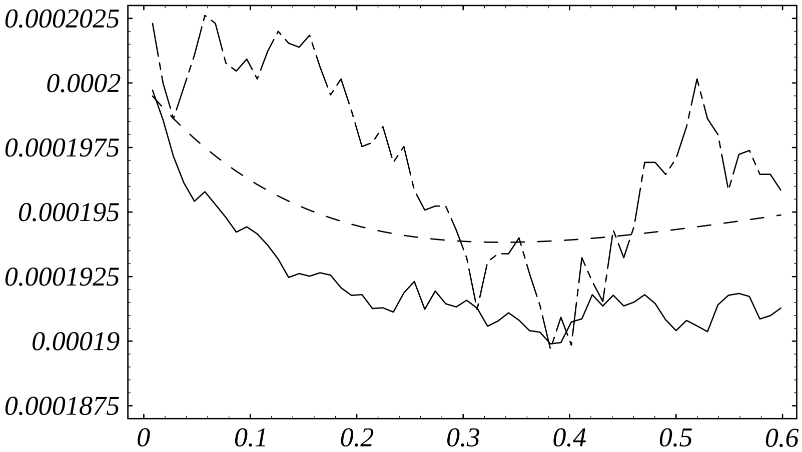
Table 1

κ_2	variance V	CPU–time T	$V * T$
0.5	23	13	299
1	19	13	247
2.5	12	15	180
5	8	20	160
10	5	32	160
20	4	66	264
50	3	311	933

In order to illustrate the powerful variance reduction, which can be achieved by the algorithm based on the function γ, we choose $\varepsilon = 0.0001$, the time interval $[0, 0.6]$, and the parameters $\kappa_1 = 1$ and $\kappa_2 = 100$. In the following figures, the solid lines correspond to the γ–algorithm and the dashed–dotted lines correspond to the standard algorithm. The dashed lines represent the exact solution, which can be calculated analytically for an appropriate choice of the initial value λ_0.

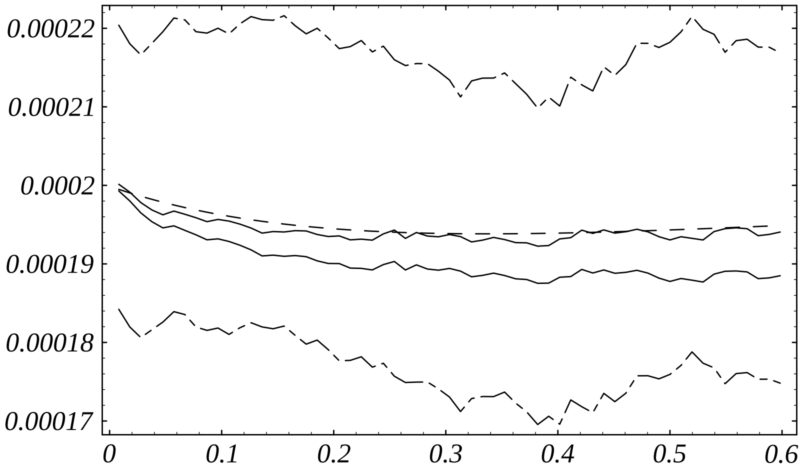
First we consider $n=100$ and $N=100000$. Figures 2 and 3 show the curves for the empirical mean values (cf. (6.3)) and the confidence intervals (with a confidence level of 0.99), respectively.

Figure 2



Empirical mean values for n=100 and N=100000

Figure 3

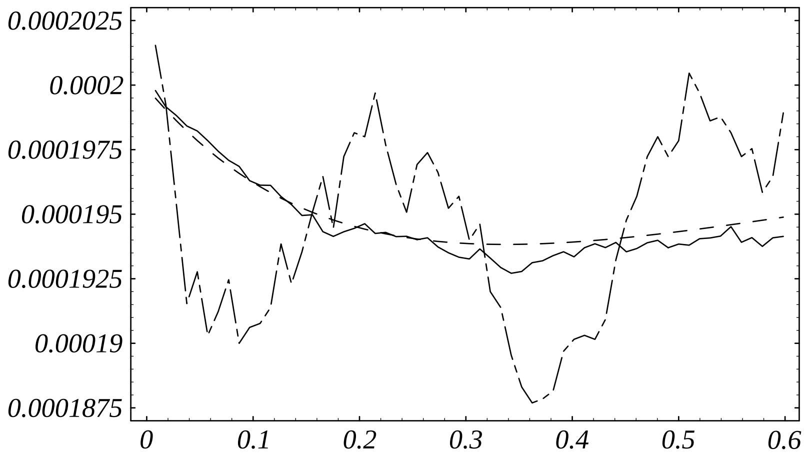


Confidence intervals for n=100 and N=100000

The small fluctuations of the γ–algorithm allow us to conclude that there is still a systematic error.

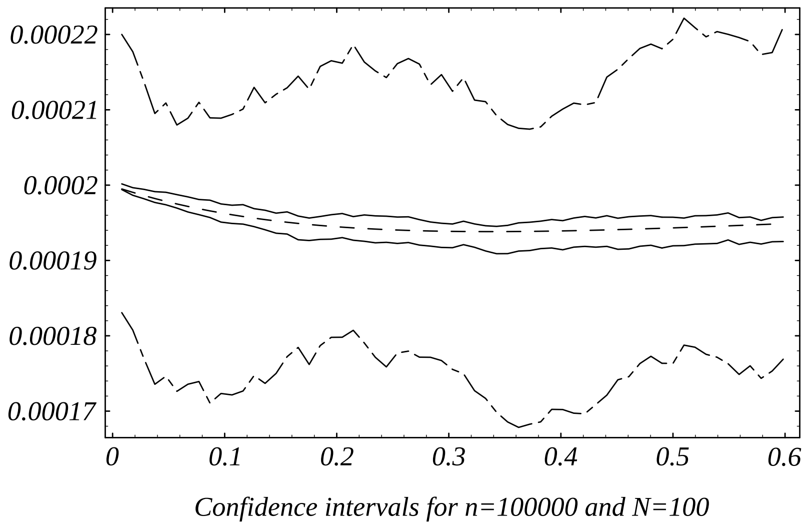
Next we consider $n = 100000$ and $N = 100$ in order to eliminate the systematic error. Figures 4 and 5 show the corresponding curves for the empirical mean values and the confidence intervals, respectively.

Figure 4



Empirical mean values for n=100000 and N=100

Figure 5



Confidence intervals for n=100000 and N=100

The reduction of the fluctuations achieved by the parameter κ_2 is approximately by a factor 10. To obtain this simply by averaging over more independent samples, one would have to increase N by a factor 100. The relation of the CPU–times for both algorithms gives a factor of about 13. So there is still a considerable advantage in using the γ–algorithm.

The test example was designed in order to illustrate the opportunities of the free parameters in the γ–algorithm. A more detailed study of various test cases will be published in a separate publication.

The partial weight transfer during the collisions causes an increase of the number of particles in the system. If there are no special effects like flow out of the region or absorption at the boundary, then after some time it will become necessary to reduce the number of particles in the system. A reduction procedure preserving mass, momentum and energy in the system was studied in [14]. We avoided this problem by restricting the test example to a relatively small time interval.

It will be of interest to apply the generalized algorithm in more realistic examples, including the Boltzmann equation. The possible dependence of the collision mechanism on the spatial cells is quite obvious. But it is also possible to work with general parameters depending on the pre–collision as well as post–collision velocities. We expect this to be useful in problems, where the particle density changes by several orders of magnitude in different regions.

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