Monte-Carlo approximations for 2d homogeneous Boltzmann equations without cutoff and for non Maxwell molecules

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Abstract

In [10], using a typically probabilistic substitution in the Boltzmann equation, we extend Tanaka's probabilistic interpretation [19] to much more general spatially homogeneous Boltzmann equations, i.e. homogeneous Boltzmann equations without cutoff and for non Maxwell molecules.

In this paper we show how this interpretation allows us to build some approximating cutoff interacting particle systems, and to derive some Monte-Carlo algorithms for the simulation of solutions of the Boltzmann equation.

Key words : Boltzmann equations without cutoff and for non Maxwell molecules, Nonlinear stochastic differential equations, Interacting particle systems, Monte-Carlo algorithm.

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1 Introduction and general setting

The Boltzmann equation we consider describes the evolution of the density $f(t,v)$ of particles with velocity $v \in I\!R^2$ at time t in a rarefied homogeneous gas:

$$\frac{\partial f}{\partial t} = Q(f,f) \tag{1.1}$$

where Q is a quadratic collision kernel preserving momentum and kinetic energy, of the form

$$Q(f,f)(t,v) = \int_{v_* \in I\!R^2} \int_{\theta=-\pi}^{\pi} \Big(f(t,v')f(t,v'_*) - f(t,v)f(t,v_*) \Big) B(|v-v_*|,\theta) d\theta dv_* \tag{1.2}$$

with

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$$v' = v + A(\theta)(v - v_*) \ ; \ v'_* = v_* - A(\theta)(v - v_*) \tag{1.3}$$

and

$$A(\theta) = \frac{1}{2} \begin{pmatrix} \cos\theta - 1 & -\sin\theta \\ \sin\theta & \cos\theta - 1 \end{pmatrix} \tag{1.4}$$

Notice that for each $\theta \in [-\pi, \pi] \setminus \{0\}$,

$$|A(\theta)| \leq K|\theta| \tag{1.5}$$

The cross-section B is a positive function, even in the θ-variable. If the molecules in the gas interact according to an inverse power law in $1/r^s$ with $s \geq 2$, then $B(z,\theta) = z^{\frac{s-5}{s-1}} d(|\theta|)$ where $d \in L^\infty_{loc}(]0,\pi])$ and $d(\theta) \sim K(s)\theta^{-\frac{s+1}{s-1}}$ when θ goes to zero, for some $K(s) > 0$. Physically, this explosion comes from the accumulation of grazing collisions.

In this general (spatially homogeneous) setting, the Boltzmann equation is very difficult to study. A large literature deals with the non physical equation with angular cutoff, namely under the assumption $\int_0^\pi B(z,\theta)d\theta < \infty$. More recently, the case of Maxwell molecules, for which the cross section $B(z,\theta) = \beta(\theta)$ only depends on θ, has been much studied without the cutoff assumption. In the Maxwell context, Tanaka, [19] was considering the case where $\int_0^\pi \theta\beta(\theta)d\theta < \infty$, and Desvillettes, [4], Desvillettes, Graham, Méléard, [5] and Fournier, [6] have worked under the general physical assumption $\int_0^\pi \theta^2\beta(\theta)d\theta < +\infty$.

The case in which B depends on z is really harder and there is just a few results on it. We can just mention the paper of Alexandre-Desvillettes-Villani-Wennberg [1] and Fournier-Méléard [9] in which a natural probabilistic approach is proposed to study the case of non Maxwell molecules under the condition $\int_0^\pi \theta B(z,\theta)d\theta < \infty$, when $B(z,\theta) = \psi(z)\beta(\theta)$ where ψ is positive and bounded and locally Lipschitz continuous. One proves in this case the existence of a measure-solution of the equation for any initial probability data with a second order moment. Moreover, we deduce of this probabilistic interpretation a stochastic particle method to approximate this solution, based on a Monte-Carlo approach.

In [10], another model is considered for which $\int_0^\pi \theta^2 B(z,\theta)d\theta < \infty$. Tanaka's probabilistic interpretation [19], who was dealing with Maxwell molecules, is extended to this case. Using a tricky transformation of the cross-section, a solution of the equation is related to the solution V_t of a Poisson-driven stochastic differential equation. That thus implies the existence of measure-valued solutions for the nonlinear equation.
Our aim in this paper is to build Monte-Carlo approximations of these solutions and to describe the corresponding algorithm. We will prove an extended law of large numbers, showing that the empirical probability measure associated with an interacting stochastic particle system tends to a solution of (1.1), in a certain sense.
We will see that the tricky transformation introduced in [10] will have a key rule in our study.
In the last part, we study numerically the behaviour of the empirical moment of order 4 associated with our particle system. We obtain numerical results which "confirm" our theoritical results, and which show that a central limit theorem might be associated with

our extended law of large numbers.

The simulation algorithm has to be compared with that of [9]. The main interest of the present algorithm is that it allows to consider the case where $B(z,\theta)$ satisfies only $\int \theta^2 B(z,\theta)d\theta < \infty$: in [9], it was assumed that $B(z,\theta)$ was of the form $\psi(z)\beta(\theta)$, with $\int \theta\beta(\theta)d\theta < \infty$. We thus get rid of two assumptions. Furthermore, the present algorithm is slightly more fast, because there were many fictive collisions in [9]. But the main objection, and this is a real limitation, is the following: we will see that the explicit computation (or numerical approximation) of the inverse of a distribution function associated with $B(z,\theta)$ has to be done.

Notation 1.1 *The terminal time $T > 0$ is arbitrarily fixed.*
$\mathbb{D}_T$ will denote the Skorohod space $\mathbb{D}([0,T],\mathbb{R}^2)$ of càdlàg functions from $[0,T]$ into $\mathbb{R}^2$. The space $\mathbb{D}_T$ endowed with the Skorohod topology is a Polish space.
$\mathcal{P}(\mathbb{D}_T)$ will denote the space of probability measures on $\mathbb{D}_T$ and $\mathcal{P}_2(\mathbb{D}_T)$ will be the subset of probability measures with a second order moment : Q belongs to $\mathcal{P}_2(\mathbb{D}_T)$ if

$$\int_{x\in\mathbb{D}_T} \sup_{[0,T]} |x(t)|^2 Q(dx) < \infty \tag{1.6}$$

K will denote a real positive constant of which the value may change from line to line.

In order to prove the existence of measure-solutions, it is assumed in [10] that

Assumption (S) : for each $x \in \mathbb{R}_+$, $B(x,\theta)$ is an even strictly positive function on $[-\pi,\pi]/\{0\}$ satisfying

$$\text{for all } x \in \mathbb{R}_+, \quad \int_{-\pi}^{\pi} B(x,\theta)d\theta = \infty \tag{1.7}$$

and

$$\sup_{x\in\mathbb{R}_+} \int_{-\pi}^{\pi} \theta^2 B(x,\theta)d\theta < \infty \tag{1.8}$$

For $X \in \mathbb{R}^2$, we will denote by $B(X,\theta)$ the quantity $B(|X|,\theta)$.

Equation (1.1) has to be understood in a weak sense, i.e. f is a solution of the equation if for each bounded test function ϕ,

$$\frac{\partial}{\partial t} < f,\phi > = < Q(f,f),\phi > \tag{1.9}$$

where $< .,. >$ denotes the duality bracket between L^1 and L^∞ functions. A standard integration by parts would give that f satisfies for each bounded ϕ

$$\frac{\partial}{\partial t}\int_{\mathbb{R}^2} f(t,v)\phi(v)dv = \int_{\mathbb{R}^2\times\mathbb{R}^2}\int_{-\pi}^{\pi}(\phi(v')-\phi(v))B(v-v_*,\theta)d\theta f(t,v)dv f(t,v_*)dv_* \tag{1.10}$$

But under (S), the form of v' and the fact that $\int |\theta| B(x,\theta)$ might be infinite necessitates to consider a compensated form of the collision term, which may explode in the previous form. This remark leads us to the following definition of solutions of (1.1).

Assume (S). First of all, we define, for $q \in \mathcal{P}_2(I\!R^2)$, each $\phi \in C_b^2(I\!R^2)$,

$$\begin{aligned} L_q\phi(v) &= \int_{I\!R^2}\int_{-\pi}^{\pi} \Big(\phi(v + A(\theta)(v - v^*)) - \phi(v) - A(\theta)(v - v^*).\nabla\phi(v)\Big) \\ &\qquad\qquad\qquad\qquad\qquad\qquad\qquad B(v - v^*, \theta)d\theta q(dv^*) \\ &\quad - \int_{I\!R^2}(v - v^*).\nabla\phi(v)b(v - v^*)q(dv^*) \end{aligned} \tag{1.11}$$

with for each $X \in I\!R^2$,

$$b(X) = \frac{1}{2}\int_{-\pi}^{\pi} B(X, \theta)(1 - \cos\theta)d\theta. \tag{1.12}$$

This kernel is well defined thanks to (1.5) and (1.8).

Definition 1.2 *Assume (S). Consider Q_0 a probability measure on $I\!R^2$. We say that a probability measure family $\{Q_t\}_{t\in[0,T]}$ is a measure-solution of the Boltzmann equation (1.1) with initial data Q_0 if for each $\phi \in C_b^2(I\!R^2)$, all $t \in [0, T]$,*

$$\langle \phi, Q_t\rangle = \langle \phi, Q_0\rangle + \int_0^t \langle L_{Q_s}\phi(v), Q_s(dv)\rangle\, ds, \tag{1.13}$$

The probabilitistic approach consists in considering (1.13) as the evolution equation of the flow of time-marginals of a Markov process, solution of the following nonlinear martingale problem.

Definition 1.3 *Let B be a cross-section satisfying (S) and let Q_0 in $\mathcal{P}_2(I\!R^2)$. We say that $Q \in \mathcal{P}_2(I\!D_T)$ solves the nonlinear martingale problem (MP) starting at Q_0 if for X the canonical process under Q, the law of X_0 is Q_0 and for any $\phi \in C_b^2(I\!R^2)$, any $t \in [0, T]$,*

$$\phi(X_t) - \phi(X_0) - \int_0^t L_{Q_s}\phi(X_s)ds \tag{1.14}$$

is a square-integrable martingale. Here, the nonlinearity appears through Q_s which denotes the law of X_s under Q.

Remark 1.4 *Taking expectations in (1.14), we observe that if Q is a solution of (MP), then its marginal flow $(Q_t)_{t\in[0,T]}$ is a measure-solution of the Boltzmann equation, in the sense of Definition 1.2.*

2 Transformation of the Boltzmann equation and main results.

This whole work is based on the following substitution in L_q.

Notation 2.1 *For each $X \in I\!R^2$, we consider the function h_X defined on $[-\pi, \pi]/\{0\}$ by*

$$h_X(\theta) = \int_\theta^\pi B(X, \varphi)d\varphi \text{ if } \theta > 0\ ;\ h_X(\theta) = -\int_{-\pi}^\theta B(X, \varphi)d\varphi \text{ if } \theta < 0 \tag{2.1}$$

Thanks to (S), it is clear that for each X, $h_X(\theta)$ is strictly decreasing from 0 to $-\infty$ between $\theta=-\pi$ and $\theta=0^-$, and from $+\infty$ to 0 between $\theta=0^+$ and $\theta=\pi$. We thus can set, for each $X\in I\!R^2$ and each $z\in I\!R^*$,

$$g(X,z)=h_X^{-1}(z), \quad \text{i.e.} \quad h_X(g(X,z))=z \tag{2.2}$$

Notice that for each X,z, the derivative $\frac{\partial}{\partial z}g(X,z)=-1/B(X,g(X,z))<0$, thanks to (S). The function $g(X,z)$ is thus strictly decreasing from 0 to $-\pi$ between $-\infty$ and 0^-, and from π to 0 between 0^+ and $+\infty$.

Notice also that $g(X,.)$ is odd and depends only on $|X|$.

Finally we remark that (1.12) can be written as

$$b(X)=\int_{I\!R^*}(1-\cos g(X,z))dz \tag{2.3}$$

that (1.8) becomes

$$\sup_{X\in I\!R^2}\int_{I\!R^*}g^2(X,z)dz<+\infty \tag{2.4}$$

We introduce again some notations.

Notation 2.2 *For $X\in I\!R^2$ and $z\in I\!R^*$, we set*

$$\gamma(X,z) \;=\; A(g(X,z)).X \;:\; I\!R^2\times I\!R^*\mapsto I\!R^2 \tag{2.5}$$

$$\delta(X) \;=\; b(X)X \;:\; I\!R^2\mapsto I\!R^2. \tag{2.6}$$

Proposition 2.3 *Assume (S). Then for each $q\in\mathcal{P}_2(I\!R^2)$, each $\phi\in C_b^2(I\!R^2)$,*

$$\begin{aligned} L_q\phi(v) \;=\; & \int_{I\!R^2}\int_{z\in I\!R^*}\Big(\phi(v+\gamma(v-v^*,z))-\phi(v)-\gamma(v-v^*,z).\nabla\phi(v)\Big)dzq(dv^*) \\ & -\int_{I\!R^2}\delta(v-v^*).\nabla\phi(v)q(dv^*) \end{aligned} \tag{2.7}$$

Proof. It suffices to use the substitution

$$\theta=g(v-v^*,z) \quad ; \quad z=h_{v-v^*}(\theta) \quad ; \quad dz=-B(v-v^*,\theta)d\theta \tag{2.8}$$

in (1.11) and (1.12) $\triangle$

Remark 2.4 *We now give an idea of the probabilistic approach we will use, following the main ideas of Tanaka, [19], who was dealing with a much more simple case of Maxwell molecules: $B(X,\theta)=\beta(\theta)$ and $\int_0^\pi\theta\beta(\theta)d\theta<+\infty$. In this case, the jump measure appearing in the analogous of (2.7) is $\beta(\theta)d\theta q(dv^*)$ independent of v. The main interest of the transformation described above is to transform the jump measure $B(v-v^*,\theta)d\theta q(dv^*)$ in a measure $dzq(dv^*)$ independent of v. That will allow us to have a probabilistic interpretation in terms of Poisson measure.*

Let us consider two probability spaces : the first one is the abstract space $(\Omega, \mathcal{F}, \{\mathcal{F}_t\}_{t\in[0,T]}, P)$ and the second one is the auxiliary space $([0,1], \mathcal{B}([0,1]), d\alpha)$ introduced to model the nonlinearity by the Skorohod representation theorem. In order to avoid any confusion, the processes on $([0,1], \mathcal{B}([0,1]), d\alpha)$ will be called α-processes, the expectation under $d\alpha$ will be denoted by E_α, and the laws $\mathcal{L}_\alpha$.

Notation 2.5 *We will denote by L^2_T the space of $I\!D_T$-valued processes Y such that*

$$E\left(\sup_{t\in[0,T]} |Y_t|^2\right) < +\infty \tag{2.9}$$

and by L^2_T-α the space of α-processes W such that

$$E_\alpha\left(\sup_{t\in[0,T]} |W_t|^2\right) < +\infty \tag{2.10}$$

Definition 2.6 *Assume (S). We will say that (V, W, N, V_0) is a solution of (SDE) if*
(i) (V_t) is an adapted L^2_T-process on Ω,
(ii) (W_t) is a L^2_T-α-process on $[0,1]$,
(iii) $N(\omega, dt, d\alpha, dz)$ is a Poisson measure on $[0,T]\times[0,1]\times I\!R^*$ with intensity measure

$$m(dt, d\alpha, dz) = dt d\alpha dz \tag{2.11}$$

(iv) V_0 is a square integrable variable independent of N,
(v) The laws of V and W on their respective probability spaces are the same, i.e. $\mathcal{L}(V) = \mathcal{L}_\alpha(W)$,
(vi) The following S.D.E. is satisfied :

$$V_t = V_0 + \int_0^t \int_0^1 \int_{I\!R^*} \gamma(V_{s-} - W_{s-}(\alpha), z)\tilde{N}(ds, d\alpha, dz) - \int_0^t \int_0^1 \delta(V_{s-} - W_{s-}(\alpha)) d\alpha ds \tag{2.12}$$

where $\tilde{N}$ denotes the compensated Poisson point process associated with N.

The following remark shows the connection between (SDE) and the Boltzmann equation (1.1).

Remark 2.7 *If (V, W, N, V_0) is a solution of (SDE), one easily proves by using the Itô formula, that $\mathcal{L}(V) = \mathcal{L}_\alpha(W)$ is a solution of the martingale problem* (1.14) *with initial law $Q_0 = \mathcal{L}(V_0)$, and thus $\{\mathcal{L}(V_s)\}_{s\in[0,T]}$ is a measure-solution of (1.13) with initial data Q_0.*

Let us now state an hypothesis, which, combined with (S), will be sufficient for proving the existence of a solution to (SDE) (and thus a solution to (MP), and hence a measure-solution to (1.1)).

> Assumption (MS) : (i) There exists a constant $K \in I\!R_+$ such that for all $X \in I\!R^2$,
>
> $$\int_{I\!R^*} \gamma^4(X, z) dz \le K(1 + |X|^4) \tag{2.13}$$
>
> (ii) There exists a function S from $I\!R^2 \times I\!R^2 \to I\!R^+$, locally bounded, such that for each $X, Y \in I\!R^2$,
>
> $$|\delta(X) - \delta(Y)|^2 + \int_{I\!R^*} (\gamma(X,z) - \gamma(Y,z))^2 dz \le |X - Y|^2 S^2(X, Y) \tag{2.14}$$
>
> (iii) The initial data Q_0 admits a moment of order 4.

Then it is proved in [10] that the following result holds.

Theorem 2.8 *Assume hypotheses (S) and (MS). Then*
1) The martingale problem (MP) with initial data Q_0 admits a solution $Q \in \mathcal{P}_2(I\!\!D_T)$.
2) Let Q be any solution of (MP). Let W be any α-process with law Q. On an enlarged probability space from the canonical space $(I\!\!D_T, \mathcal{D}_T, Q)$ there exist a Poisson measure N with intensity m and an independent square integrable variable V_0 with law Q_0 such that (X, W, N, V_0) is solution of (SDE), where X is the canonical process.

Remark 2.9 *Let us remark that there is no assumption on Q_0, except to have a forth order moment, and that allows us to consider degenerate initial data, as Dirac measures. Theorem 2.8 exhibits in particular a measure-solution to the Boltzmann equation (1.1) for every initial data $Q_0 \in \mathcal{P}_4(I\!\!R^2)$.*

Remark 2.10 *Assume that the cross-section is of the form $B(X,\theta) = \psi(X)/|\theta|^\alpha$, with ψ positive and $\alpha \in [1,3[$.*
Then (S) and (MS) are satisfied if ψ is strictly positive, bounded, and locally lipschitz continuous on $I\!\!R^2$.

Proof. Observing that when $\alpha = 1$, $g(X,z) = sign(z)e^{-|z|/\psi(X)}$, and when $\alpha > 1$, $g(X,z) = sign(z)\left(\frac{\pi^{\alpha-1}\psi(X)}{(\alpha-1)|z|\pi^{\alpha-1}+\psi(X)}\right)^{\frac{1}{\alpha-1}}$, the remark can be proved by using simple computations. $\triangle$

3 The stochastic particle approximation

In this part, we introduce some stochastic particle systems and prove the convergence of the empirical measures of the system to a solution of the nonlinear martingale problem (MP). This will be the theoretical basis of the Monte-Carlo algorithm given in the next section.
To define the particle system, we firstly need to "cutoff" the cross-section, in order to obtain a finite number of collisions during each finite time-interval. Namely, for each fixed real number l, we consider

$$B_l(x,\theta) = B(x,\theta)\mathbf{1}_{|\theta|\geq\frac{1}{l}}.$$

Now, we consider transformations as described in Section 2. The real number l is fixed.

Notation 3.1 *For each $X \in I\!\!R^2$, we define the function h^l_X on $[-\pi,\pi]/\{0\}$ by*

$$h^l_X(\theta) = \int_\theta^\pi B_l(X,\varphi)d\varphi = \int_{\frac{1}{l}\vee\theta}^\pi B(X,\varphi)d\varphi \text{ if } \theta > 0 \; ; \quad (3.1)$$

$$h^l_X(\theta) = -\int_{-\pi}^\theta B_l(X,\varphi)d\varphi = -\int_{-\pi}^{(-\frac{1}{l})\wedge\theta} B(X,\varphi)d\varphi \text{ if } \theta < 0 \quad (3.2)$$

Thanks to (S), it is clear that for each X, $h^l_X(\theta)$ is strictly decreasing from 0 to $-A_l(X)$ between $\theta = -\pi$ and $\theta = -\frac{1}{l}$, and from $A_l(X)$ to 0 between $\theta = \frac{1}{l}$ and $\theta = \pi$, where

$$A_l(X) = \int_{\frac{1}{l}}^\pi B(X,\varphi)d\varphi.$$

We thus can set, for each $X \in I\!R^2$ *and each* $z \in [-A_l(X), 0[\cup]0, A_l(X)]$,

$$g_l(X,z) = (h^l_X)^{-1}(z), \quad \text{i.e.} \quad h^l_X(g_l(X,z)) = z \tag{3.3}$$

Notice that for each $X \in I\!R^2$, all $|\theta| > \frac{1}{l}$,

$$h^l_X(\theta) = h_X(\theta) \tag{3.4}$$

and that for all $0 < |z| < A_l(X)$,

$$g_l(X,z) = g(X,z). \tag{3.5}$$

We extend $g_l(X,z)$ by 0 for $|z| \geq A_l(X)$.

Notation 3.2 *As before we denote*

$$\gamma_l(X,z) = A(g_l(X,z)).X \tag{3.6}$$
$$\delta_l(X) = b_l(X)X \tag{3.7}$$

where

$$b_l(X) = \int_{[-A_l(X),0[\cup]0,A_l(X)]} (1 - \cos g_l(X,z))dz.$$

Let us remark that for all l, $X, z \in I\!R^2 \times I\!R^*$,

$$\begin{aligned} |\gamma_l(X,z)| &\leq K|X||g_l(X,z)| \\ \int_{I\!R_*} |\gamma_l(X,z)|^2 dz &\leq K|X|^2 \int_{-\pi}^{\pi} \theta^2 B(X,\theta)d\theta \leq K|X|^2. \end{aligned} \tag{3.8}$$

Assumption (SA) : We will assume that

$$\sup_{X\in I\!R^2} \int_{\frac{1}{l}}^{\pi} B(X,\theta)d\theta = A_l < +\infty \ ; \ \sup_{X\in I\!R^2} \int_0^{\frac{1}{l}} \theta^2 B(X,\theta)d\theta \mapsto 0 \text{ for } l \mapsto \infty. \tag{3.9}$$

For example, if $B(X,\theta) = \psi(X)\beta(\theta)$, this assumption is satisfied as soon as the function ψ is bounded. Let us remark that since $A(0) = 0$, then $A(g_l(X,z))$ is well defined for all $z \in [-A_l, 0[\cup]0, A_l]$, and then also $\gamma_l(X,z)$.

Let us now define our approximating systems. The natural interpretation of the nonlinearity in (1.14) leads to a simple mean field interacting system but a physical interpretation of the equation leads also naturally to a binary mean field interacting particle system. In both cases, these n-particle systems are pure-jump Markov processes with values in $(I\!R^2)^n$ and with generators defined for $\phi \in C_b((I\!R^2)^n)$ by

$$\frac{1}{n} \sum_{1\leq i,j\leq n} \int_{[-A_l,0[\cup]0,A_l]} \left(\phi(v^n + \mathbf{e_i}.\gamma_l(v_i - v_j, z)) - \phi(v^n)\right) dz \tag{3.10}$$

for the simple mean-field interacting system and by

$$\frac{1}{n} \sum_{1\leq i,j\leq n} \int_{[-A_l,0[\cup]0,A_l]} \frac{1}{2}\Big(\phi(v^n + \mathbf{e_i}.\gamma_l(v_i - v_j, z) + \mathbf{e_j}.\gamma_l(v_j - v_i, z)) - \phi(v^n)\Big) dz \tag{3.11}$$

for the binary mean-field interacting system. In these formulas, $v^n = (v_1, ..., v_n)$ denotes the generic point of $(\mathbb{R}^2)^n$ and $\mathbf{e_i} : h \in \mathbb{R}^2 \mapsto \mathbf{e_i}.h = (0, ..., 0, h, 0, ..., 0) \in (\mathbb{R}^2)^n$ with h at the i-th place.
Both cases can be treated indifferently in a probabilistic point of view. The first particle system can be related to the Nanbu algorithm (cf. [16]) and is as simple as possible. The second one can be related to the Bird algorithm (cf. [20]). Its main interest is that it conserves momentum and kinetic energy. Moreover a set of numerical experiments shows it looks faster and more precise. We thus consider from now on the **binary mean-field system**. We denote by

$$V^{l,n} = (V^{l,1n}, ..., V^{l,nn})$$

the Markov process defined by (3.11).
We consider as in the previous section a pathwise representation of such processes using Poisson point measures. In this cutoff case, we could write a pathwise representation of the interacting systems in terms of solutions of SDEs driven by Poisson point measures (without compensation), but in order to obtain the tightness below, we need to use as in the previous section the corresponding representation using compensated Poisson point measures.
More precisely, we introduce a family of independent Poisson point measures $(N^{l,n,ij})_{1 \leq i < j \leq n}$ on $[0,T] \times [-A_l, 0[\cup]0, A_l]$ with intensities $\frac{1}{2n} dz dt$ and $(\tilde{N}^{l,n,ij})_{i,j}$ the compensated martingales. For $i > j$, we set $N^{l,n,ij} = N^{l,n,ji}$. Now we consider the process $(V^{l,in})_{1 \leq i \leq n}$ solution of the following stochastic differential equation:

$$V_t^{l,in} = V_0^i + \sum_{j=1}^n \int_0^t \int_{[-A_l, 0[\cup]0, A_l]} \gamma_l(V_{s-}^{l,in} - V_{s-}^{l,jn}, z) \tilde{N}^{l,n,ij}(dz, ds) - \int_0^t \delta_l(V_{s-}^{l,in} - V_{s-}^{l,jn}) ds. \tag{3.12}$$

We construct it easily by working recursively on each interjump interval of the point process $(N^{l,n,ij})_{1 \leq i,j \leq n}$. It is a n-dimensional Markov process with generator the one described above.
Let us denote by

$$\mu^{l,n} = \frac{1}{n} \sum_{i=1}^n \delta_{V^{l,in}}$$

the empirical measure of this system and by $(\pi^{n,l})_n$ the sequence of laws of $\mu^{l,n}$, which are probability measures on $\mathcal{P}(\mathbb{D}([0,T], \mathbb{R}^2))$.

Theorem 3.3 *Assume (S), (MS), (SA). Let $(V_0^i)_{i \geq 1}$ be i.i.d. Q_0-distributed random variables. Then the sequence $(\pi^{n,l})_{l,n}$ is uniformly tight for the weak convergence and any limit point charges only probability measures which are solutions of (MP). Thus any limit point (for the convergence in law) of the sequence $(\mu^{l,n})$ is a.s. a solution of (MP).*

Proof. To prove this theorem, we will show
1) the tightness of $(\pi^{n,l})_n$ in $\mathcal{P}(\mathcal{P}(\mathbb{D}([0,T], \mathbb{R}^2)))$,
2) the identification of the limiting values of $(\pi^{n,l})_{l,n}$ as solutions of the nonlinear martingale problem (MP).
One knows (cf. [15] Lemma 4.5) that the tightness of $(\pi^{n,l})_{l,n}$ is equivalent to the tightness of the laws of the semimartingales $V^{l,1n}$ belonging to $\mathcal{P}(\mathbb{D}([0,T], \mathbb{R}^2))$. This tightness can

be proved by showing the tightness of the law of the supremum of $|V_t^{l,1n}|$ on $[0,T]$ and the the Aldous criterion for $V^{l,1n}$.
One easily proves by a good use of Burkholder-Davis-Gundy and Doob's inequalities for (3.12) and thanks to (2.4), (2.3) and (MS) that

$$\sup_{l,n} E(\sup_{t\leq T}|V_t^{l,1n}|^2) < +\infty \tag{3.13}$$

from which we deduce without difficulty the tightness of the laws of $V^{l,1n}$ and hence the tightness of the sequence $(\pi^{l,n})$.
Let us now prove that all the limit values are solutions of the nonlinear martingale problem (MP). Consider $\pi^\infty \in \mathcal{P}(\mathcal{P}(I\!D([0,T],I\!R^2)))$ a limit value of $(\pi^{l,n})$. It is the limit point of a subsequence we still denote by $(\pi^{l,n})$.
For $\phi \in C_b^1(I\!R^2)$, $0 \leq s_1,...,s_k \leq s < t$, $g_1,...,g_k \in C_b(I\!R^2)$, $Q \in \mathcal{P}(I\!D([0,T],I\!R^2))$ and for X the canonical process on $I\!D([0,T],I\!R^2)$, we set

$$\begin{aligned} F(Q) &= \left\langle g_1(X_{s_1})...g_k(X_{s_k})\Big(\phi(X_t)-\phi(X_s)-\int_s^t L_{Q_u}\phi(X_u)du\Big),Q\right\rangle \\ &= < g_1(X_{s_1})...g_k(X_{s_k})(H_t^\phi - H_s^\phi),Q > \end{aligned} \tag{3.14}$$

where $L_q\phi$ is defined in (2.7) and then

$$\begin{aligned} H_t^\phi &= \phi(X_t)-\phi(X_0)+\int_0^t\int_{w\in I\!R^2}\nabla\phi(X_u)\delta(X_u-w)Q_u(dw)du \qquad (3.15)\\ &- \int_0^t\int_{I\!R^*}\int_{w\in I\!R^2}\left(\phi(X_u+\gamma(X_u-w,z))-\phi(X_u)-\gamma(X_u-w,z).\nabla\phi(X_u)\right)Q_u(dw)dzdu. \end{aligned}$$

Our aim is to prove that $< |F|,\pi^\infty >= 0$. The mapping F is not continuous since the projections $X \mapsto X_t$ are not continuous for the Skorohod topology. However, for any $Q \in \mathcal{P}(I\!D([0,T],I\!R^2))$, $X \mapsto X_t$ is Q-almost surely continuous for all t outside an at most countable set D_Q, and then F is continuous at the point Q if $s,t,s_1,...,s_k$ are not in D_Q. Here we use the continuity and the boundedness of $\phi, g_1,...,g_k$ and also the continuity of $(q,v) \mapsto \int_{I\!R^2}\nabla\phi(v)\delta(v-w)q(dw) - \int_{I\!R^*}\int_{w\in I\!R^2}\left(\phi(v+\gamma(v-w,z))-\phi(v)-\gamma(v-w,z).\nabla\phi(v)\right)q(dw)dz$ on $\mathcal{P}(I\!D([0,T],I\!R^2)) \times I\!R^2$. Now one can show that the set D of all t for which $\pi^\infty(Q, t \in D_Q) > 0$ is again at most countable. Thus, if $s,t,s_1,...,s_k$ are in D^c, F is π^∞-a.s. continuous. Then,

$$\left\langle F^2,\pi^\infty\right\rangle = \lim_{l,n}\left\langle F^2,\pi^{l,n}\right\rangle$$

But $\left\langle |F|,\pi^{l,n}\right\rangle \leq \left\langle |F^l|,\pi^{l,n}\right\rangle + \left\langle |F-F^l|,\pi^{l,n}\right\rangle$ where F^l is defined as F with δ_l and γ_l instead of δ and γ.
Firstly,

$$\begin{aligned} &\left\langle (F^l)^2,\pi^{l,n}\right\rangle = E((F^l(\mu^{l,n}))^2) \\ &= E\left(\left(\frac{1}{n}\sum_{i=1}^n(M_t^{l,i\phi}-M_s^{l,i\phi})g_1(V_{s_1}^{l,in})...g_k(V_{s_k}^{l,in})\right)^2\right) \\ &= \frac{1}{n}E\left(\left((M_t^{l,1\phi}-M_s^{l,1\phi})g_1(V_{s_1}^{l,1n})...g_k(V_{s_k}^{l,1n})\right)^2\right) \qquad (3.16)\\ &+\frac{n-1}{n}E\left((M_t^{l,1\phi}-M_s^{l,1\phi})(M_t^{l,2\phi}-M_s^{l,2\phi})g_1(V_{s_1}^{l,1n})...g_k(V_{s_k}^{l,1n})g_1(V_{s_1}^{l,2n})...g_k(V_{s_k}^{l,2n})\right) \end{aligned}$$

where $M^{l,i\phi}$ is the martingale defined by

$$\begin{aligned}M_t^{l,i\phi} &= \phi(V_t^{l,in}) - \phi(V_0^i)\\ &-\frac{1}{n}\sum_{j=1}^n \int_0^t \int_{[-A_l,0[\cup]0,A_l]} \Big(\phi(V_s^{l,in} + \gamma_l(V_s^{l,in} - V_s^{l,jn}, z)) - \phi(V_s^{l,in})\Big) dzds\end{aligned}$$

and with Doob-Meyer process given by

$$< M^{l,i\phi} >_t = \frac{1}{n}\sum_{j=1}^n \int_0^t \int_{[-A_l,0[\cup]0,A_l]} \Big(\phi(V_s^{l,in} + \gamma_l(V_s^{l,in} - V_s^{l,jn}, z)) - \phi(V_s^{l,in})\Big)^2 dzds$$

and for $i \neq j$,

$$\begin{aligned}< M^{l,i\phi}, M^{l,j\phi} >_t &= \frac{1}{n}\int_0^t \int_{[-A_l,0[\cup]0,A_l]} \Big(\phi(V_s^{l,in} + \gamma_l(V_s^{l,in} - V_s^{l,jn}, z)) - \phi(V_s^{l,in})\Big)\\ &\Big(\phi(V_s^{l,jn} + \gamma_l(V_s^{l,jn} - V_s^{l,in}, z)) - \phi(V_s^{l,jn})\Big) dzds.\end{aligned}$$

The right terms in (3.16) go to 0 thanks to the expression of the Doob-Meyer process, to the uniform integrability proved in (3.13) and thanks to (2.4) and (3.8). Moreover the convergence is uniform on l. Hence

$$\lim_n \langle |F^l|, \pi^{l,n}\rangle = 0, \text{uniformly in } l.$$

Otherwise, it is not hard to check that

$$\langle |F - F^l|, \pi^{l,n}\rangle = E(|F - F^l|(\mu^{l,n})) \leq K_l \sup_{l,n} E(\sup_{t\leq T}\langle |v|^2, \mu_t^{l,n}\rangle)$$

The last term is finite by (3.13) and

$$K_l \leq K \int_0^{\frac{1}{l}} \theta^2 B(X,\theta)d\theta, \tag{3.17}$$

which tends to 0 as l tends to infinity thanks to (SA).
We have then proved that

$$\langle |F|, \pi^\infty\rangle = 0.$$

Thus, $F(Q)$ is π^∞-a.s. equal to 0, for every $s, t, s_1, ..., s_k$ outside of the countable set D_Q. It is sufficient to assure that π^∞-a.s., Q is solution of the nonlinear martingale problem (MP). △

Corollary 3.4 *Assume (S), (MS), (SA) and consider a sequence μ^{l_r,n_r} which converges to Q. Then the probability measure-valued process $(\mu_t^{l_r,n_r})_{t\geq 0}$ converges in probability to the flow $(Q_t)_{t\geq 0}$ in the space $\mathbb{D}([0,T], \mathcal{P}(\mathbb{R}^2))$ endowed with the uniform topology.*

Proof. We first check that the limit point Q is deterministic. This is not obvious, since the uniqueness for (MP) is not known, and the only information we have about Q is that it a.s. satisfies (MP). However, the uniqueness of a solution Q_l holds for $(MP)_l$, the martingale problem $(MP)_l$ being defined as (MP), but with the cross section with cutoff B_l. Thus any (random) probability measure satisfying a.s. $(MP)_l$ is a.s. equal to Q_l, and thus is

deterministic. But one can check that the limit point Q of μ^{l_r,n_r} is equal to the limit of Q_{l_r}, and hence is deterministic.
The flow $(Q_t)_{t\geq 0}$ is thus deterministic and continuous, the continuity (for the weak convergence topology) being obvious from the expression of (MP). Then the convergence to $(Q_t)_{t\geq 0}$ is the same for the Skorohod or for the uniform topology. We use an intermediary lemma, proved in Méléard [15], Lemma 4.8, (see also Léonard [14]).

Lemma 3.5 *Let $(\mu^n)_n$ be a sequence of random probability measures on $I\!D_T$ which converges in law to a deterministic probability measure Q in $\mathcal{P}_2(I\!D_T)$. Let us assume moreover that*

$$\lim_{r\to 0} \sup_{0\leq t\leq T} E_Q\left(\sup_{t-r<s<t+r} |\Delta X_s| \wedge 1\right) = 0 \tag{3.18}$$

where X is the canonical process on $I\!D_T$, then the flow $(\mu^n_t)_{t\geq 0}$ converges in probability to $(Q_t)_{t\geq 0}$ in $I\!D([0,T],\mathcal{P}(I\!R^2))$ endowed with the uniform topology.

This result is not obvious since in $I\!D_T$ the projections are not continuous for the Skorohod topology.
Let us verify (3.18) in our context. We know by the point (ii) of Theorem 2.8 that X can be obtained on an enlarged probability space as solution of (2.12). Then

$$\begin{aligned}
E_Q\left(\sup_{t-r<s<t+r} |\Delta X_s| \wedge 1\right) &\leq E_Q\left(\sum_{s\in[t-r,t+r]} |\Delta X_s|^2 \wedge 1\right)^{\frac{1}{2}}\\
&\leq \left(\int_{t-r}^{t+r}\int_0^1\int_{I\!R_*} E_Q|\gamma(X_{s-}-W_{s-}(\alpha),z)|^2 dz d\alpha ds\right)^{\frac{1}{2}}\\
&\leq K\left(\int_{t-r}^{t+r}\int_0^1 E_Q((|X_{s-}-W_{s-}(\alpha)|^2) d\alpha ds\right)^{\frac{1}{2}}\\
&\leq KrE_Q\left(\sup_{t\leq t}|X_t|^2\right)^{\frac{1}{2}}.
\end{aligned}$$

But this last quantity tends to 0 as r tends to 0 since $E_Q(\sup_{t\leq T}|X_t|^2)$ is finite. Indeed, since $Q\in\mathcal{P}_2(I\!D_T)$, the canonical process X is a L^2_T-process under Q. We have the result. △

We will now explicit the algorithm of simulation.

4 The Monte-Carlo algorithm

We deduce from the above study an algorithm associated with the binary mean-field interacting particle system (Bird's approach). We could do the same thing with the simple mean-field interacting particle system (Nanbu's approach), but the numerical results seem less efficient.
¿From now on, the cross-section B, the initial distribution Q_0, the terminal time $T>0$, the size $n\geq 2$ of the particle system and the cutoff parameter $l>0$ are fixed. We denote by $B_l(z,\theta)$ the cross-section with cutoff. Because of Theorem 3.3, we simulate a particle system following (3.11), i.e. the whole path $(V^n_t)_{t\in[0,T]}\in I\!D([0,T],(I\!R^2)^n)$.

First of all, we assume that V_0^n is simulated according to the initial distribution $Q_0^{\otimes n}$. Then, we denote by $0 < T_1 < ... < T_k$ the successive jump times until T of a standard Poisson process with parameter nA_l. For example, one simulates independent exponential laws with this rate which describe the inter-collision time-intervals.
Before the first collision, the velocities do not change, so that we set $V_s^n = V_0^n$ for all $s < T_1$. Let us describe the first collision. We choose at random a couple (i,j) of particles according a uniform law over $\{(l,m) \in \{1,...,n\}^2;\ m \neq l\},$. We choose z uniformly on the interval $[-A_l, A_l]$, and we finally choose the collision angle following the law $\frac{1}{2A_l}dz$. Then we set

$$\begin{aligned} V_{T_1}^{n,i} &= V_0^{n,i} + \gamma_l(V_0^{n,i} - V_0^{n,j}, z) \\ V_{T_1}^{n,j} &= V_0^{n,j} + \gamma_l(V_0^{n,j} - V_0^{n,i}, z) \\ V_{T_1}^{n,l} &= V_0^{n,l} \quad \text{if } l \neq \{i,j\} \end{aligned}$$

Since nothing happens between T_1 and T_2, we set $V_s^n = V_{T_1}^n$ for all $s \in [T_1, T_2[$.
Iterating this method, we simulate $V_{T_1}^n, V_{T_2}^n, ..., V_{T_k}^n$, i.e. the whole path $(V_t^n)_{t\in[0,T]}$, which was our aim.
Notice that this algorithm is very simple and takes a few lines of program and does not require to discretize time. It furthermore conserves momentum and kinetic energy.

5 Numerical study.

We now would like to give an idea about the speed of convergence of the previous (Bird) algorithm. We consider the case of interactions in $1/r^3$, for which the cross section is given by $B(z,\theta) = z^{-1}\theta^{-2}$. Unfortunately, this collision kernel does not satisfy our assumptions. We thus consider a cross section of the form $B^M(z,\theta) = (z^{-1} \wedge M)\theta^{-2}$, which satisfies (S), (MS), and (SA).
Notice that $B^M(z,\theta)$ does not integrate θ, so that the method used in [9] does not allow to consider such a cross section.

The associated cross section with cutoff is given by $B^{M,l}(z,\theta) = (z^{-1} \wedge M)(\theta^{-2} 1_{\{|\theta| \geq 1/l\}})$. We also consider the initial distribution $Q_0(dv) = 1_{[-1,1]^2}(v)dv$. Then explicit computations of $g^M(x,z)$, $A_l^M(X)$, A_l^M, and $\gamma_l^M(X,z)$ (corresponding to the cross sections B^M and $B^{M,l}$) can be done.

For each M, l, we denote by $\{Q^{M,l}\}$ the solution of the martingale problem with the cross section $B^{M,l}$, obtained by Theorem 2.8. We know that for each M, each l, $\{Q^{M,l}\}$ is the limit, as n tends to infinity, of the empirical measures $\mu^{M,l,n}$ associated with the simulable empirical particle system. We also know that for each fixed M, $\{Q^{M,l}\}_l$ is tight, and that any limit point Q^M is solution of the martingale problem with the cross section B^M.

In order to test our algorithm, we decide to study the behaviour of the following moments of order 4, at the instant $t_0 = 1$:

$$m^M = \int_{\mathbb{R}^2} |v|^4 Q_{t_0}^M(dv) \quad ; \quad m^{M,l} = \int_{\mathbb{R}^2} |v|^4 Q_{t_0}^{M,l}(dv)$$

$$\text{and} \quad m^{M,l,n} = \int_{\mathbb{R}^2} |v|^4 \mu_{t_0}^{M,l,n}(dv)$$

Testing algorithms with the moments of the solution to the Boltzmann equation was great in the case of Maxwell molecules, in which case explicit computations of these moments are known. The moment of order 2 $\int |v|^2 Q_t(dv)$ being constant in t (it represents the kinetic energy of the system), people traditionally study the moment of order 4, which is the first non-trivial moment. We thus carry on studying this quantity, even if no explicit computation may be done in our context.

First of all, we make simulations, in order to choose M in such a way that the error due to this (spatial) cutoff seems to be small.
With $l = 64$, $n = 50000$, taking each time the mean over 100 simulations, denoting by $< m^{M,64,50000} >$ the mean over 100 experiences, we obtain with quite a good precision (the empirical mean error $\left\langle \left| m^{M,64,50000} - < m^{M,64,50000} > \right| \right\rangle$ is of the order of 5.10^{-3}):

M	1	4	8	16	32
$< m^{M,64,50000} >$	0.7870	0.7906	0.7908	0.7909	0.7910

The quantity $m^{M,64}$ does thus seem to converge very fastly, and we decide, from now on, to consider the cross section B^{16}.
We now study, for $M = 16$ fixed, the convergence of $m^{16,l}$ as l tends to infinity. With $n = 50000$, taking each time the mean over 100 simulations, we obtain with quite a good precision (the empirical mean error is again of the order of 5.10^{-3}):

l	1	2	4	8	16	32	64	128
$< m^{16,l,50000} >$	0.7075	0.7535	0.7740	0.7828	0.7868	0.7890	0.7912	0.7910

One might remark that $m^{16,l}$ goes to $0,791$ when l tends to infinity, with a speed of convergence in $|m^{16,l} - 0,791| \simeq 0.07/l$. This speed of convergence in $1/l$ is known for the Maxwell cross section $1/\theta^2$, see for example [7] for a proof in the $3D$ case.

We finally choose to study the speed of convergence of $m^{16,64,n}$ to $m^{16,64}$, when n tends to infinity. We obtain the figure 1.
It thus seems that a central limit theorem holds, at least for M and l fixed. See [8] for the proof of such a result in the Maxwell context. We of course could not hope a better speed of convergence, since the method we use is a Monte Carlo method.

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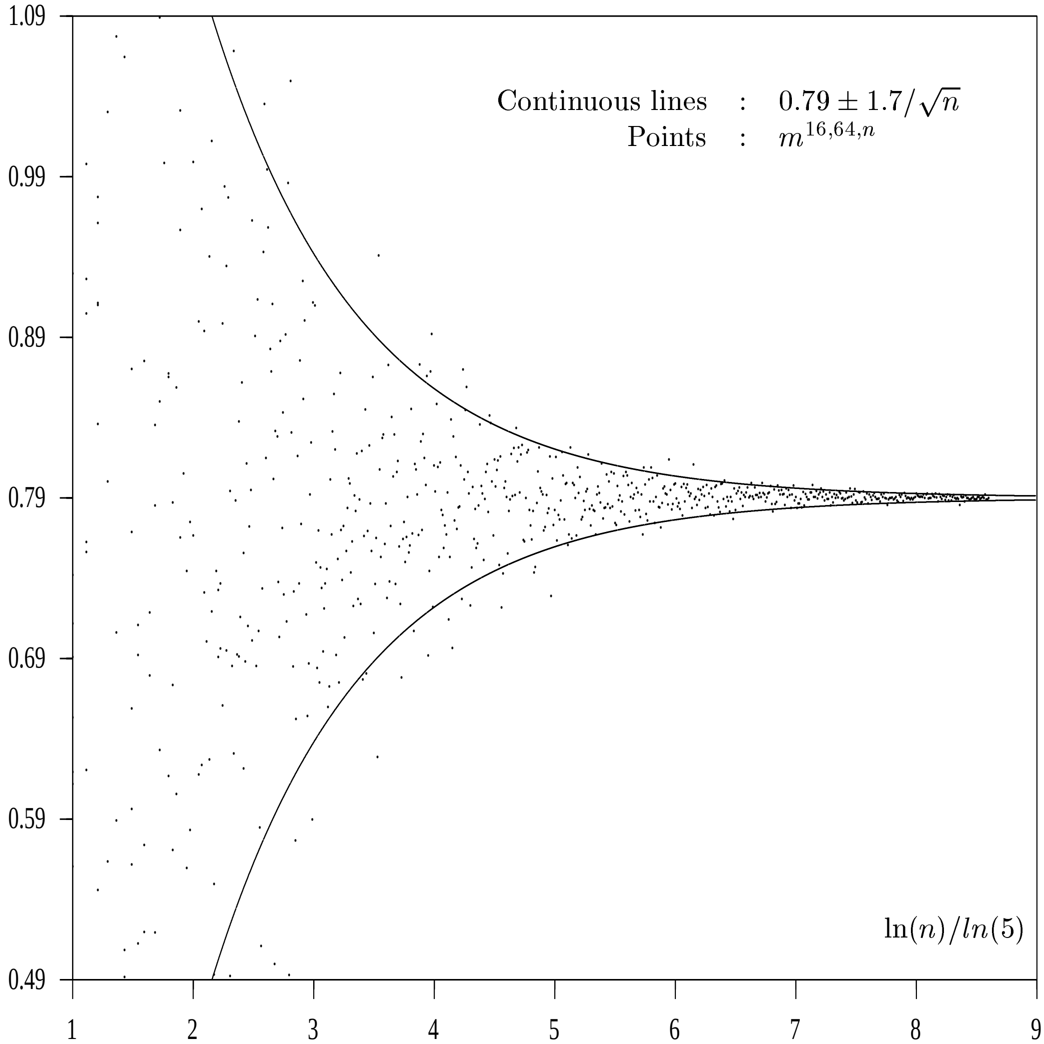
Figure 1: Result due to one simulation as a function of $\ln(n)/ln(5)$.



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