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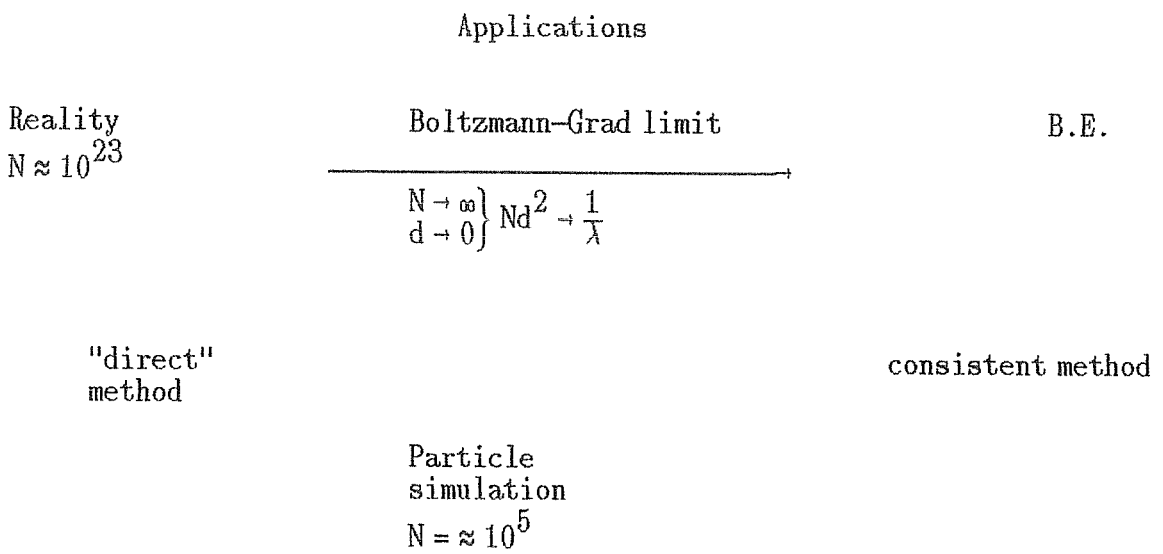
Abstract. We describe the mathematical structure of a recently developed family of consistent and convergent particle simulation methods for the Boltzmann equation.

1. The setting. Particle simulation methods for the Boltzmann equation have recently found wide-spread interest, in particular because new projects in spaceflight and in very high flying aircraft have created a new demand for computational rarefied gas dynamics. Because rarefied gases are believed to be well described by the Boltzmann equation, it is desirable that any such numerical scheme be consistent with this equation. In [1] and [2], we gave a convergence proof for a method which has been developed during the last 5 years and is a modification of a scheme originally suggested by Nanbu ([3], [4]). The objective of this article is to give a concise mathematical description of this method and of a more recent and more efficient variant. Our emphasis is on clarity and simplicity, and we avoid the technical details which were essential for the convergence proof in [2].

First, we clarify the concept "particle simulation". It is best explained by a simple diagram, which summarizes realistic, analytical and computational rarefied gas dynamics:



A realistic gas cloud consists of an astronomically large number of particles, far too large to track each particle individually. The Boltzmann equation is believed to be a good description because it emerges (formally) in the Boltzmann-Grad limit for the density distribution of a tagged particle. The idea of particle simulation is really to just return to the particle description, with a particle number N that is sufficiently large to guarantee "closeness" to the physical situation, but small enough to make the situation tractable from a computational point of view. Given the physical background of the problem, the particle simulation approach seems completely natural. There is, however, a second, analytical reason why particle simulation is reasonable here. We have to take a look at the Boltzmann equation to see it.

Let $f = f(t,x,v)$ be the particle density of the rarefied gas. It depends on time t, position x and velocity v, and its time evolution is given by the Boltzmann equation

$$\partial_t f + v \cdot \nabla_x f = \mathcal{J}(f,f) \tag{1}$$

The collision operator $\mathcal{J}(f,f)$ is defined by

$$\mathcal{J}(f,f)(t,x,v) = \frac{1}{\lambda} \int_{\mathbb{R}^3} \int_{S^2_+} k(|v-w|,\theta)\{f(v')f(w')-f(v)f(w)\}dn\, dw, \tag{2}$$

where $S^2_+ = \left\{n \in S^2;\ n \cdot (v-w) > 0\right\}$,

θ is the acute angle between n and $v-w$,

$v' = v - n(n\cdot(v-w))$

$w' = w + n(n\cdot v-w))$

are the post-collisional velocities associated with the (ingoing) collision configuration (v,w,n), and $k(|v-w|,\theta)$ is the collision kernel (for hard spheres, $k(|v-w|,\theta) = |v-w| \cdot \cos\theta$). λ is proportional to the mean free path between collisions – for the rest of this article, we set $\lambda = 1$.

The integration in (2) is 5-dimensional, and this is the second reason why particle simulation is a sensible way to solve the Boltzmann equation numerically – except in isotropic situations where $\mathcal{J}(f,f)$ could be evaluated with low-dimensional integrals, it would be just too inefficient to evaluate (2) by quadrature formulas. Monte Carlo simulation is a well-known alternative, and we shall see that it arises quite naturally (but not necessarily) in particle simulation.

2. Reduction of the Boltzmann equation. We now go through a series of fairly elementary steps which will reduce the Boltzmann equation to a form which is readily accessible to an approximation by point measures (particle simulation). These are

a) time discretization

b) separation of free flow and interaction ("splitting")

c) local homogenization

d) weak formulation

e) measure formulation.

To start, suppose that a particle at (x,v) in state space will go to $\phi_t(x,v)$ after time t, provided there is no collision with another particle (if the particle does not interact with the boundary of the confining container, $\phi_t(x,v) = (x+tv,v)$; otherwise, we assume that the trajectory is defined by some reasonable deterministic boundary condition, like specular reflection).

Choose a time step $\Delta t > 0$, then a first order discrete counterpart to the derivative

$$\left[\partial_t f + v \cdot \nabla_x f\right]\left[j \cdot \Delta t,\ \phi_{\Delta t}(x,v)\right]$$

is

$$\frac{1}{\Delta t}\left\{f((j+1)\Delta t,\ \phi_{\Delta t}(x,v)) - f(j\Delta t,\ x,\ v)\right\} \tag{3}$$

Substitute (3) for the left hand side in (1), let $(y,w) = \phi_{\Delta t}(x,v)$ and evaluate. The result is

$$f((j+1)\Delta t,\ y,\ w) = f(j\Delta t,\ \phi_{-\Delta t}(y,w)) + \Delta t \cdot \mathcal{J}(f,f)\left[j\Delta t,\ \phi_{-\Delta t}(y,w)\right] \tag{4}$$

The discretized equation (4) suggests to split the approximation into the collision simulation

$$\tilde{f}((j+1)\Delta t, y, w) = f(j\Delta t, y, w) + \Delta t \; \mathcal{J}(f,f)(j\Delta t, y, w) \tag{5}$$

and the free flow step

$$f((j+1),\Delta t, y, w) = \tilde{f}\Big[(j+1)\Delta t, \phi_{-\Delta t}(y,w)\Big]. \tag{6}$$

The numerical simulation of (6) will be obvious once we have understood the collision simulation. We therefore focus on that. Notice that the position variable y is not operated on in (5) – effectively, (5) is a discretized version of the spatially homogeneous Boltzmann equation.

To continue, we have to introduce a concept of "spatial cell" which already Boltzmann used in the classical derivation of his equation (his cell was just defined by $(x, x+dx)$, $(y, y+dy)$ etc.). The key idea is that such a cell is small from a macroscopic point of view, but large enough to contain many particles, and certainly large enough to keep a collision count for any particle in the cell during $\Delta t(dt)$ by just counting collisions with other particles in the same cell. In this collision count, the spatial variation of the gas density over the cell is neglected, i.e. spatial homogeneity over the cell is assumed (in fact, the numerical procedures we are about to describe allow to keep the exact positions of the approximating particles, but the collision partners needed for the collision simulation are assumed to be homogeneously distributed in each cell; see [2]).

Specifically, suppose that the gas in question is confined to a container $\Lambda \subset \mathbb{R}^3$, and that this container is partitioned into cells by

$$\Lambda = \cup C_i, \qquad C_i \cap C_j = \emptyset, \qquad i \neq j,$$

and we assume that the cells are such that $f(j\Delta t, \cdot)$ is on C_i well approximated by its homogenization

$$\frac{1}{\lambda^3(C_i)} \int_{C_i} f \, dy$$

(we replace $f(j\Delta t, \cdot)$ by its homogenization, but keep writing $f(j\Delta t, \cdot)$). If $f(j\Delta t, \cdot)$ is locally homogeneous in this sense, so is $\tilde{f}((j+1)\Delta t, \cdot)$; however, the free flow step will destroy the homogeneity, and one has to homogenize again before the next collision simulation. We note that the cells need not be the same size and that the partition of Λ can actually be changed with time (refined, for example) to gain better adjustment to the hypothesis of local homogeneity.

We have now reduced the Boltzmann equation to the remaining key question of doing the collision simulation (5) on an arbitrary but fixed cell C_i, where $f(j\cdot\Delta t, \cdot)$ is supposed to be independent of y. To simplify notation, we write $f_j(v)$ for $f(j\cdot\Delta t, y, v)$ and $f_{j+1}(v)$ for $\tilde{f}((j+1)\Delta t, y, v)$. Then (5) reads, explicitly

$$\begin{aligned} f_{j+1}(v) = &\left[1 - \Delta t \iint k(|v-w|, \theta) d\eta \, f_j(w) dw\right] f_j(v) \\ &+ \Delta t \iint k(|v-w|, \theta) f_j(v') f_j(w') d\eta \, dw. \end{aligned} \tag{7}$$

We next make the crucial assumption that there is an $A > 0$ such that

$$\int k(|v-w|,\theta)dn \leq A < \infty \tag{8}$$

for all v, w. Unfortunately, this means that k has to be truncated even for the hard sphere case; a little thought shows that we have to cut off k for large $|v-w|$, i.e. the collisions between particles with large relative velocity are neglected. Fortunately, for any reasonable gas cloud only few particles are affected.

Also, we renormalize $f_j(v)$ such that $\int f_j\, dw = 1$ (assuming that we have $\iint_A f_j(y,v)dv\, dy = 1$ and $\int_{C_i}\int f_j(y,v)dv\, dy = \lambda^3(C_i)\int f_j(v)dv = \gamma_{j,i}$, this means that we have to replace f_j by $f_j \cdot \frac{\lambda^3(C_i)}{\gamma_{j,i}}$; for this paper, we simply set $\frac{\lambda^3(C_i)}{\gamma_{j,1}} = 1$). Then, if $\Delta t < \frac{1}{A}$, $f_j \geq 0$ implies that $f_{j+1} \geq 0$.

Thus the truncation (8) is necessary to keep the density nonnegative, an essential feature. This is an artifact of the explicit nature of our approximation scheme; (8) can be avoided by starting from an alternative formulation of the Boltzmann equation, but this would lead to serious problems later on.

The next step is a transition to a weak formulation of (7). To this end, multiply (7) with a test function $\varphi \in C_b(\mathbb{R}^3_v)$, integrate, use the involutive property of the collision transformation and that $|v'-w'| = |v-w|$. The result is

$$\int \varphi(v)f_{j+1}(v)dv = \iint K_{v,w}\varphi\, f_j(v)f_j(w)dv\, dw, \tag{9}$$

where $K_{v,w}\varphi = \left[1 - \Delta t \int k\, dn\right]\varphi(v) + \Delta t \int k\, \varphi(v')dn$ (we have also used the renormalization $\int f_j\, dw = 1$).

Finally, before we rewrite (9) in measure formulation, we introduce a convenient representation for $K_{v,w}\varphi$. Let v and w be given. Then, we define a continuous function $T_{v,w}: S^2_+ \to \mathbb{R}^3$ by $T_{v,w}(n) = v'$. Moreover, let $B^1 = \left\{y \in \mathbb{R}^2; \|y\| \le \frac{1}{\sqrt{\pi}}\right\}$ be the circle of area 1, and assume that $\Delta t < \frac{1}{A}$.

Lemma 2.1. (see [1]) For all $v, w \in \mathbb{R}^3$, there is a continuous function $\phi_{v,w}: B^1 \to S^2_+$ such that

$$K_{v,w}\varphi = \iint_{B^1} \varphi\left[T_{v,w} \circ \phi_{v,w}(y)\right] d^2y$$

Remarks and Sketch of the Proof. This lemma, which is extremely useful for the sequel, is proved in detail in [1]. The function $\phi_{v,w}$ can actually be computed in terms of the collision kernel k.

The purpose of the function $\phi_{v,w}$ is a) to decide whether the particles with velocities v and w collide at all, and b) if they collide, with what collision parameter.

The idea of the proof is as follows. We represent B^1 by polar coordinates as $\left\{(r,\beta);\ 0 \le r \le \frac{1}{\sqrt{\pi}},\ 0 \le \beta \le 2\pi\right\}$. There is an $r_0 < \frac{1}{\sqrt{\pi}}$ such that

$$\pi r_0^2 = \Delta t \int k\, dn.$$

Let $n \in S^2_+$ be represented by (θ,ψ) $(\theta \in [0, \frac{\pi}{2}],\ \psi \in [0, 2\pi))$, where θ is the polar angle with respect to the axis in direction of $v-w$, and ψ is an azimuthal angle.

For $r \geq r_0$, let $\phi_{v,w}(r,\beta) = \left[\frac{\pi}{2}, \beta\right]$, i.e. $\theta = \frac{\pi}{2}$, $\psi = \beta$. These angles correspond to a grazing collision, and therefore $T_{v,w} \circ \phi_{v,w}(r,\beta) = v$; this happens on a set of measure $1 - \Delta t \int k\, dn$.

For $r < r_0$, the collision result is nontrivial. We set again $\psi(r,\beta) = \beta$, but $\theta(r,\beta) = \theta(r)$ is defined as the inverse of a function $r(\theta)$ which satisfies

$$\frac{d}{d\theta}\left[\frac{1}{2} r^2(\theta)\right] = \Delta t \cdot k(|v-w|, \theta) \sin\theta.$$

Clearly $r^2\left[\frac{\pi}{2}\right] = 2\Delta t \int_0^{\pi/2} k(|v-w|,\theta)\sin\theta\, d\theta = r_0^2$, and $\Delta t \int \varphi(v')k\, dn =$

$\int_0^{2\pi} \int_0^{r_0} \varphi\left[T_{v,w}(\theta(r),\beta)\right] r\, dr\, d\beta$. This completes the proof.

Now define probability measures $d\mu_j = f_j\, dv$, and let $\Psi(v,w,y) = T_{v,w} \circ \phi_{v,w}(y)$. By the lemma, (9) reduces to

$$\int \varphi(v) d\mu_{j+1} = \int_v \int_w \int_y \varphi \circ \Psi(y,v,w) d^2y\, d\mu_j(v) d\mu_j(w) \tag{10}$$

or, if we set $dM_j := d^2y \times d\mu_j \times d\mu_j$ (dM_j is a probability measure on $B^1 \times \mathbb{R}^3_v \times \mathbb{R}^3_w$),

$$\int \varphi\, d\mu_{j+1} = \int \varphi\, d\left[M_j \circ \Psi^{-1}\right] \tag{11}$$

In other words, we have identified the measure μ_{j+1} with $M_j \circ \Psi^{-1}$! (11) is the reduced Boltzmann equation which is most useful for the particle simulation idea.

3. The essence. We have now arrived at the central point of particle simulation. It is best summarized as follows: Suppose we have a sequence of discrete probability measures

$$\mu_j^N = \frac{1}{N} \sum_{i=1}^{N} \delta_{V_i^N(j)}$$

such that $\mu_j^N \to \mu_j$ as $N \to \infty$ weak–* in the sense of measures, how do we find a corresponding sequence of discrete probability measures μ_{j+1}^N such that $\mu_{j+1}^N \xrightarrow[w]{*} \mu_{j+1}$? μ_j^N will be called an N–particle approximation of μ_j.

Suppose next that $\Psi(v,w,y)$ is continuous as a function of v, w and y (this is certainly true if k is bounded and continuous; since we had to truncate k anyway, it is not unreasonable to enforce boundedness and continuity), and that we are given a sequence of probability measures M_j^N on $B^1 \times \mathbb{R}_v^3 \times \mathbb{R}_w^3$ such that

$$M_j^N \xrightarrow[w]{*} M_j \quad \text{as} \quad N \to \infty.$$

It is then elementary that $M_j^N \circ \Psi^{-1} \xrightarrow[w]{*} M_j \circ \Psi^{-1} = \mu_{j+1}$ (see [5]). Suppose next that we have found triples (y_i^N, v_i^N, w_i^N) $(i = 1, \ldots, N)$ such that

$$M_j^N = \frac{1}{N} \sum \delta_{y_i} \times \delta_{v_i} \times \delta_{w_i} \xrightarrow[w]{*} M_j, \tag{12}$$

then $M_j^N \circ \Psi^{-1} = \frac{1}{N} \sum \delta_{\Psi(y_i,v_i,w_i)}$ is an N–particle approximation of μ_{j+1}. $v_i(j+1) = \Psi(y_i,v_i,w_i)$ are the velocities of the N approximating particles after the collision simulation step, where v_i was the ingoing velocity, w_i the velocity

of the collision partner, and y_i a collision parameter. The remaining question now is this: Given $v_i^N(j)$, $i = 1, \ldots, N$, how do we choose the y_i^N, w_i^N such that (12) holds?

We describe two methods. The first one, discussed in detail in [1, 2], is a Monte Carlo method, because it involves random choices: Given $v_1, \ldots, v_N$, choose sequences of independent and equidistributed random variables $(r_i)_{i\in\mathbb{N}}$ on $[0, 1]$, $(y_i)_{i\in\mathbb{N}}$ on B^1. Then, define an index $c_i \in \{1,\ldots,N\}$ by $c_i = [N\cdot r_i] + 1$, let $w_i = v_{c_i}$, $v_i(j+1) = \Psi(y_i, v_i, w_i)$. That's all. Notice that the w_i are taken from the same set $\{v_1,\ldots,v_N\}$. The same velocity can be chosen repeatedly for collision partners! In particular, we have no guarantee that the total energy and momentum are conserved in this process (however, the expected values are conserved). It was shown in [1] and [2] that by the central limit theorem $M_j^N \circ \Psi^{-1}$ converges indeed w^* to μ_{j+1} almost surely.

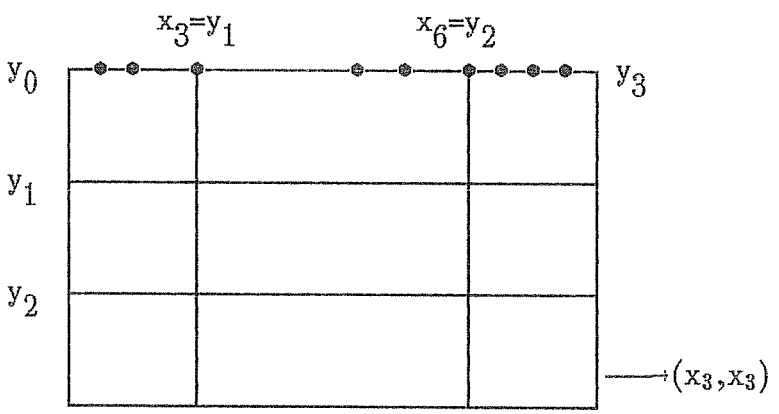
We present a second idea that has been successfully applied. Observe that there is no reason to keep the velocities v_i^N fixed; instead, our target is to find efficient N-atomic approximations to the product measure M_j. In doing this, we may even vary N a little if this helps our approximation (the only reason to keep N approximately constant is computational efficiency).

We demonstrate the mentioned idea for the simpler case of a probability measure μ_j on a real interval, say $I = [0, 1]$. Suppose that $\mu_j^N = \frac{1}{N}\sum_{i=1}^{N} \delta_{x_i}$ is a sequence of atomic measures, and that $\mu_j^N \xrightarrow[w]{*} \mu_j$ as $N \to \infty$. If $N = k^2$, $k \in \mathbb{N}$, the following idea, due to M. Bäcker [6], yields a good approximation to $\mu_j \times \mu_j$: order the x_i such that $x_1 < x_2 < x_3 < \ldots < x_N$, let $y_0 = 0$, $y_1 = x_k$,

$y_2 = x_{2k}, \cdots, y_{k-1} = y_{(k-1)k}, y_k = 1$, and define intervals I_j by $I_j = [y_{j-1}, y_j)$ for $1 \le j \le k$, $I_k = [y_{k-1}, 1]$. Then all the I_j contain exactly k of the x_i's.

The set of rectangles $R_{i,j} = I_i \times I_j$ is a cover of $[0, 1]^2$ of exactly $k^2 = N$ elements. If we choose $\bar{x}_i$ as the center if I_i, then the N-atomic measure $\frac{1}{N} \sum_{i,j=1}^{k} \delta_{(\bar{x}_i, \bar{x}_j)}$ will be a reasonable discrete approximation to $\mu_j \times \mu_j$ – the quality of the approximation depends of course on the quality of approximation of μ_j^N to μ_j. Figure 1 below displays the idea graphically (for $N = 9$).

Figure 1



The idea readily generalizes to the higher-dimensional situation which we face with the measure M_j – of course, rather than with $N = k^2$, one has to work with numbers N which factor in a more convenient way.

It is clear that this approach should eliminate statistical fluctuations prevalent in the Monte Carlo simulation (for an unkikely possibe choice of the

r_i's and y_i's, one can get very poor approximations of M_j – for example, if $c_i = i$ for all i). This has been confirmed by numerical experiments.

4. Remarks. There are some positive and some negative features of the methods outlined above. First, observe that a consistent scheme must reflect the essential properties of a rarefied gas, which enter into the derivation of the Boltzmann equation. The most fundamental of these assumptions is the propagation of molecular chaos, which is believed to hold in general, and proved to be true for special situations ([7, 8, 9)]. The numerical counterpart to this is the requirement (12) that

$$M_j^N \xrightarrow[w]{*} M_j$$

as $N \to \infty$, and this was exactly what we called "the essence"! Therefore, we can say that (12) means that we choose the w_i, y_i such that molecular chaos is satisfied in the limit.

On the negative side, the methods described here do not guarantee the strict conservation of momentum, energy etc. (mass, of course, is conserved). However, for the Monte Carlo method, these conservation laws are satisfied in the mean, and consistency and convergence will of course guarantee that these laws hold in the limit $\Delta t \to$, $\Delta x \to 0$ (Δx is the diameter of the largest cell) and $N \to \infty$ (Clearly, N will have to grow much faster than the number of cells). We emphasize that the consistency with molecular chaos is more important than these conservation laws on the discrete level (it is possible to modify the first method such that momentun and energy are conserved, see [1].)

5. A technical detail, convergence, and outlook. In this final section we give a few comments on the convergence proof from [2]. First, it is highly desirable to have a metric which will control the weak–*–convergence used in Section 3. The discrepancy between two measures is an efficient way to do this. We explain it for the case of probability measures on $\mathbb{R}^2$:

Let Q, P be arbitrary points in $\mathbb{R}^2$, then "$\leq$" denotes the usual semi–order, i.e. $Q \leq P$ if and only if $Q_i \leq P_i$, $i = 1, 2$. Moreover, let $R(P) = \{Q \in \mathbb{R}^2, Q \leq P\}$.

Definition. Let μ, ν be two probability measures on $\mathbb{R}^2$. The discrepancy $D(\mu,\nu)$ between them is

$$D(\mu,\nu) = \sup_{P\in\mathbb{R}^2} \left| \int_{R(P)} d\mu - \int_{R(P)} d\nu \right|.$$

The useful link between D and the w*–convergence is the theorem below (for the proof see [2]).

Theorem. Let μ be an absolutely continuous probability measure on $\mathbb{R}^n$. Then

$$\mu_N \xrightarrow[w]{*} \mu \text{ if and only if } D(\mu_N,\mu) \xrightarrow[N\to\infty]{} 0.$$

This theorem, the central limit theorem and the Borell–Cantelli lemma were three of the most essential tools of the convergence proof in [2]. We conclude with a short synopsis of this result.

The most crucial assumption in [2] is the hypothesis that the Boltzmann equation has a unique solution f on the time interval $[0, T]$ in question) such that for some $\alpha > 0$, $C > 0$

$$\operatorname*{ess\,sup}_x \int f(t,x,v)e^{\alpha v^2}\,dv \le C,\ t \in [0, T].$$

There is also the truncation assumption (8) on the collision kernel k, and a regularity assumption (with respect to x) of the solution. The result is then this:

Given a sequence of particle approximations $\mu_0^N = \frac{1}{N}\sum_{i=1}^{N} \delta_{(x_i,v_i)}$ to the initial value f_0, and given sequences of time steps $(\Delta t)_n$ and cell sites $(\Delta x)_n$ such that $(\Delta t)_n \searrow 0$ $(\Delta x)_n \searrow 0$, there is a sequence $N(n) \to \infty$ such that

$$D\left[\mu^{N(n)}_{k\cdot(\Delta t)_n},\ f\left[k(\Delta t)_n, x, v\right]dx\,dv\right] \longrightarrow 0$$

as $n \to \infty$, almost surely with respect to the γ_i, $i = 1, 2, 3, \ldots$, for $k \circ (\Delta t)_n \in [0, T)$. The $\mu^{N(n)}_{k\cdot(\Delta t)_n}$, of course, are the discrete measures computed from $\mu_0^{N(n)}$ via the procedures from sections 2–4.

There are several aspects of the described methods which call for further investigation. We formulate a few questions which concern some of these aspects:

Is it possible to modify the methods such that the truncation error with respect to Δt will be of higher order, without having to increase the particle number at every step?

What criteria should be applied to design an optimal partition into cells? What is an optimal number of particles per cell from a computational point of view? What can be said about convergence rates?

These and other questions leave us a lot to think about for the future. Meanwhile, the methods described here are being successfully used to model rarefied gases.

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