Numerical Study of the Uchiyama particle model

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The physical context that we are interested in is the one of the kinetic theory of gases. There exists several levels of description for this one: the microscopic, the mesoscopic and the macroscopic scales. The famous sixth problem of Hilbert is about linking these different scales. More specifically, it suggests to use the Boltzmann equation as an intermediate step in the transition between atomistic and continuous models for gas dynamics. The historical result addressing this question is due to Lanford [10] who established the convergence in the low density limit to the Boltzmann equation, starting from the particle system called hard spheres (only for short times). Until the end of the 90’s, the proof of Lanford has been completed by many authors. More recently, the proof has been improved by means of quantitative estimates by Gallagher, Saint-Raymond, Texier [8], Pulvirenti, Saffirio, Simonella [12]. Recent improvements regarding the linear setting have been also made (Bodineau, Gallagher, Saint-Raymond[4], Ayi [2], ...).

We take an interest in a variant of this setting: discrete velocity models (DVM). It consists in models involving particles which can take only a finite number of velocities. The model we are interested in is the Broadwell one [5]: we define the set

\[ S := \{v_1, v_2, v_3, v_4\}, \]  

(0.0.1)

with \( v_1 := (1, 0), v_2 := (-1, 0), v_3 := (0, 1), v_4 := (0, -1) \) and we study the equation

\[
\partial_t f(t, x, v) + v \cdot \partial_x f(t, x, v) = a\left[f(t, x, iv)f(t, x, -iv) - f(t, x, v)f(t, x, -v)\right]
\]  

(0.0.2)

with \( t \in \mathbb{R}^+, x \in \mathbb{R}^2, v \in S, a \) a nonnegative constant and where \( i \) denotes the \( \pi/2 \) rotation operator.

The two natural microscopic models which would be the equivalent of the hard spheres for discrete velocities are the HPP model [9] introduced by de Hardy, Pomeau et de Pazzis and the Uchiyama model [13]. The first one is a lattice model while the second one is continuous. The HPP model describes the evolution of particles on a lattice in dimension two with particles which have their velocities living in \( S \). The description of the dynamics is the following: during one unit of time, each particle jumps in the direction of its velocity. At each site where the number of particles is two and where two particles have opposite velocities, there is a collision, and each velocity turns with an angle of \( \pi/2 \). For all the other sites, nothing changes.

The Uchiyama model describes the evolution of “hard” squares in \( \mathbb{R}^2 \) whose diagonals are of length \( \varepsilon \) and parallel (or orthogonal) to the coordinate axes. Particles move freely with velocities belonging to \( S \) until they undergo a collision. We distinguish two types of collision: the “head-on” collisions and the “side-to-side” ones. The collision rules are the following: in case of a “side-to-side” collision, the particles involved exchange their velocities while in case of a “head-on”, the velocities undergo a rotation of angle \( \pm \pi/2 \). Surprisingly, Uchiyama proved in [13] that, except for very particular situations, in the low density limit, starting from his model, we do not obtain the Broadwell equation. The same applies to the HPP model. The question of the limit model associated with the Uchiyama one is then open.

Indeed, one of the inherent difficulties of those DVM models is the appearance of a phenomenon of recollisions between the particles which cannot be controlled. Therefore, if a kinetic equation exists, it should contain a memory term associated with this phenomenon. Nevertheless, up to now, it is a very difficult problem and there is not much more which is known. This is why we have decided, in a first place, to adopt a numerical approach.

We carry out the molecular dynamics simulation for the Uchiyama’s particle system using an Event-Driven algorithm. The Event-Driven method is concerned with the times at which events, in
this case collisions, take place. The algorithm is the following: you establish a list of the collisions to come if the particles moved only in straight lines. This list is ordered according to the time at which the collisions will take place, the first element being the closest collision in time. The particles are then displaced until this time and the collision is carried out. The list of future collisions is then updated. Indeed, some of them may be invalidated by the collision that has just taken place since the velocities and therefore the direction of the two particles involved have changed, new ones may also become possible for the same reasons. Then, again, we move to the nearest collision in time and so on . . .

First, we take an interest in the low density limit, the one for which we fail to obtain the Broadwell equation. In that case, in the spirit of the paper of Aoki et al [1] in the hard spheres case, we study the backward cluster. A backward cluster is defined as the group of particles involved directly or indirectly in the backwards-in-time dynamics of a given tagged sphere. We denote $J_i = \{i_1, i_2, \ldots, i_n\}$ with $i_s \neq i_i$ for $i \neq s$ the backward cluster of the particle $i$, $K_i = |J_i|$ the cardinality of $J_i$. We are interested in $< K >_t$ the average with respect to the initial position of the cardinality of the backward cluster of a tagged particle at time $t$. We focus on the quantity

$$r = \lim_{t \to \infty} \frac{1}{t} \log(< K >_t + 1).$$

Our preliminary result shows that, as in [1], we should obtain an exponential estimate of the growth in time of $< K >_t$, for the Uchiyama model, with a different $r$ than for the hard spheres.

We introduce the notion of internal and external recollisions: internal recollisions (recollision in the pseudo-trajectory sense in the backward trajectory of a particle), and external recollisions (when the two backward clusters of two particles have a non-empty intersection). Thus, for $N$ particles and $M$ trajectories, we are interested in the two quantities:

$$P^{i.r.} = \frac{1}{N} \frac{1}{M} \sum_{m=1}^{M} \sum_{i=1}^{N} 1\{\text{particle } i \text{ presents a recollision on the } m\text{-th trajectory}\}$$

and

$$P^{e.r.} = \frac{1}{M} \frac{1}{N(N-1)} \sum_{m=1}^{M} \sum_{1 \leq i < j \leq N} 1\{\text{particle } i \text{ and particle } j \text{ undergo an external recollision}\}.$$  

We think that, most of the time, there is propagation of chaos, except exactly where we would need to have it to obtain the Broadwell equation. Therefore, we expect $P^{i.r.}$ not to be small and, on the contrary, $P^{e.r.}$ to be small for the Uchiyama model, while it is clear that it is small in both cases for the hard spheres model. The results numerically obtained goes exactly in that direction.

<table>
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<th>Uchiyama</th>
<th>Hard Spheres</th>
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<tr>
<td>3000</td>
<td>2.8</td>
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Finally, in a last part, we observe a regime which seems close enough from the diffusive limit. We recall that for the hard-spheres, the limit process is a Brownian motion. Of course, regarding
our previous remarks, we have no hope to obtain such a process for our diffusive limit. We numerically test a wider class: fractional Brownian motion. Our preliminary results indicate that the limit process does not belong to that class either.

From a theoretical point of view, there are many paths that we plan to explore.

- We could as in [6] work in an extended phase space. The good new set of parameters would be given by the one which allows to make appear the pathological structures (two particles moving one ahead of the other one in the same direction).
- We could put an additional term catching all the pathological situations (like the “flowers” appearing in the case of the Two-Dimensional Magnetotransport equation, see [3]).
- We could also rescale in time and take an interest in the super diffusion limit as in [11] to obtain the usual limit process.
- We could study a version with randomness of the Uchiyama model for which one we could hope to obtain the Broadwell equation (as it is the case for the HPP model, see [7]).

References