Report on:

Efficient Algorithms for the Periodic Lorentz Gas in Two and Three Dimensions

1. Summary

In this paper, the authors describe a method for computing a particle's first collision in a periodic Lorentz lattice gas. The particular lattice gas, that is considered, is one in which each site of the lattice is at the center of a disk (sphere) in two-dimensions (three-dimensions). The lattice that is specifically considered in this paper is the square lattice $\mathbb{Z}^2$ in 2D and the cubic lattice $\mathbb{Z}^3$ in 3D.

The goal of the paper is to describe how it is possible to *efficiently* calculate the particle's first collision time with a disk or sphere. The authors use the term "efficiently" to mean that the method they develop is better than the *classical* or standard method for determining this first collision time. They go on to show numerically, that the algorithm they proposed is "efficient" in the case in which the gas is very dilute, i.e. the radii of the disks (spheres) are small.

In $2D$, this new method is built up using (1) a number of geometric properties of the lattice gas that improve upon the original classical method and (2) the use of continued fractions. In $3D$, this $2D$ method is employed to find the particle's first collision time by projecting the particle's path to each of the xy- xz- and yz-planes. Although this technique of projection may detect some false collisions, the authors show that it is still possible to determine which collisions are genuine by checking the collision using the classical method.

The main improvements over the original algorithm are (1) by modifying the geometric approach to finding collisions it is only necessary to solve a linear equation vs. two linear and one quadratic and (2) by use of continued fractions, one can *skip* through parts of the lattice in which the classical method would need to check for a possible collision. The authors conclude with a number of numerical simulations, which illustrate to what extent this new method outperforms the original classical method for various radii of the corresponding disks or spheres.

2. Evaluation

As the authors point out, there has been and continues to be quite a bit of interest in the study of Lorentz lattice gas models, in particular in those models with a periodic structure, mainly due to the fact that such systems are more mathematically tractable than those with an irregular structure. This specifically includes the study of lattice gas models in the plane and in higher dimensional settings.

Moreover, knowledge of a particle's first collision time allows one to inductively recreate the particle's entire trajectory, since after every collision one can look for the next "first" collision. That is, an "efficient" algorithm for detecting first collisions, at least in the case of dilute gas models, is helpful for both developing mathematical theories and numerically verifying conjectures regarding such systems.

With this in mind, the subject material in this paper is a good fit for the *Journal of Physic A*. However, the writing and exposition in the paper could use some work. In particular, the precision in describing and summarizing the distinctions and interplay of the various algorithms, used throughout the paper, could be improved.

Since this makes up the bulk of the paper, what may, in fact, be needed is a rewrite of the main parts of the paper. More to the point, since these are algorithms, it would help if the paper was written in such a way that one could more clearly see the step by step process involved in each algorithm and the distinctions between the different algorithms. Some comments and suggestion regarding how the paper could be improved are described in more detail in section 4.

3. Recommendation

The recommendation is that the paper be rewritten to be more precise in the description of the various algorithms mentioned therein. In particular, the authors should take care in formally naming and describing each algorithm, on which their new "efficient" algorithm is based. To guide the authors, a number of comments and suggestions are given below.

4. Comments & Suggestions

The following is a list of comments and suggestions related to the paper. The list is likely incomplete and in this sense is intended to give an idea of what could be improved.

4.1. **Precision** & **Clarity.**

- There are a number of algorithms mentioned in the paper, i.e. the *classical*, the *new* in $2D$ and $3D$, the algorithm of *Caglioti and Glose* (CG), the *continued fraction* algorithm. To some degree, these algorithms are intertwined. For instance, the new and CG algorithms rely on the continued fractions algorithm, etc. If these could disentangled from one another and more clearly stated, each as a step by step process, this would be helpful for paper's exposition.
- In quite a few places, the *new* more efficient algorithm is compared to the method in which "periodic boundary conditions" are applied. The way the paper is written, it may be unclear as to which algorithm checking these conditions applies. Moreover, for those who do not know what it means to apply periodic boundary conditions or what a *cell* is, a quick explanation, figure, etc. would be useful in helping the reader understand how and why the *new* algorithm is more efficient for dilute gases. Moreover, this would help explain why we need to use these boundary conditions in the *new* algorithm when the particle reaches an obstacle. Additionally, this would help the reader understand the phrase "per cell" in the section on numerical measurements, etc.
- Some comments on generating continued fraction along with some properties are given in *Appendix A*. Unless I missed it, it does not appear that this is referenced in the main text of the paper. Also, it should probably be stated what the *connection* is between what is referred to in the paper as the "continued fraction algorithm" and Appendix A.
- Introduction: The paragraph "However, Glose's algorithm..." seems to infer that the *new* algorithm can do all the things mentioned that the CG algorithm cannot. However, in the following paragraph, the *new* algorithm is stated to work for disks and spheres on (simple) $2D$ and $3D$ lattices. It would be helpful from the beginning to clear up what cases the algorithm can handle efficiently, which the other algorithms cannot.

4.2. **Grammar, Phrasing, and Additional Questions.**

- Since the proposed algorithm is more "efficient" only when the gas is *dilute*, i.e. the disks or spheres are small, it may be worth mentioning this in the title and/or abstract.
- Page 3, line 12: The sentence "At each step..." may be confusing.
- Figure 1: It may be helpful to label the various lines in this figure, etc.
- Page 3, line 6: In the degenerate case that either v_1 or v_2 is zero, can the rotations and reflections mentioned in section 3 be used to get both of these components positive?
- Page 3, line 8: Based on equation (1) the particle has the trajectory $\mathbf{x}_0 + t\mathbf{v}_0$ until it collides with a disk. It would help to relate this to the equation $y = \alpha x + b$.
- Page 4, line 12: In the sentence "Furthermore, now we do not..." is the number $\alpha \in \mathbb{N}$?
- Page 6, line 5: It should be stated whether the "standard method" part of the classical algorithm.
- Section 5: Can any mathematical arguments be made as to why the new algorithm will outperform the classical method if $r << 1$ for a typical $\mathbf{x}_0$ and $\mathbf{v}_0$?