INFLUENCE OF PARTICLE SHAPE IN THE STATISTICAL MECHANICS OF CLASSICAL GASES

F. Alonso-Marroquin*, & S. Luding**
*ESSCC, The University of Queensland, South Australia, 5005,Santa Lucia, Qld. 4068 Australia,
** Multi Scale Mechanics, University of Twente (UT), P.O. Box 217, 7500 AE Enschede, the Netherlands

Summary The evolution towards statistical equilibrium of a classical system of non-spherical particles is studied using molecular dynamics. Simulations with a large number of particles comply with the basic assumptions of classical statistical mechanics, such as the principle of equipartition of energy, and the Maxwell-Boltzmann statistics for energy distribution.

INTRODUCTION

Rapid advances in computer simulations have led to many new developments in the non-equilibrium statistical mechanics of particulate systems [1]. These systems represent different real physical systems at different scales, such as the small scale of liquid crystals [2], geological scales of snow and debris flow, and the astronomical scales of planetary rings or dynamics evolution of precursors of planets [3]. Although particle shape plays an important role, theoretical and numerical developments have been restricted to particles with spherical shape. In this paper we investigate the existence of a statistical equilibrium in a system of non-spherical particles in the collisional regime. Collisions allow the system to evolve towards the different microstates of the system. The limit state is consistent with the ergodic hypothesis, where the energy distribution satisfies the Maxwell-Boltzmann distribution and each quadratic term of the kinetic energy contributes the same amount of averaged energy to the system. These simulations are the starting point to investigate the statistical mechanical properties of different particulate systems where particle shape plays an important role, such as liquid crystals, complex fluids, granular gases and jammed granular materials.

SHAPE REPRESENTATION

Systems with different particle shapes are modeled using the concept of the Minkowski sum of a polygon (or polyline) with a disk. This mathematical operation is equivalent to sweeping a disk around the profile of the polygon (or polyline) without changing the relative orientation, see Fig. 1. This simple concept allows us to generate complex shapes, including non-convex bodies, without need to decompose the complex object into simple spherical or convex parts. A conservative interaction between the particles is obtained from the repulsive interaction between each vertex of one polygon and each edge of another. The number of floating point operations used to calculate interaction forces is drastically reduced by using a neighbor list and a contact list for each pair of neighbor particles. The details of the algorithm are presented elsewhere [5]. Here we will investigate the relaxation of systems of non-spherical particles towards the classical statistical equilibrium.

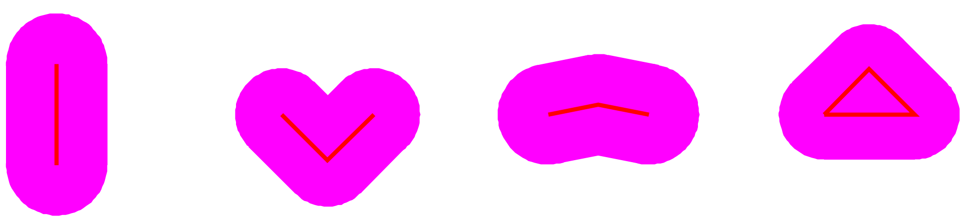

Figure 1. The Minkowski sum of a polygon (polyline) with a disk is used to represent different shapes. From left to right: $rice = line + disk$; $hearth = polyline + disk$; $peanut = polyline + disk$; and $pebble = triangle + disk$.

SIMULATION RESULTS

Simulations with a large number of particles show that elastic interactions allow the particles to exchange energy and momentum, whereas its contribution to the energy budget is negligible. This property leads us to investigate the existence of a statistical equilibrium in a gas of non-spherical particles. It is expected that the system will reach the statistical equilibrium, which is characterized by a Maxwell-Boltzmann statistics for energy distribution [6]:

$$\rho(E_k)dE_k = 2\sqrt{E_k/\pi(kT)^3}\exp(-E_k/k_BT)dE_k, \tag{1}$$

here $E_k = \frac{1}{2}(mv_x^2 + mv_y^2 + I\omega^2)$ is the kinetic energy of the particle; T the temperature; and k_B the Boltzmann constant. The mean energy of the particles leads to $\bar{E}_k = \int_0^\infty \rho(E_k)E_k dE_k = \frac{3}{2}k_BT$.

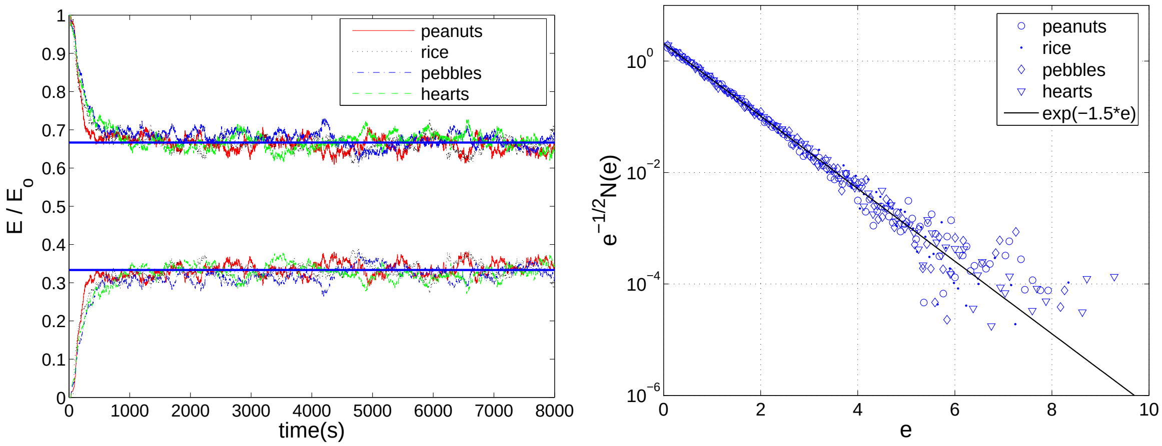

Figure 2. Left: Time evolution of the mean value of linear and rotational kinetic energy, The horizontal lines correspond to the expected value from classical statistical mechanics. Right: energy distribution $N(e)$ for the particles, where $e = E_k/E_k$. The line corresponds to the best fit $n(e) = 2\beta\sqrt{e\beta/\pi}\exp(-\beta e)$, with $\beta = 1.5$

The limit of statistical equilibrium is investigated by performing a series of simulations with many non-spherical particles interacting via elastic forces. Each test consists of 391 particles confined by four fixed rectangular walls. Each particle occupies an area of $1cm^2$ and the confining area is $46cm \times 46.25cm$. These dimensions lead to a volume fraction of $\Phi = 0.186$. Gravity is not taken into account in the simulations. Each sample consists of identical particles with a specific shape as shown in Fig. 1: rice, peanuts, hearts and pebbles.

Initially, each particle has zero angular velocity and a linear velocity of $1cm/s$ with random orientation. Due to collisions, the linear momentum of each particle changes and part of it is transferred to angular momentum. Elastic energy has a negligible contribution to the energy budget, as it differs from zero only for short times during collisions. In consequence almost all energy of the system consist of rotational and translational kinetic energy. At the beginning of the simulations the rotational kinetic energy is zero, and it increases during the simulations due to collision, see left part of the Fig. 2. For all the samples, we observe the same stationary regime, where the average of rotational kinetic energy reaches the limit of $1/2$ of the linear kinetic energy. This is in agreement with the theorem of equipartition of energy [6], which states that each quadratic term in the energy should contribute the same weight in the mean energy of the system.

We also calculate the energy distribution of the particles in the stationary regime. Independent of particle shape, all distribution collapses onto the same curve, as shown the Fig. 2. We observe an excellent agreement between this theoretical distribution and the simulations data. This result suggests that the gas non-spherical particles satisfy the ergodic hypothesis, where the particles explore all accessible phase space during the simulation time. Simulations with particles having different degrees of non-sphericity [4], show that energy distribution for all samples collapse onto the theoretical expected value. It is also shown that the relaxation time for the statistical equilibrium is very sensitive to the degree of non-sphericity of the particle.

CONCLUSIONS

Using numerical simulations we have shown that systems of non-spherical particles in the collisional regime evolves towards a statistical equilibrium. This equilibrium is characterized by a Maxwell-Boltzmann distribution of energy and a equipartition of energy and holds for all particle shapes. This investigation will allow us to investigate how these systems relax to the statistical equilibrium. Simulations which are presented elsewhere [4] show that the relaxation time decreases as the sphericity of the particles increases. Detailed analysis of the relevant shape parameters on the relaxation time will allow us to develop mean field evolution equations for dense system of collisional particles.

References

[1] M. P. Allen, D. J. Tildesley, Computer Simulation of Liquids, Oxford University Press, Oxford, 1987.
[2] G. Pelzl, S. Diele, W. Weissflog, Banana-shaped compounds - a new field of liquid crystals, Advanced Materials 11 (9) (1999) 707–724.
[3] T. Pöschel, S. Luding, Granular Gases, Springer, Berlin, 2000.
[4] F. Alonso-Marroquin, S. Luding, Effect of grain shape in the statistical mechanics of granular gases, in preparation (2008).
[5] F. Alonso-Marroquin, An efficient algorithm for computing conservative interaction between two-dimentional, complex-shaped rigid bodies, submitted to Journal of Computational Physics.
[6] R. Tolman, The principles of statistical mechanics, Dover Publications, Inc., New York, 1979.