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Homogeneous cooling state of frictionless rod particles

S.M. Rubio-Largo [a,*], F. Alonso-Marroquin [b], T. Weinhart [c], S. Luding [c], R.C. Hidalgo [a]

[a] Department of Physics and Applied Mathematics, University of Navarra, 31080 Pamplona, Navarra, Spain
[b] School of Civil Engineering, The University of Sydney, Sydney NSW 2006, Australia
[c] Multi Scale Mechanics, CTW, UTwente, 7500 AE Enschede, Netherlands

HIGHLIGHTS

- A granular gas of rods has been simulated with DEM implemented on GPU.
- A homogeneous cooling state of frictionless 3D rods has been identified.
- Haff's Law is satisfied when introducing of a novel characteristic time.
- The energy equipartition between degrees of freedom has been clarified.

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ABSTRACT

In this work, we report some theoretical results on granular gases consisting of frictionless 3D rods with low energy dissipation. We performed simulations on the temporal evolution of soft spherocylinders, using a molecular dynamics algorithm implemented on GPU architecture. A homogeneous cooling state for rods, where the time dependence of the system's intensive variables occurs only through a global granular temperature, has been identified. We have found a homogeneous cooling process, which is in excellent agreement with Haff's law, when using an adequate rescaling time $\tau(\xi)$, the value of which depends on the particle elongation ξ and the restitution coefficient. It was further found that scaled particle velocity distributions remain approximately Gaussian regardless of the particle shape. Similarly to a system of ellipsoids, energy equipartition between rotational and translational degrees of freedom was better satisfied as one gets closer to the elastic limit. Taking advantage of scaling properties, we have numerically determined the general functionality of the magnitude $\mathcal{D}_c(\xi)$, which describes the efficiency of the energy interchange between rotational and translational degrees of freedom, as well as its dependence on particle shape. We have detected a range of particle elongations $(1.5 < \xi < 4.0)$, where the average energy transfer between the rotational and translational degrees of freedom results greater for spherocylinders than for homogeneous ellipsoids with the same aspect ratio.

1. Introduction

Granular materials are commonly handled in everyday life and are involved in many industrial processes. For this reason, the study of their kinetic and mechanical properties is a very active research field [1,2]. Nevertheless, although these systems have been thoroughly examined in the past, they still reveal relevant and unexpected results [1,2].

* Corresponding author.
E-mail address: srubio.4@alumni.unav.es (S.M. Rubio-Largo).

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Granular gases are very dilute systems of macroscopic grains, which move randomly loosing energy through inelastic collisions. Thus, in the absence of any external driving force, their energy uniformly decreases towards an homogeneous cooling state (HCS). In that condition, the time dependence of all its intensive variables results only from the global granular temperature [3,4]. For highly dissipative systems, however, the HCS rapidly becomes unstable and the system subsequently evolves into an inhomogeneous state where the cooling process notably slows down [5,6]. Consequently, the correlation between the particles' motion determines the rate of energy loss and large inhomogeneities in the density field are observed [5,7].

A number of theoretical studies have carefully analyzed particle–particle interactions during collision, explaining how inelasticity emerges from such interactions [8–10]. For soft grains, in which the repulsion force depends linearly on deformation, a constant restitution coefficient can be recovered [11,12] and, consequently, cooling kinetics following Haff's law would be expected. There is also experimental evidence of materials with variable restitution coefficients that depend on the relative velocity of the interacting particles. For instance, assuming nonlinear elastic repulsive forces (Hertzian contact) leads to a notably different algebraic decay of the system energy during the HCS [9].

On the other hand, in granular gases of spherical particles roughness leads to correlations between the translational and rotational degrees of freedom [13–15]. In general, both translational and rotational kinetic energies decrease with the same power law but differ from each other due to the breakdown of energy equipartition. Years ago, these correlations were quantified for a system of agitated rough spheres [16,17]. More recently, simulations of 3D gases of rough spheres shed light on the nontrivial process of energy interchange between the translational and rotational degrees of freedom, showing that the spin of a single grain can be correlated with the particle linear velocity [18,19].

The effect of particle shape on the kinetic evolution of granular gases has been studied by Aspelmeier and other researchers [20]. They developed a kinetic theory of hard needles based on the assumption of a homogeneous cooling state, in the very dilute limit. Hence, it was found that energy interchange between rotational and translational degrees of freedom is controlled by the macroscopic restitution coefficient and by the particle spatial distribution of mass. In recent years, there has been an increasing interest in the behavior of non-spherical grains both experimentally [21–26] and numerically [27–30]. Here, the primary interest is also focused on the evolution in time of the translational kinetic energy and rotational energy. Thus, it has been commonly found that in granular gases of elongated particles equipartition is not obeyed. Moreover, several details of the cooling process depend on particle aspect ratio, mass distribution of the grains and the driven mechanisms.

In the present work, we investigate the free cooling of a granular gas of elongated 3D particles, and both the role of inelasticity and the particle shape in the overall kinetic processes are analyzed. The paper is organized as follows: in Section 2 we introduce some basic concepts about the kinetics of granular gases, in Section 3 we described the numerical model and implementation of our algorithm, Section 4 discusses the results of the homogeneous cooling state of a system of frictionless rods. At the end, conclusions and outlook are drawn.

2. Homogeneous cooling state of rods

In a gas of spherical particles of radius a in HCS, the kinetic energy decreases homogeneously and the time evolution of all variables occurs only through their global temperature. By introducing the dimensionless translational temperature T and rotational temperature R as well as a characteristic time τ, Luding et al. [31] found that the kinetics of a granular gas of rough spheres is governed by the system of equations,

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}\tau}T &= -AT^{3/2} + BT^{1/2}R \\ \frac{\mathrm{d}}{\mathrm{d}\tau}R &= BT^{3/2} - CT^{1/2}R \end{aligned} \tag{1}$$

where A, B and, C are constants that depend on space dimensionality (see details in Ref. [31]). In $3D$, $A = \frac{1-e_n^2}{4} + \eta(1-\eta)$, $B = \frac{\eta^2}{q}$ and $C = \frac{\eta}{q}\left(1 - \frac{\eta}{q}\right)$, where $\eta = \frac{q(1+e_t)}{(2q+2)}$ (in 3D $q = \frac{2}{5}$ for spheres) and e_n and e_t are the restitution coefficients in normal and tangential directions respectively. The equilibrium Enskog's collision rate for the initial temperature $T(0)$ reads as

$$G_{sph}(a) = 8(2a)^2 \frac{N}{V}\sqrt{\frac{\pi}{m}}\, g(2a)T^{1/2}(0) \tag{2}$$

where N is the number of particles per unit of volume, m and V are the mass and volume of the particles, respectively.

This variable is commonly used to rescale time according to $\tau = \frac{2}{D}G_{sph}t$, where D accounts for the number of translational degrees of freedom. It has been found that in general the principle of equipartition does not necessarily apply, resulting asymptotically in $T_{tr}(\tau)/T_{rot}(\tau) \neq 1$.

The HCS of systems consisting of frictionless oblate and prolate ellipsoids has been recently examined [27,28]. There, it was introduced a granular temperature $T_{tot}(t)$ of the gas as a weighted average of $T_{tr} = \frac{2}{3N}\sum_{i=1}^{N}\frac{1}{2}mv_i^2$ and