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On the relevance of "molecular chaos" for granular flows

With numerical simulations of dissipative, spherical particles the assumption is tested, that the velocities and the positions of colliding particles are uncorrelated ("molecular chaos"). This assumption is a basic ingredient of all theoretical approaches based on a kinetic theory or a pseudo-Liouville operator formalism. The numerical model is an event-driven method for the simulation of rigid spherical particles in two dimensions. In elastic systems, the impact parameter is uniformly distributed or, with other words, the molecular chaos assumption is valid independent of the density. In freely cooling systems, the molecular chaos assumption fails as soon as dissipation becomes strong enough so that convective shear modes are created.

1 Introduction

In the last years, granular media have attracted more and more attention in physics, engineering and applied mathematics. Experimental, theoretical and numerical studies are used to understand the fascinating and complex behavior of granular media. For a recent review see the conference proceedings edited by Herrmann, Hovi and Luding [7]. For the theoretical treatment classical kinetic theories have been extended to account for dissipation and rather high densities [1-3, 5, 8, 15]. However, most of the classical but also the more advanced approaches are based on the assumption of molecular chaos, i.e. the fact that the velocities and positions of all colliding pairs of particles in a gas are uncorrelated. In an elastic gas, the errors introduced by this assumption are small. Since in granular systems, correlations between colliding particles may be important, the validity of the molecular chaos assumption is checked by event driven (ED) "hard sphere" simulations as frequently applied for the simulation of granular media [11,13,16].

2 System and Simulation Method

The system we study in the following is a periodic square in two dimensions (2D), where each side has length L and, due to the periodic boundaries, we need not to specify wall interactions. Inside the system N particles of diameter $2a$ and mass m exist with the global volume fraction $\nu = N\pi a^2/L^2$.

In the event driven (ED) method the particles follow a linear trajectory, until a collision occurs, where the duration of a collision is implicitly zero. We introduce dissipation on contact in normal direction via the restitution coefficient r. The limits $r = 1$ and $r = 0$ correspond to elastic and completely inelastic collisions respectively. The optimized serial algorithm used here, was proposed by Lubachevsky [9]. For details concerning the interaction model used in the ED method see refs. [10, 13, 14]. The ED method readily handles the excluded volume constraint of the particles, when the collision rules

$$\mathbf{v}'_{1,2} = \mathbf{v}_{1,2} \pm \frac{1+r}{2} \left[(\mathbf{v}_2 - \mathbf{v}_1) \cdot \hat{\mathbf{n}} \right] \hat{\mathbf{n}} \ , \ \text{with} \ \ \hat{\mathbf{n}} = (\mathbf{r}_2 - \mathbf{r}_1)/|\mathbf{r}_2 - \mathbf{r}_1| \tag{1}$$

are applied. In Eq. (1), $\hat{\mathbf{n}}$ is the unit vector pointing from center to center and $\mathbf{v}_i$ is the velocity of particle i with $i = 1, 2$, which is located at position $\mathbf{r}_i$. Since the particles dissipate energy at each collision and there is no energy input the total energy decreases with time.

3 The impact parameter

One basic assumption connected to molecular chaos is a uniform probability distribution of the impact parameter $b = |(\mathbf{r}_2 - \mathbf{r}_1) \times (\mathbf{v}_2 - \mathbf{v}_1)| / |\mathbf{v}_2 - \mathbf{v}_1|$ which is schematically displayed in Fig. 1. We define $P(b/d)$, the probability

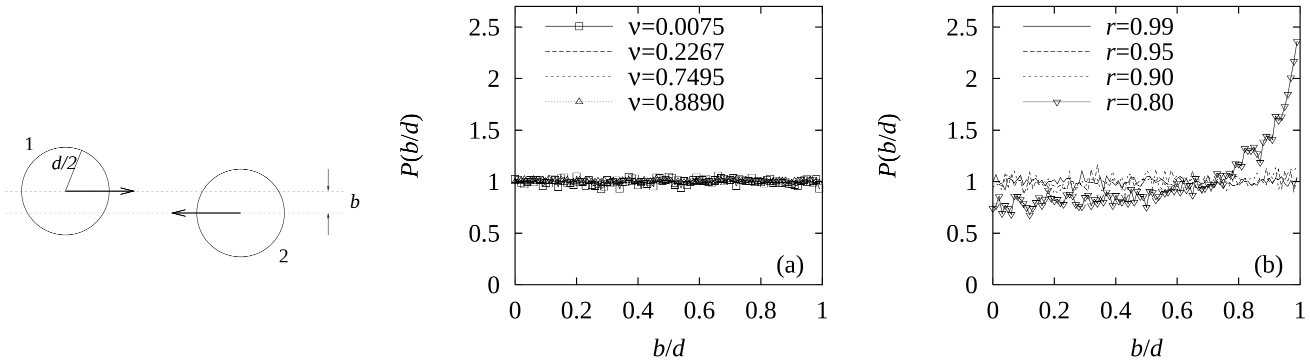

Figure 1: (Left) Schematic drawing of the collision parameter. (a) Probability distribution $P(b/d)$ for elastic systems of different volume fractions. (b) $P(b/d)$ for inelastic systems with different restitution coefficients r.

distribution of b, and normalize it such that $\int_0^1 \mathrm{d}(b/d)P(b/d) = 1$. We find from ED simulations with elastic particles and with different volume fractions, see Fig. 1(a), that $P(b/d) = 1$ in 2D and $P(b/d) = 2b/d$ in 3D (not shown here), as expected for the case of molecular chaos. The systems with high volume fractions are ordered, i.e. the particles are arranged on a triangular lattice, where the normal unit vectors $\hat{\mathbf{n}}$ takes discrete values only. A random collision parameter b thus implies that the relative velocities of the particles are uncorrelated even if the positions are strongly correlated.

Furthermore, dissipation alone is not sufficient to cause the probability distribution to deviate from uniformity. Only when the restitution coefficient is small enough (when dissipation is large enough) one observes a noticeable deviation from $P(b/d) = 1$, see Fig. 1(b). This effect is connected to shear in the granular assembly [11, 16], where the probability for grazing contacts is increased whereas central collisions occur with a lower probability.

4 Simulation Results

In this section, several simulations are presented, starting with the same initial condition and using the same parameters, except for the value of the restitution coefficient r. The simulations involve $N = 99856$ dissipative particles in a system with volume fraction $\nu = 0.25$, and the values $r = 0.9$, 0.8, 0.6, and 0.2 are used. In order to reach an equilibrated initial situation, the system was first allowed to evolve with $r = 1$ for about 10 collisions per particle, so that a Maxwellian velocity distribution and a homogeneous density is achieved. Then, at $t = 0$s, dissipation is switched on and the quantities of interest are calculated as functions of time.

In a homogeneous cooling state [3, 4, 6, 13, 16] one expects that the normalized kinetic energy $K(t) = E(t)/E(0)$ decays with time and follows the functional form

$$K(t) = \left(1 + \frac{1-r^2}{4}\,\tau\right)^{-2} \quad , \quad \text{with} \;\; \tau = 4a\frac{N}{V}\sqrt{\pi\frac{E(0)}{M}}\, g_{2a}(\nu)\, t \ , \tag{2}$$

with the dimensionless time $\tau = t_E^{-1} t$ rescaled by the Enskog collision rate (in our case $t_E^{-1} \approx 252\,\mathrm{s}^{-1}$) at time $t = 0$, with the system volume V, the total mass $M = Nm$, and the particle-particle correlation function at contact $g_{2a}(\nu) = (1 - 7\nu/16)/(1-\nu)^2$ [8, 13]. The decay of energy in the rescaled time frame depends only on r, and all dependencies on quantities like system size, kinetic energy and density are hidden in τ.

In Fig. 2 the normalized kinetic energy $K(t)$ is plotted against the normalized time τ. At the beginning of the simulation we observe a perfect agreement between the theory for homogeneous cooling and the simulations. The simulations show substantial deviations from the homogeneous cooling behavior after some time. The snapshot in Fig. 2 shows that density inhomogeneities build up due to dissipation. The smaller r the faster the clusters grow [11-13] and the earlier the deviation from the HCS begins. Note that the so-called TC model [13] has to be used in order to avoid the inelastic collapse [2, 16]. For all simulations presented, a value of $t_c = 10^{-5}\,$s is used as contact duration. In Fig. 3, $P(b/d)$ is plotted for the simulation with $r = 0.8$ at different times. One has $P(b/d) = 1$ for short times only. For larger times one obtains an increasing (decreasing) probability of grazing (central) collisions. The assumption of a homogeneous probability distribution of the impact parameter is violated if the system is viewed in total. When zooming into the system, see Fig. 3, one obtains local shear modes, fact which explains that the global probability distribution deviates from the equilibrium distribution.

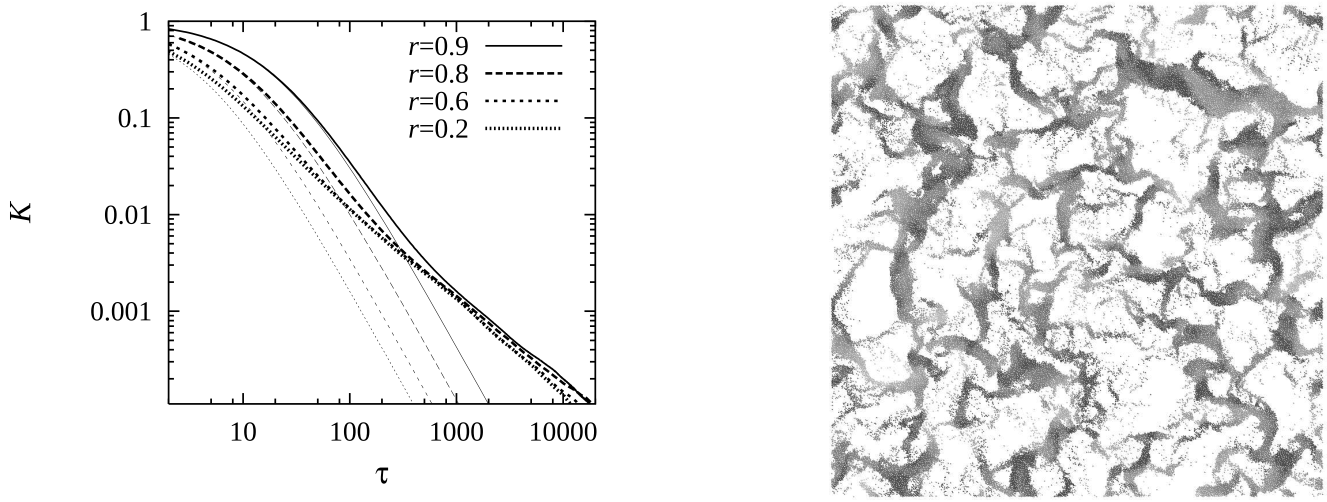

Figure 2: (Left) The normalized kinetic energy is plotted against the normalized time from ED simulations in 2D with $N = 99856$, $\nu = 0.25$, and different $r = 0.9$, 0.8, 0.6, and 0.2. The thick lines are simulation results, the thin lines represent Eq. (2). (Right) snapshot from the simulation with $r = 0.2$ at time $\tau = 2583$. The greyscale indicates the kinetic energy of individual particles – lighter particles move faster.

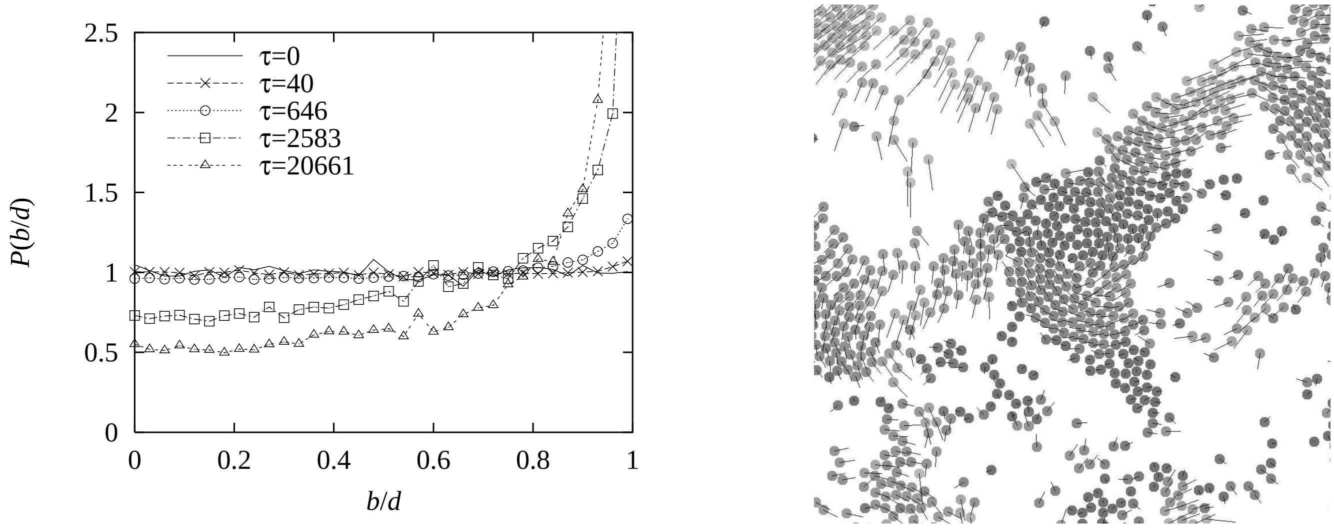

Figure 3: (Left) Normalized probability distribution of the contact parameter from an ED simulation in 2D with $N = 99856$, $\nu = 0.25$, and $r = 0.8$ at different times τ. (Right) Snapshot from a part of a typical simulation at $\tau = 322$; individual particles are visible and the solid lines from the particle centers indicate the particle velocity, the greyscale corresponds to the kinetic energy.

5 Conclusion

We performed numerical experiments of freely cooling granular systems with the ED method, where no assumption about the probability distribution of the collision paramter is made. We find that the molecular chaos assumption, i.e. uncorrelated relative velocities of colliding particles, is valid for arbitrary density and weak enough dissipation.

For sufficiently strong dissipation the probability of grazing collisions increases. This can be understood by the existence of a convective shear motion, where many particles graze rather than colliding with uncorrelated relative velocities.

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