The validity of "molecular chaos" in granular flows

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We investigate with numerical simulations the validity of the assumption that the velocities and positions of colliding particles are uncorrelated ("molecular chaos") in systems of dissipative particles. This assumption is an essential part of all theories which are based on kinetic theory. We compare two simulational techniques: an "event driven" method which calculates exactly the collisions of each particle, and a Monte-Carlo method which assumes molecular chaos. This comparison isolates effects depending on particle correlations. In freely cooling granular media, the event driven simulations dissipate energy more slowly, due to a violation of molecular chaos: the impact parameter is not uniformly distributed. Examination of the structure function shows that the two methods yield distributions of mass which are similar long length scales, but very different at small length scales.

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I. INTRODUCTION

In the last years, granular media have attracted a lot of attention [1]. Dissipative, many-particle systems, far from equilibrium are another description of this fascinating granular "state of matter". For their description classical kinetic theories have been extended to account for dissipation and rather high densities (see for example refs. [2,3] and references therein). However, most of the classical and advanced approaches for a theoretical description of granular flow are based on the assumption of molecular chaos – the assumption that the velocities and positions of all colliding pairs of particles in a gas are uncorrelated. In a gas, the errors introduced by this assumption are small. In dense granular flows, correlations between colliding particles may be important, leading to qualitative changes in behavior. Therefore, we examine the validity of the molecular chaos assumption in granular flows by comparing event driven (ED) "hard sphere" simulations to those performed with the Direct Simulation Monte Carlo (DSMC) method. The ED method is capable of reproducing velocity correlations – even in the limit of rather large densities, whereas DSMC assumes molecular chaos. Comparison of these two models could guide theoreticians, because if the two methods give different results, then the breakdown of molecular chaos is significant.

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II. SIMULATION METHODS

The system we study in the following is a periodic square in two dimensions (2D), where each side has length L. Due to the periodic boundaries we need not specify wall interactions. Inside the system we have N particles of diameter d, so that the volume fraction is calculated as $V_0 = N\pi(d/2)^2/L^2$. The particles dissipate energy during each collision and there is no energy input, so that the total energy decreases monotonically.

A. ED simulation method

In the event driven (ED) method the particles follow a linear trajectory, until a collision occurs. 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 [4]. For details concerning the interaction model used in the ED method see refs. [5,6]. Since the ED method readily handles the excluded volume constraint of the particles, we use it to check the validity of molecular chaos.

B. DSMC simulation method

Direct simulation Monte Carlo (DSMC) is a method first proposed by Bird for the simulation of rarefied gas flows [7], and was also used for liquid-solid flow simulations (see Ref. [8] and references therein). One of the algorithm's advantages is its suitability for parallelization. It is also faster than ED.

In DSMC the evolution of the system is integrated in time steps τ. At each time step every particle is first moved without interaction with other particles. The particles are then sorted into spatial cells with length L_c and volume $V_c = L_c^2$. The quantity L_c is set to one half of the mean free path, but never smaller than two bead diameters. The time step τ is chosen small enough to assure that even the fastest particle needs several time steps to cross a cell. Between particles in the same cell stochastic collisions take place. The rules for this collisions are taken from kinetic theory. First we choose

$$M_c = \frac{N_c(N_c-1)\sigma v_{max}\tau}{2V_c} \tag{1}$$

collision pairs in each cell. N_c is the number of particles in the cell, v_{max} is an upper limit for the relative velocity between the particles, $\sigma = 2d$ is the scattering cross section of discs. To get v_{max} we sample the velocity distribution from time to time and set v_{max} to twice the maximum particle velocity found. In order to account for the actual relative velocities we apply an acceptance-rejection method: For a pair of particles i and j the collision is performed if

$$\frac{|\vec{v}_i - \vec{v}_j|}{v_{max}} < Z, \tag{2}$$

where Z is independent uniformly distributed in the interval $[0,1]$. This method leads to a collision probability proportional to the relative velocity of the particles.

Since the collision takes place regardless of the position in the cell, we have to choose an impact parameter b in order to calculate the post collision velocities. The impact parameter is defined as

$$b = \left| (\mathbf{r}_1 - \mathbf{r}_2) \times \frac{(\mathbf{v}_1 - \mathbf{v}_2)}{|\mathbf{v}_1 - \mathbf{v}_2|} \right| = d \sin\gamma, \tag{3}$$

where γ is the angle between $(\mathbf{v}_1 - \mathbf{v}_2)$ and $(\mathbf{r}_1 - \mathbf{r}_2)$. For central collisions $b = 0$, and $b = d$ for grazing collisions. Following molecular chaos, b is drawn from a uniform distribution in the interval $[-d, d]$. The rest of the collision scheme is identical to the event driven procedure, so that the normal component of the post collision velocity is $\vec{u}^{(n)} = -r\vec{v}^{(n)}$, whereas the tangential component remains unchanged.

To get better results at higher densities we changed the DSMC method in two respects. First we increased the number of collisions M_c in equation (1) by replacing the volume V_c of a cell with the effective free volume $V_c - V_0$, where V_0 is the volume the particles in that cell would need in a random close packing with packing fraction 0.82 in 2D [9]. Second we added an offset of d to the particle distance along the direction of the momentum transfer [10].

III. COMPARISON OF ED AND DSMC SIMULATIONS

In this section we present two simulations, starting with the same initial condition, using the same parameters, but carried out with the two different methods ED and DSMC. In ED the probability distribution may deviate from the case expected for molecular chaos, whereas DSMC always uses the function $P(b/d) = 1$. The simulation involves $N = 99856 = 316^2$ dissipative particles in 2D with restitution coefficient $r = 0.8$ in a periodic quadratic system with volume fraction $V_o = 0.25$. In order to reach an equilibrated initial condition, the system is first allowed to evolve with $r = 1$ for about 10 collisions per particle, so that a Maxwellian velocity distribution and a rather homogeneous density distribution exists. Then, at $t = 0$s, dissipation is set to $r = 0.8$ and the quantities of interest are calculated as functions of time.

A. The cooling of granular materials

In the homogeneous cooling state [11–14] we expect that the energy $K(t)$ of the system decays with time and follows the functional form

$$\frac{K(t)}{K(0)} = \left(\frac{1}{1 + t/t_0} \right)^2 \quad . \tag{4}$$

The theoretically expected time scale

$$t_0 = \frac{\sqrt{\pi} d s_*(V_0)}{2(1 - r^2) V_0 \bar{v}} \tag{5}$$

is a function of the initial energy $\bar{v} = \sqrt{2K(0)/Nm}$, the particle diameter d, the restitution coefficient r, the volume fraction V_0, with $s_*(V_0) = (1 - V_0)^2/(1 - 7V_0/16)$. Inserting the corresponding parameters $1 - r^2 = 0.36$, $s_*(V_0) \approx 0.63158$, $d = 0.001$m, and $\bar{v} = 0.2047$m/s, we have $t_0^{-1} = 23.24\text{s}^{-1}$.

B. Simulation Results

In Fig. 1(a) we present the normalized kinetic energy $K(t)/K(0)$ as a function of the normalized time t/t_0.

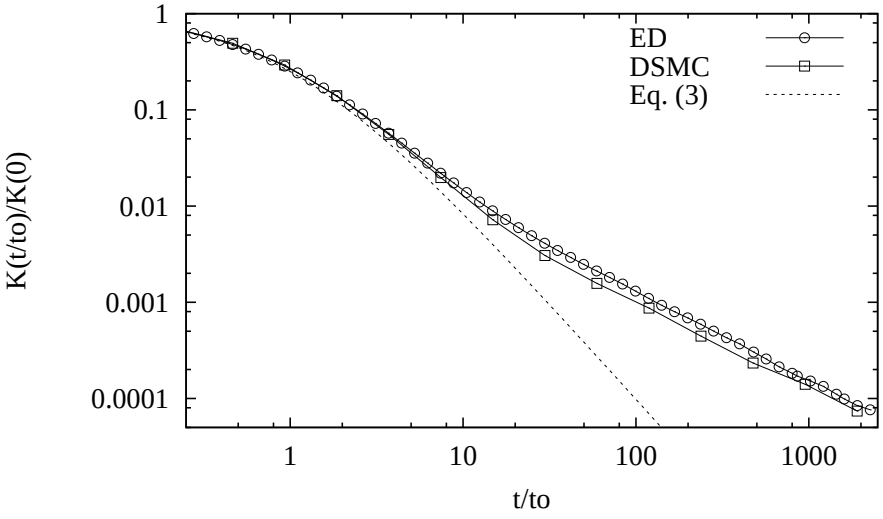

FIG. 1. Normalized kinetic energy vs. normalized time from an ED and a DSMC simulation in 2D with $N = 99856$, $V_o = 0.25$, and $r = 0.8$. The dotted line represents Eq. 4.

At the beginning of the simulation we observe a perfect agreement between the theory for homogeneous cooling and the simulations. At $t/t_0 \approx 2$ both simulation methods show substantial deviations from the homogeneous cooling behavior, and only at $t/t_0 \approx 10$ we evidence a difference between ED and DSMC. After that time, the kinetic energy obtained from the DSMC simulation is systematically smaller than $K(t)$ from the ED simulation. We relate this to the fact that the molecular chaos assumption of a constant probability distribution of the impact parameter b is no longer valid. Since dissipation acts only at the normal component of the relative velocity, DSMC dissipates more energy than ED as soon as the number of central collisions is overestimated. To verify this assumption we take a closer look at the impact parameter and its probability distribution in section IV.

IV. THE IMPACT PARAMETER

One basic assumption connected to molecular chaos is a uniform probability distribution of the impact parameter. We define $P(b/d)$ to be the probability 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 the normalized probability distributions $P(b/d) = 1$ in 2D and $P(b/d) = 2b/d$ in 3D, as expected for the case of molecular chaos.

A. The inhomogeneous probability distribution

The ED simulation of Fig. 1 leads to $P(b/d) = 1$ for short times only. For larger times we observe an increasing (decreasing) probability of grazing (central) collisions. In Fig. 2 we present data of the probability distribution at different times during the simulation. As obvious from the data, more and more grazing collisions occur with increasing simulation time. Evidently, the assumption of a homogeneous probability distribution of the impact parameter is violated.

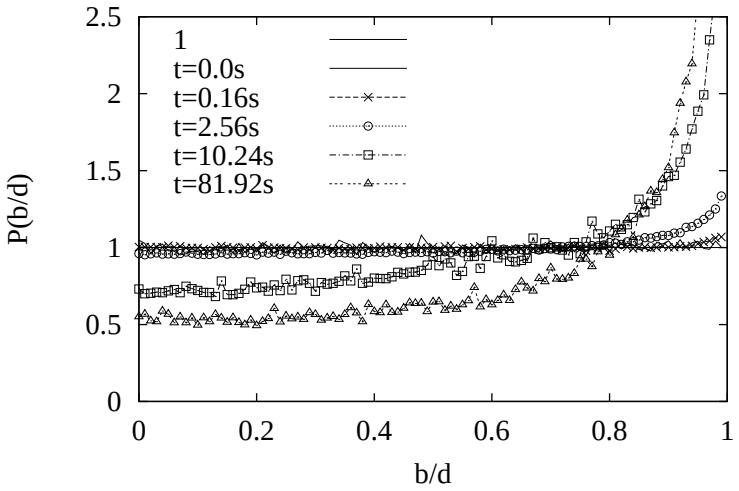

FIG. 2. Normalized probability distribution of the contact parameter from an ED simulation in 2D with $N = 99856$, $V_o = 0.25$, and $r = 0.8$ at different times.

B. The reason for the breakdown of molecular chaos

One can imagine at least two possible reasons for the deviation of $P(b/d)$ from the constant value. The first is, that $P(b/d)$ might be a function of the density, and that due to density fluctuations, the form of $P(b/d)$ changes. Thus we calculate $P(b/d)$ in smaller systems with $N = 240$, $r = 1$, and different volume fractions, ranging from very dilute to extremely dense systems. From Fig. 3(a) we learn that $P(b/d)$ is not sensitive to the density, as long as the system is elastic. The stronger fluctuations for low density come only from a comparatively worse statistics. The second reason for $P(b/d)$ to deviate from unity might be dissipation. In Fig. 3(b) the restitution coefficient is varied for fixed $V_0 = 0.7495$. For weak dissipation, i.e. $r \geq 0.9$, the distribution is homogeneous. For stronger dissipation $r = 0.80$ we find, as in the previous subsection, an increasing probability of grazing contacts.

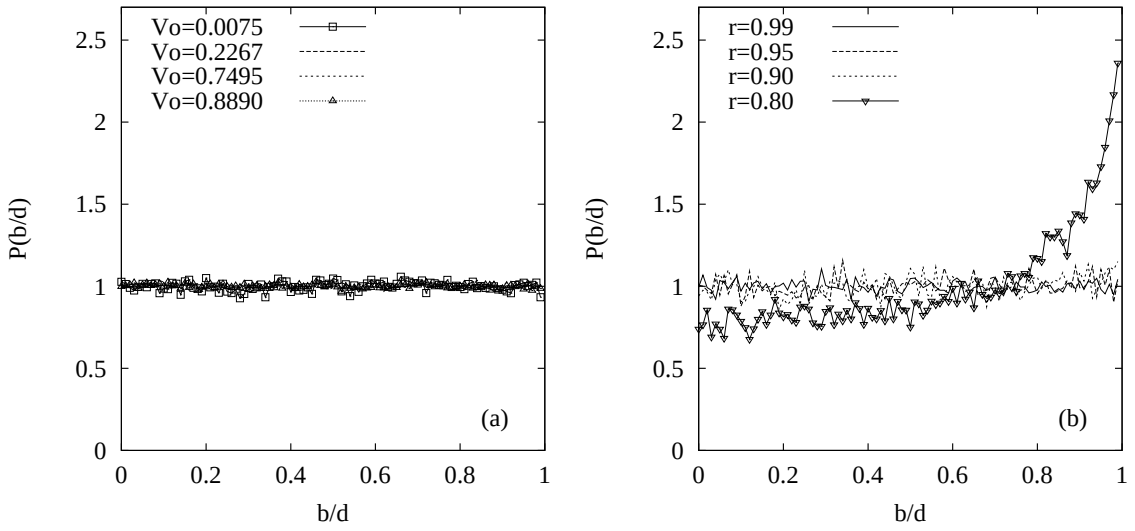

FIG. 3. (a) Normalized probability distribution of the contact parameter from ED simulations in 2D with $N = 240$, $r = 1$, and different V_o. (b) Normalized probability distribution from ED simulations in 2D with $N = 240$, $V_o = 0.7495$ and different r.

The assumption $P(b/d) = 1$ is true in elastic systems for arbitrary density. For inelastic systems, $P(b/d)$ is constant for sufficiently weak dissipation but is no longer fulfilled for strong dissipation. The breakdown of molecular chaos is *not* due to high density. Furthermore, dissipation alone is *not* the reason for an inhomogeneous probability distribution, since the dissipation must be strong enough to cause the inhomogeneous distribution.

The remaining question is, why we observe this increasing probability of grazing contacts. Looking in more detail at the simulations in Fig. 3(b), we observe that the inhomogeneous distribution for $r = 0.8$ is connected to shear motion of the particles, whereas no visible shear motion occurs for $r \geq 0.9$. The shear motion, can be understood as the geometrical reason for the higher probability for grazing contacts.

V. THE STRUCTURE FACTOR

One difference between ED and DSMC simulations is the handling of excluded volume by the two methods. While the ED method models hard spheres with a well defined excluded volume, the DSMC method models point particles and excluded volume is introduced by the approximations described in subsection II B. As expected we obtain dramatic differences in the particle-particle correlation function $g(r)$: At large times ED simulations lead to a $g(r)$ with a rich structure for short distances, indicating a rather close packing of monodisperse spheres. In contrast, the DSMC simulations show no short range correlations between particle positions throughout the whole simulation.

We would like to know if this difference has consequences at longer length scales. The formation and growth of large clusters [12–14] is quantified by $g(r)$ at large r, or equivalently, the structure factor $S(k)$ at small k. We calculate $S(k)$ by a direct FFT of the two dimensional density. Before we apply the FFT we map the particles onto a $M \times M$ lattice, where M is the closest power of 2 that gives a lattice box size of about one diameter.

We plot the structure factors obtained by ED in Fig. 4(a) and those obtained by DSMC in Fig. 4(b). Different symbols correspond to different times. We observe an increase of $S(k)$ for short wavenumbers $k < 25$, until the structure factor ceases to change for $t \geq 20$.

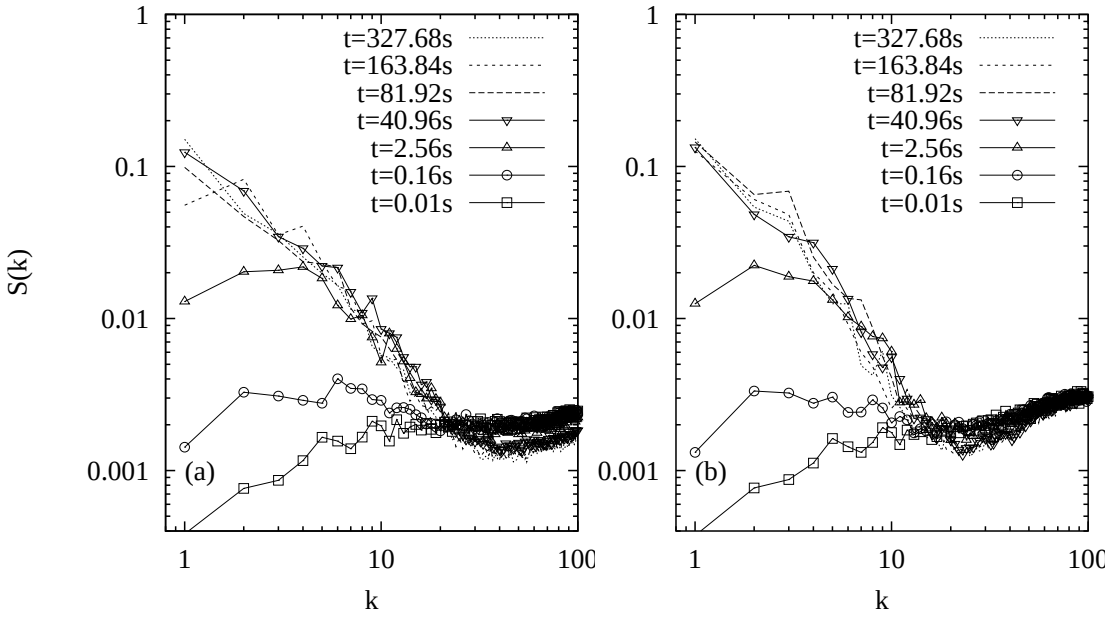

FIG. 4. (a) Structure factor obtained from the ED simulations of Fig. 1 as function of the wavenumber $k = L/\lambda$, with wavelength λ and system size L. (b) Structure factor obtained from the corresponding DSMC simulation.

The structure factor agrees reasonably well for both simulation methods, and for large enough times it does not change further. This proves that the DSMC simulation is capable to reproduce the more realistic, but computationally more expensive, ED results that account for the excluded volume by construction. Even without short-range correlations, the information about large wavelengths is well reproduced by DSMC simulations.

VI. CONCLUSION

We performed numerical experiments using ED and DSMC simulations. While for ED no assumptions about the collisions parameter are made, DSMC assumes a constant probability distribution. This is one part of the molecular chaos assumption often used in kinetic theory. We find that it is valid for arbitrary density and weak dissipation. For sufficiently strong dissipation the probability of grazing collisions increases. This can be understood by the existence of shearing motion, where many particles graze, rather than colliding with uncorrelated relative velocities.

Even with no short range correlation in DSMC, both methods agree well with respect to long range correlations quantified by the structure factor. This indicates that kinetic theories can succeed in describing the formation and growth of clusters, even though the assumption of molecular chaos is not satisfied. Furthermore, the faster DSMC method can

be used to study cluster formation in larger or three dimensional systems. We are optimistic that DSMC can be used to study other problems in granular materials, but more study is needed to be sure.

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