The Breakdown of Kinetic Theory in Granular Shear Flows

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We examine two basic assumptions of kinetic theory–binary collisions and molecular chaos–using numerical simulations of sheared granular materials. We investigate a wide range of densities and restitution coefficients and demonstrate that kinetic theory breaks down at large density and small restitution coefficients. In the regimes where kinetic theory fails, there is an associated emergence of clusters of spatially correlated grains.

For granular materials, kinetic theory has been the primary strategy used to systematically derive hydrodynamics equations, starting from elementary assumptions about grain-grain interactions. This has led to much interest in applying predictions from the theory to realistic granular flows (for reviews, see [2]), and recent work continues in this direction [3, 4, 5]. However, kinetic theory strictly applies only to dilute gases, and the extent that it applies to the dense regime remains unclear.

In this Letter we perform tests of the fundamental assumptions of kinetic theory, using the Contact Dynamics (CD) algorithm. We find that kinetic theory is severely limited by the assumption that only binary interactions occur between grains. Instead, an effective many body interaction arises that is a direct consequence of persistent contacts in the dense regime. In Fig. 1 we characterize the failure of the binary collision assumption, using spatial force correlations to approximate the average number of grains \( N_c \) that form a cluster in contact. As we see, the cluster size increases when going to low restitution coefficient and high density, which should limit the relevance of kinetic theory. This Letter provides quantitative estimates of this breakdown.

Most kinetic theory research starts with the Boltzmann equation, which is derived from the BBGKY hierarchy, and then finds its solutions [1, 4, 5]. However, certain assumptions are necessary to derive the Boltzmann equation. We begin by discussing two of these assumptions.

Consider a system of \( N \) grains and the evolution equation for the \( N \)-body probability distribution function (pdf) \( f^{(N)}(\vec{r}, \vec{p}) \), where \( \{\vec{r}\} \) denotes the set of all positions and momenta for the system (with the notation \( \vec{r} = \{\vec{r}_i\} \)). This equation is simply a statement of conservation of probability and reads

\[
\frac{\partial f^{(N)}}{\partial t} + \sum_i \frac{\partial f^{(N)}}{\partial \vec{r}_i} \cdot \frac{\vec{p}_i}{m} = -\sum_{ij} \frac{\partial f^{(N)}}{\partial \vec{p}_i} \cdot \vec{F}_{ij} \quad (1)
\]

where we have decomposed the force on each grain as a sum over pairs: \( \vec{F}_i = \sum_j \vec{F}_{ij} \).

The BBGKY hierarchy is derived from Eq. (1) by integration [6]. This hierarchy is the set of \( N-1 \) equations for the evolution of the \( n \)-body pdfs \( f^{(n)} \), with \( 1 \leq n < N \). If the force resulting from a pair interaction depends only on the positions and velocities of the interacting pair, then the evolution equation of each \( f^{(n)} \) depends only on \( f^{(n+1)} \). This is the classical form of the BBGKY hierarchy.

When applying the derivation of the BBGKY hierarchy to granular materials, additional care must be taken. For dilute hard-sphere gases the derivation applies since interactions result from binary collisions and thus pair forces depend only on the positions and velocities of the interacting pair. However, in dense systems of dissipative grains the situation is different. In this case there may be clusters of grains in persistent contact, as illustrated in Fig. 2. If clusters have formed, the force between any pair in the cluster will depend not only on the positions and velocities of the interacting pair, but also on the positions and velocities of all other grains in the cluster. In this case, the hierarchical structure of the BBGKY equations is not guaranteed. Therefore, in order to derive the BBGKY hierarchy for granular materials, we must make the binary collision assumption. This stipulates that only binary collisions occur, thereby assuring that pair forces depend only on the positions and velocities of the interacting pair.

The Boltzmann equation follows from the first equation \((n = 1)\) of the BBGKY hierarchy, which relates \( f^{(1)} \) to \( f^{(2)} \). A second assumption is also required, the molecular chaos assumption, which simplifies this equation by...
setting
\[ f^{(2)}(r_1, r_2, v_1, v_2) = \chi(r_1, r_2)f^{(1)}(r_1, v_1)f^{(1)}(r_2, v_2), \] (2)
where \( \chi \) describes possible correlations in the positions of particles. This assumption allows us to approximate the first equation of the BBGKY hierarchy as a non-linear equation for \( f^{(1)} \); this is the Boltzmann equation.

The Boltzmann equation relies on the assumptions of binary collisions and molecular chaos. In the rest of this Letter we test these fundamental assumptions, using two-dimensional CD simulations of frictionless granular materials in simple shear flow at constant volume. The simulations are performed using Lees-Edwards boundary conditions, which ensure translational invariance. The density, restitution coefficient, and shear rate are prescribed and other observables are measured.

In Fig. 2, we show two representative screenshots from our simulations, in steady state, for identical shear rate and density, but different restitution coefficients, \( e = 0.92 \) and \( e = 0 \). A small time interval is chosen, and in both cases grains that collide during this time interval are colored. Different colors corresponding to separate contact networks. For \( e = 0.92 \) the interacting grains are well spaced and tend to occur in pairs, whereas for \( e = 0 \) the interacting grains tend to form large clusters. These clusters indicate the emergence of persistent contacts for small values of \( e \) (high inelasticity).

FIG. 2: (Color online). Steady state screenshots of sheared granular materials at two different restitution coefficients: \( e = 0.92 \) (left) and \( e = 0 \) (right). Grains involved in a collision during a small time period are colored, with different colors denoting different contact networks. Interactions are binary for \( e = 0.92 \) whereas large clusters form for \( e = 0 \).

We now test the binary collision assumption, which is primarily a statement about the forces between pairs of grains. The idea is to measure the relative contribution to momentum transport from binary collisions and from clusters in persistent contact. A quantitative measure of these contributions can be obtained by measures of the stress tensor. The “static” stress \( \Sigma^s \) reads:
\[ \Sigma^s_{\alpha\beta} A = \frac{1}{2} \sum_{i>j} (D_i + D_j) \hat{n}_{ij} \cdot \hat{n}_{ij} \cdot \hat{F}_{ij} \] (3)
where \( \alpha, \beta \) denote components and \( i, j \) denote grains, \( D_i \) is the diameter of grain \( i \), \( \hat{n}_{ij} \) the unit normal vector at contact between the pair \((i,j)\), and \( A \) is the area of the simulation cell. This quantity measures the true momentum transport in a microcanonical configuration. At each time step, the CD algorithm determines the contact forces \( \hat{F}_{ij} \) by upholding constraints relevant to perfectly rigid contact between grains.

When a binary collision occurs, the final relative velocity of the colliding pair is set equal to the initial relative velocity, multiplied by \(-e\). The CD algorithm calculates the force between the pair based on the instantaneous impulse that produces this final relative velocity. Because of the time-discretization, this “binary collision force” is approximated over a time interval \( \Delta t \) by a constant force equal to the instantaneous impulse divided by \( \Delta t \):
\[ \hat{F}_{ij}^{bc} = \frac{\hat{F}_{ij}}{2\Delta t} \] (4)
where \( \hat{F}_{ij} \) is the reduced mass of grains \( i \) and \( j \), and \( \hat{V}_{ij} \) is the pre-collisional velocity of grain \( i \). However, when multiparticle collisions occur, the total forces \( \hat{F}_{ij} \) differ from the binary collision forces \( \hat{F}_{ij}^{bc} \). Replacing \( \hat{F}_{ij} \) by \( \hat{F}_{ij}^{bc} \) in Eq. (3) provides the flux of momentum that would be transported if all forces resulted from binary collisions:
\[ \Sigma^{bc}_{\alpha\beta} A = \frac{1}{2} \sum_{i>j} \mu_{ij}(D_i + D_j) \hat{n}_{ij} \cdot \hat{n}_{ij} \cdot (v_i - v_j) \cdot \hat{F}_{ij} \] (4)
We call this tensor the “collisional” stress tensor: it is defined at any time, even in the presence of multi-contact interactions, and is an approximation to the static stress.

A theory that assumes binary collisions and is capable of taking into account all correlations and providing an exact expression for the distribution of velocities between incoming pairs of grains would only account for \( \Sigma^{bc}_{\alpha\beta} \), but never \( \Sigma^{s}_{\alpha\beta} \). Because most kinetic theories assume binary collisions, the core question is whether \( \Sigma^{bc}_{\alpha\beta} \) is a reasonable approximation to \( \Sigma^{s}_{\alpha\beta} \).

To answer this question, we further decompose stresses into pressure \( p \) and shear stress \( s \). Pressure is one-half of the trace of the tensor and the shear stress is defined as either of the off-diagonal elements of the symmetric stress tensor. In Fig. 3, we plot data from our simulations for the static pressure divided by the collisional pressure \( p^s/p^{bc} \) and the static shear stress divided by the collisional shear stress \( s^s/s^{bc} \) as a function of packing fraction, for a variety of restitution coefficients. For restitution coefficients near unity and relatively low packing fraction, the static values are equal to the collisional values and the ratios in Fig. 3 are close to unity. However, for large packing fractions and small restitution coefficients, the static values become larger than the collisional values. This signals a breakdown of the binary collision assumption.

This first numerical test quantitatively demonstrates that the collisional stress tensor is not an adequate approximation of the true static stress tensor in certain regimes of granular shear flow. It rules out the possibility that a theory based on the binary collision assumption can be applied to predicting the static stress at high density or low restitution.
Next, we examine the molecular chaos assumption: we test whether a broad array of kinetic theories succeed in accounting for the collisional stress. In two dimensions, kinetic theories that assume both binary collisions and molecular chaos make a prediction for the collisional pressure. In two dimensions, kinetic theories that assume both binary collisions and molecular chaos make a prediction for the collisional pressure $p^{bc}$:

$$p^{bc} = (1 + e)\nu p^*$$

where $\nu$ is the packing fraction and $\chi$ is the pair correlation function at contact. This prediction is proportional to $p^* = \frac{nm}{2} \delta v^2 / \bar{\delta v}$ where $n$ is the number density, $m$ is the average mass, and $\delta v$ is the average square of the fluctuating velocity (the granular temperature).

Our second numerical test compares the prediction for the collisional pressure to the actual collisional pressure measured in the simulations. We determine all parameters in Eq. (5) directly from the simulations: $e$ and $\nu$ are prescribed, $\chi$ and $p^*$ are measured. Following other studies, we measure $\chi$ using the collision frequency $\omega$ and the following formula from kinetic theory:

$$\omega = \sqrt{2\pi\delta v^2} \chi m$$

where $\sigma$ is the average grain diameter.

Using Eqs. (5) and (6), we measure, without any fitting parameters, the approximation to the collisional pressure resulting from the molecular chaos assumption. This is reported in solid lines on Fig. 3, where we have also plotted raw data for both the collisional and static pressure. For $e = 0.92$ there is excellent agreement between the kinetic theory prediction and the collisional pressure, even for large values of packing fraction. For $e = 0$ the molecular chaos assumption leads to an overestimate of pressure at all packing fractions.

We expect this overestimate to result from correlations of the pre-collisional velocities: if the velocities of two incoming grains are positively correlated then their relative velocity is smaller, and the collisional pressure is thereby reduced. Because the molecular chaos assumption does not incorporate these correlations, it overestimates the collisional pressure.

The insets of Fig. 3 contain measurements of the pre-collisional velocity correlations $\langle \delta v_1 \delta v_2 \rangle$, where $\delta v$ is the fluctuating part of the velocity in the direction parallel to the vector connecting the grain centers $\hat{n}$. We measure correlations in this direction because only these velocity components contribute to the collisional stress in Eq. (5). The average is performed over a disk centered on one grain with a radius of $1.8\sigma$, although the results do not depend on the size of the averaging disk. Pairs of
grains that collided in the previous time step are excluded from the average in order to ensure the correlations are truly pre-collisional. We observe that large values of the correlation correspond to packing fractions where kinetic theories based on the molecular chaos assumption overestimate the collisional pressure. However, the value of the correlation does not correspond to whether the collisional stress is a good approximation to the static stress – this seems to be related only to the breakdown of the binary collision assumption.

In order to further understand how the binary collision assumption breaks down, we return to the observation that dense granular flows organize into clusters of interacting grains, as illustrated in Fig. 2. The failure of the binary collision assumption is related to the formation of these clusters and the fact that the stress tensor is not determined solely by two particle interactions.

A cluster of grains may be defined as a region in the material over which forces are correlated. To determine the average number of grains $N_c$ in these correlated clusters, we measure the spatial force-force correlations $C(\ell) \equiv \langle \vec{F}(0) \cdot \vec{F}(\ell) \rangle$, where $\ell$ is a positive distance measured in grain diameters and $\vec{F}$ is the total vector force acting on a grain. If a grain is isolated, so that there are no forces acting on it, it is not included in this average. We then define $N_c$ proportional to the square of the correlation length

$$\sqrt{N_c} \propto \langle \ell \rangle = \int \frac{\ell C(\ell) d\ell}{\int C(\ell) d\ell}$$

and normalize so $N_c = 2$ for $e = 0.92$ and low density. We choose this normalization because we have observed (see Fig. 3) that the binary collision assumption, which corresponds to $N_c = 2$, is appropriate for dilute, nearly elastic granular materials.

Our measurements of $N_c$ are presented in Fig. 5 along with measurements of $C(\ell)$. The force correlations fluctuate at small distance and exhibit an exponential decay at large distance. The values of $\langle \ell \rangle$ determined from Eq. (7) match the exponential decay (when we plot $e^{-\ell/\langle \ell \rangle}$) for the densities and restitution coefficients we have investigated. We notice from Fig. 5 that the divergence of $N_c$ close to jamming nicely echoes the divergence of pressure and shear stress ratios in Fig. 3. This confirms that the formation of clusters is directly related to the breakdown of the binary collision assumption.

The measurement of $N_c$ allows us to partition the phase space of granular shear flow into regions where kinetic theory applies ($N_c = 2$) and regions where it does not ($N_c > 2$). In Fig. 4 we plot contours of $N_c$ as a function of restitution coefficient and packing fraction. Although numerical noise prevents us from plotting the contour $N_c = 2$, Fig. 4 provides an estimate of the regime where kinetic theory applies.

We have presented two numerical tests of the fundamental assumptions of kinetic theory in granular materials: first we have observed the breakdown of the binary collision assumption for large densities and small restitution coefficients; second we have demonstrated that the molecular chaos assumption is not valid for small restitution coefficients, due to pre-collisional velocity correlations. In order for an approach based on kinetic theory to be useful at high density, the deficiencies in these core assumptions must be addressed. Although the molecular chaos assumption can in principle be addressed by incorporating velocity dependent terms in Eq. (2), it seems to us that the failure of the binary collision assumption may be much more difficult to overcome in a standard kinetic theory. Successful theories of granular materials in the dense regime must incorporate clustering.

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