

## Emergence of multi-contact interactions in contact dynamics simulations of granular shear flows

G. LOIS<sup>1</sup>, A. LEMAÎTRE<sup>1,2</sup> and J. M. CARLSON<sup>1</sup>

<sup>1</sup> *Physics Department, University of California - Santa Barbara, CA 93106, USA*

<sup>2</sup> *Institut Navier-LMSGC - 2 allée Képler, 77420 Champs-sur-Marne, France*

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**Abstract.** – We examine the binary collision assumption of hard-sphere kinetic theory in numerical simulations of sheared granular materials. For a wide range of densities and restitution coefficients we measure collisional and non-collisional contributions to the stress tensor and find that non-collisional effects dominate at large density and small restitution coefficient. In the regimes where the non-collisional contributions disappear, we test kinetic theory predictions for the pressure without any fitting parameters and find remarkable agreement. In the regimes where the non-collisional contributions become large, we observe groups of simultaneously interacting grains and determine the average multi-contact cluster size using measurements of spatial force correlations.

Flows of granular materials occur in many natural settings and challenge conventional theories of hydrodynamics and statistical physics [1, 2]. Kinetic theory provides a systematic derivation of hydrodynamic equations for granular media [3–5], but relies on methods originally designed for dilute systems. For this reason it is not expected to apply in dense granular flows [6, 7]. Nevertheless, several tests of kinetic theory have been performed [8–15] that include moderate to high densities and present strong agreement between the predictions of kinetic theory and numerical simulations. It has also been suggested that kinetic theory may provide a starting point to study the rheology of dense granular flows [15].

These surprising results challenge our expectations about the range of validity of kinetic theory and suggest that further quantitative tests are needed to clarify its domain of applicability. The limits of kinetic theory have attracted considerable attention over the years, but most work has focused on moderately dense granular gases with moderately dissipative collisions. In these situations, the so-called clustering instability leads to the emergence of short-range correlation [16–18], the molecular chaos assumption loses relevance [19], and kinetic theory is no longer applicable [20]. This picture has shaped our notions about the breakdown of kinetic theory, but it is based on simulations and analyses of granular gases at intermediate densities and restitution coefficients. It remains unclear how this can be used to help us interpret attempts to test kinetic theory in dense flows.

Realistic granular materials consist of irregularly shaped grains, each with a finite stiffness (or Young’s modulus). Hard-sphere kinetic theory makes the simplifying approximation that grains are infinitely stiff and spherical. In this approximation, an important assumption is

required in the derivation of kinetic theory. This is the “binary collision assumption”<sup>(1)</sup>, which postulates that momentum transport is entirely realized by collisions between pairs of grains [5, 13, 21–23]. In this paper we carry out hard-sphere simulations of granular shear flow and find that this assumption does not always hold since *dissipative* hard spheres can form contacts that last for a finite amount of time. These persistent contacts facilitate the emergence of multi-contact interactions, which carry a fraction of the total stress. Although hard-sphere kinetic theory becomes formally invalid when multi-contact interactions occur, its predictions do not suddenly become entirely inaccurate. Instead, persistent contacts begin to carry part of the momentum transfer, while another part continues to be carried by collisions.

The crossover between contact and collisional transport is an essential feature in the progression of granular flows toward jamming. However, the emergence of multi-contact forces in dense granular flows and its *quantitative* effects on momentum transport has received little attention in comparison with, *e.g.*, the clustering instability. This is perhaps because separating “persistent” and collisional forces is difficult, even in simulations of granular flows.

Here, we use contact dynamics (CD) simulations to test the binary collision assumption in hard-sphere granular shear flows. In agreement with previous simulations [24] we find that there is indeed a regime where an increasing part of the stress is carried by “static” forces, while Bagnold’s scaling still holds. We find that the development of non-collisional stress in dense regimes is accompanied by the emergence of force-force correlations, instead of the velocity-velocity correlations seen at intermediate densities.

*Contact dynamics simulations.* – CD simulations have been instrumental in determining properties of static forces in dense granular packings [25, 26], but have not been carefully compared with the kinetic theory formalism in flowing regimes. The CD algorithm models dynamics of perfectly rigid grains by integrating Newton’s equations of motion over a fixed time step. For every contact that occurs in each time step, the relative normal velocities of the contacting grains are updated using a constant restitution coefficient  $e$ . This allows the contact forces to be deduced as the solution of a set of coupled algebraic equations [27, 28]. Although the CD algorithm is equipped to incorporate friction between grains, we concentrate here on the frictionless case. A detailed account of the algorithmic techniques we use can be found in ref. [29]. In the simulations presented here, the granular medium consists of a polydisperse sample of grains with diameters evenly distributed between  $0.74\sigma$  and  $1.26\sigma$ , where  $\sigma$  is the average diameter. We simulate between 2500 and 10000 grains in a two-dimensional shear cell using Lees-Edwards boundary conditions.

To concretely illustrate the methodology underlying CD, and to highlight important differences between CD and event-driven simulations or molecular dynamics, we consider each algorithm in the context of a simple example: a single grain falling under gravity and coming to rest on a horizontal plane. In reality, the grain hits the plane with a non-zero initial velocity and bounces back with a lower velocity. The fractional decrease is roughly represented by a restitution coefficient  $e < 1$ . A series of rebounds follows, each dissipating a fraction ( $e^2$ ) of the kinetic energy, until other microscopic dissipation processes take over, and the grain eventually comes to rest (in a finite time).

A precise simulation of the dynamics in this example would account for the finite elasticity of the grain and of the plane. In this case, each impact takes a fixed time and involves motions over a finite length scale, corresponding to the size of asperities on both solids. Energy decreases roughly exponentially with the number of collisions, as does the height of successive rebounds. After a few bounces the grain does not jump sufficiently high for the

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<sup>(1)</sup>It appears at a very early stage in the derivation of the pseudo-Liouville formalism, prior to inferring the Boltzmann-Enskog equation via the molecular chaos assumption [23].

asperities to separate and a contact is formed. Once that occurs the grain will vibrate with a small amplitude, which is damped by various mechanisms. Careful molecular dynamics simulations could in principle account for this delicate motion, but the small-scale and short-time description comes with a large computational cost that severely limits the range of accessible parameters.

If we instead model the grain as a hard-sphere and the plane as perfectly rigid, the contact time and the contact thickness are both approximated as zero. Keeping the restitution coefficient fixed, a straightforward calculation shows that the rigid particle comes to rest with the plane in a finite time, but after an infinite number of collisions (this is called inelastic collapse). This does not create any mathematical inconsistency: the rigid grain motion is well defined and matches the time- and energy-scales of the physical dynamics. The accumulation of collisions, however, introduces significant problems for numerical simulation. In particular, the relaxation of a rigid grain *a priori* cannot be solved using event-driven simulations. In an effort to represent dense systems, event-driven simulations often bypass inelastic collapse by assuming the restitution coefficient is itself a dynamical variable, becoming equal to unity in certain circumstances, *e.g.*, low-velocity impacts, or two collisions occurring in a small cut-off time  $t_c$  [30,31]. In our elementary case—a grain bouncing on the floor—this class of models would predict that at long times the grain rebounds indefinitely on the horizontal plane and, in this latter stage, the system no longer dissipates energy.

CD offers an alternative approach to the same numerical puzzle by coarse-graining time. In our example of a grain bouncing on the floor, CD sacrifices an accurate representation of the very fast vibrations at small scales during the latest stages of collapse, while maintaining the correct inference that a persistent contact has been created and simultaneously accounting for the dissipated energy [28]. In the case of simple shear flow, which we investigate here, the CD algorithm accurately represents experimental granular flows in the regimes where inertial scalings are dominant. Additionally, since the CD algorithm treats grains as perfectly rigid spheres, it is well suited to test the assumptions and predictions of hard-sphere kinetic theory, which is our primary aim.

*Testing the binary collision assumption.* – We now numerically test the binary collision assumption. The idea is to measure the contribution of binary collisions and persistent contacts to the stress tensor. The static stress  $\Sigma^s$  is defined as

$$\Sigma_{\alpha\beta}^s A = \frac{1}{2} \sum_{i>j} (\sigma_i + \sigma_j) \hat{n}_{ij\alpha} \mathbf{F}_{ij\beta}, \quad (1)$$

where  $\alpha, \beta$  denote components and  $i, j$  denote contacting grains,  $\sigma_i$  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, based on the contact forces  $\mathbf{F}_{ij}$  that are determined from the CD algorithm.

When a binary collision occurs, the momentum exchange is determined by the incoming grain velocities and by the restitution coefficient  $e$ . The CD algorithm approximates this “binary collision force” by a constant force over the interval  $\Delta t$ :  $\mathbf{F}_{ij}^{bc} = \frac{\mu_{ij}}{\Delta t} (1 + e) \hat{n}_{ij} \cdot (\mathbf{v}_i - \mathbf{v}_j) \hat{n}_{ij}$ , where  $\mu_{ij}$  is the reduced mass of grains  $i$  and  $j$ , and  $\mathbf{v}_i$  is the pre-collisional velocity of grain  $i$ . When multi-particle collisions occur, the total forces  $\mathbf{F}_{ij}$  may differ from the binary collision forces  $\mathbf{F}_{ij}^{bc}$ . Replacing  $\mathbf{F}_{ij}$  by  $\mathbf{F}_{ij}^{bc}$  in eq. (1) provides the fraction of momentum that is transported from binary collisions:

$$\Sigma_{\alpha\beta}^{bc} A = \frac{1 + e}{2\Delta t} \sum_{i>j} \mu_{ij} (\sigma_i + \sigma_j) \hat{n}_{ij\alpha} \hat{n}_{ij\beta} (\mathbf{v}_i - \mathbf{v}_j) \cdot \hat{n}_{ij}, \quad (2)$$

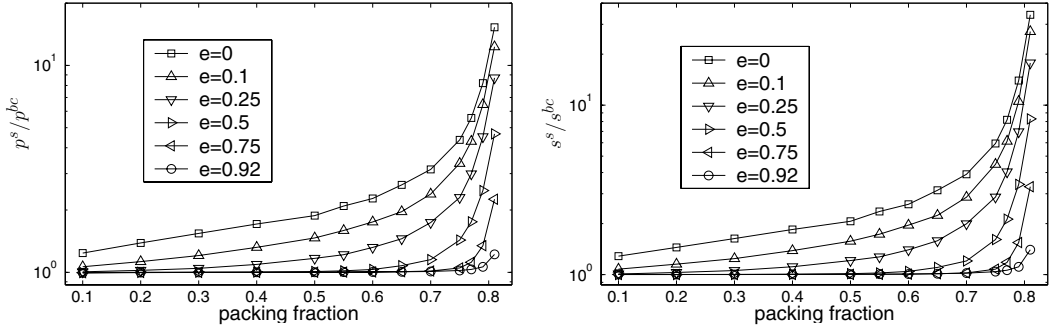


Fig. 1 – The static pressure divided by the collisional pressure ( $p^s/p^{bc}$ ) and the static shear stress divided by the collisional shear stress ( $s^s/s^{bc}$ ) as a function of packing fraction, for a variety of restitution coefficients  $e$ . Values larger than unity reveal the presence of non-collisional stresses.

where the sum runs over newly contacting grains only. We call this tensor the “collisional” stress tensor: it is defined at any time, even in the presence of multi-contact interactions. The emergence of multi-contact interactions should be signaled by the relative importance of the collisional contribution  $\Sigma_{\alpha\beta}^{bc}$  to the total stress tensor  $\Sigma_{\alpha\beta}^s$ .

To compare these quantities, we further decompose stresses into pressure  $p$  and shear stress  $s^{(2)}$ . In fig. 1 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 fractions, the static values are equal to the collisional values and the ratios in fig. 1 are close to unity. However, for large packing fractions and small restitution coefficients, the static values become larger than the collisional values. These results are independent of the simulation time step [32]. This signals the breakdown of the binary collision assumption and reveals that multi-particle interactions become a significant source of momentum transport. For high density and/or large dissipation, the collisional stress tensor is not an adequate approximation of the static stress tensor.

*Testing the predictions of kinetic theory.* – For flows where the collisional pressure is equal to the static pressure, it is relevant to test the predictions of kinetic theory. In two dimensions, kinetic theories that assume both binary collisions and molecular chaos make a prediction  $p^{kt}$  for the collisional pressure [5, 13, 21, 22] that has been verified by directly simulating the Enskog equation [13]:

$$p^{kt} = (1 + e)\chi\nu p^*. \quad (3)$$

In this equation,  $\nu$  is the packing fraction,  $\chi$  is the equilibrium pair correlation function at contact, and  $p^*$  is the streaming pressure.

Our second numerical test compares the prediction for the collisional pressure to the actual collisional pressure measured in the simulations. For this test, we measure the actual collisional pressure  $p^{bc}$  and compare it to the kinetic theory prediction from eq. (3). We determine all parameters in eq. (3) directly from the simulations:  $e$  and  $\nu$  are prescribed;  $\chi$  and  $p^*$  are measured. Following other studies [33] we measure  $\chi$  using the collision frequency  $\omega$  found in simulations on an equilibrium system with  $e = 1$  and zero shear rate. The formula

<sup>(2)</sup>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.

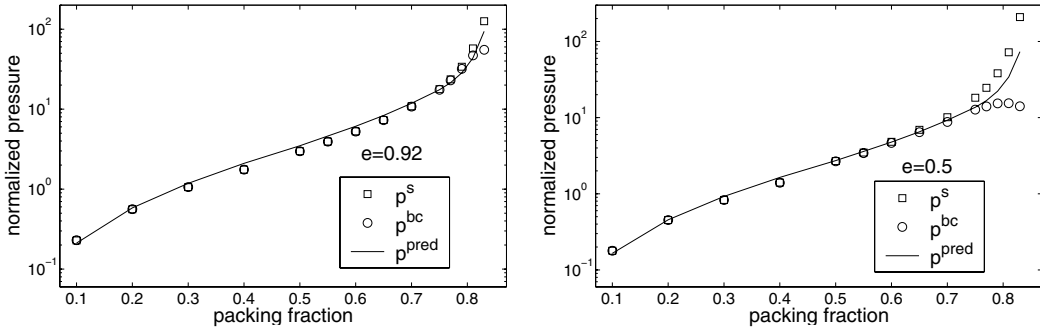


Fig. 2 – The static pressure  $p^s$ , collisional pressure  $p^{bc}$ , and kinetic theory prediction  $p^{kt}$ , all normalized by  $p^*$ , for  $e = 0.92$  (left) and  $e = 0.5$  (right).

$\omega = \chi n \sigma \sqrt{2\pi \delta v^2}$  relates the collision frequency to  $\chi$ , where  $\sigma$  is the average grain diameter,  $n$  is the number density, and  $\delta v^2$  is the average square of the fluctuating velocity. The streaming pressure is measured in the normal way as  $p^* A = \sum_i m_i (\mathbf{v}_i - \mathbf{U})^2 / 2$ , where  $m_i$  and  $\mathbf{v}_i$  are the mass and velocity of grain  $i$ ,  $\mathbf{U}$  is the average velocity, and  $A$  is the area of the simulation cell. The sum is over all grains.

Using eq. (3) we measure, without any fitting parameters, the prediction of the collisional pressure. This is reported in solid lines in fig. 2, where we have also plotted raw data for both the collisional and static pressure.

When collisional and static pressures are equal, there is excellent agreement between the kinetic theory prediction and the collisional pressure, for both values of restitution. This compares well to earlier tests of eq. (3), using both event-driven [12] and soft-sphere simulations [9,10,15]. It is important to note that, although the simulated granular material consists of a polydisperse collection of grains, we use the kinetic theory prediction for a monodisperse granular material and find excellent agreement at low density. This suggests that more elaborate calculations are not required for polydisperse systems [13] and the average grain diameter sets the relevant microscopic length scale.

When the collisional and static pressures are not equal, the kinetic theory prediction overestimates the collisional pressure. In this situation i) the collisional stress badly approximates the total stress and ii) kinetic theory badly approximates the collisional stress. However, kinetic theory may seem to match reasonably well the total stress if these two quantities are directly compared. This observation is striking and cautions against the direct comparison of macroscopic quantities [15].

*The emergence of multi-contact clusters.* – In order to further understand the breakdown of the binary collision assumption, we examine how dense granular flows organize into clusters of simultaneously contacting grains. These “clusters” should not be mistaken for the fluctuations of density which arise in the so-called “clustering” instability [11, 34, 35]. In regimes displaying a clustering instability the binary collision assumption usually holds, but velocities become correlated<sup>(3)</sup>. Our measurements of velocity-velocity correlations, however, do not seem to account for the growing importance of static forces close to jamming [32]. Here we define multi-contact clusters as sets of simultaneously contacting grains. We now show that these clusters can be characterized by measurements of force-force correlations.

<sup>(3)</sup>For example, ref. [11] links the length-scale of density fluctuations with the value of the streaming (or kinetic) part of the stress tensor.

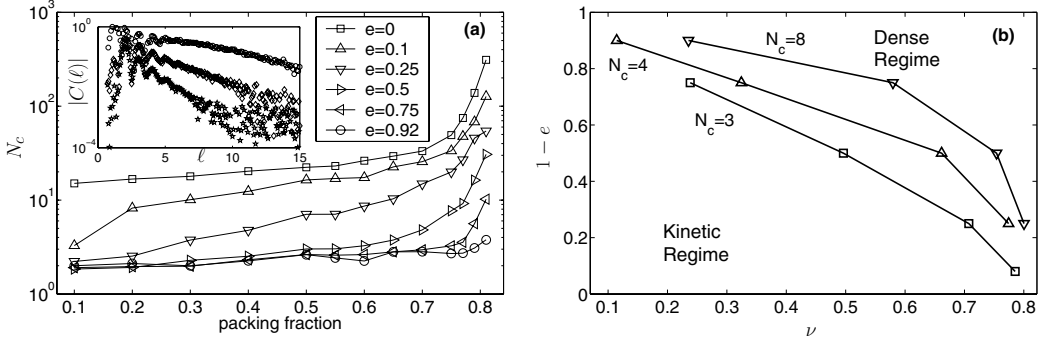


Fig. 3 – (a) Average multi-contact cluster size  $N_c$  as a function of packing fraction, for many values of the restitution coefficient  $e$ . Inset: spatial force-force correlations  $|C(\ell)|$  (in arbitrary units on a log scale) for  $e = 0$  and  $\nu = 0.7$  (bottom)  $\nu = 0.77$  (middle) and  $\nu = 0.81$  (top). (b) Contours of the average multi-contact cluster size  $N_c$  as a function of restitution coefficient  $e$  and packing fraction  $\nu$ . Kinetic theory applies to binary interactions between grains ( $N_c = 2$ ).

To determine the average number of grains  $N_c$  in correlated clusters, we measure 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 has no contacts, it is not included in this average. We observe that  $C(\ell)$  decays exponentially, as shown in the inset of fig. 3a. We then define  $N_c \propto \langle \ell \rangle^2$ , where  $\langle \ell \rangle$  is determined such that  $e^{-\ell/\langle \ell \rangle}$  matches the exponential decay of  $C(\ell)$ , and normalize so  $N_c = 2$  for  $e = 0.92$  and low density. We choose this normalization because we have observed that the binary collision assumption is appropriate for dilute, nearly elastic granular materials.

Our measurements of  $N_c$  are presented in fig. 3a. We notice that  $N_c = 2$  in dilute regimes and increases as jamming is approached. The growth of  $N_c$  for large packing fraction also nicely echoes the increase of pressure ratios in fig. 1. This confirms that the formation of multi-contact clusters is directly related to the breakdown of the binary collision assumption.

At this point we would like to stress that the existence of multi-contact clusters does not render our system inhomogeneous. Indeed, many such clusters exist in each simulation—they are created due to dissipation between grains and destroyed by the overall shear flow. However, over scales larger than  $N_c$ , the local values of macroscopic variables are not spatially dependent. This suggests that a granular system with  $N_c > 2$  is best described as a homogeneous collection of multi-contact grain clusters.

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. 3b 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. 3b provides an estimate of the regime where kinetic theory applies—for  $N_c \geq 3$ , we would not expect kinetic theory to hold.

We have investigated the assumptions and predictions of kinetic theory using simulations of granular shear flow. We find that clusters of simultaneously contacting grains form in the dense regime and limit the applicability of hard-sphere kinetic theory, which assumes that only binary collisions occur. For dilute systems where the multi-contact cluster size is small, momentum transport is entirely carried out by binary collisions and the predictions of kinetic theory are accurate. For dense systems where the multi-contact cluster size is large, there are

non-collisional contributions to the stress tensor and kinetic theory cannot be applied. This presents new challenges to modeling hard-sphere granular flow, and any successful theory must incorporate the effects of simultaneous contacts.

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