Detection of Inelastic Collapse in 3-D Shear Flow

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Inelastic collapse has been observed in a wide range of granular simulations. Very little work, however, has been done in the area of detection of inelastic collapse in couette flow hard sphere simulations. Only recently has the occurrence of inelastic collapse been investigated for such systems.[1] That work has shown that the probability of detecting inelastic collapse increases with a decrease in the coefficient of restitution. In this paper we show that the traditional method for detection of inelastic collapse, based on separation distance, is too strict for couette flow systems. We show this by first performing a 3-D simulation of a granular system in planar shear where the traditional detection method finds what is considered to be inelastic collapse at a current time in the simulation. Unlike in previous work, the simulation is then allowed to continue beyond this point, and eventually reaches a steady state where inelastic collapse is not detected. Therefore the initial indication of inelastic collapse is a false positive, suggesting that the probability of inelastic collapse detection is too high. Furthermore, in a different granular system with a lower coefficient of restitution, however, when the simulation is allowed to continue beyond the detection of inelastic collapse, a steady state flow is not reached. Instead the system ceases to move forward in time. Based on the above results, we propose a new detection method for inelastic collapse in driven hard sphere simulations in order to avoid false positives.

[1] Alam, M., Hrenya, C. M., Phys. Rev. E, **63**, 2001, 061308

I. Background

Inelastic granular materials exhibit certain phenomena that are not observed in fully elastic systems. One example is known as inelastic collapse,[1] which is when a group of particles undergo an infinite number of collisions in a finite time. Inelastic collapse has been observed both in granular flow simulations and in granular flow theory.

There has been a significant amount of theoretical investigation of inelastic collapse in systems of only three particles. For example, Zhou and Kadanoff determined conditions when inelastic collapse would occur between three particles where one particle is bouncing between the other two.[2] Also, Schorghofer and Zhou extended these results to cases where the three particles are rotating.[3]

Most simulations attempting to study inelastic collapse have been conducted on cooling systems where energy is lost through particle-particle collisions. Simulations studying inelastic collapse were first done by McNamara and Young using one-dimensional cooling systems.[4] McNamara and Young then also found inelastic collapse in two-dimensional cooling systems.[5] To detect inelastic collapse in these cooling systems, McNamara and Young suggested a detection criterion for dynamic hard sphere simulations.[6] After a binary collision, if the pair of particles in the next collision are then separated by a distance, scaled by the particle diameter, that is numerically less than machine precision, then inelastic collapse is assumed to have occurred. This definition is commonly used as the criteria for detection of inelastic collapse in hard sphere simulations.

In dynamic simulation investigations of inelastic collapse, simulations are run for a predetermined number of collisions per particle. If inelastic collapse is detected, the simulation typically terminates. McNamara and Young, however, allowed their cooling simulation to continue after inelastic collapse was detected as shown in Figure 2 of their paper.[6] In this figure, the separation distance decreases to the limit of machine precision, indicating inelastic collapse. The subsequent collisions are then a series of inaccurately resolved collisions, with separation distance at the limit of machine precision. Afterwards, the particles disperse, and the separation distance actually increases.

Simulations, where there is energy input, used to counteract dissipation due to particle-particle collisions, are known as driven systems. Most simulation studies of inelastic collapse have been conducted in driven systems where energy has been added through random particle accelerations. For example, Cornell, Swift, and Bray showed that inelastic collapse can occur in one-dimensional versions of these types of driven systems.[7] Very little has been done in shear flow simulations. One exception being that Alam and Hrenya observed inelastic collapse in two-dimensional systems where energy is added using Lees-Edwards boundary conditions.[1] Furthermore, using the criterion of McNamara and Young, they charted how likely inelastic collapse is to occur given the 2D simulation conditions.

While the separation distance criterion is often used to detect inelastic collapse in a hard sphere simulation, the significance of this detection is unclear, as indicated by Alam and Hrenya.[1] It is also not clear, as suggested by Kadanoff, if the inelastic collapse found in a hard sphere simulation is related to natural collapse phenomena such as the decaying bounces of a ball.[8]

In this work, we examine inelastic collapse in a driven system. We investigate the validity of the separation distance as a criterion for inelastic collapse in a driven system. We do so by allowing our simulations to proceed in time beyond the point where inelastic collapse is detected based on this separation distance criterion. Our results indicate that reliance on just the separation distance is not sufficient to determine if inelastic collapse has been found.

II. Simulation Description

The driven system of interest is a three-dimensional cubic shear flow system. The system is fully periodic, with Lees-Edwards boundaries used to maintain the shear.[1] The hard sphere algorithm, which assumes instantaneous binary collisions, is used to simulate the particle movement.[9] A one parameter coefficient of restitution model of Walton, is used to handle the collisions between particles.[10] Particles are otherwise assumed to be smooth, inelastic spheres of constant density.

Monodisperse, hard sphere simulations are conducted for two sets of conditions of varying coefficient of restitution, e. The conditions are: (1) $e = 0.6$, $\phi = 0.3$, (2) $e = 0.2$, $\phi = 0.3$, where ϕ is the solids volume fraction. The number of particles, N, in each simulation is 4000. Also, the occurrence of inelastic collapse, based on the criterion of McNamara and Young, will be monitored by the simulation.[6] If the separation distance, scaled by the particle diameter, is less than or equal to 10^{-16}, then the criterion for inelastic collapse will have been met. In our results, discussed below, any dimensionless separation distance that is 10^{-17} is considered to be associated with an inelastically collapsed system. The actual value of the separation distance may be less than or equal to 10^{-16}, negative, or zero, but it was set to 10^{-17} to show the same value for any separation distance that is numerically imprecise. The reported dimensionless simulation time is the actual simulation time multiplied by the shear rate.

III. Results and Discussion

For the first set of conditions $e = 0.6$, $\phi = 0.3$, Figure 1 shows that inelastic collapse is detected before the system reaches steady state and after less than ten collisions per particle. As expected, the separation distance in Figure 1 decreases below the limit of numerical precision reaching a state of inelastic collapse. Also, unlike most studies of inelastic collapse, the simulation, in the present work, is continued after inelastic collapse is observed. Similar to what was shown by McNamara and Young,[6] a series of inaccurately resolved collisions occur until the particles finally separate, and the separation distance increases. The collisions are inaccurately resolved because the pre-collision separation distance between the particles is numerically too small. Therefore the time until the collision cannot be accurately calculated. This will cause the resulting outgoing velocities to be inaccurately calculated, which is why the collisions are referred to as inaccurately resolved.

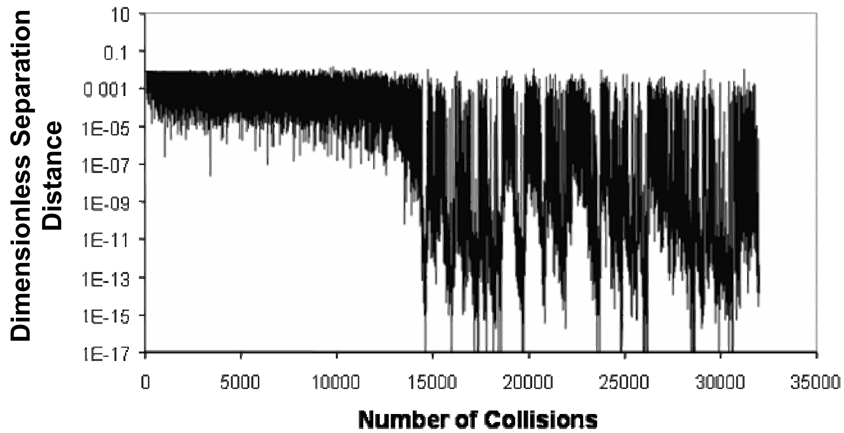

Figure 1: Dimensionless Separation Distance vs. Number of Collisions (N = 4000, e = 0.6, ϕ = 0.3)

McNamara and Young stopped their simulation at this point, in part because their investigation was for a cooling system.[6] Our driven simulations are allowed to continue further in time. After a few more collisions, the separation distance again drops below the threshold of numerical precision, resulting in more inaccurately resolved collisions. Again, the separation distance eventually increases. There is then a time period where the separation distance repeatedly bounces between being numerically precise and numerically imprecise. As shown by Figure 2, this period of repeatedly dropping below the limit of numerical precision only continues temporarily. Eventually, the separation distance increases and then does not again decrease down to the limit of numerical precision. Figure 3a shows the overall evolution of the

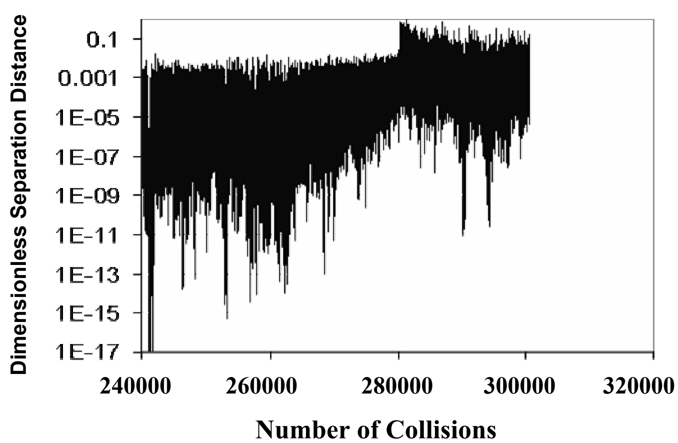

Figure 2: Dimensionless Separation Distance vs. Number of Collisions (N = 4000, e = 0.6, ϕ = 0.3)

simulation time with the number of collisions and indicates that the simulation time increases at a constant slope through most of the simulation. Based on the number of collisions, the region shown in Figures 1 and 2 is highlighted in Figure 3b. Initially, the simulation time grows very slowly with the number of collisions. Thus the system in Figure 1 is not at steady state because the initial slope in Figure 3b is much smaller than the eventual slope after a larger number of collisions. Once the average amount of time per collision attains the constant slope as shown in Figure 3a, the simulation is considered to be at steady state. Therefore these results show a case where inelastic collapse is initially "detected" using the separation distance criterion. However, when the simulation is then allowed to proceed beyond that point in time, the system, through a series of inaccurately resolved collisions, eventually reaches steady state.

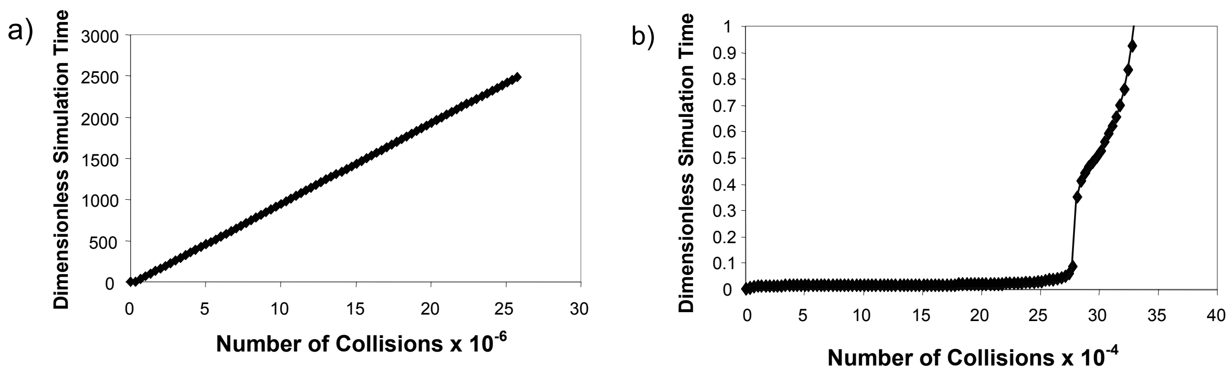

Figure 3: Dimensionless Simulation Times vs. Number of Collisions (N = 4000, e = 0.6, ϕ = 0.3) (a) Entire Simulation (b) Initial Part of Simulation

For the low coefficient of restitution case, e = 0.2, ϕ = 0.3, inelastic collapse is also observed, using the current detection method, as shown in Figure 4. As with the previous case, the simulation is allowed to continue in time after inelastic collapse is detected. Unlike the previous case, however, there is not an eventual increase in time per collision. Instead, as shown in Figure 5, the system moves forward an amount of time that is less than machine precision, and is essentially zero. Once the transition occurs, all of the repeating collisions are

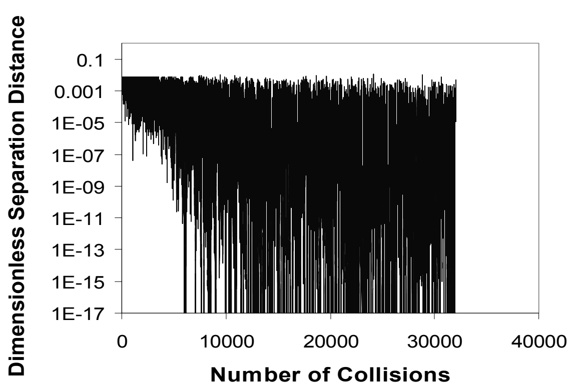

Figure 4: Dimensionless Separation Distance vs. Number of Collisions (N = 4000, e = 0.2, ϕ = 0.3)

separated by a distance less than machine precision. Eventually there is only once repeating collision. Figure 6 shows the change in separation distance behavior once the system stops moving forward in time. We consider this to be a "truly" collapsed state.

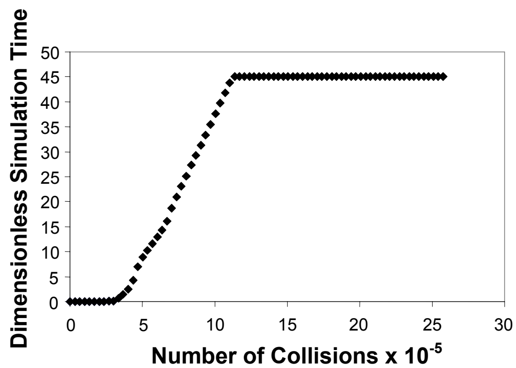

Figure 5: Dimensionless Simulation Time vs. Number of Collisions (N = 4000, e = 0.2, ϕ = 0.3)

Given the above results, it is necessary to distinguish between the two methods of inelastic collapse detection, especially in a driven system. In the e = 0.6 case, using the traditional detection method, based on detection of very small dimensionless separation distances, inelastic collapse appears very quickly during the course of the simulation. However, since the simulation is allowed to continue in time, it eventually exits this collapsed state as a result of a significant number of inaccurately resolved collisions. It is likely that there is enough energy being added to the system such that the "very close" particles eventually come apart. Furthermore, it is possible (although highly unlikely), that inelastic collapse, using this traditional detection method, could be detected for elastic particles. This is because this detection criterion only examines the separation distance between two particles that are about to collide. Clearly in the case of a three particle collision, where their centers form an equilateral triangle, inelastic collapse would be detected even though the three particles would eventually move apart assuming that the simulation was allowed to continue.

The present criterion does, however, ensure that no collision will be resolved inaccurately. Yet, as discussed previously by McNamara and Young,[6] it is unclear as to what effect a series of inaccurately resolved collisions has on the overall simulation results (for a cooling system). It is possible that the effect could be negligible because these inaccurately resolved collisions typically do not dissipate a lot of energy. For a driven system, issues of energy dissipation are not as significant because energy is being added to the system. Furthermore, for the e = 0.6 case discussed above, inelastic collapse is detected only before the system reached steady state. Therefore the effects of inaccurately resolved collisions do not directly influence the overall steady state results of the simulation for this case.

Clearly our results show that inelastic collapse detected by the traditional detection method does not guarantee the identification of a "truly" collapsed state. We propose a new detection method that examines both the separation distance and the simulation time. If there is an observed separation distance that is less than machine precision, unlike the previous method, the simulation should be allowed to continue. A "truly" collapsed state is then detected with this improved method if the particle pairs repeat for a significant amount of collisions, there is no change in separation distance, and the simulation time does not increase (at the level of machine precision) with increasing number of collisions. As with the traditional method, the probability of inelastic collapse eventually occurring will depend on e, ϕ, and N.

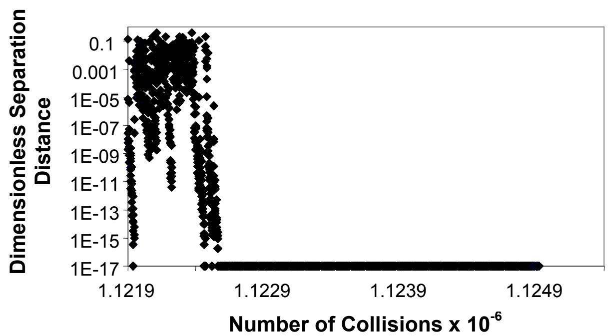

Figure 6: Dimensionless Separation Distance vs. Number of Collisions (N = 4000, e = 0.2, ϕ = 0.3)

IV. Conclusions

In this paper, we put forth an improved method for detection of inelastic collapse based on simulation time and tracking the particles involved in each collision as well as particle separation distance. The traditional detection method based on particle separation distance is unable to distinguish between particle systems which are in a truly collapsed state versus systems which may only be "temporarily" in a collapsed state. The more comprehensive detection method put forth here involves continuing to integrate forward in time systems which initially show inelastic collapse based on separation distance. This continued integration shows that systems, which for a period in time exhibit a series of inaccurately resolved collisions, may move to a new timeline, or effectively a new set of initial conditions, for which inelastic collapse based on separation distance no longer occurs. With this new detection method, the inability of a system to move to a new timeline indicates a truly collapsed state.

Acknowledgements

This work was supported in part by the Graduate Assistance in Areas of National Need Fellowship, by the NSF Industry/University Cooperative Center for Pharmaceutical Processing Research, and by Procter & Gamble.

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