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Simulation of Gravity Flow and Packing of Spheres*

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ABSTRACT

In the past decade discrete particle simulations of macroscopic particles have advanced from being a curiosity that 'might provide some insight into the mechanisms occurring in the deformation and flow of granular materials,' to become a viable predictive technique that is now *leading* in predicting new phenomena and explaining the mechanisms behind the new observations. A number of calculational studies have examined the rheology of rapidly shearing flows of inelastic, frictional, particles (Walton and Braun, 1986a,b; Walton *et al.*, 1991; Walton, 1990; Walton, 1992a). These simulations were compared with annular shear cell results and with kinetic theory predictions. In most cases they reproduced experiments and/or theoretical predictions; however, in some areas, significant new findings resulted from the simulations. At low solids fractions the simulations produced large first-normal stress differences. Once the anisotropic velocity distribution was recognized in the simulations, as a key mechanism causing this effect, it was incorporated into newly developing kinetic theories and good correlations were, again, obtained between theory and simulations. Subsequently, clustering was observed in simulations of low density shearing flows (Hopkins and Louge, 1991; Walton et al., 1991). Currently, new statistical mechanical theories are being developed, incorporating mode coupling to account for inelastic effects, and they are confirming that such clustering is to be 'expected' for inelastic particles (Oppenheim, 1992).

The work reported here is concerned with the movement of cohesionless, inelastic, frictional spheres under the influence of a constant body force (e.g., gravity). Both static and steady-state dynamic situations have been simulated. The models employed are described in detail elsewhere (Walton, 1992a and 1992b). The trajectory-following technique utilizes nearly-rigid particles interacting via contact forces and gravity. Energy losses in the simulations occur only via displacement-dependent hysteretic loading/unloading paths and sliding friction. One series of simulations examined the flow of small spheres through a close packed bed of larger spheres. Figure 1 shows the initial configuration of one of these simulations with four large spheres (two blue and two red) in a calculational cell with periodic boundaries on all six sides. Two hundred fifty (250) smaller spheres (with diameters 1/10 of the large spheres' diameter) are randomly placed 'floating' in the interstitial space between the large spheres. The small spheres are released and they establish a nearly steady flow pattern. Figure 2 is a 'snapshot' of the configuration during this steady flow. The large spheres occupy 74.04% of the volume in the calculational cell. The mean solids fraction of the small spheres in the remaining interstitial void space is approximately $\nu = 0.178$ making the total solids faction 0.787. The interaction force models

used in this simulation produce an effective coefficient of restitution of 0.85, and a coefficient of sliding friction of 0.20 – values similar to measured properties for glass beads or metal spheres. Figures 3 and 4 show snapshots from a similar calculation; only in this calculation, the number of small spheres has been increased to 322. This makes the solids fraction of small spheres in the interstitial void space, $\nu = 0.230$, and the total solids fraction approximately 0.800. In this case the flux of small spheres is high enough for frictional arches or bridges to form just above the narrowest points of the channels connecting the interstitial voids between the large spheres. When this calculation was repeated using lower coefficients of friction (*i.e.*, $\mu = 0.0$, or 0.1, or 0.15), no permanent arches formed, and nearly steady flows developed. The average flux of small particles in these simulated flows decreased as the coefficient of friction increased.

Another series of simulations examined the effects of walls on the packing of spheres between two parallel, vertical planar surfaces. These packing simulations did not use any artificial prescription to determine when to stop moving one particle and to start the next (as is quite often done in computer 'simulations' of packing). Instead, the full dynamics of Newton's equations of motion, including inertia, operated during the *filling* of a simulated container. In addition, the filling is done in a gravity field, similar to a real experimental configuration. The only somewhat artificial, or arbitrary, aspect of the simulations is the choice of starting conditions. For this series of simulations a calculational cell was selected with two vertical planar walls (perpendicular to the x-axis). The other two vertical planar sides of the calculational cell were made *periodic* to simulate a long, narrow channel using only a limited number of particles. The height of the calculational cell was chosen to be approximately 25 particle diameters tall. The number of particles was set to correspond to approximately 15 particles per unit area of the cell (floor), where a 'unit area' is equal to a square of one particle diameter on a side. The particles were initially randomly placed throughout the volume of the cell and released, to fall under the influence of gravity. Two types of particles were modeled. Particles in the first set were frictionless and nearly elastic (with a coefficient of restitution of 0.97). Those in the second set were less elastic (restitution = 0.85) and frictional (with a coefficient of friction of 0.4). The frictional particles were additionally dropped with a slightly viscous drag force acting between the particles and an assumed stationary 'massless fluid' filling the cell. These two sets of simulations, then, were expected to span the range of behavior that might be observed for particles slowly added to a bed and for particles that were vibrated (effectively lowering the contact friction) after being deposited. Gap widths ranging from one to ten diameters were examined.

A very significant structure was observed in the distribution of particles in the vicinity of each bounding wall. For the frictionless particles the overall packing was higher than for frictional particles, but the wall effect also extended much further into the assembly, affecting packing as much as five diameters from the planar walls. The less elastic, frictional particles tended to form bridges or arches and, thus, produced assemblies with significantly lower average solids packings. For both sets of particles a definite periodic pattern of average density changes occurred as the width of the cell was varied; however, this was much more pronounced with the frictionless particles. Whenever there was enough room between the walls to just accommodate another hexagonal layer nestled into an existing hexagonally packed layer the observed packing dramatically increased. For subsequent small increments in gap width (significantly less than a particle diameter) the average solids packing would decrease, until enough space existed for the next layer to fit between the walls. This effect was much more pronounced with the frictionless particles, and was also observed for many more layer thicknesses with the frictionless particles. It is expected that physical tests of packing between two close walls would result in solids fractions between the values obtained with the two 'extreme' sets of particles used in these simulation. Figure 5 summarizes the packings obtained in these simulations.

We also simulated flows on inclined surfaces. Initial scoping calculations examined flows on an incline tilted 17 degrees from the horizontal. Assemblies of inelastic spheres with interparticle friction coefficients less than the tangent of the inclination angle were found to accelerate unboundedly. Those with friction coefficients somewhat greater than the tangent of the inclination angle developed steady velocity and density profiles for a variety of flow depths but resulted in arrested flow for coefficients of friction greatly exceeding the inclination angle tangent (e.g. by more than a factor of 2). Conversely, a significant range of inclination angles is expected to exist that will result in steady flows for a given set of assembly properties.

The mean velocities of the simulated flows increased as the number of particles per unit area increased. Shallow flows (i.e. those with fewer than 5 particles per unit diameter squared surface area) usually exhibited monotonically increasing velocity profiles. Deeper flows often exhibited a non-shearing region riding over the top of a relatively thin shearing layer. The shallowest flows (fewer than 2.5 per unit area) exhibited monotonically decreasing density profiles with height above the incline. Intermediate depth flows exhibited a maximum solids fraction somewhere inside the flow region, while the deepest flows exhibited an essentially uniform (random close packed) non-shearing region above a lower density shearing region.

Gravity-driven flows of inelastic, frictionless spheres down inclined planar surfaces, to which a monolayer of identical inelastic spheres are fixed, were also simulated. In contrast to the frictional-particle simulations which produced a variety of steady flow conditions, initial simulations with frictionless but relatively inelastic spheres (*i.e.*, $e = 0.7$) have generally resulted in accelerating or decelerating conditions. The apparent 'dynamic friction coefficient' for the simulated flowing layer (determined by observing the rate of change of the mean flow velocity down the incline) decreased almost monotonically as the mean flow velocity increased. This appears to be a consequence of the fact that particles traveling with a significant velocity parallel to the bumpy layer are precluded from 'penetrating' sufficiently into the 'valleys' to receive significant reversing tangential impulses when they encounter the bottom layer. In effect then, the bumpy boundary appears somewhat *smoother* to particles in a flow with a high 'slip velocity' over the bumpy bottom layer than it does for a flow with a relatively low 'slip velocity'. As a consequence, for inclination angles between about 14^o and 17^o it is possible to obtain a nearly steady flow velocity (albeit highly unstable) if and only if the initial conditions have a mean flow velocity that produces a 'dynamic friction coefficient' essentially equal to the tangent of the inclination angle. If the mean velocity increases, even momentarily, above this critical value then the effective resistance to the flow decreases and the flow accelerates unboundedly. Conversely, if the mean velocity decreases slightly, then the mean resistance increases and the flowing layer decelerates and comes to rest on the bumpy incline. Thus, over a narrow range of inclination angles (spanning about 2 degrees, the specific values of which depend on the configuration of the 'bumpy' layer) two non-steady solutions are observed, one accelerates unboundedly, the other decelerates and comes to rest.

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References:

Hopkins, M.A. and M.Y. Louge (1991), *Phy. Fluids A*, 3(1), p47-57.

Oppenheim, I. (1992) in *proceedings: Joint DOE/NSF Workshop on Flow of Particulates and Fluids*, Gaithersburg, MD (to appear).

Walton, O.R., and R.L. Braun (1986a) *J. Rheology*, **30** (5), p949-980.

Walton, O.R., and R.L. Braun (1986b) *Acta Mechanica* **63**, p73-86.

Walton, O.R., H. Kim, and A.D. Rosato (1991) *Mechanics of Computing in 1990's and Beyond*, ASCE pub., Vol. 2, p.1249.

Walton, O.R. (1990) in *Science on Form*, S. Ishizak, ed., KTK Sci. Pub, Tokyo, p125-189.

Walton, O.R. (1992a) in *Two Phase Particulate Flow*, M. Roco, ed., Butterworth-Heinemann, Boston, Chapter 25.

Walton, O.R. (1992b) "Numerical Simulation of Inclined Chute Flows of Monodisperse Inelastic, Frictional Spheres," *Mech. of Mat*, (to appear).

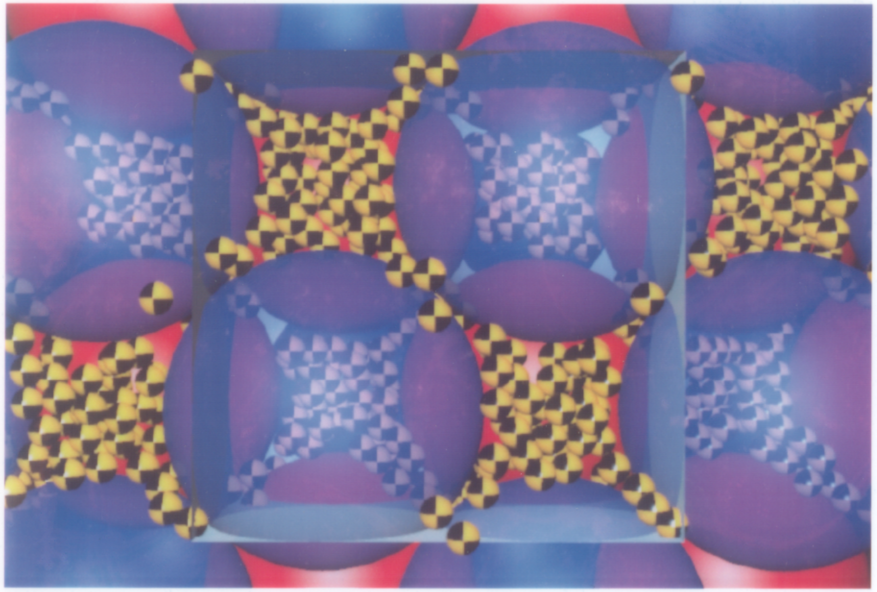

Figure 1. Four large spheres, HCP packing. 250 small (1/10 diameter) spheres, random initial positions.

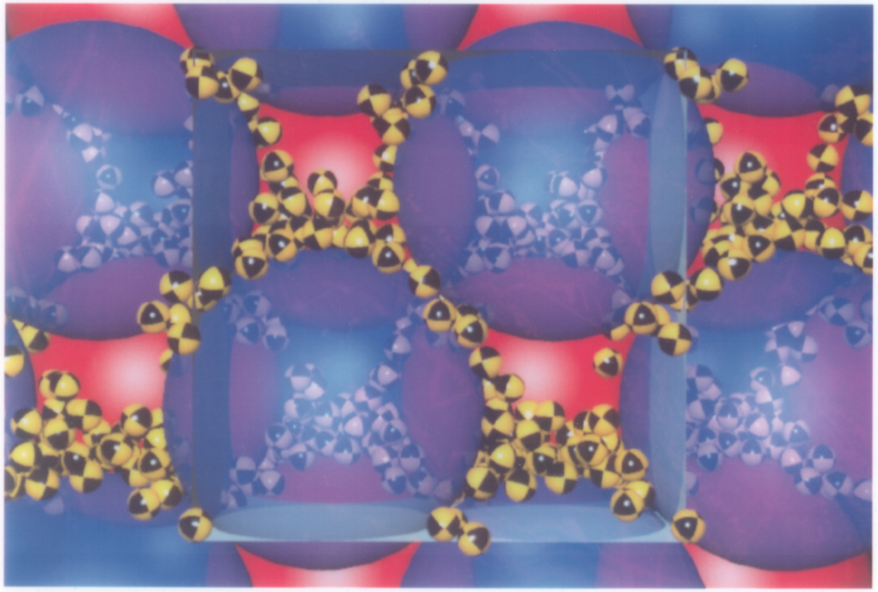

Figure 2. 250 small spheres, steady gravity flow, mean solids fraction=0.7867.

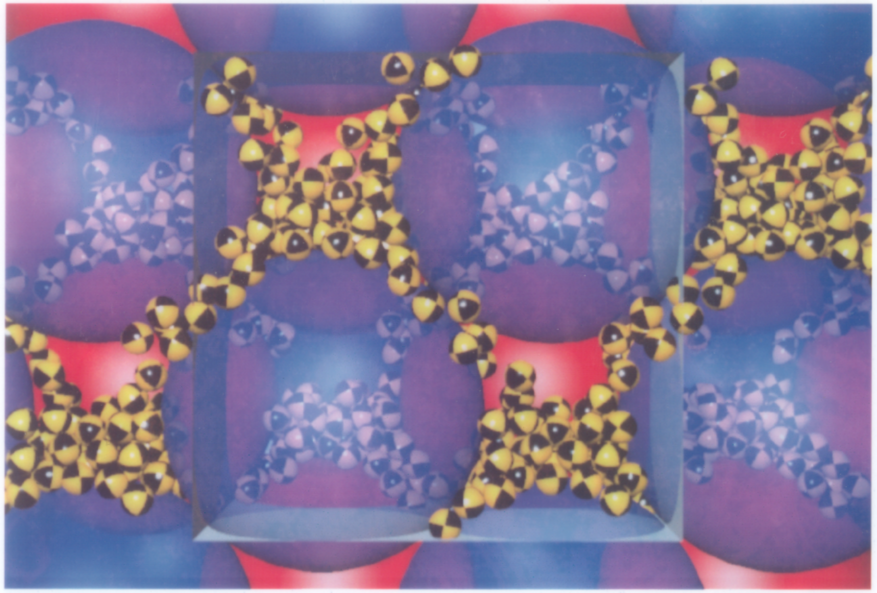

Figure 3. 322 small spheres, nearly steady flow, ν=0.800.

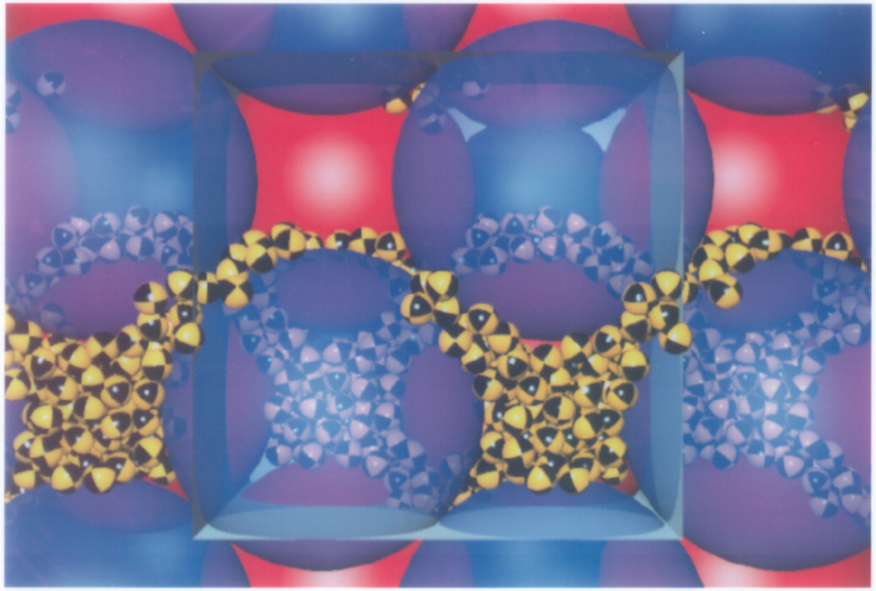

Figure 4. 322 small spheres, flow stopped due to bridging, ν=0.800.

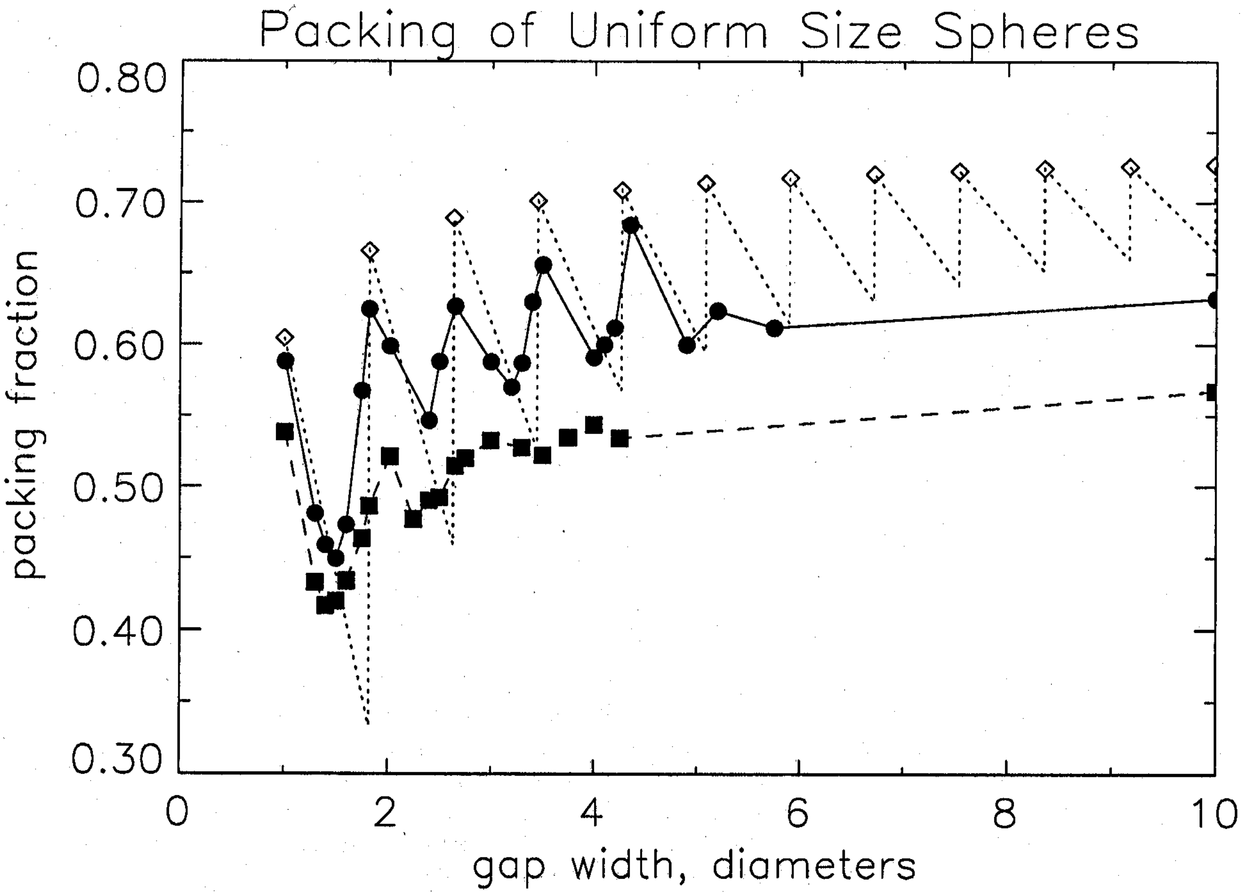

Figure 5. Average packing fraction of uniform sized spheres dropped between two walls. Open diamonds – theoretical packing if only hexagonal layers are allowed. Filled circles – frictionless spheres with coefficient of restitution of 0.97. Filled squares – frictional spheres with coefficient of restitution of 0.85 and coefficient of friction of 0.4.

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