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MD Simulations of a granular medium

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Abstract
The purpose of this article is twofold: to present the physics of granular media, to emphasise modern principles and research topics, and to discuss the models most applicable to the simulation of these phenomena by machine. There is a thorough discussion of soft-particle molecular dynamics, event-driven molecular dynamics, Moreau and Jean's touch dynamics, and the bottom-to-top-restructuring model.

Keywords: Tangential velocity, granular flow, binary collision

Introduction

While fluids can be accurately modelled using the Navier-Stokes equations on the mesoscopic or macroscopic scale, studying microscopic scale phenomena such as diffusion and phase transitions is still fascinating. Many natural events may be attributed to granular flows involving diffusion mechanisms, such as avalanches, landslides, and soil fluidisation. Broadly speaking the individual molecules of a fluid build-up a granular medium through interparticle ‘contacts’ [1, 2, 3]. Mixing is an important process in these processes that happens due to the diffusive motion of the particles. The kinetic theory of swift granular flows, laboratory studies and numerical simulations studied this diffusion [4, 5]. Lack of diffusion is recorded for solid volume fractions above 0.56 in Campbell's analysis of findings prior to 1990 regarding diffusion in molecular dynamics simulations of dense granular media. This implies that high densities can suppress the diffusive motion of particles. Campbell's conclusion was based on a series of unbounded granular shear flow computer simulations. However in later computer simulations on small fast granular flows, this absence of diffusion was not found [6]. It was therefore necessary to explore this problem further and we examined it by simulating a flow of inelastic, rugged, hard spheres from Couette. Under periodic boundary conditions in the y and x directions, our simulations were performed in a cell, with a velocity gradient applied in the z direction. Two large walls were fixed to travel in opposite directions, similar to the x direction, with the same properties as the inner particles.

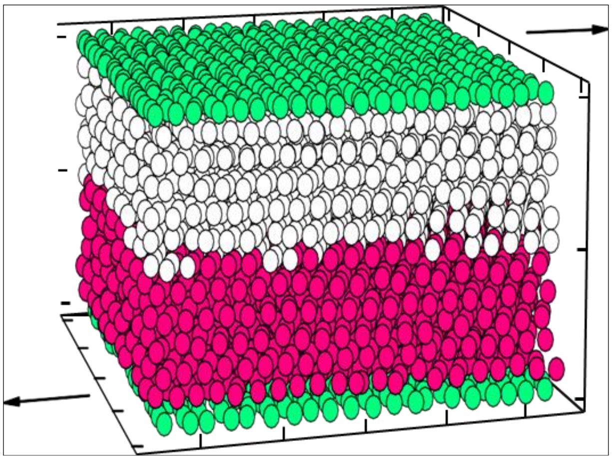

Fig 1: A schematic picture of the initial configuration of dark and light particles in the computational box which includes the wall particles

The number of particles in the interior and walls ranged from 4296 to 4824, respectively, and from 400 to 625. This meant that they ranged from 0.5 to 0.6 for concentration. With an initial collection of random interacting spheres using the process, all the simulations started. Then once the overlaps were gone, the actual spheres were arbitrarily moved [7].

Results and Discussion

Stress fluctuations, diffusion coefficient tensors, velocity curves, density profiles, functions of radial distribution, and correlation functions were calculated from the simulations.

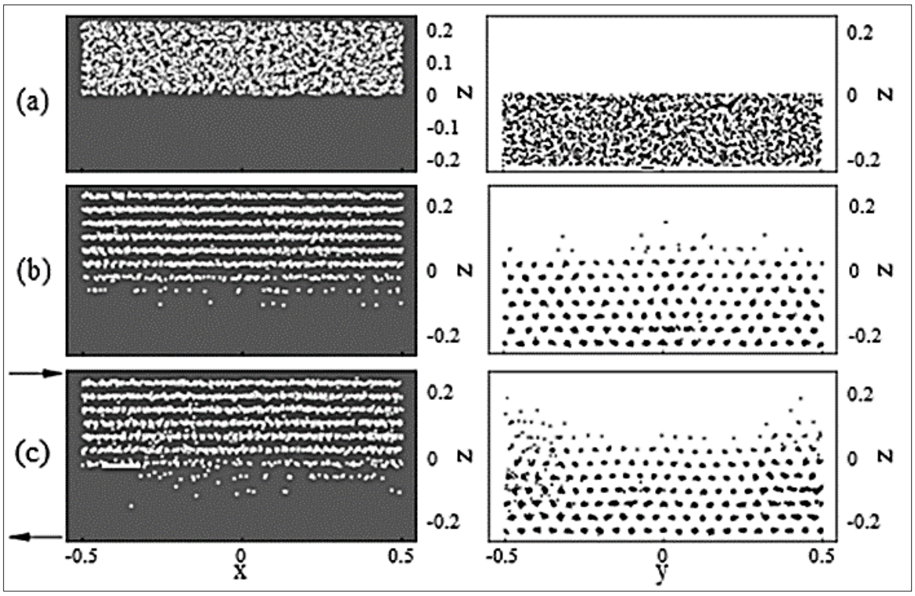

Fig 2: Snapshots of a system with solid volume fraction *f* = 0.565 and shear rate *g* = 4 *s*-1

On the lack of diffusion, Campbell reported. An ordered initial structure in their simulations could have caused the absence of self-diffusion. From a near hexagonal pattern in the yz plane, the ordered layers in the xz plane (the structure is very similar to icosahedral) [6].

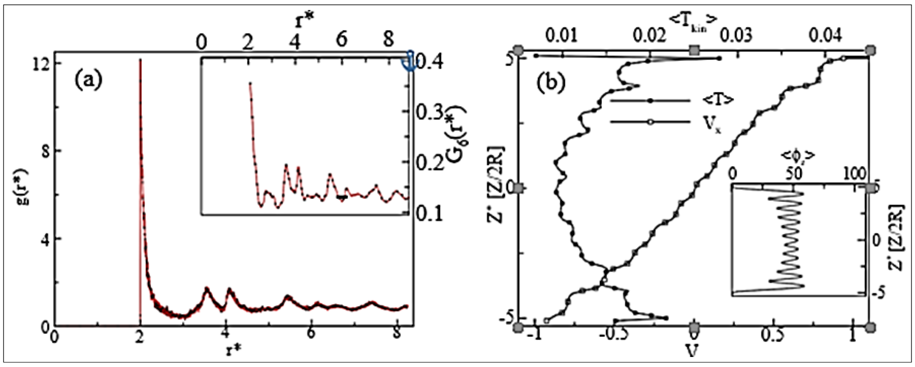

Fig 3: Radial distribution function in the equilibrium situation

It is seen in the inset of Figure 3, which also shows that the system is similar to an icosahedral-oriented liquid with an intermediate degree of symmetry between a crystal and a liquid. In conclusion, the system of inelastic, raw, hard spheres reveals the symmetry of imperfect icosahedral or hexagonal liquid for solid volume fractions at a high average shear rate. We display the velocity and density profiles and the local granular kinetic temperature in Figure 3b. From the density profile, a layered structure in the yz plane is visible, and an S-shaped velocity profile can also be detected and a high granular temperature close to the walls. In the opposite case, by increasing the coefficient of restitution to e = 0.93, and decreasing the surface friction coefficient to *m* = 0.123 the result was closer to those in the annular shear cell tests of [8].

With the solid volume fraction, the stress variations on the walls rose as the latter was lifted from 0.56 to 0.58 (c.f. Figure 3.a). Meanwhile the self-diffusion coefficient (measured for dimensionless time intervals from the slope of the mean square displacement curve *t* * > 1) decayed further, reaching a value similar to that of recent experimental observations. The increased stress fluctuations may be the result of higher dissipation at 0.58 leading to the decrease in the transverse self-diffusion coefficients. At ϕ 0.582, diffusion decays rapidly with time (at t* = 245) to D* ≈ 10-5 (the diamonds in Figure 3.b). This also is an evidence of a phase transition to an ordered state or to a structural arrest. In an ordered system fluctuations induced changes in the geometry of the cage formed by the nearest neighbours around a particle become infrequent. This could result in a dramatic decay of the long-time transverse self-diffusion coefficient [9, 10].

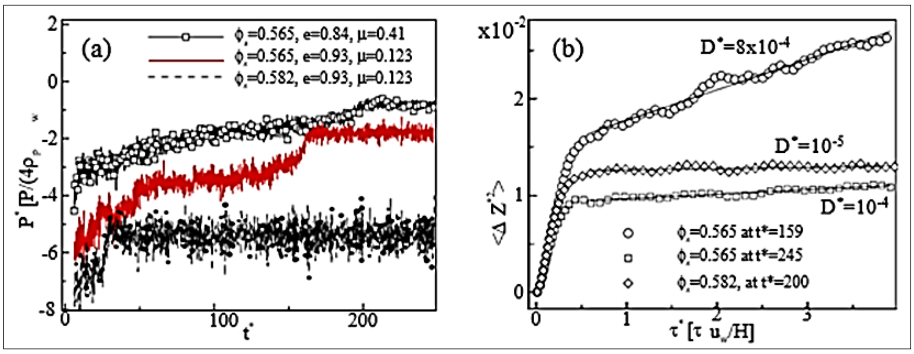

Fig 4: Dimensionless normal stress, exerted by the particles on the bottom wall as a function of dimensionless time *t* *, for three indicated sets of parameters

Also shown in Figure 4b are the self-diffusion coefficients for the cases ϕ = 0.565, t* = 159, 245. The coefficients decay from ~ 10–3 up to 10–4 when t* increases from 159 to 245. This is consistent with the result presented in Figure 4.

Shearing of particles with rough surfaces tends to produce lower normal stress than shearing of smooth particles in a related way. This can be translated as tending to have more rotational energy for rough particles than for smooth particles. In comparison, particles lack transverse diffusional motions of rough surfaces. This finding confirms the findings of the Menon and Durian in that collisions rather than sliding interactions control the dynamics of grains in a thick granular flow [11]. A comparison between diffusion coefficients in granular media for various volume fractions showed that the velocity autocorrelation function also decays exponentially for dilute systems, as expected by kinetic theory. The findings for a diluted and dense device. The velocity autocorrelation decays quicker with the higher volume fraction, ~ 0.51, and there is a lower diffusion coefficient correspondingly [12]. Our findings also indicate that the self-diffusion coefficient was much higher in the stream direction than for both smooth and rough particles in the transverse directions, in line with Hsiau and Shieh's experimental results [13].

Conclusion

In conclusion, our numerical simulations of a sheared, dense, monosized granular substance show that there is a long-term phase change for rugged particle systems, inducing a sharp decrease in the particle's dimensionless, long-term transverse self-diffusion coefficient. However, also more than 0.56, the method is diffusive at solid volume fractions. It was observed that the composition of the ordered state is similar to that of a plain hexagonal lattice rather than an icosahedral liquid. In the smooth particle method, a related behaviour may be observed, such that the coefficient of self-diffusion decreased by increasing concentration. In this case, the coefficient of self-diffusion in the direction of the stream was much higher than in the transverse direction, and much lower than for rough particles.

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