



Simulations of granular materials on different scales

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Abstract

Granular materials have very special properties as well in the solid state (packing) as in the fluidized state (e.g., under vibrations). To describe and predict their behaviour, computer simulation methods have been developed on different scales. Collision models take into account individual particle contacts and although once over 10^9 particles have been simulated for several microseconds in real time, these methods typically cannot treat more than 10^4 particles. On intermediate scales stochastic models and lattice models have been introduced in which details of the collisions are lost but particle numbers are high. © 2000 Elsevier Science B.V. All rights reserved.

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1. Introduction

Granular material can exhibit astonishing phenomena [1,2]. Examples are the so-called “Brazil nut” segregation, heap formation under vibration, density waves emitted from outlets and $1/f$ noise in the power spectra of local forces. All these effects originate in the ability of granular materials to form a hybrid state between a fluid and a solid: When the density exceeds a certain value, the critical dilatancy [3,4], it is resistant to shear, like solids, while below this density it will “fluidify”. This fluidified state can be rather complex, specially in the presence of density fluctuations and density gradients.

In order to formalize and quantify the complicated rheology of granular media various attempts have been made. Continuum equations of motion, a kinetic theory [5], and thermodynamic formulations [6–8] have

been proposed. But many of the above mentioned effects, such as size segregation or density fluctuations, have so far eluded a satisfactory explanation. This is because it is very difficult to incorporate into these theories static friction, local rotations and other relevant microscopic mechanisms.

To gain a better understanding of the rheological effects of granular media it is therefore very useful to do computer simulations [9,10]. For over a decade discrete methods have been used where instead of a continuum one treats the granular material as an assemblage of particles interacting through their contacts. This technique was introduced by Cundall [11] to study the motion of rock masses. Since then it has been applied to statistical micromechanics [12, 13], constitutive behaviour of granular soils [14], creep of soils [15], analysis of rock-support interaction [16] and other applications of soil mechanics [17]. These techniques have also been applied to model size segregation [18], outflow from a hopper [19,20], shear flow [21] and flow down an inclined chute [22].

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In the following we will discuss these techniques. In particular we will present Molecular Dynamics (MD) [23,24] simulations of inelastic particles with an additional shear friction.

2. Molecular Dynamics technique

As opposed to usual molecular gases the elementary units of granular materials are mesoscopic grains each consisting of many atoms (10^{15} – 10^{25}). When these objects interact (collide) the attractive potentials of the individual atoms are unimportant and completely different mechanisms must be considered. It is important that on a microscopic scale the surface of the grains is rough. Solid friction is the immediate consequence: When two touching grains are at rest with respect to each other a finite force F_s is needed to trigger relative motion (*static friction*), while moving against each other a finite force F_d is needed to maintain the motion (*dynamic friction*). $F_d < F_s$ and both only depend on the normal force and neither on the velocity nor on the area of contact (*Coulomb law*). No doubt, this picture is idealized and an entire discipline, called tribology, has evolved to study solid friction in depth [25]. For our purpose it is, however, more convenient to concentrate only on the basic mechanisms because we are interested in explaining the generic effects of granular rheology without entering into material-dependent details. Friction has a crucial consequence on the level of the grains, namely that the system does *not* conserve energy as opposed to what happens on the molecular level. Another source of dissipation can be plastic deformation of grains due to the normal force acting at collisions. Again it seems most important that dissipation does occur and the complications arising from the non-linearities of plasticity seems less relevant. We will therefore in the following assume very simple dissipation laws. In fact more complicated laws have been used increasing the number of parameters without giving qualitatively different answers.

Let us consider a system of N spherical particles of equal density and with diameters d chosen randomly from a homogeneous distribution of width w around d_0 . When two particles i and j overlap (i.e. when their distance is smaller than the sum of their radii) three forces act on particle i :

- (1) An elastic restoration force

$$\vec{f}_{\text{el}}^{(i)} = k_n m_i \left(\frac{1}{2} (d_i + d_j) - |\vec{r}_{ij}| \right)^\beta \frac{\vec{r}_{ij}}{|\vec{r}_{ij}|}, \quad (1a)$$

where k_n is the elastic modulus (normalized by the mass), m_i the mass of particle i and \vec{r}_{ij} points from particle i to j . For Hooke's law $\beta = 1$ but in the case of spheres in three dimensions one has to choose $\beta = 3/2$ [26] and for conical contacts one should take $\beta = 2$.

- (2) A dissipation due to the inelasticity of the collision

$$\begin{aligned} \vec{f}_{\text{diss}}^{(i)} &= -\gamma_n m_i (\vec{v}_{ij} \cdot \vec{r}_{ij}) \frac{\vec{r}_{ij}}{|\vec{r}_{ij}|^2} \\ &= -\gamma m_i v_{ij}^n, \end{aligned} \quad (1b)$$

where γ_n is a phenomenological dissipation coefficient and $\vec{v}_{ij} = \vec{v}_i - \vec{v}_j$ the relative velocity.

- (3) A shear friction force which in its simplest form can be chosen as

$$\begin{aligned} \vec{f}_{\text{shear}}^{(i)} &= -\gamma_s m_i (\vec{v}_{ij} \cdot \vec{t}_{ij}) \frac{\vec{t}_{ij}}{|\vec{r}_{ij}|^2} \\ &= -\gamma_s m_i v_{ij}^t, \end{aligned} \quad (2a)$$

where γ_s is the shear friction coefficient and \vec{t}_{ij} is the vector \vec{r}_{ij} rotated by 90° . Eq. (2a) is a rather simplistic description of shear friction. In many applications (arching, heap formation) it is important to include real static friction [27] which can be done by a static friction force [12]: When two particles start to touch each other, one puts a “virtual” spring between the contact points of the two particles. If δs is the *total* shear displacement of this spring during the contact the restoring frictional force is $k_s \delta s$ (static friction). The maximum value of the restoring force is then according to Coulomb's criterion proportional to the normal force F_n and the proportionality constant is the friction coefficient μ . Cast into a formula this gives a friction force

$$\vec{f}_{\text{friction}}^{(i)} = -\text{sign}(\delta s) \min(k_s \delta s, \mu F_n), \quad (2b)$$

where δs is the shear displacement integrated over the entire collision time. When particles are no longer in contact with each other the

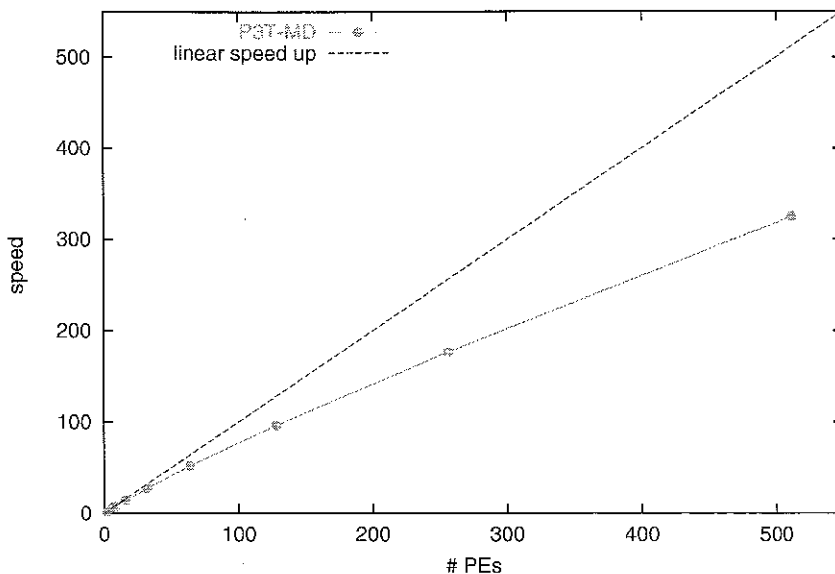


Fig. 1. Speed-up of the molecular dynamics program, i.e. the inverse execution time versus the number of processors used to parallelize the problems. The lower curve is measured and the upper curve shows the upper theoretical limit.

spring is removed. Main source of static friction is the geometrical roughness of the surfaces [28] and the same effects of particle stopping can be obtained also without Eq. (2b) by using particles of complicated shapes, like crosses or polygons [29,30]. It is not straightforward to implement the above technique when the particles are allowed to rotate, i.e. able to roll on each other.

When a particle collides with a wall the same forces act as if it would have encountered another particle of diameter d_0 at the collision point. One force that acts on all particles pulling them down is gravity, $g \approx -10 \text{ m/s}^2$. In most simulations presented here we use a fifth order predictor-corrector MD with 10^3 – 10^5 iteration steps per cycle depending on the largest velocities appearing in the application. This algorithm vectorizes on the Cray-YMP, running at about $10 \mu\text{sec}$ per particle-update for $N = 200$. The programs were also run on 8 or 16 processors of an Intel iPSC/860 or on an IBM RS/6000. For massive parallel systems with distributed memory, MPI (Message Passing Interface) offers a convenient way to implement parallel programs. On the Cray T3E-900 it takes about $50 \mu\text{s}$ per particle update on

a single CPU. The program shows good speed-up to 512 CPU's (Fig. 1). In a metacomputing testbed it was running on 1258 CPU's coupling two T3E's at NIC/ZAM Jülich with a T3E at HLRS, Stuttgart. In a transatlantic metacomputing effort the same program set a world record for the largest particle number with 1 399 440 000 particles [31].

3. Angle of repose and angle of marginal stability

As opposed to fluids the surface of granular media at rest is usually not flat but can show undulations (ripples, dunes) or form mountains (sand piles, heaps). This is due to the fact that up to a maximal angle, the so called angle of maximal stability θ_m , grains can arrange in a statically stable way. The angle of a heap of granular material can fluctuate between θ_m and a dynamic angle θ_r . Various experiments can be devised to obtain these angles.

Numerical studies have been made to investigate the angles θ_r and θ_m in two dimensions [28]. They start by putting N particles randomly in a box and wait sufficiently long until under the action of gravity they have all settled on top of each other and come to rest.

Next one side wall is removed. The particles violently fall out forming a big avalanche and after some time only a few remain inside the box. The pile that is left forms a certain angle which is what is called the angle of repose θ_r .

In principle the static friction coefficient μ defined in Eq. (2c) should determine the slope of the pile. Since the angle of repose can easily be determined experimentally it is of interest to find the relation between θ_r and μ . This relation is essentially linear for $\mu < 0.2$. Recently [32] in fact these calculations have been extended to larger values of μ and a curvature was observed which is close but not identical to the theoretical relation $\mu = \tan \theta_r$. For the range of parameters which interest in practice, however, the linear relation is a very good fit.

Molecular dynamic simulations for granular media have been performed for nearly all technologically relevant configurations: silos, pipe flow, vibrated beds, deformation of soils, segregation, rotating drums, heap formation and so on. Let us just cite two review articles of those applications [33,34].

4. Direct Simulation Monte Carlo (DSMC)

The most time consuming part of a MD simulation is the calculation of the forces between the particles. For hard spheres the so called hard sphere MD or event driven (ED) algorithm offers a possibility to avoid this calculation. In contrast to MD it is however not well suited for parallelization. A method that avoids calculating forces and is very well suited to run on parallel computers is DSMC. This method was first proposed by Bird [35] for the simulation of rarefied gas flows, recently it was also applied to dry granular media [36,37].

One of the basic assumptions of DSMC is that the movement of the particles can be decoupled from their interaction. The system is integrated in time steps τ . At each time step every particle is first moved, according to the equation of motion, without interaction with other particles. External forces, such as gravitation, are taken into account.

Next, one takes the collisions into account. In contrast to ED simulations, the exact times and places of these collisions are not calculated, but a stochastic algorithm is applied as described in the following:

The particles are sorted into spatial cells of linear size L and volume $V_c = L^d$, where d is the dimensionality of the system. Collisions occur only between the particles in the same cell, which ensures that only particles which are close to each other may collide. In every cell with more than one particle, we choose randomly

$$M_c = \frac{N_c(N_c - 1)\sigma v_{\max}\tau}{2V_c} \quad (1)$$

pairs of particles. Here, N_c is the number of particles in the cell, σ the scattering cross section (for spherical particles, $\sigma_{2D} = 4R$, $\sigma_{3D} = 4\pi R^2$) and v_{\max} is an upper limit for the relative velocity between the particles. In order to determine the correct number of collisions, one applies an acceptance-rejection method: For a pair of particles i and j the collision is performed if

$$\frac{|\vec{v}_i - \vec{v}_j|}{v_{\max}} < Z,$$

where Z is independent uniformly distributed in the interval $[0; 1]$. This method leads to a collision probability proportional to the relative velocity of the particles.

Since the collision takes place regardless of the particle positions in the cell, we have to choose an impact parameter b in order to calculate the post collision velocities. Molecular chaos is assumed here; b is drawn from a uniform distribution in the interval $[-2R, 2R]$ in 2D or in a circle with radius $2R$ in 3D.

Finally, dissipation can be introduced by changing the normal component of the post collision velocity to $\vec{u}^{(n)} = -e\vec{v}^{(n)}$, whereas the tangential component remains unchanged.

So far only ideal gas properties have been considered; the particles have a scattering cross section but no real volume. One consequence of the excluded volume is an increase in the number of collisions. Several approaches exist to take this into account. One possibility is to multiply the right hand side of Eq. (1) with the Enskog factor χ . We take a different approach by replacing V_c in Eq. (1) with an effective free volume $\tilde{V} = V_c - V_b/v_{\text{tcp}}$, where V_b is the volume of the beads in that cell and v_{tcp} is the packing fraction of a random close packing.

Like every simulation method, DSMC is based on certain approximations. To keep the error small, three conditions must be fulfilled:

- (i) the system should be in the collisional regime,

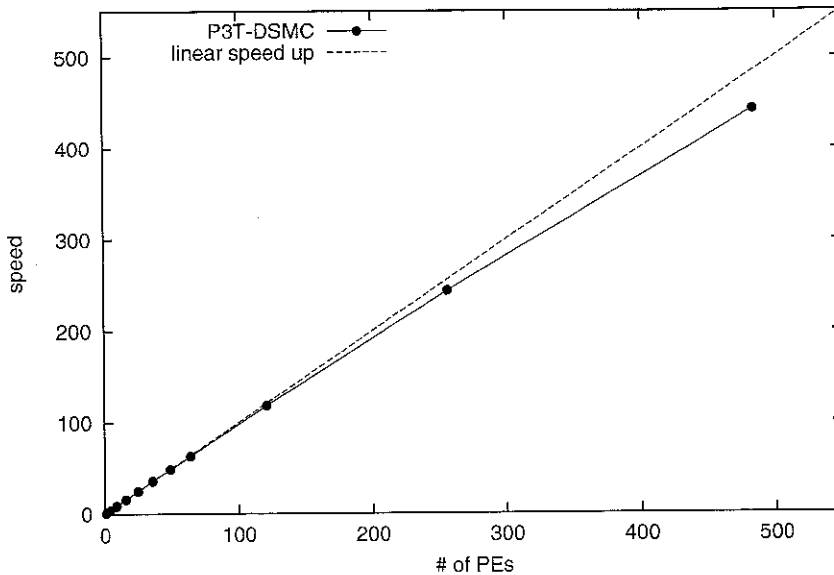


Fig. 2. Speed-up of the DSMC program, i.e. the inverse execution time versus the number of processors. The lower curve is measured and the upper curve shows the upper theoretical limit. Measurements have been performed on a CRAY T3E with a two-dimensional system with $N = 500\,000$ particles and volume fraction $\nu = 0.1$.

(ii) the mean free path should be larger than the cell size,

(iii) the mean time between two collisions should be larger than the time step.

In particular these limitations restrict the validity of the method to relatively low densities.

Because the interaction of the particles is of short range, domain decomposition is the method of choice. Unlike in MD simulations the particles interact only with particles of the same cell, therefore no shadow rows have to be communicated. The reduced communication demand results in a better speed up (see Fig. 2).

A second advantage of DSMC is the low memory demand. Only the position and velocity of every particle have to be stored. On two coupled Cray T3Es (one at HLRS/Stuttgart the second at PSC/Pittsburgh) we were able to simulate 1 759 165 695 particles of a granular gas.

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