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Granular material flowing down an inclined chute: a molecular dynamics simulation

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Abstract. — Two-dimensional Molecular Dynamics simulations are used to model the free surface flow of spheres falling down an inclined chute. The interaction between the particles in our model is assumed to be subjected to the Hertzian contact force and normal as well as shear friction. The stream of particles shows a characteristic height profile, consisting of layers of different types of fluidization. The numerically observed flow properties agree qualitatively with experimental results.

1. Introduction.

Flows of granular material such as sand or powder reveal macroscopic behaviour far from the behaviour of flowing liquids. Examples of astonishing effects are heap formation under vibration [1-9], size segregation [10-12], formation of convection cells [13-15] and density waves emitted from outlets [16, 17] or from flows through narrow pipes [18] and on surfaces [19-22] and displacements inside shear cells [23-30]. For its exotic behaviour granular materials have been of interest to physicists over many decades.

Recently highly sophisticated experimental investigations were carried out concerning the two-dimensional free surface flow of plastic spheres generated in an inclined glass-walled chute [31]. The observed flows at sufficiently low inclination consists of layers of different types of fluidization. The flow generally can be divided into frictional and collisional regions. At least in the case of a rough bed the frictional region typically consists of a quasi-static zone at the bottom and above of the so called block-gliding zone where blocks of coherent moving particles move parallel to the bed.

In the current paper we want to present the results of our numerical investigations concerning the problem mentioned above. Beginning at an initial state of particle positions, velocities and angular velocities the dynamics of the system will be determined by integrating Newton's equation of motion for each particle for all further time steps. In our case the forces acting upon the particles are exactly known for each configuration of our system. For this reason we have chosen a sixth order predictor–corrector molecular dynamics simulation [32] for the evaluation of the positions of the particles and a fourth order predictor–corrector method for the calculation of the particles angular movement to be the appropriate numerical methods to solve our problem.

The height profiles of the particle's velocities, of the particle density and the segregation of the particle flow into different types of fluidization were the essential points of interest of our investigations. As shown below the properties of the particle flow varies sensitively with the smoothness of the bed surface. As we will demonstrate, the numerical results are in qualitative accordance with the experimental data.

2. Numerical model.

The system consists of $N = 400$ equal two-dimensional spherical particles with radius R moving down a chute of length $L = 50 \cdot R$ inclined by an angle ($\alpha = 10° \; ..30°$) which is assumed to have periodic boundary conditions in the direction parallel to the bed. Our results did not vary qualitatively with the number of particles provided that they are enough to yield reliable statistics ($N \geq 250$). In simulations with more particles ($N = 1000$) we observed the same effects, the profiles of the averaged particle density, the cluster density and the particle velocity became slightly smoother, while the calculation time rose substantially. In figure 1 the setup of our computer simulations is drawn.

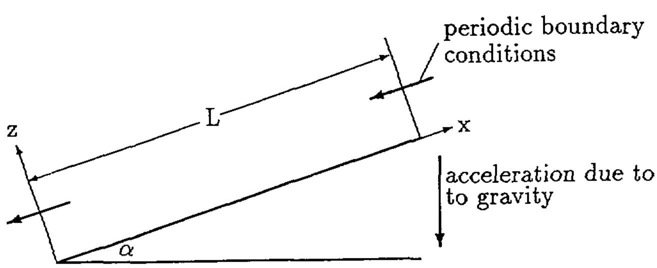

Fig.1. — Computer experimental setup.

The particles were accelerated with respect to the acceleration due to gravity ($g = -9.81$ m/s^2, the mass M was set to unity):

$$F_Z = M \cdot g \cdot \cos(\alpha) \tag{1}$$

$$F_X = M \cdot g \cdot \sin(\alpha) \tag{2}$$

where F_Z and F_X are the forces acting upon each particle in the directions normal to the inclined chute and parallel to it respectively.

The surface of the chute was built up of smaller spherical particles ($R_S = 0.66 \cdot R$) of the same material as the moving particles, i.e. with the same elasticity and friction parameters. These spheres were arranged at fixed positions either regularly and close together in order to simulate a smooth bed or randomly out of the interval $[2 \cdot R_S; 2 \cdot \sqrt{R \cdot R_S + {R_S}^2}\;)$ to simulate a rough bed (Fig. 2).

Fig.2. — Rough and smooth beds both consist out of spheres with diameter $R_S = 0.66 \cdot R$. In the case of the smooth bed these spheres are arranged close together while in the case of the rough bed they are arranged irregularly.

To describe the interaction between the particles and between the particles and the bed we applied the ansatz described in [33] and slightly modified in [10]:

$$\mathbf{F}_{ij} = \begin{cases} F_N \cdot \dfrac{\mathbf{x}_i - \mathbf{x}_j}{|\mathbf{x}_i - \mathbf{x}_j|} + F_S \cdot \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \cdot \dfrac{\mathbf{x}_i - \mathbf{x}_j}{|\mathbf{x}_i - \mathbf{x}_j|} & \text{if } |\mathbf{x}_i - \mathbf{x}_j| < 2 \cdot R \\ 0 & \text{otherwise} \end{cases} \tag{3}$$

with

$$F_N = k_N \cdot (r_i + r_j - |\mathbf{x}_i - \mathbf{x}_j|)^{1.5} \ + \ \gamma_N \cdot M_{\text{eff}} \cdot (\dot{\mathbf{x}}_i - \dot{\mathbf{x}}_j) \tag{4}$$

and

$$F_S = \min\{-\gamma_S \cdot M_{\text{eff}} \cdot v_{\text{rel}} \ , \ \mu \cdot |F_N|\} \tag{5}$$

where

$$v_{\text{rel}} = (\dot{\mathbf{x}}_i - \dot{\mathbf{x}}_j) + R \cdot (\dot{\Omega}_i - \dot{\Omega}_j) \tag{6}$$

$$M_{\text{eff}} = \frac{M_i \cdot M_j}{M_i + M_j} = \frac{M}{2} \tag{7}$$

The terms $\mathbf{x}_i$, $\dot{\mathbf{x}}_i$, $\dot{\Omega}_i$ and M_i denote the current position, velocity, angular velocity and mass of the ith particle. The model includes an elastic restoration force which corresponds to the microscopic assumption that the particles can penetrate slightly each other. In order to mimic three-dimensional behaviour this force rises with the power $\frac{3}{2}$ which is called "Hertzian contact force" [34]. The other terms describe the energy dissipation of the system due to collision between particles according to normal and shear friction. The parameters γ_N and γ_S stand for the normal and shear friction coefficients. Equation (5) takes into account the fact that the particles will not transfer rotational energy but slide upon each other in case the relative velocity at the contact point exceeds a certain value depending on the normal component of the force acting between the particles (Coulomb-relation [35]. For all our simulations we have chosen the constant parameters $\gamma_N = 1000 \text{ s}^{-1}$, $\gamma_S = 300 \text{ s}^{-1}$, $k_N = 100 \frac{N}{m^{1.5}}$ and $\mu = 0.5$. For the integration time step we used $\Delta t = 0.001$ s to provide numerical accuracy. When doubling the time step we got exactly the same results.

3. Results.

3.1 Initialization. — In the simulations, the particles are placed initially on a randomly disturbed lattice above the bed so that they do not touch each other at the beginning. In order to obtain periodic boundary conditions of the bed we have to fit the length of the bed in a way such that the center of the first sphere of the bed is at $x = 0$ and can reappear at $x = L$

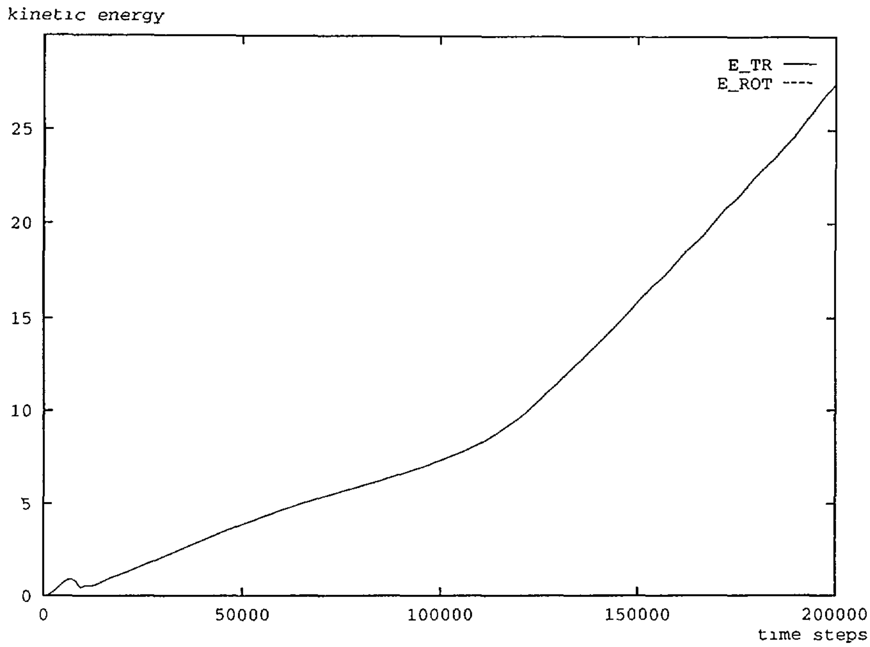

Fig.3. — Evolution of the kinetic (transversal) and rotational energy for the particle flow on a smooth bed. The sharp kink separates two different regimes of the particle movement called the low energy regime and the high energy regime.

without colliding with its neighbours. Suppose the length of the chute was chosen to be L_0 it was fitted to L with $L \in [L_0, L_0 + R_S)$ to hold periodic boundary conditions. The particles' initial velocities were zero. After starting the simulation the particles gain kinetic energy since they fall down freely without any collisions, i.e. without dissipation. This is the reason for a peak of the kinetic energy at the very beginning of the simulation.

3.2 SMOOTH BED. — For the case of the smooth bed figure 3 shows the kinetic energy of the system. The chute was inclined by an angle $\alpha = 20°$. The curve shows a significant kink which separates two different regimes of the particle movement as shown below. The numerical simulations reported in 3.2. and 3.3. run while the particles are accelerated due to gravity, their kinetic energy rises. After waiting enough time the system comes into saturation and finds its steady state as we will demonstrate in 3.4. below. In figure 4 a snapshot of the grains' movement before the kink of the energy is displayed. The small line drawn within each particle shows the direction and the amount of the velocity of the particle, its length was scaled due to the fastest particle. In all our simulations the rotational energy is negligible. In figure 3 the evolution of the rotational energy coincides with the time-axis.

As indexed by the velocity arrow drawn inside the particles the flux divides into the lower block gliding zone, where nearly all the particles move coherently with an equal velocity forming a single block of particles. The particles which belong to one block are drawn bold faced. More precisely to identify which particles form a block we applied the following rule: each two particles moving in the neighbourhood ($|\mathbf{r}_i - \mathbf{r}_j| < \lambda \cdot R$) for a time of at least 5000 time steps which corresponds to a covered distance of $(10 \ldots 30) \cdot R$ approximately belong to the same

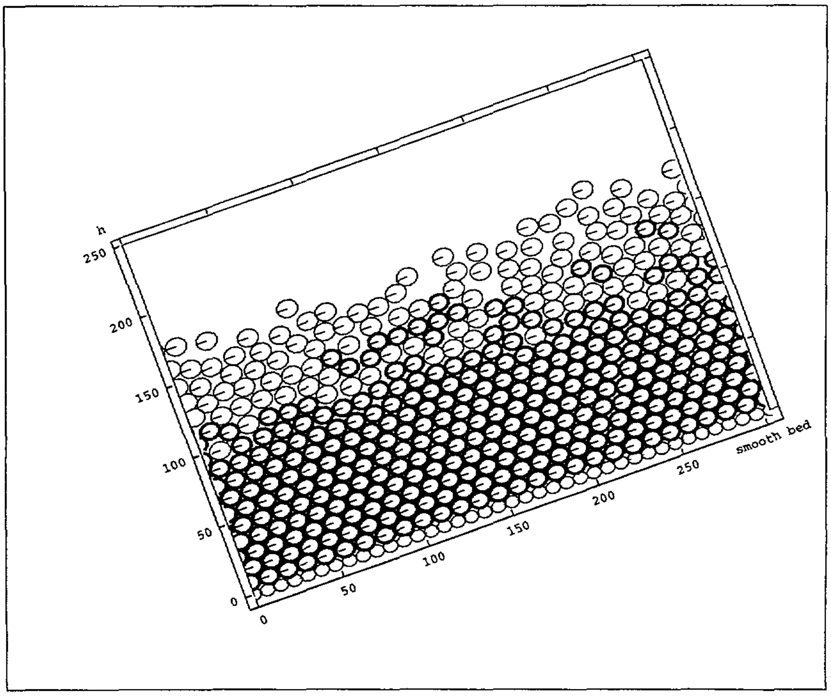

Fig.4. — Snapshot after 90.000 timesteps within the low energy regime. Particles which belong to a cluster are drawn bold faced. All grains at the bottom ($h < 100$) form one large block. Only few of them above the block belong to clusters.

block. If λ was chosen very small ($\lambda < 2.1$) then even very small elastical bouncing of two neighbouring particles leads to the wrong interpretation that the particles are not neighboured anymore while two particles moving with a small relative velocity were detected to belong to a cluster when λ was chosen too large. With the value $\lambda = 2.2$ we got correct results. As visible the grains in the lower part move coherently as a block in the case of low energy distinct from the high energy behaviour as shown below in figure 8. The upper particles move irregularly.

Figures 5, 6 and 7 show the particle-density, velocity in horizontal direction due to the bed and cluster-density depending on the vertical distance from the bed h corresponding to the snapshot given in figure 4.

The velocity distribution in horizontal direction separates into two regions, the lower particles including the block and the grains close to the block move with nearly the same velocity. The particles on the surface of the flow move with larger velocity. There is a sharp transition between the velocities of particles which belong to the block and the grains moving at the surface. The term cluster density means the portion of particles which belong to one of the clusters. The cluster density as a function of the distance from the bed h does not vary from the bed to the top of the block and lowers then fastly as expected from the snapshot (Fig. 4) because there are almost no smaller clusters except the block. The velocities in figure 6 have negative sign because the particles move from the right to the left i.e. in negative direction.

As pointed out above the sharp kink of the energy in figure 3 corresponds to different regimes. Figures 8-11 are analogous to figures 4-7 for a snapshot short time after the transition into the high velocity regime at time step 110.000.

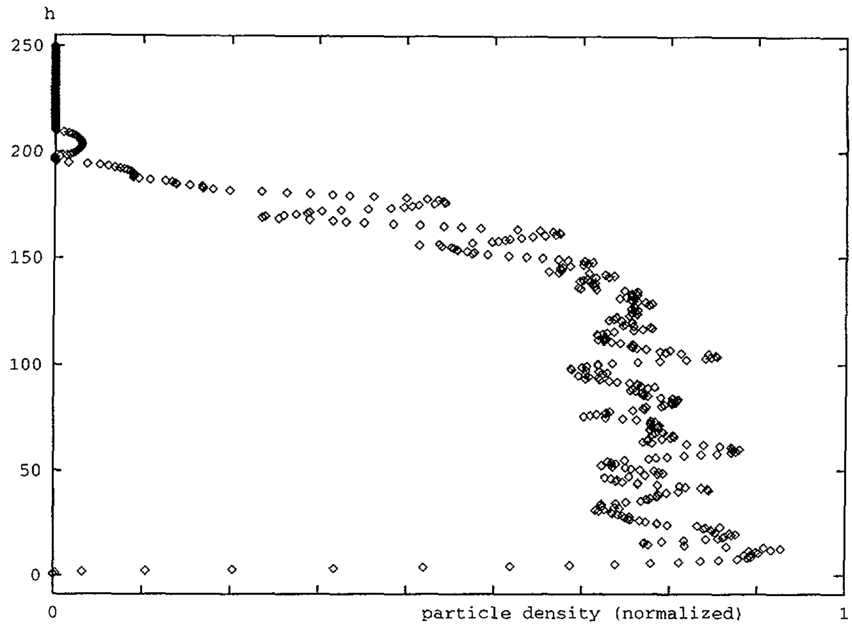

Fig.5. — Particle density depending on the vertical distance from the bed h (low energy regime). Within the block the partical density does not vary.

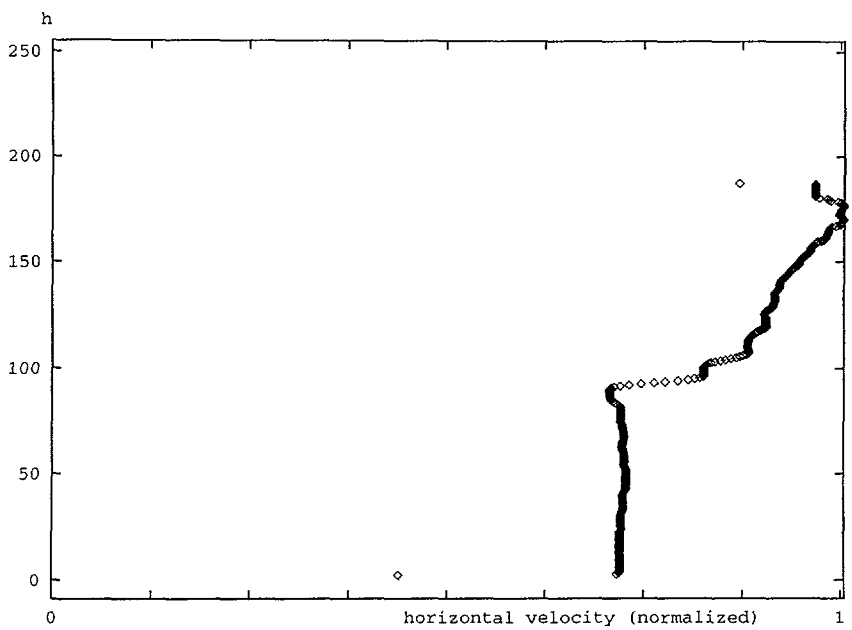

Fig.6. — Averaged horizontal velocity (low energy regime). The grains which belong to the block move with equal velocity, i.e. there is really only one block but not different blocks gliding on each other. The velocity changes desultory at the upper boundary of the block ($h \approx 100$), the free moving particles are 1.3 to 1.5 times as fast as the block.

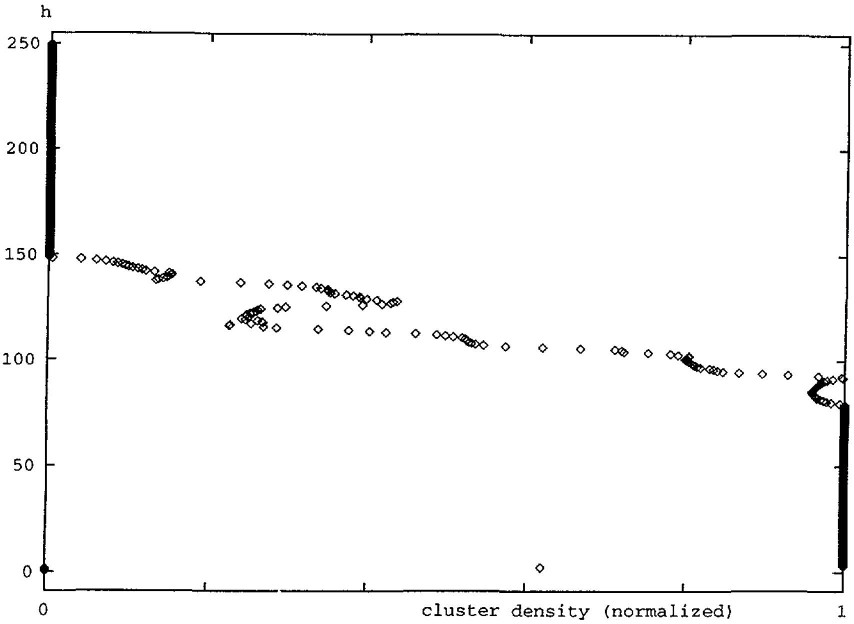

Fig.7. — Cluster density (low energy regime). Above the block the cluster density vanishes. There are almost no particles which belong to a cluster except of the block at the bed.

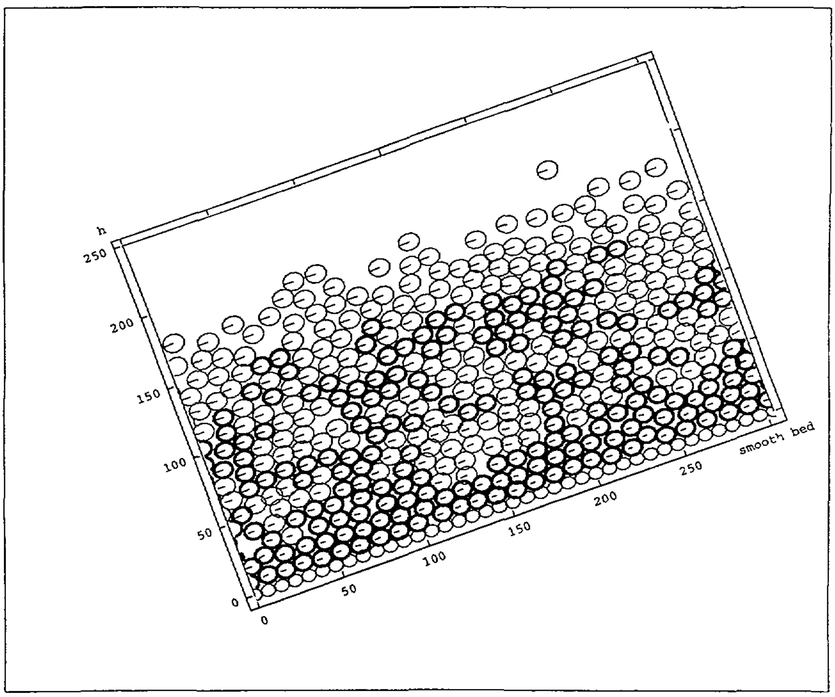

Fig.8. — Snapshot after 110.000 timesteps in the high energy regime. The block (Fig. 4) separated within a relatively short time into many independently moving smaller clusters. The rest of the block lies still close to the bed. It also vanishes after some time.

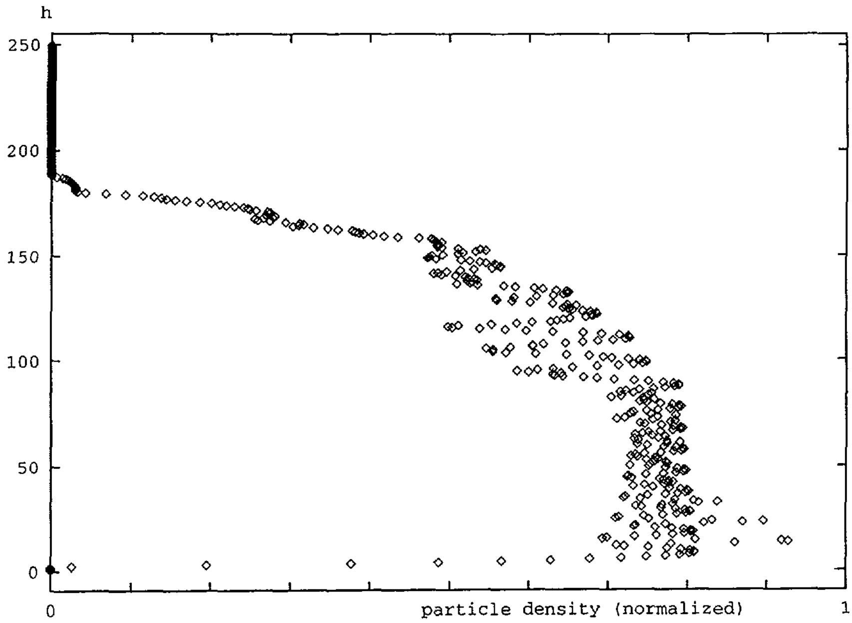

Fig.9. — Particle density depending on the vertical distance from the bed h (high energy regime). Although the properties of the flow are very different from the flow in the low energy regime the profile of the particle density differs not significantly.

If the energy rises over a critical value while the grains move accelerated due to gravity the particle flow does not any longer divide into the block and the free moving particles but the block separates into independently moving smaller clusters. This transition occurs within a short energy interval which corresponds to a short time from the beginning of the simulation. As shown in figure 9 the density as a function of the distance from the bed h varies only slightly from the same function at low energy (Fig. 6). Nevertheless the profile of the horizontal velocity (Fig. 10) differs significantly from the corresponding profile in the low energy regime (Fig. 6). The velocity of the grains rises continually from the bed to the top of the partical flow. The profile of the horizontal velocity shows the transition into another regime of movement. Between the small block of grains near the chute and the freely moving particles in the collisional zone there is a region with an approximately constant cluster density (Fig.11). This behaviour is also observed in the experiment [31]. Neighbouring clusters move with relative velocities between each other.

3.3 Rough bed. — In this section we want to discuss the results of the simulations with the same set of parameters as in the previous section but with the rough bed. As shown in figure 12, the energy-time-diagram for this case does not show the same behaviour as for the case of the rough bed but has roughly a parabolic shape. This shape is maintained qualitatively over a long time corresponding to a wide range of kinetic energy of the particles until the kinetic energy comes into the region of saturation. The problem of energy saturation will be discussed in more detail in section 3.4.

Corresponding to the previous section, figure 13 shows a snapshot of a typical situation of the flow, figures 14-16 show the particle-density, the averaged velocity in horizontal direction

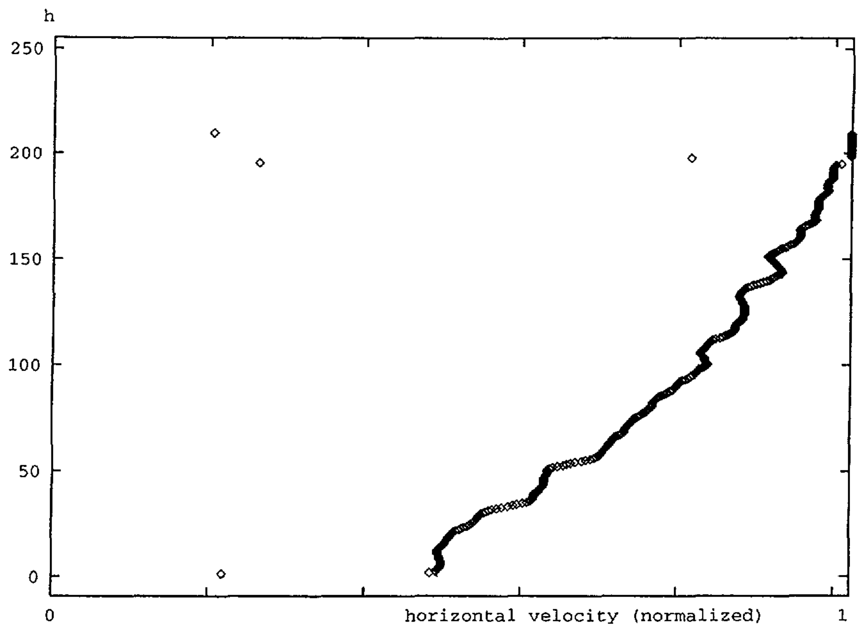

Fig.10. — Averaged horizontal velocity (high energy regime). It is the most noticeable index to the fact that the particle flow changed into an other regime.

and the cluster-density as a function of the distance from the bed h.

The snapshot figure 13 shows the situation as it can be observed over a wide range of energy values. These layers were found experimentally [31]. The flow divides into three different zones (Fig. 15) the slow particles close to the chute whose velocity rises continously with the distance from the chute h, the particles in the block gliding zone which have approximately the same velocity and a few fast moving particles in the collisional zone at the top of the flow. Also figure 16 shows evidently that the flow divides into three regions of different types of fluidization. The slow particles close to the bed and the fast particles in the collisional zone are separated by a zone, where clusters occur. This zone we call block gliding zone. It was first investigated experimentally in [31].

3.4 Steady state. — The numerical experiments shown above were performed in the accelerated regime. Since our model includes friction the system will of course reach a steady state after waiting a long enough time. For the parameter sets we used in the simulations above, this steady state is incident to very high particle velocities. To obtain numerical accurate results in the steady state regime therefore one has to choose a very high time resolution i.e. a very small time step Δt. Hence the computation time rises strongly with the kinetic energy of the system.

To demonstrate that our model is able to reach the steady state regime we have chosen the angle of inclination $\alpha = 10°$ and the time step $\Delta t = 0.001$ s. Figure 17 shows the evolution of the energy of the system as a function of time.

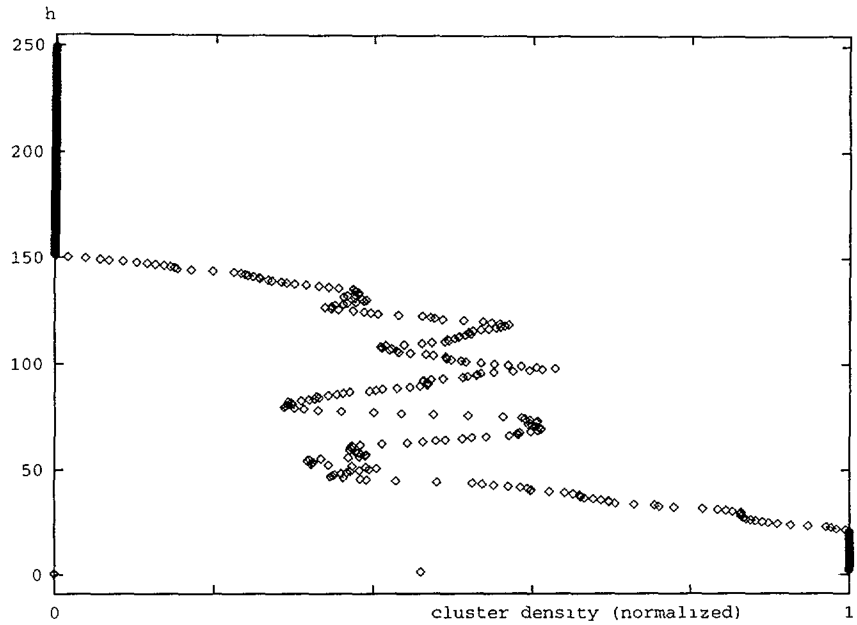

Fig.11. — Cluster density (high energy regime). Between the rest of the block gliding on the chute and the free moving particles on the top of the flow lies a region of constant cluster-density.

4. Discussion.

The flow of granular material on the surface of an inclined chute was investigated through a two-dimensional molecular dynamics simulation. For the case of a smooth bed simulated by regularly arranged small spheres on the surface of the chute we found two qualitatively different regimes of particle movement corresponding to low and high kinetic energies. The velocity as well as the density profiles agree with experimental results [31]. For the case of the rough bed we did not find such a behaviour. As in the case of the smooth bed the density and velocity profiles agree with the measured data. In both cases we observed a coherent motion of groups of grains, so called clusters, which has also been observed in the experiment. Of particular interest seems to us the fact that the behaviour of the flow on a chute with regular (smooth) surface differs significantly from the flow on a chute with irregular (rough) surface.

By simulating a system with a smaller inclination angle we gave evidence that our numerical model is able to reach a steady state at a constant kinetic energy.

The numerical results show that our two dimensional ansatz for the force acting on the grains which does not include static friction is able to describe the experimentally measured scenario qualitatively correctly for the system considered.

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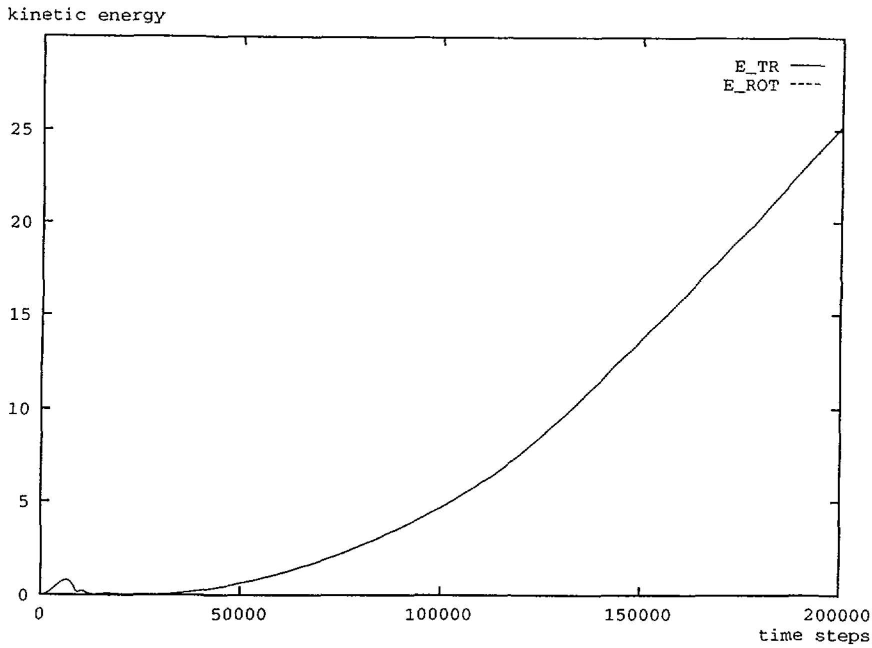

Fig.12. — Evolution of the kinetic (transversal) and rotational energy for the case of the rough bed. The energy shows no kink as in the flow on the smooth bed (Fig. 4) but its shape is close to parabolic over a wide range.

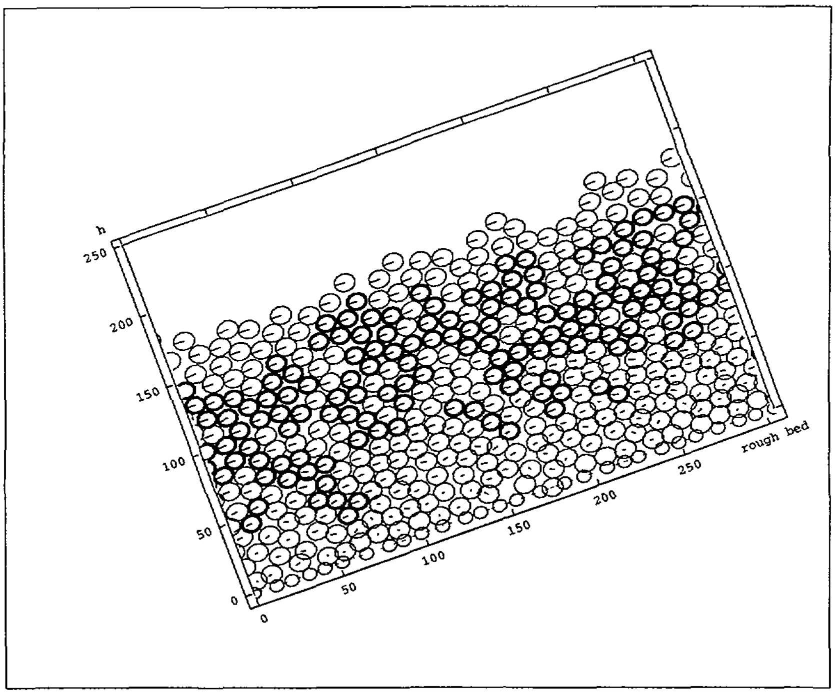

Fig.13. — Snapshot after 80.000 timesteps. As in figure 4 the particles which belong to one of the blocks are drawn bold.

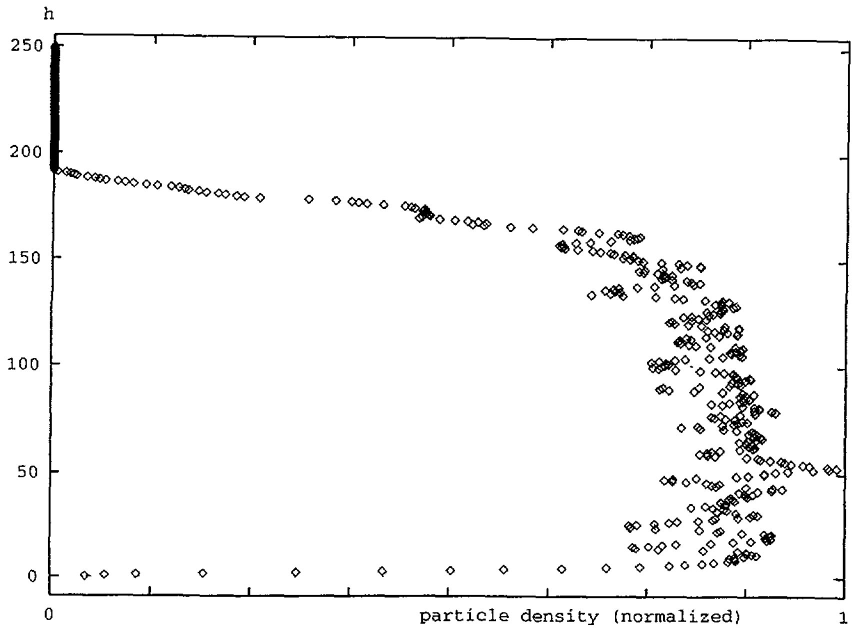

Fig.14. — Particle density depending on the vertical distance from the bed h. It shows no very different behaviour than the corresponding figures (Figs. 5,9) for the case of the smooth bed.

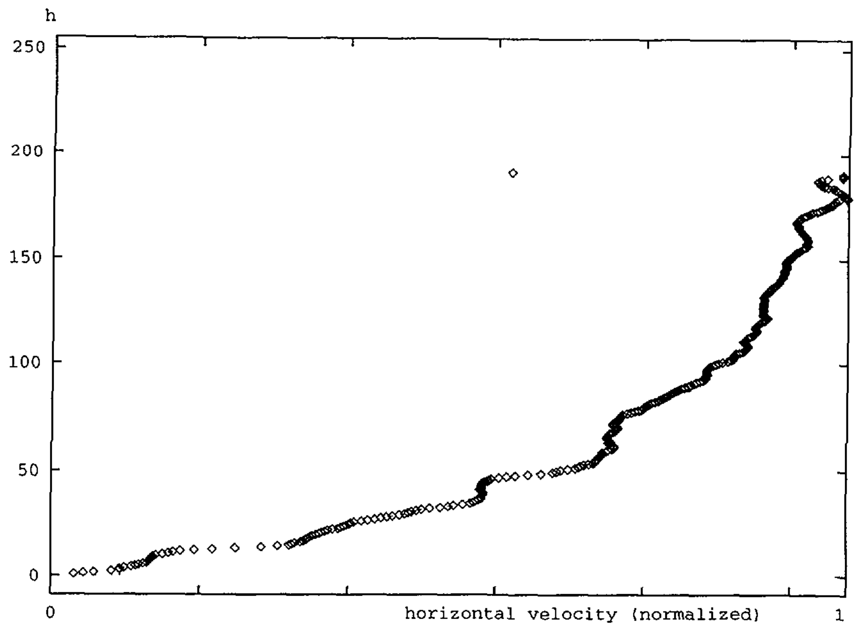

Fig.15. — Averaged horizontal velocity. The flow consists of different regions: the slow particles close to the chute, the block gliding zone and the collisional zone near the top of the flow. The velocity rises continually with the distance from the bed h.

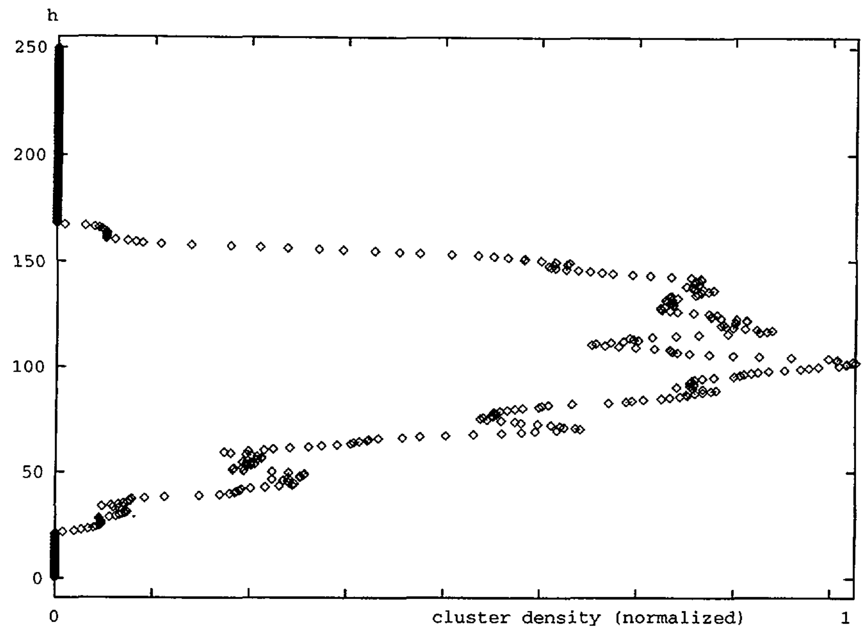

Fig.16. — Cluster density. There is a zone of significiant higher cluster density. This region will be called block gliding zone.

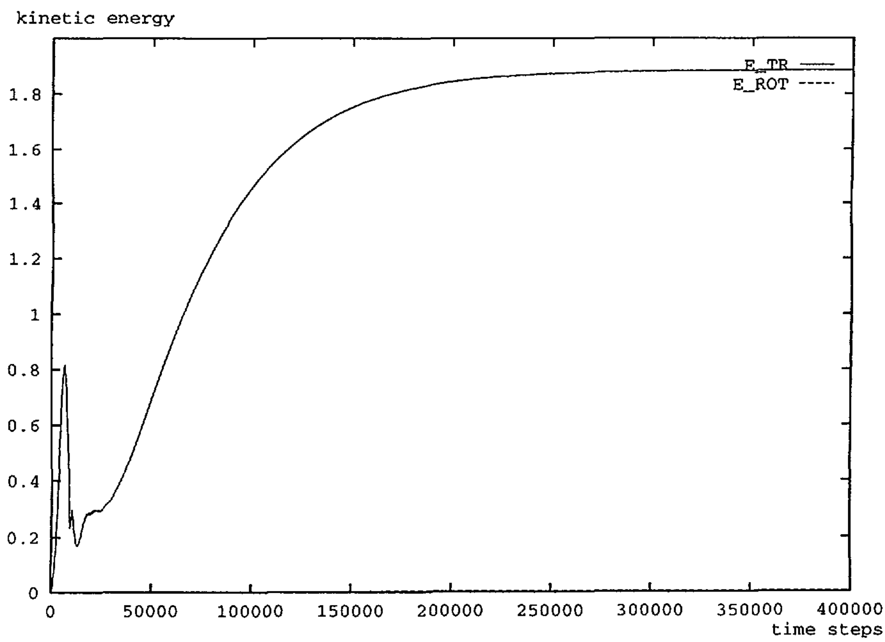

Fig.17. — Saturation of the kinetic energy after long time for a flow of particles down a chute which was inclined by an angle of $\alpha = 10°$ only.

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