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"Microscopic Modelling of Sound Waves in Granular Material"

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Introduction

Our work over the past several years has been directed toward a detailed examination of the transmission of sound through dry granular materials at the microscopic level. Such a granular system consists of a contact network along which, and only along which, the momentum impulses which comprise the sound wave may travel.

In the past several years we have studied two such systems. In one of these [Haff, 1987] grains cascaded down an incline, and the pressure impulses recorded on the bed were studied using computer simulation. These studies indicated that there were systematic characteristics of the bed pressure excursions which might serve as diagnostics of granular flow conditions. We looked at both thin and thick flows. The thick flows, corresponding to dense granular assemblies in which contact between grains was retained for times long compared to typical collision times, were characterized by the spontaneous appearance in the flow of stress-columns, or arches, which seem to play a role similar to turbulence in fluid flow, i.e., they are coherent structures responsible for long range transmission of stress through the deforming granular medium. These simulated flows generated synthetic bed-pressure spectra in which the effect of the stress-columns was clearly visible. We therefore suggest that instrumentation of particle transport equipment with high resolution transducers might provide a way to assess remotely the state of granular flows either in dry transport or in dense slurries, (although fluid effects were not included in the

simulation).

The second type of system studied [Haff, 1988] was a collection of quasi-static grains subjected to compressive loading. Again the walls were equipped with high-resolution simulated pressure transducers. Point sources of elastic deformation were selected and localized impulses applied to the sample. The spatial and temporal spreading of the signal, resulting from the multiplicity of contact pathways, and the attenuation effects resulting from friction were analyzed. Microscopic inhomogeneities in packing and stress-state were also examined, and it was shown how such irregularities could lead to wave speed and attenuation anomalies. We argued that pressure measurements at the microscale (i.e., with resolution on the order of a grain diameter) ought to be investigated further as a possible probe of the state of static granular masses. We also emphasized the phenomenon of super-acoustic transmission, by which information could be propagated through a small granular system at speeds exceeding the nominal speed of sound in the material. This peculiar effect is evidently grain-size dependent, and we recommend that it be further investigated as a possible means of determining grain size distributions in situations where it was otherwise either impossible or inconvenient to measure grain physical dimensions in situ.

Our static-grain system studies have also led to a preliminary, and so far inconclusive, investigation of mode-localization in granula media, wherein an effective acoustic attenuation appears by virtue of repeated reflections of

wavelets.

More Grain-Flow Studies

We return here to a consideration of flowing systems. One limitation of the particle dynamics method [Haff, 1987,1988] used earlier to simulate grain motion lies in the number of particles it can treat in a given simulation, with perhaps a few thousand being the maximum number which can be done routinely today with desktop computing power. In this particle-number range care must be taken to ask the correct questions of the simulations, and to set up the boundary conditions properly, so that edge effects don't dominate the calculation and confuse or distort the results.

There are times when it would be helpful and interesting to be able to compute the motion of a much larger number of particles, say a hundred thousand or even a million grains. There were several ways to pursue this goal. One, which we have explored a bit already, is the lattice-grain-model. It takes its name from the lattice gas models currently under development in fluid mechanics [e.g., Frisch, et al., 1986; Margolis et al., 1986].

The standard lattice gas model of fluid mechanics involves the manipulation of large numbers of cellular automata, which are constrained to lie on the vertices of a two-dimensional triangular lattice, Figs. 1a,b, and which evolve according to the following set of rules:

1. Each automata has a unit velocity vector which points in one of six directions corresponding to the lattice directions.
2. A single vertex may have at most only one automata for each velocity direction; thus the occupancy of a vertex may be stored using only six bits.
3. Each equal time step consists of two stages: an updating of the positions of the automata and an evaluation of their "collisions" (a "collision" occurs when two automata simultaneously occupy a single site).
4. Each automata advances exactly one lattice spacing in each time step in a direction determined by its velocity vector.
5. Two or more automata on the same vertex may collide according to a simple set of rules. Collision results are usually stored in the form of a lookup table.

These evolution rules are not arbitrary but are determined by a number of considerations, i.e., the triangular lattice is chosen instead of the simpler square lattice since in the latter case it can be shown that the pressure tensor will not have the correct symmetry properties [Frisch et al., 1986]. The single value of velocity magnitude and the limited number of velocity directions are designed to keep the position updating and the collision rules as simple as possible, and so on. We will not

detail the "collision rules" themselves, which describe what happens when two automata come together at the same lattice point, but they are designed simply to reflect the conservation of energy and momentum at each encounter.

The appeal of the lattice model of fluid mechanics revolves around the fact that repetitive manipulations of very simple entities (the automata) according to simple rules leads to average automata velocities which converge to solutions of the Navier-Stokes equation of fluid dynamics. The algorithm is stable, is relatively easy to program, and can handle both time-dependent problems and problems with irregular geometries. By the statement "converging to the Navier-Stokes equation" we mean that, in addition to the laws of conservation of energy and momentum inherent in this equation, the averaged lattice gas model also gives the correct constitutive behavior of Newtonian fluids. Correspondingly, the lattice gas model has stimulated intense interest in the fluid mechanics community.

We consider the following task: to design a lattice model, with suitably chosen displacement and collision rules, which, in its average behavior, will represent dynamically evolving granular materials.

The formulation of the lattice-grain-model is based upon considerations similar to those arising in lattice gas models of fluids, except for two distinguishing characteristics of granular systems: the inelasticity of grain-grain contact forces and the (usually) short length of the grain mean free path relative to a particle diameter. A short mean free path means

that the impact parameter in a collision is determined by the relative locations of the particles involved and can no longer be set arbitrarily. This, as well as the inelasticity of collisions, forces us to allow for a range of velocity magnitudes rather than a single magnitude. In addition, it is no longer possible to permit more than one particle on a lattice point; instead we must allow for collisions between particles on adjacent lattice points. Although these considerations mean that the model is slower to compute than the standard lattice gas model, it is nonetheless more efficient than particle dynamics methods which solve Newton's equations of motion.

Several interpretations of lattice-grain particles are possible. Like the automata in lattice gas models, they may be considered fictitious entities with no direct physical meaning, only their average behavior being of interest and physically relevant. This would correspond to problems where great masses of material were in motion. Each lattice particle then has a mass and size many times that of any real particle in the system, and it is only the average motion of many lattice particles that has a direct physical meaning. Alternatively, unlike in LGM, the lattice-grain particles may be thought of as representing "real" particles. This is the point of view adopted here.

Preliminary studies of the lattice-model [Gutt, 1989] show interesting time-dependent flow patterns around obstacles which bear resemblance to patterns observed in corresponding laboratory studies of grain flow in channels [Nedderman et al., 1980]. Figs. 2a,b represent snapshots of computed vertical flow between

parallel confining walls with a fixed circular obstruction lodged in the center of the pipe. Beneath the obstacle is an orifice whose function is to regulate the flow. The chamber at the bottom collects the "used" grains. In Fig. 2a the material has not yet commenced flowing. The little dingus marked by two points in the middle of the collection chamber serves to scatter the falling grains off to the side so that a mound which could potentially block the orifice does not build up. Fig. 2b shows the granular material flowing out of the orifice, while Fig. 2c shows several characteristic particle trajectories.

Several features of this test-case flow are interesting and instructive. 1) It is time-dependent. The upper cell of the hopper starts full and empties through time; 2) the confining geometry is irregular. The LGrM is not slowed down by either of these flow characteristics, but a more standard differential equation model would be difficult to solve; (3) the "constitutive law", although never made explicit, is inherent in the automata rules we invoke, e.g., inelasticity of collisions, grain size (the particles are not points) and so forth; (4) the model can handle free surfaces, i.e., at the top as the upper cell empties, in the bottom cell, and in the "gap" beneath the obstruction. The "gap" is not perfectly empty, as it would be for a real grain system, because of the high value of the coefficient of restitution chosen for this run; (5) although the LGrM is inherently a collisional model, as indicated in the descriptive discussion at the beginning of this section, it possesses the remarkable ability to simulate static or quasi-static granular

masses where the grain contacts are enduring and not ephemeral. A discussion of the technical issues [Gutt, 1989] which underlie this important fact is beyond the scope of this report; (6) there is little slip of granular material past the bounding walls because the walls are rough. This fact, plus the presence of an obstacle to the flow in the center of the channel accounts for the two "dimples" in the upper free surface. Our present implementation of LGrM does not simulate the slope of free surfaces accurately because of the strong directional influence of the fixed lattice directions. Adjustments to the automata evolution and collision rules will hopefully be able to correct this defect. 7) Finally, a typical and fascinating feature of LGrM is illustrated in the presence of the bottom collection chamber, i.e., it is easier to collect in a box the "spent" grains which have exited the orifice than to reprogram the code to "erase" automata once they have exited the region of physical interest. A close correspondence like this between LGrM and experimental (or natural) configurations is frequently encountered in automata-based models.

Figs. 3 a,b show flow around a square obstacle and Figs. 4 a,b flow around a triangular obstacle, by way of illustrating that variations in geometry are easy to implement. In Fig. 4b a recirculating "eddy" beneath the obstacle is evident. This fluid-like behavior evidently results from using a large value for the coefficient of restitution.

Other simulations of this nature have also been performed [Gutt, 1989]. For example, Figs. 5a and 5b show granular flow

out of an hourglass or hopper. The hourglass empties out through a central "pipe" or core region, with grains on the free surface sliding down to the top of the pipe, a rather typical hourglass-type flow [Tuzun and Nedderman, 1982]. Additionally, this simulation replicates the well-known observation that the hopper flow rate is independent of the pressure head (unlike the case of a Newtonian fluid).

LGrM seems to be a promising, if unproven, new tool for studies of moving granular material. Even if only in its overall qualitative flow pattern, lattice models seem to be able to provide a useful visual picture of the kind of granular flow phenomena which may be expected in certain confining geometries. In the channel flows just discussed, all the features exhibited in the simulation correspond to features seen in laboratory investigations of vertical chute flows around obstacles [Nedderman et al., 1980].

Additional work is needed to improve the calculation of the angle of repose, which is not treated adequately in the present model, and to assess more quantitatively flow velocity profiles and stress distributions in the deforming grain mass.

References

- Frisch, U., Hasslacher, B., and Pomeau, Y., 1986, Lattice-Gas Automata for the Navier-Stokes Equation, *Physical Review Letters* 56, 1505.
- Gutt, G. M., The Physics of Granular Systems, Caltech Ph.D. thesis (unpublished) 1989.
- Haff, P. K., Micro-Stresses and Their Distributions and Effects in Discrete Media, Proc. Solid Transport Contractor's Review Meeting, Sept. 1988, Pittsburgh, USDOE, PETC.
- Haff, P. K., Micromechanical Aspects of Sound Waves in Granular Material, Proc. Solid Transport Contractors' Review Meeting, Sept. 1987, Pittsburgh, USDOE, PETC, p. 41.
- Hui, K. and Haff, P. K., 1986, Kinetic Grain Flow in a Vertical Channel, *Int. J. Multiphase Flow*, 12, 289-298.
- Margolis, N., Tommaso, T., and Vichniac, G., 1986, Cellular-Automata Supercomputers for Fluid-Dynamics Modelling, *Physical Review Letters*, 56, 1694.
- Nedderman, R. M., Davies, S. T., and Horton, D. J., 1980, The Flow of Granular Materials Around Obstacles, *Powder Technology*, 25, 215.
- Tuzun, V. and Nedderman, R. M., 1982, An Investigation of the Flow Boundary During Steady-State Discharge from a Funnel-Flow Bunker, *Powder Technology*, 31, 27.

Figure Captions

Fig. 1. (a) Triangular lattice. Arrows indicate six possible displacements of a lattice particle located at tail of arrows. (b) Several representative particles residing on the lattice.

Fig. 2. (a) Circular obstacle in vertical channel. Dots represent lattice particles. The restrictor plate regulates the flow rate of particles, which collect in the lower chamber. Note dinging in lower chamber which serves to scatter particles sideways so they don't build up in a pile and block outlet. (b) Snapshot of flow. Note dimples in upper surface and cavity beneath obstacle. (c) Representative trajectories of particles in channel.

Fig. 3. (a) Same as for 2b,c but for square obstacle.

Fig. 4. Same as for 2b,c but for triangular obstacle.

Fig. 5. (a) Full hourglass, (b) Snapshot of hourglass emptying.

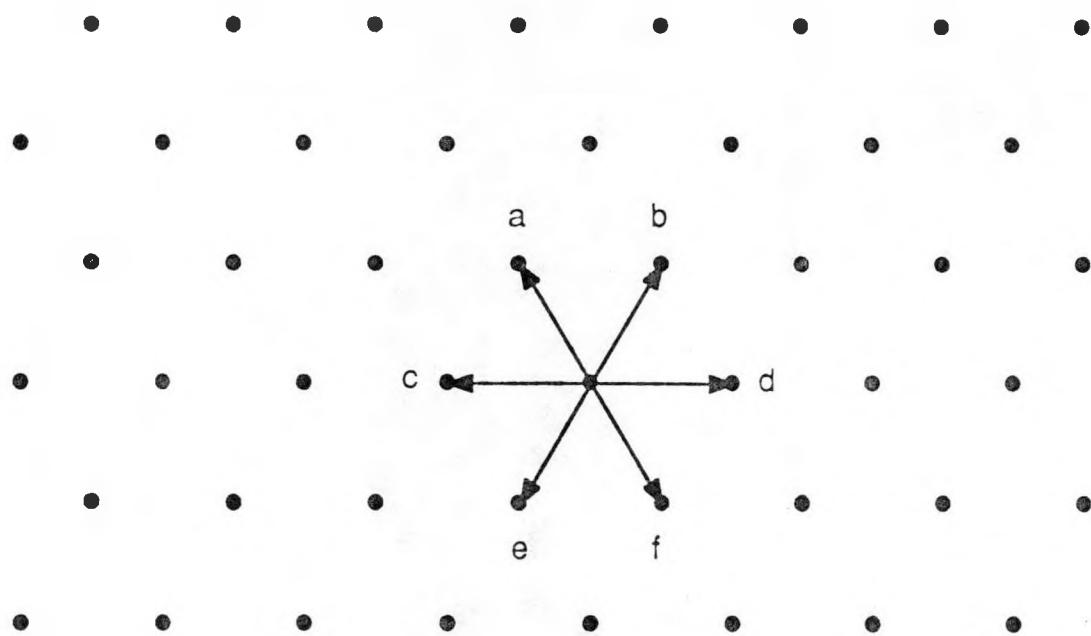


Fig. 1a

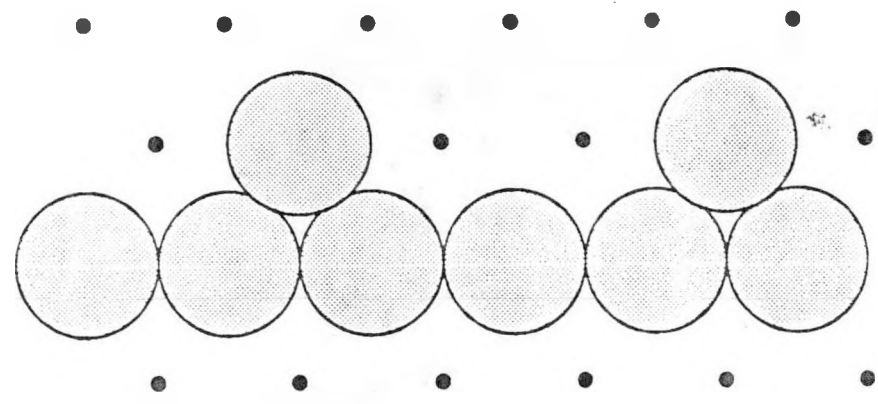


Fig. 1b

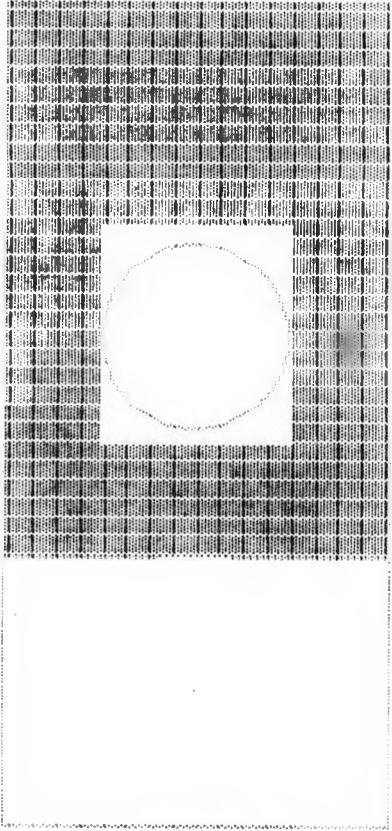


Fig. 2a

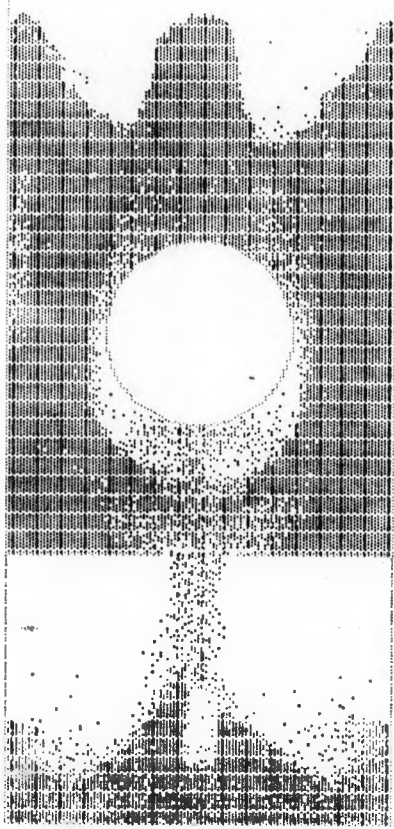


Fig. 2b

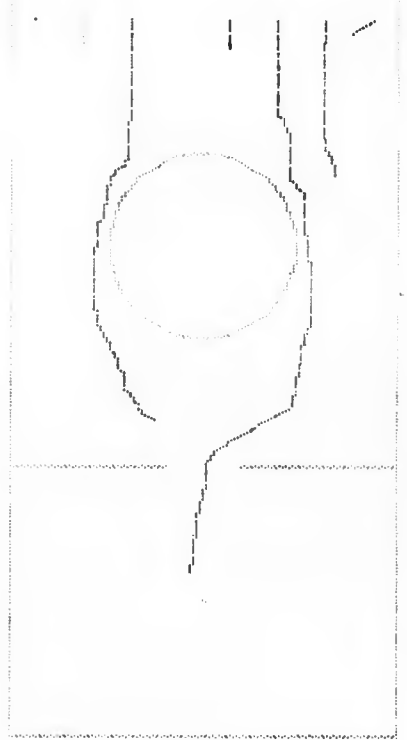


Fig. 2c

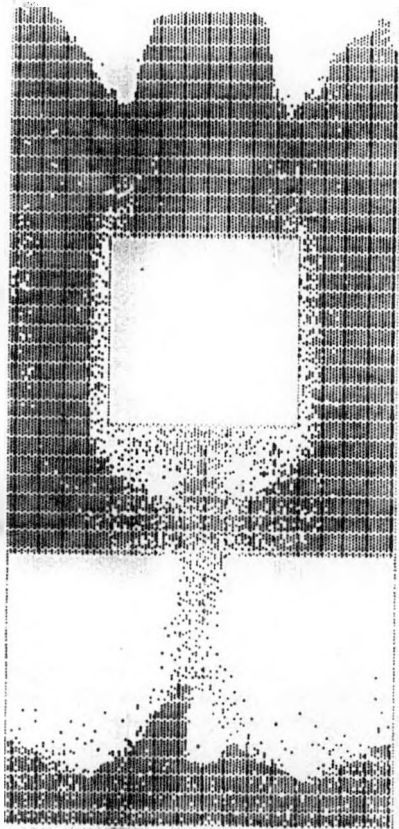


Fig. 3a

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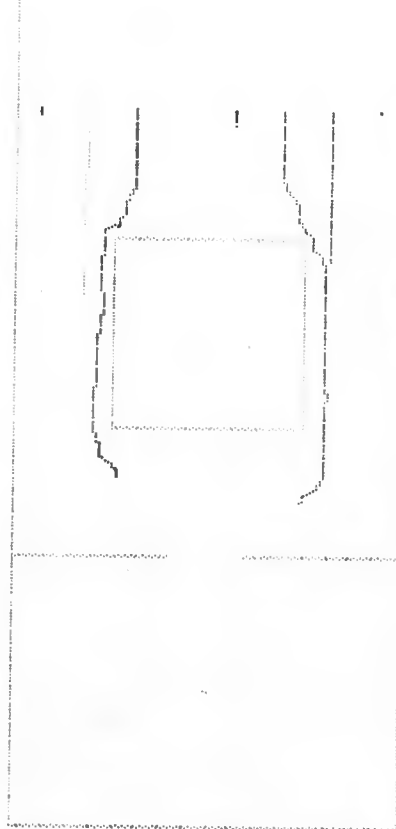


Fig. 3b

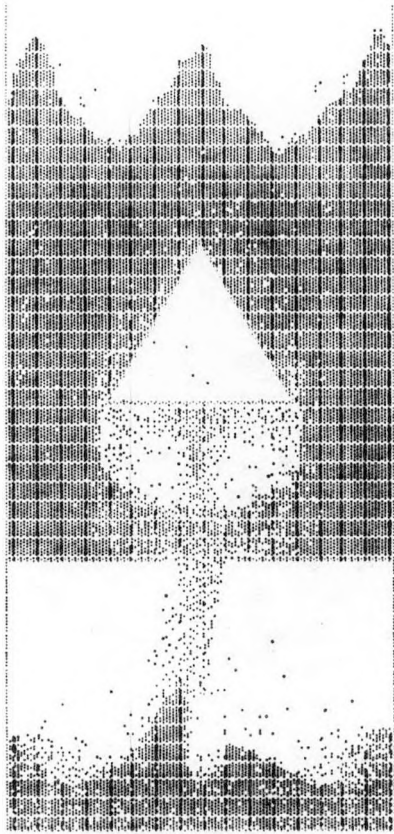


Fig. 4a

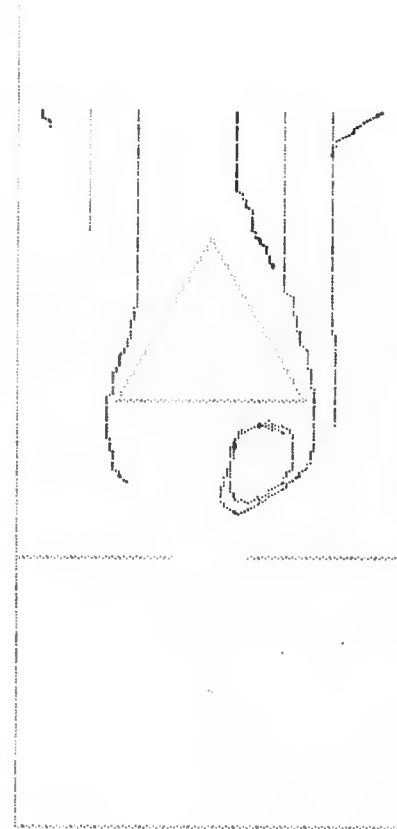


Fig. 4b

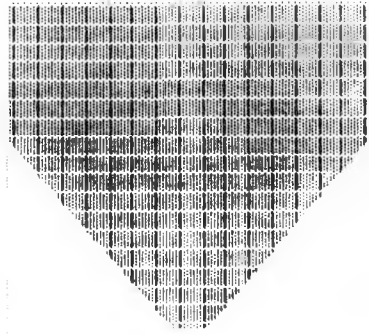


Fig. 5a

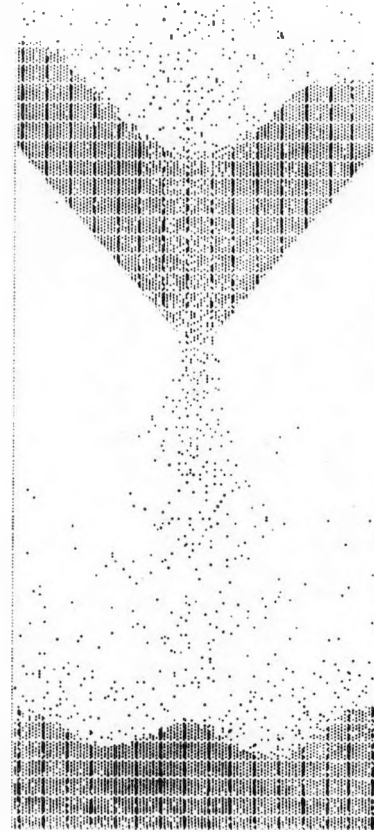


Fig. 5b