Granular Media Lattice Gas

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Due to the lack of a general continuum theory the main theoretical approach to investigate granular flow has been computer simulation. As an alternative to molecular dynamics and in analogy with hydrodynamics recent lattice gas models have been used to model flow in granular media. We present the details and the discussion of one such automaton.

Hydrodynamic lattice gas (HDLG) cellular automata (CA) have been introduced to simulate the behavior of a viscous fluid, especially in two dimensions. The basic idea behind the HDLG is the following: The continuum equation of hydrodynamics, the Navier-Stokes (NS) equation expresses basically the conservation of momentum. Microscopic dynamics with the appropriate conservation laws should lead to the NS equation, irrespective of whether it is the real molecular dynamics or some properly defined cellular automaton. The solution was found on the triangular lattice by using particles on the bonds with unit velocity[1].

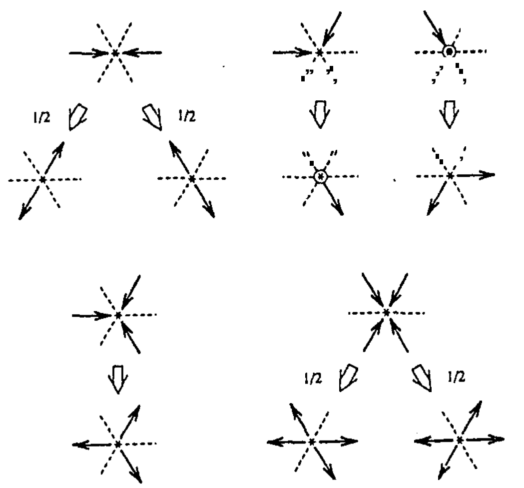

Figure 1: Collision rules of the FHP-II model. The empty arrows indicate the state after collision. Note that there are collisions with rest particles involved (circles), where energy is not conserved but on the average these cancel out (first row middle and last collisions). If there are two final states one of them is chosen with probability 1/2.

The complex physics of granular media has attracted recently much attention[2]. These systems consist of many particles each of them having a large number of degrees of freedom (they have temperature, there is friction between the grains). Therefore, granular systems show very complex behavior, including clogging, segregation, avalanches, kinematic waves, piling due to vibrations, difference between angle of repose and maximal angle of stability, etc.[2]. An apparent feature is that granular systems can behave both as fluids (they flow) and as solids (they build piles).

Since the fundamental hydrodynamic equations of granular media are not known, the basic theoretical approaches are either molecular dynamics[3] or simplified models concentrating on some features of the systems[4,5]. It is tempting to try to extend the method of HDLG to granular flow for several reasons[6,7]. Cellular automata are flexible enough to incorporate the important characteristics of granular media and at the same time they are much more 'computer friendly' than molecular dynamics.

In this contribution we give a short account of our simulations of granular media based on hydrodynamic-type cellular automata[7]. Throughout the paper we shall deal with two dimensional systems and we do not consider effects due to difference in the particles.

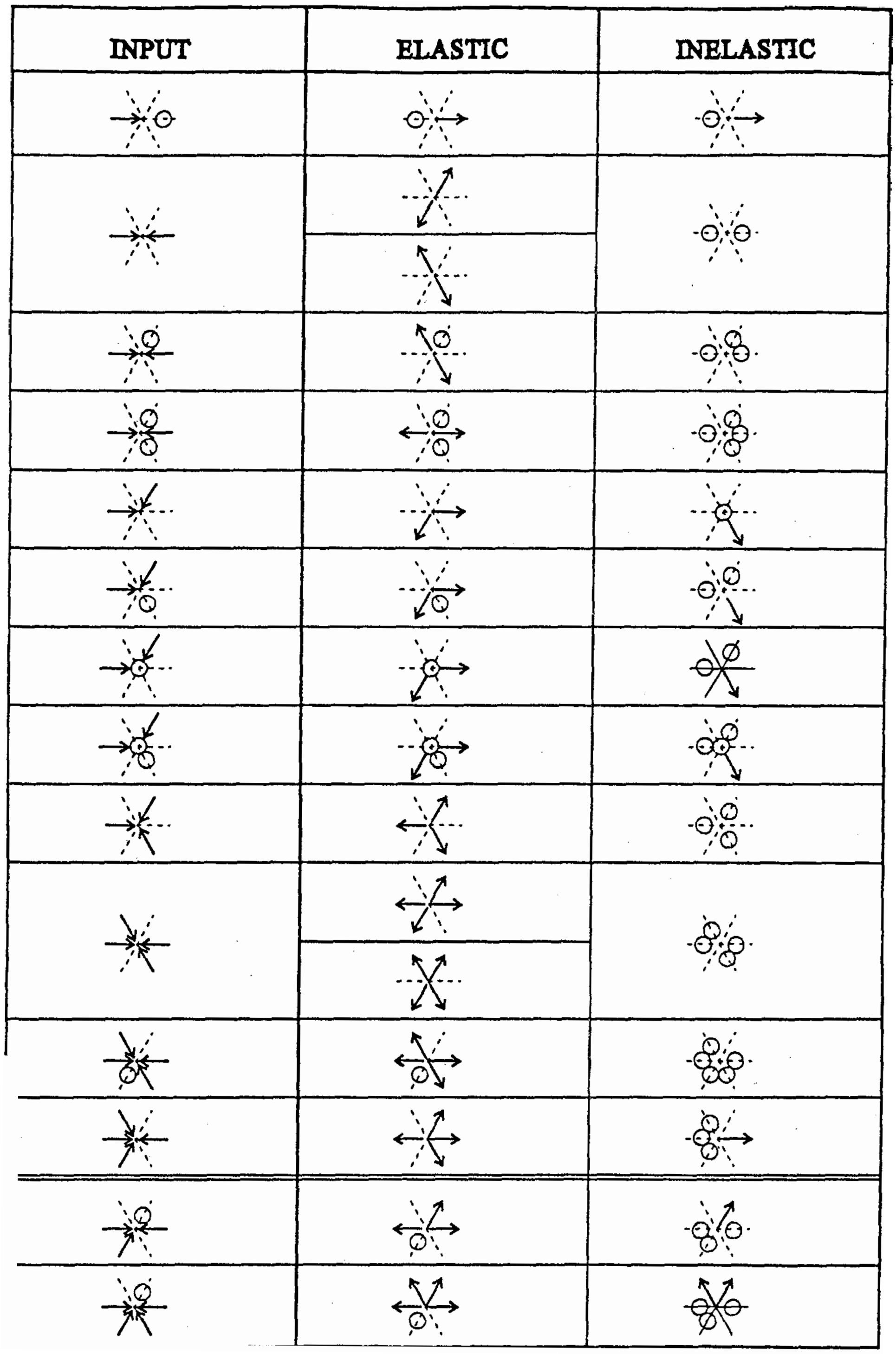

Figure 2: Table of collisions in the GMLG. The inelastic (elastic) output is chosen with probability $k(1-k)$. The last two lines are examples showing how general collisions can be treated using the table.

Let us start with a short summary of the HDLG algorithm. Identical particles move on the edges of a triangular lattice with appropriately chosen collision rules. These rules assure the momentum and energy conservation and also sufficient mixing in the phase space. In Fig. 1 the rules of the so called FHP-II model are shown[1].

For granular media three main differences have to be taken into account:

i) Gravity

ii) Dissipation

iii) Static friction

iv) Dilatancy

The first problem has been already discussed in the context of fluids[1]. The particles change their travelling directions downward with probabilities proportional to the gravity parameter.

Dissipation is naturally introduced in the FHP-II rules: All we have to do is to choose higher probability for the collisions with energy loss than with energy gain. However, if these rules are applied an unphysical effect occurs in a closed system under gravity: After some time all particles will be at rest but - since particles can only sit on the nodes - the volume of the system will increase when approaching this assymptote! This is just the opposite to what happens in a real granular system. The flow is related to dilatancy: Due to shear induced tensile stress the system expands when it starts to flow. (The physical reason for this effect is the simple fact that no flow can take place in *a* closely packed system).

In order to take into account this dilatancy effect we introduced rest particles on the bonds. As a result the number of particles at rest per node increased to 7 instead of 1. The particles can move only if they have space - just in reality, causing the desired dilatancy.

The table of collision rules is shown in Fig. 2. The inelasticity of the collisions is described by a parameter k, the probability that in a collision the inelastic output has to be chosen (and with probability $1-k$ the elastic one). Finally, static friction is taken into account in the following way. If two particles are at rest next to each other then gravity alone is not enough to let a particle to roll down: A collision with a moving particle is needed (Fig. 3). This rule violates conservation of momentum but this is legitimate since static friction is related to gravity and to the container in a dry granular medium. We do not consider here cohesion (wet sand).

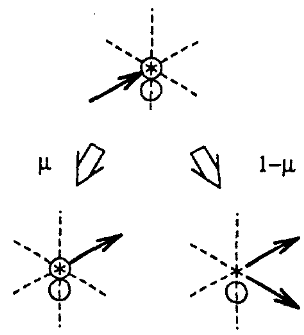

Figure 3: Rules corresponding to the static friction. The different final states are taken with the indicated probabilities a parameter.

These rules define the model we call granular medium lattice gas (GMLG) automaton. We have finally three parameters characterizing gravity, dissipation and static friction and the model is expected to describe both static limit and rapid flow phase of granular media. It should be noted that - as usual for HDLG models - the rules are not unique.

Of course, the number of states and therefore the possible collisions have increased as compared to the simple hydrodynamic case. However, multispin coding and parallelization still work and make the algorithm very efficient. For example, using a RISC-6000 it takes about 5 minutes to empty the 'hour glass' with 20 000 particles shown in Fig. 4. Note that on the workstation only the advantages of multi-spin coding could be utilized.

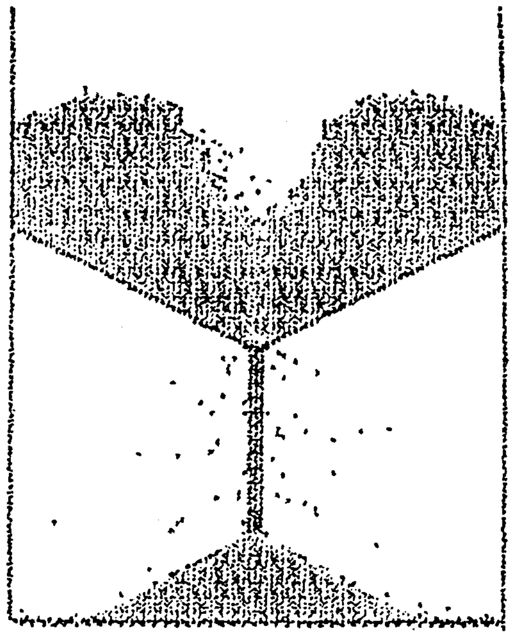

Figure 4: Simulation of granular material flowing out of a container.

Such a simplified model has its liinitations as well. There are only two values the velocity of a particle can take: 0 or 1. Therefore an isolated particle in gravitational field and in vacuum will behave unphysically because it is not accelerated without limits. This is usually not a serious problem because under flow conditions the particles are hindered in their motion by dissipative collisions with the wall and with each other. However, GMLG cannot be expected to describe the so called plug flow where in a vertical tube a part of the medium is accelerated by gravity in the middle of the tube.

As an illustration Fig. 4 shows a snapshot of a granular material flowing out of a conic container with a hole in the middle of the bottom ('hour glass'). It is clearly seen that the angle of repose (lower container) is different from the angle of stability (upper container). The angle of stability can be influenced by the parameters of the model while the angle of repose is given by the lattice symmetry. Many other geometries and physical situations have been sirnulated by the GMLG[7] and we consider the model as a promising alternative to molecular dynamics simulations.

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