Density Waves in Granular Flow

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Abstract: Ample experimental evidence has shown the existence of spontaneous density waves in granular material flowing through pipes or hoppers. Using Molecular Dynamics Simulations we show that several types of waves exist and find that these density fluctuations follow a 1/f spectrum. We compare this behaviour to deterministic one-dimensional traffic models. If positions and velocities are continuous variables the model shows self-organized criticality driven by the slowest car. We also present Lattice Gas and Boltzmann Lattice Models which reproduce the experimentally observed effects. Density waves are spontaneously generated when the viscosity has a nonlinear dependence on density which characterizes granular flow.

1 Introduction

As shown already in Daniel Bideau’s talk, moving dry granular media, like sand, show a rich variety of rather astonishing and scarcely understood phenomena [1,2]. Famous are the so-called “Brazil nut” segregation [3–5] and the heap formations that occur under vibrations [6–8]. A series of experiments have given evidence that under certain circumstances density patterns are generated inside the flowing medium. D. Bideau and collaborators, for instance, visualized wave-like patterns emanating from the outlet of a two dimensional wedge-shaped hopper. Also previous authors [9–12] had noted the formation of similar structures. Similarly rather erratic shock-like density waves have been observed in flow through pipes [13] and down inclined planes [14]. Another experimentally observed ubiquitous phenomenon in granular media seems to be 1/f noise. Baxter [15] also observed power law decay in the frequency dependent forces that act on the wall of a hopper. For avalanches going down the slope of a sand pile theoretical considerations of self-organized criticality [16] led to the proposal that their size and life time distributions were power laws which in fact only verified experimentally on very small piles [17].
We will present Molecular Dynamics simulations\cite{13,16} showing complex density patterns with a power law spectrum. Then we present traffic jam models\cite{19} showing similar behaviour. Finally we will reproduce the effects using a lattice gas with dissipation\cite{20} and a Boltzmann lattice model\cite{21}.

2 Molecular Dynamics simulations

We present Molecular Dynamics (MD) simulations of inelastic particles with static and dynamic friction in two dimensional systems\cite{13,18}. In fact, MD simulations \cite{22} have already been applied to granular media to model segregation \cite{6}, outflow from a hopper \cite{23,24}, shear flow \cite{25}, convection cells on vibrating plates \cite{26,27}, avalanches on a sand pile \cite{28} and others.

We consider a system of $N$ spherical particles of equal density and with diameters $d$ either all equal or chosen randomly from a Gaussian distribution of width $\sigma$ around $d_0 = 1$ mm. These particles are placed into a hopper having an opening angle $\theta$ and at the bottom an opening of diameter $D$. In the case $\theta = 0$ we have a pipe. 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

$$f^{(i)}_{e} = Y(\frac{1}{2}(d_i + d_j)) \frac{r_{ij}}{r_{ij}} , \tag{1a}$$

where $Y$ is the Young modulus and $r_{ij}$ points from particle $i$ to $j$; 2.) a dissipation due to the inelasticity of the collision

$$f^{(i)}_{diss} = -\gamma m_{eff} \langle v_{ij} \cdot r_{ij} \rangle \frac{r_{ij}}{r_{ij}} = -\gamma m_{eff} v_{ij}^0 , \tag{1b}$$

where $\gamma$ is a phenomenological dissipation coefficient and $v_{ij} = v_i - v_j$ the relative velocity between the particles; 3.) a shear friction force which in its simplest from can be chosen as

$$f^{(i)}_{shear} = -\gamma_s m_{eff} \langle v_{ij} \cdot t_{ij} \rangle \frac{t_{ij}}{t_{ij}} = -\gamma_s m_{eff} v_{ij}^t , \tag{2a}$$

where $\gamma_s$ is the shear friction coefficient and $t_{ij} = (-r_{ij}^x, r_{ij}^y)$ is the vector $r_{ij}$ rotated by $90^\circ$. Eq. 2a is a rather simplistic description of shear friction which is proportional to the relative velocity of the particles. In order to allow for static situations of blocking in a hopper due to arching it is important to include real static friction, i.e. which does not depend on the velocities but rather the relative angle of the surfaces \cite{29}. When two particles start to touch each other, one puts a "virtual" spring between the contact points of the two particles. Be $\delta s$ the total shear displacement of this spring during the contact and $k_s \delta s$ the restoring frictional force (static friction). The maximum possible value of the restoring force is then, according to Coulomb's criterion, proportional to the normal force $F_n$ multiplied by the friction coefficient $\mu$ \cite{5,29}. Cast into a formula this gives a friction force

$$f^{(i)}_{friction} = -\text{sign}(\delta s) \min(k_s m_{eff} \delta s, \mu F_n) \tag{2b}$$
where $\delta s$ is the shear displacement integrated over the entire collision time. When particles are no longer in contact with each other the spring is removed.

When a particle collides with a wall the same forces act as if it would have encountered another particle of diameter $d_0$ with infinite mass at the collision point. The walls are in fact made out of small particles themselves and in order to introduce roughness on the wall these particles are chosen randomly from a distribution of two radii. The only external force acting on the system is gravity $g \approx -10\text{m/s}^2$.

In fig. 1 we see a space-time diagramm of the density inside a pipe with 600 particles and periodic boundary conditions. The particles initially have homogeneously randomly distributed initial positions and velocities (left pipe). After some time spontaneously various patterns appear in the density: On one hand one has very dark regions, nearly constant in time. Then one sees black diagonal strips of constant velocity down the pipe. Finally there are also some lighter horizontal lines. We want to try in the following to explain these rather complex structures.

![Fig. 1: Vertical pipe plotted at regular time steps next to each other. Time goes from left to right. Gravity acts from top to bottom. For more details see ref. 13.](image)

Similar effects have also been observed in hoppers of opening angles of $\theta = 30^\circ$ and the density at a position six particles diameters above the outlet has been measured as a function of time. In fig. 2 we see the Fourier transformation of this density in a log-log plot. Clearly the data fall on a straight line over nearly two decades. The slope is about $\alpha = -1.35 \pm 0.1$ obtained by a least square fit. That means that we have a power law spectrum of the form $1/f^\alpha$. 
3 Traffic models

We have shown that similar to the avalanches that one observes on the surface of a sandpile also inside the bulk of granular material one has avalanche behavior which like the ones on the surface shows self-organized criticality on small scales \[16\]. The mechanisms that generate the patterns are similar but not identical to the original sandpile models. While the static friction similarly generates waiting times with a threshold it is not the motion of the sand itself that constitutes the avalanches but it is the group velocity of the holes between them: An individual particle can easily go from one dense region to the other by flying fast through a region of low density. There is therefore a backflow of information similar to the jamming on highways \[30\].

Everybody knows of the seemingly erratic motions of cars jammed on highways. One wonders whether they are due to a random behaviour of the individual drivers or if there is an intrinsic chaotic mechanism. In favour of the first hypothesis is the existence of regular kinematic waves in dissipative systems with excluded volume \[31\]. For this reason many traffic models include rather important statistical noise in time \[30\]. In favour of the second hypothesis are measurements performed on Japanese highways showing a 1/f spectrum in the Fourier transformed density fluctuations \[32\] which might stem from some self-organized criticality \[16\]. It is therefore interesting to see if a traffic model without noise is able to give the observed erratic behaviour and its 1/f spectrum.

In ref. 19 we consider a continuous one-dimensional model. The system has length \( L \) with periodic boundary conditions; and velocity \( v_i \) and position \( z_i \) of a vehicle \( i \) are continuous variables. The update rule is as follows:
If the velocity is high with respect to the gap, then the car slows down:

\[ v > \Delta z - \alpha \Rightarrow v \to \max(0, \Delta z - 1) \]  \hspace{1cm} (3a)

(the "max" is only necessary to prevent negative velocities);

else if the velocity is low with respect to the gap and slower than five, then the car accelerates:

\[ v < \Delta z - \beta \& v < v_{max} \Rightarrow v \to v + \min(1, \gamma \cdot \Delta z) \]  \hspace{1cm} (3b)

Note that this rule allows maximum speeds up to nearly six.

After the velocity has been updated for all vehicles according to the last two rules, we move all vehicles simultaneously by a distance equal to their velocities.

In our simulation we used \( \alpha = 0.5 \), \( \beta = 3.0 \), and \( \gamma = 0.1 \). We initially placed \( N = [\rho \cdot L] \) vehicles on sites 1 to \( N \), all with velocity zero, where \( \rho \) was chosen small enough to prevent the first car hitting the first one through the periodic boundary conditions. Starting from this totally ordered initial state, the system was allowed to evolve according to the above rules, with the exception of the first vehicle, the speed of which was kept fixed at \( v_{lead} = 4.99999 \) after its initial acceleration. This is a simplification of the well known situation where a number of fast vehicles follow a slower one which they cannot pass.

In Fig.3a we see the time evolution of a system which had been transformed to the coordinates of the first vehicle, i.e. the positions of all cars are given relative to the first car. We see that equally spaced cars rapidly evolve into a fluctuating state (right hand side). In this new state density increases give rise to very short bursts (traffic jams) of very different sizes which redistribute the cars backwards such that in some cases they even start again in equally spaced patterns.

In order to clarify that this behaviour is an intrinsic consequence of the dynamics and not just the enhancement of numerical round-off errors, we have compared single precision with double precision calculations. The behavior of the model (i.e. the formation of the collective shocks) is robust with respect to parameter changes. More precisely, we could not find a qualitatively different behavior for changes of the parameters \( \alpha, \beta, \gamma \), and \( v_{lead} \) within the following range \( 0.1 \leq \alpha \leq 0.6, 2.0 \leq \beta \leq 5.0, 0.08 \leq \gamma \leq 0.12, 4.5 \leq v_{lead} \leq 4.99999 \).

We measured the distribution of times \( \tau \) between consecutive "braking" events for the last vehicle (\( \tau \) is the time from the end of one braking to the beginning of the next). Braking is defined as a slowing down according to the rules for the velocity update. system sizes on up to 512 processors and averaging the results. For instance for \( N = 1900 \) vehicles, we waited about \( 3 \cdot 10^5 \) time steps to let the transients die out, and then measured the distribution of \( \tau \) during about \( 1.1 \cdot 10^6 \) further time steps. As seen in Fig. 3b, this distribution displays a remarkable straight line on a log-log plot, fulfilling a power law relation

\[ n(\tau) \propto \tau^{-\alpha} \]  \hspace{1cm} (4)
with $\alpha = -2.2 \pm 0.1$. This non-trivial exponent is a strong indication for the existence of self-organized criticality\cite{16} for this model.

Many aspects of this model are reminiscent of the so-called train model for earthquake dynamics\cite{35}. Instead of pulling at one end, the slower car may be seen as pushing against the other cars which want to move faster. This leads to a slowly increasing average density, and at some time this density locally exceeds a critical threshold. The reaction is a more or less drastic slowing down of the corresponding vehicle, which may or may not force the next vehicle to slow down as well. By this mechanism, avalanches of all sizes are generated, which may propagate through the entire traffic jam.

4 Lattice Gas and Boltzmann Models

It seems natural to describe the flow of granular media using the concepts of fluid mechanics. One must, however, consider that as opposed to classical fluids there is local dissipation of energy. Taking into account the dissipation rate in the energy balance equations it has been possible\cite{34,35} to predict the existence of an instability: Slightly denser regions have more dissipation and therefore lower pressure which itself generates a flow that will enhance the density. So, the dissipation will be responsible for the formation of clusters of high density and these have been observed\cite{34}. Also has it been possible to derive from this kinetic gas theory\cite{35–37} that the viscosity increases very sharply with density.
One alternative to the direct solution of the equations of motion of fluids are the so called Lattice Gas (LG)\textsuperscript{[38]} Lattice Boltzmann Models (LBM)\textsuperscript{[38]}. These models are defined on a lattice with velocity vectors that can only point into few discrete directions and all have the same length. For the LG this simplification is somewhat compensated by the fact that on each site one has more real degrees of freedom (six on a triangular lattice) than in the classical numerical techniques allowing for the definition of a local shear or a local rotation.

Let us first describe the Lattice Boltzmann Model as used in ref. 20. We consider a triangular lattice, and on each site $x$ we have six real variables $N_i(x, t), i = 1, \ldots, 6$, representing (counted counter clockwise) the densities of the particles going in the direction $i$ of the lattice. (For convenience we will in the following omit the site index $x$ and denote by $N_i$ the value of the particle density after collision.) One updating of the system ($t \to t + 1$) is given by two steps: (1.) The collision step at which the six $N_i$ are updated at each site through

$$N_i' = N_i + \lambda(N_i - N_i^{eq})$$  \hfill (5)

and (2.) the propagation step at which each $N_i$ is shifted to the site of the nearest neighbor in direction $i$. Eq. (5) produces a relaxation towards the equilibrium densities $N_i^{eq}$ which is numerical stable provided the relaxation constant $-2 < \lambda < 0$. The value of $\lambda$ sets the kinematic viscosity of the fluid. The equilibrium densities are given by

$$N_i^{eq} = \frac{\rho}{6}(1 + 2u \cdot c_i + 4(u \cdot c_i)^2 - 2u^2)$$ \hfill (6)

where $\rho$ is the mass density at site $x$

$$\rho = \sum_i N_i$$  \hfill (7)

c$_i$ the unity vector along direction $i$ and $u$ the velocity vector at site $x$ defined through the momentum density per site

$$\rho u = \sum_i c_i N_i$$  \hfill (8)

The equilibrium distribution $N_i^{eq}$ given in Eq. (6), is chosen to give mass and momentum conservation in the collision step. The flow will be forced into the direction of the gravity $g$, which is pointing parallel to the walls of the pipe. For that purpose an additional step is added after the collision step which is defined by $N_i'' = N_i' + \frac{1}{2}c_i \cdot (\rho g)$. Periodic boundary conditions are imposed in the direction of gravity in which the system has a length of $L_1$. In the perpendicular direction one has walls separated by $L_2$ lattice spacings. The lattice orientation is such that one of the lattice directions is parallel to the walls. At the beginning of the simulation the average density $\bar{\rho}$ is fixed. It is an important parameter of the model which because of mass conservation stays constant in time. We initialize the system by having the same values of the $N_i$ on each site and then let the system evolve to its steady state. In the case of the stable flows steady state is reached after 2000
or 3000 time steps. In the case of the unstable flows that develop density waves, the simulations might take up to 20000 time steps to reach steady state. At the walls we used no-slip conditions.

The relaxation parameter \( \lambda \) depends on the material properties including the kinematic and the bulk viscosities. Since an exact relation between \( \lambda \) and the material constants is not known we will lean on some approximative arguments\(^{(38)}\) that predict a vanishing bulk viscosity. In that case one can relate \( \lambda \) directly to the kinematic viscosity \( \nu \) through \( \lambda = -\frac{1}{2} (0.25 + 2 \nu)^{-1} \). We will consider that \( \nu \) is a function of the local density \( \rho \).

A salient feature of granular media is the spontaneous formation of density waves, similar to traffic jams on highways. One possibility to explain the effect that generates these waves is to assume that the viscosity depends on density. Within the kinetic gas theory of granular media\(^{(35\text{-}37)}\) the relation \( \nu \propto (\rho - \rho_c)^{1/3} \) has been derived. Since the above relation imposes a maximum density \( \rho_c \) it is rather difficult to implement it directly within the context of the LBM where the particles do not have an exclusive volume. We therefore chose a piecewise linear relation of the form \( \nu = \nu_{\text{min}} \) if \( \rho \leq \rho_t \) and \( \nu = \nu_0 + \gamma (\rho - \bar{\rho}) \) for \( \rho > \rho_t \) (see fig. 4a). \( \bar{\rho} \) is the average density and the threshold density \( \rho_t \) is chosen to make \( \nu \) a positive continuous function of the density.

![Graph showing density dependence of viscosity](image)

**Fig. 4.** (a), i.e. left: density dependence of the viscosity chosen in the simulations. (b), i.e. right: density in the center of the channel as a function of the position \( X \) along the channel for \( \rho_t = 2.862, \bar{\rho} = 3.0, \gamma = 3.33 \times 10^{-6} \) and \( L_2 = 64 \). The curve of crosses is for \( L_1 = 256 \) and 60,000 iteration steps after the initial perturbation. The other curves correspond to \( L_1 = 512 \) and 5000 (thick line), 60,000 (full line) and 60,025 (dashed line) iterations after the perturbation was applied. The slope \( \gamma = 6.25 \) and the minimum viscosity \( \nu_{\text{min}} = 0.01 \). (From ref. 20)

In order to generate density waves we found it necessary to introduce a small perturbation producing a 0.3% relative density difference. This perturbation was performed by introducing a small amount of momentum on one line across the pipe, keeping the mass unchanged. In fig. 4b we
see that this initially very weak perturbation dramatically builds up and develops into a density wave of over 10% density contrast. For a pipe of same width but half the length, i.e., a different aspect ratio the wave has a less pronounced profile. This dependence on the aspect ratio is not to be confounded with finite size effects.

By triggering the density wave by two spatially separated perturbations, rather than just a single one, we checked that the complex shape of the waves does not reflect the detailed way in which they were initiated. We also observe that there seems to be no characteristic wavelength: Fig. 4b shows that the waves have roughly the same shape on the scale of the channel length although the amplitude depends on the system size.

Fig. 5 shows this amplitude as a function of time during 60,000 time steps. The insert shows the initial unstable phase leading to the rather drastic increase of the amplitude at the time 10,000. The first small increase in the density is due to the acceleration of the flow and can be understood from the velocity dependence in the pressure. The small jump at the time 2500 results from the perturbation. Before the instability is triggered at the time 10,000, small oscillations in the amplitude are observed. It was checked that the amplitude indeed has its steady state value at the time 60,000 by running the simulations ten times longer. The complicated relaxation towards the fully developed density wave indicates that strong non-linear effects come into play rendering a linear stability analysis meaningless. It would be interesting to understand this behaviour further.

![Figure 5](image.png)

**Fig. 5.** The amplitude, i.e., difference between largest and smallest density, along the center of the pipe as a function of time measured in units of 100 iteration steps for \( L_1 = 256 \) and otherwise the same parameters as in fig. 4b. The insert is a blow-up of the behavior at early times. (From ref. 20)

A Lattice Gas model\[^{as}\] can be formulated such as to include local dissipation of energy by introducing rest particles and special collision rules. For all details we refer to ref. 21. In fig. 6 we
see the result for the power spectrum of the time evolution of the density in pipe flow. On top of a $1/f^\alpha$ spectrum with $\alpha = 1.33 \pm 0.02$ we see a peak which corresponds to kinematic waves. Its position depends on the length of the pipe.

![Log-log plot of the Fourier transformation of the density in a pipe of length 220 and width 11. The straight line is a least square fit with slope $-1.33 \pm 0.02$. (From ref. 21)](image)

5 Conclusion

We have observed in various modelizations that complicated density patterns are generated. In Molecular Dynamics simulations two ingredients were found\(^{18}\) essential to generate them: static friction and a large enough surface roughness of the walls. The static friction tends to align the particles, i.e. to form fronts of particles moving exactly with the same vertical velocity. These fronts are nucleated randomly at the walls and their size distribution (density contrast) goes by itself into a critical state namely a power law distribution. It therefore has the properties of self-organized criticality (SOC)\(^{16}\). Traffic jam models show\(^{16}\) similar behaviour due the same effect, namely local dissipation of energy. In a fluid picture, a Lattice Boltzmann model shows\(^{20}\) that the density dependence of the viscosity that one encounters in granular media generates waves of low density. A lattice gas model with local dissipation gives both, kinematic waves and SOC in the power spectrum.

Concluding, the following picture emerges: Due to the inelastic collisions between particles (also cars) an instability\(^{34,36}\) tends to form clusters of high density (probably, the dark horizontal stripes in fig. 1). These clusters self-organize into a critical state giving a power law spectrum. As in classical traffic models the density dependence of the flux generates kinematic waves (probably, the dark tilted lines in fig. 1). The density dependence of the viscosity as predicted by kinetic gas theory builds up waves of low density (probably, the light horizontal lines in fig. 1). We see that
simply introducing dissipation to a gas of particles produces many interesting phenomena, that occur in granular materials.

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References

1. Disorder and Granular Media eds. A. Hansen and D. Bideau (North-Holland, Amsterdam, 1992)
3. J.C. Williams, Powder Techn. 15, 245 (1976)
13. T. Pöschel, preprint HLRZ 89/92, J. de Physique, in press
14. D. Bideau, private communication
15. G.W. Baxter, PhD thesis
18. G. Ristow and H.J. Herrmann, preprint HLRZ 2/93


