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Towards a continuum theory of clustering
in a freely cooling inelastic gas

B. Meerson[1] and A. Puglisi[2]

[1] *Racah Institute of Physics, Hebrew University of Jerusalem - Jerusalem 91904, Israel*
[2] *Laboratoire de Physique Théorique (UMR 8627 du CNRS), Bâtiment 210*
Université de Paris-Sud - 91405 Orsay Cedex, France

Abstract. – We performed molecular-dynamics simulations to investigate the clustering instability of a freely cooling dilute gas of inelastically colliding disks in a quasi–one-dimensional setting. We observe that, as the gas cools, the shear stress becomes negligibly small, and the gas flows by inertia only. Finite-time singularities, intrinsic in such a flow, are arrested only when close-packed clusters are formed. We observe that the late-time dynamics of this system are describable by the Burgers equation with vanishing viscosity, and predict the long-time coarsening behavior.

Introduction. – A gas of hard spheres is a standard model of statistical physics and kinetic theory [1]. It is surprising that a minor change in this model —the introduction of energy loss in the binary collisions— leads to consequences so dramatic. Among the many fascinating properties of the gas of *inelastically* colliding hard spheres [2], the clustering instability [3,4] plays a special role. No matter how small (but finite) is the inelasticity of collisions, the homogeneous cooling state (HCS) of this gas is always unstable if the system size L is large enough. When studying macroscopic properties of matter, a physicist deals, first of all, with the thermodynamic limit $L \to \infty$. From this perspective the gas of *elastically* colliding hard spheres is a singular limit of the inelastic gas problem. The practical importance of the inelastic gas model stems from its being the simplest model of granular flow [2,5,6].

The clustering instability of a freely cooling inelastic gas involves the formation of clusters of particles and the generation of vortices [3,4,7]. The basic physics of the initial stage of cluster formation is simple: the inelastic cooling of the gas causes a pressure drop in the regions of enhanced density. This pressure drop drives an inflow of gas from the periphery and therefore provides a positive feedback to the instability. A traditional framework for quantitative theory here is *granular hydrodynamics* (GH), which assumes scale separation and is derivable from the Boltzmann equation, properly modified to account for the inelasticity of collisions [2]. Though the general criteria of its validity remain controversial [8], GH is well established at least when the following two criteria are met: i) the granular gas is dilute, $n\sigma^D \ll 1$, and ii) the particle collisions are nearly elastic, $q \ll 1$. Here n is the local number

density of the gas, σ is the particle diameter, $D > 1$ is the dimension of space, $q = (1 - r)/2$ is the inelasticity of collisions, and r is the coefficient of normal restitution (assumed constant throughout this paper). In this case the GH equations, linearized around the HCS, provide an accurate theory of the initial stage of the instability in terms of the (linear) hydrodynamic modes of the system: the shear mode (spontaneous formation of vortices) and the entropy, or clustering mode (formation of clusters) [3, 4, 7].

The further evolution of the instability is a hard problem. One difficulty here is technical, as the growing nonlinear shear and clustering modes become strongly coupled. Another difficulty is conceptual: GH breaks down in high-density regions. All previous attempts to develop a theory beyond linearization of the GH equations attempted to circumvent these difficulties. Ben-Naim *et al.* [9] considered *point-like* particles inelastically colliding on a *line*. This strictly one-dimensional (1D) geometry makes a GH description problematic [8]. Still, Ben-Naim *et al.* observed that, at long times, the 1D system is describable by the Burgers equation with vanishing viscosity. Ernst *et al.* [10] considered a small two-dimensional (2D) system, where the entropy mode is suppressed, and dealt with the unstable shear mode. Baldassarri *et al.* [11] also studied the instability of the velocity field in a homogeneous gas, by introducing a lattice model.

Focusing on the entropy, or clustering, mode, Efrati *et al.* [12] had the shear mode suppressed, by working with a *quasi*-1D setting, see below. They solved numerically the low-density GH equations and found that, as the unstable system cools down, the shear stress becomes negligibly small, and a *flow by inertia* sets in. Formally, this flow develops a finite-time singularity: the velocity gradient and the gas density diverge at some location. Efrati *et al.* argued that the flow by inertia is an important intermediate stage of the clustering instability. However, they did not address still later stages of the instability, when finite-density effects come into play. We report here the first MD simulations which probe the quasi-1D clustering of a dilute inelastic gas. We find that the simulated low-density stage of the clustering instability is in excellent agreement with the hydrodynamic predictions of ref. [12]. What happens at later times? We observe that the attempted singularities are arrested only when hexagonally packed clusters are formed. The still later dynamics are describable by the Burgers equation with vanishing viscosity, in a striking analogy with the purely 1D result by Ben-Naim *et al.* [9]. Based on this observation, we predict the very-late-time coarsening dynamics of the system, all the way to its simple final steady state.

Model system and clustering instability. –   Consider an assembly of N identical hard disks of mass $m = 1$, diameter $\sigma = 1$, and inelasticity $0 < q \ll 1$ in a 2D box with dimensions L_x and L_y ($L_x \gg L_y$). The initial number density of the gas $n_0 = N/(L_x L_y)$ is very small compared to the hexagonal close-packing density $n_c = 2/(\sqrt{3}\sigma^2) \simeq 1.155$. The initial particle velocity distribution is Gaussian with temperature $T_0 = 1$. The parameters are chosen so that the low-density GH equations [5] are accurate until relatively late times, when the local value of $n\sigma^2$ is not a small parameter anymore. The boundary conditions are periodic at $x = 0$ and $x = L_x$ and elastic (specular reflection) at $y = 0$ and $y = L_y$. Assuming a homogeneous cooling, one arrives at Haff's law [5] $T(t) = T_0(1 + t/t_0)^{-2}$, where $t_0 = (2\pi^{1/2}\sigma n_0 q T_0^{1/2})^{-1}$ is the characteristic cooling time. The GH equations, linearized around the HCS, show that the HCS is unstable if L_x and/or L_y are large enough [3, 4, 7]. The density perturbations grow in time algebraically. The temperature and velocity perturbations decay, but the decay rates are smaller than that described by Haff's law. As a result, the flow tends to become supersonic [7]. A strong quasi-1D instability requires two criteria: $\sigma n_0 L_x q^{1/2} \gg 2\pi^{1/2}$, and $\sigma n_0 L_y q^{1/2} \ll \pi^{1/2}$; the latter one guarantees suppression of the shear and clustering modes in the y-direction [3, 4, 7, 12].
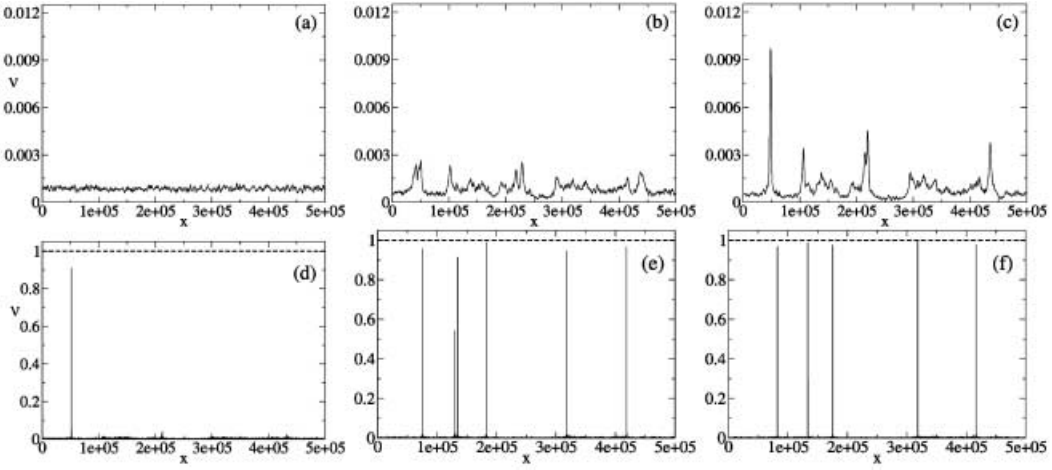
Fig. 1 – The local area fraction $\nu(x,t) = n(x,t)/n_c$ at times 0 (a), 274 622 (b), 549 554 (c), 771 055 (d), 2.14972×10^6 (e), and 2.53252×10^6 (f).

Flow by inertia. – We performed extensive event-driven MD simulations in this regime of parameters. We verified that no structure in the y-direction appears, as expected. Therefore, our diagnostics focused on 1D coarse-grained fields: the density $n(x,t)$, the mean velocity $\boldsymbol{v}(x,t) = (v_x, v_y)$ and the x and y components of the velocity fluctuations: $T_x(x,t)$ and $T_y(x,t)$. We report here a typical simulation with $N = 12500$, $q = 0.04$, $L_x = 5 \times 10^5$ and $L_y = 25$. The initial gas density is $n_0 = 10^{-3}$, while $t_0 \simeq 7.05 \times 10^4$. Strong clustering instability is clearly seen in fig. 1, which exhibits formation of multiple clusters, and fig. 2, which shows an inflow of gas into the forming clusters. Meanwhile, the gas temperature $T = T_x + T_y$ (not shown) rapidly decays with time. Throughout the simulated dynamics, T_x
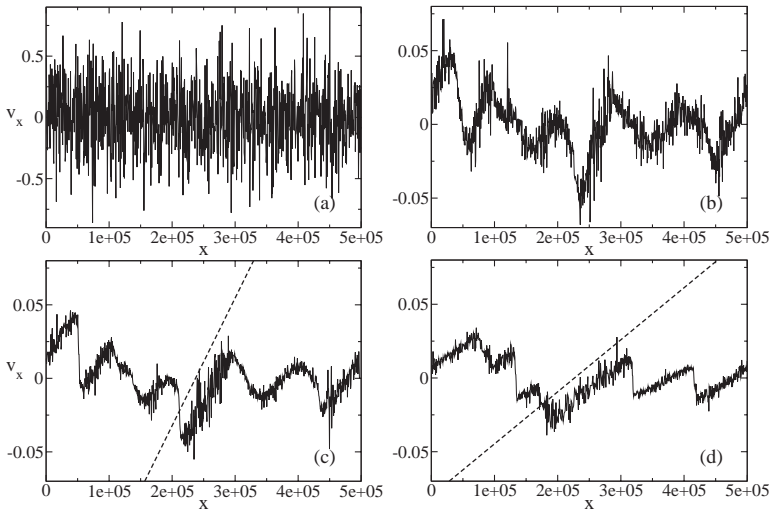

Fig. 2 – The horizontal velocity profiles at times 0 (a), 274 622 (b), 771 055 (c), and 2.53252×10^6 (d). The straight lines in (c) and (d) have a slope $1/(t + C)$, where $C = 3.8 \times 10^5$.
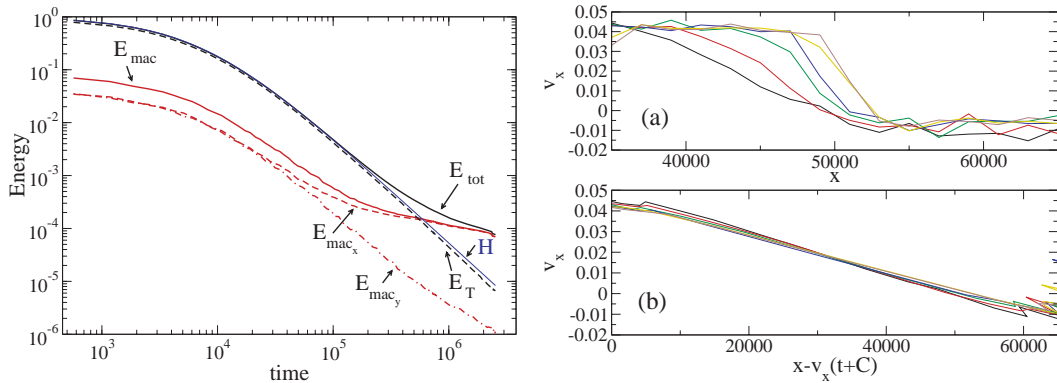
Fig. 3 – Left: the energy balance of the system *vs.* time. E_{tot} is the average kinetic energy of the particles, E_T is the average thermal energy, and E_{mac} is the average energy of the macroscopic motions. Haff's law is indicated by H. Right: the horizontal velocity profiles in a region around the leftmost peak. Shown are (a) v_x *vs.* x and (b) v_x *vs.* $x - (t + C)\,v_x(x, t)$ at times 294518, 410692, 549554, 636990, 658371, 680869 and 701507 with $C = 3.8 \times 10^5$.

and T_y remain close to each other, while their spatial inhomogeneity is small compared to the strong inhomogeneity of v_x and n.

The average particle energy *vs.* time, $E_{tot}(t)$, follows Haff's law at early times, but deviates from it at later times, when strong hydrodynamic motions develop, see fig. 3 (left). In the hydrodynamic description $E_{tot}(t) = (n_0 L_x)^{-1} \int_0^{L_x} (E_T + E_{mac})\,\mathrm{d}x$, where $E_T = nT$ is the thermal energy density, and $E_{mac} = nv^2/2 \equiv n(v_x^2 + v_y^2)/2$ is the macroscopic kinetic energy density. The role of each term is elucidated in fig. 3. Both $E_T(t)$, and $E_{mac}(t)$ initially decay; $E_T(t)$ decays faster. At later times $E_T(t)$ and the y-component of $E_{mac}(t)$ continue to decay rapidly, while the x-component of $E_{mac}(t)$ decays much slower. As a result, $E_{tot}(t)$ is dominated by E_T at early times and by the x-component of $E_{mac}(t)$ at later times. Remarkably, $E_T(t)$ continues to follow Haff's law quite closely until the latest simulated times.

Figure 4a shows the time history of a typical cluster (the leftmost density peak in fig. 1c-f). The rapid density growth is saturated when n_{max} approaches n_c. A snapshot of the density peak region (fig. 5) indeed shows almost perfect hexagonal packing. The rapid density growth is shown in more detail in fig. 4b which depicts $1/n_{max}$ *vs.* time. The linear dependence, observed at intermediate times, indicates an "attempted" finite-time singularity $n_{max} \sim (\mathrm{const} - t)^{-1}$. The same density singularity was observed in hydrodynamic simulations [12]; it is caused by a flow by inertia which develops when the forces acting on a fluid element vanish. The reason for it in the freely evolving inelastic gas is the continued rapid cooling, which makes the pressure and viscous stresses negligible [12]. The flow-by-inertia equations read

$$\frac{\partial v_x}{\partial t} + v_x \frac{\partial v_x}{\partial x} = 0, \tag{1a}$$

and

$$\frac{\partial n}{\partial t} + \frac{\partial (n v_x)}{\partial x} = 0. \tag{1b}$$
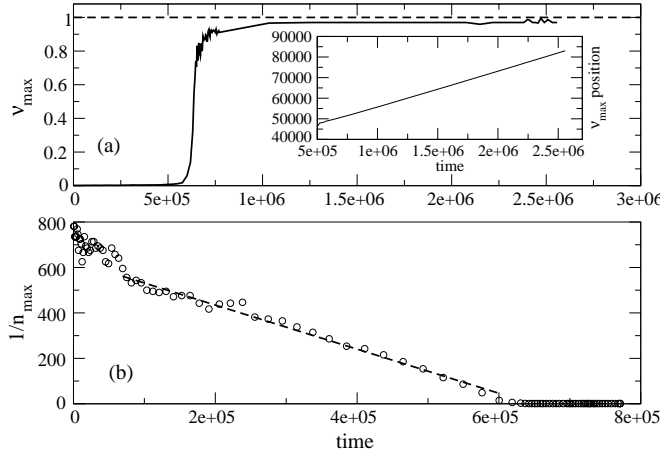
Fig. 4 – Evolution of the leftmost peak in fig. 1f. (a) shows ν_{max} vs. time. (b) shows n_{max}^{-1} vs. time and a linear fit. The inset shows the x-coordinate of the peak vs. time.

These equations are soluble analytically in Lagrangian coordinates [13, 14]:

$$v_x(x,t) = v_0(\xi), \tag{2a}$$

$$n(x,t) = \frac{n_0(\xi)}{1 + (t+C)\,v_0'(\xi)}, \tag{2b}$$

where C is an arbitrary constant, $v_0'(\xi) \equiv \mathrm{d}v_0(\xi)/\mathrm{d}\xi$, while $v_0(\xi)$ and $n_0(\xi)$ are the v_x and n, respectively, at the "initial" moment of time $t = -C$. The relation between Eulerian coordinate x and Lagrangian coordinate ξ is $x = \xi + v_0(\xi)\,(t+C)$. The finite-time singularities of both the velocity gradient, and the density occur when the denominator in eq. (2b) vanishes for the first time; it requires $v_0'(\xi) < 0$.

The results of our MD simulations quantitatively agree with the flow-by-inertia scenario. Using in eq. (2b) the straight-line fit, shown in fig. 4b, we obtain $C \simeq 3.8 \times 10^5$ and $|v_0(\xi_*)| \simeq 1.0 \times 10^{-6}$, where ξ_* is the Lagrangian coordinate of the density peak. Now we verify eq. (2a)
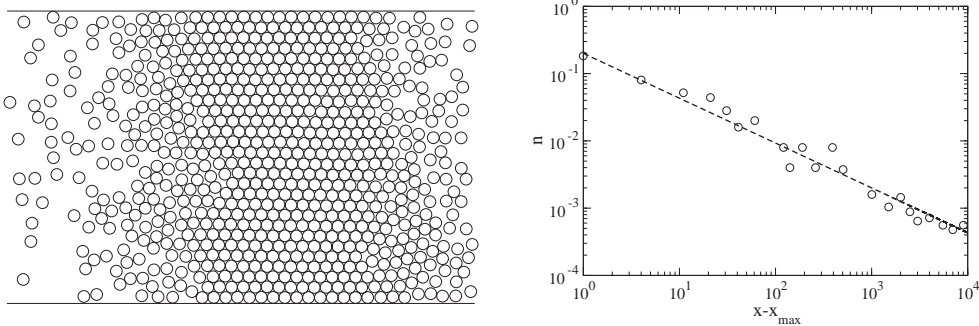

Fig. 5 – Left: a snapshot of the system in the region of the leftmost peak at time 771 055. Right: the right tail of the density peak close to the time of attempted singularity. Shown is the log-log plot of the density profile n of the leftmost density peak vs. $x - x_{max}$ at time 732 951. The dashed line is a power law $0.2 \times (x - x_{max})^{-2/3}$.

by observing (see fig. 3 (right)) the collapse of $v_x(x,t)$ *vs.* $\xi = x - (t+C)\,v_x(x,t)$, at different times, in the region of the leftmost density peak. The slope of the obtained straight line yields an independent estimate of $|v_0(\xi_*)|$ which agrees within 3 percent with the value of 1.0×10^{-6} found earlier. Still another prediction deals with the shape of the density peak close to the time of attempted singularity. The flow-by-inertia theory predicts a density profile $n \sim |x - x_{max}|^{-2/3}$ [14]. The simulations confirm this prediction, see fig. 5 (right).

As we observed, the density growth in the clusters is suppressed only when the density approaches n_c. At a fixed temperature, the pressure of an assembly of nearly elastic hard spheres diverges like $(n_c - n)^{-1}$ as n approaches n_c. Is there a pressure "revival" at $n \to n_c$? We used the empiric relation $p = nT(n_c + n)/(n_c - n)$, which interpolates between the dilute limit and the close-packing limit [15], to calculate the pressure field $p(x,t)$. We found that, though n_{max} approaches n_c, $p(x,t)$ continues to decay with time, apparently because of the very rapid temperature decay. Therefore, the pressure revival mechanism can be ruled out.

The Burgers model. – As the system approaches close packing it gets jammed. Faster particles cannot overrun slower ones, and the singular growth of the velocity gradient and density is arrested. A natural continuum model for a jammed flow is the Burgers equation [13]

$$\frac{\partial v_x}{\partial t} + v_x\,\frac{\partial v_x}{\partial x} = \nu\frac{\partial^2 v_x}{\partial x^2} \tag{3}$$

in the limit of vanishing viscosity $\nu \to 0$, together with the continuity equation (1b). We shall call this model "the Burgers model". Equation (3) is soluble exactly by the Hopf-Cole transformation [16,17]. The zero-viscosity limit of the solution, which is the subject of our interest, has the following properties. The solution is *identical* to that predicted by the flow-by-inertia model until the time moment when the flow by inertia would have developed a singularity. The attempted singularity gives way, in the Burgers model, to a "shock": a jump in the velocity field which carries a density peak (cluster). In this coarse-grained description, the close-packed clusters have zero sizes but finite masses. At long times, when the shocks have "matured" [17], the quantitative predictions of the Burgers model are especially simple and can be conveniently tested in our MD simulations. One prediction is that $\partial v_x/\partial x$ is equal to $1/(t+C)$ everywhere between the shocks, where C is the same constant ($\simeq 3.8 \times 10^5$ in the reported simulation) as above. This prediction is tested in fig. 2c and d. While the agreement in fig. 2c is only fair (as the shocks have not yet matured), it improves considerably in fig. 2d. Another prediction that we verified (see the inset of fig. 4a) is that each shock moves with a constant speed until it collides with another shock. Furthermore, a collision between two shocks leads to their merger, without any thermalization of the system. Such a merger event can be seen in the left part of figs. 1e and f. Finally, we verified that the zeros of v_x, belonging to the "ramps", stay at rest as expected [17].

Late-time coarsening dynamics. – Event-driven MD simulations become very slow once the hexagonal close packing in the clusters is achieved. Fortunately, the times reached in our simulations were large enough to have verified the Burgers model as a proper late-time continuum model of the quasi-1D clustering process. Therefore, we can give a detailed prediction of the still later *coarsening* dynamics of the system, without a need to simulate it. If the number of clusters is large, the coarsening dynamics, which proceed via cluster mergers, can be addressed statistically. At this level of description the problem coincides with that of the decaying Burgers turbulence [16,17], or the ballistic agglomeration model [18]. For uncorrelated initial conditions, the average cluster mass grows with time like $t^{2/3}$, the average velocity decreases like $t^{-1/3}$, and the average distance between two neighboring clusters grows like $t^{2/3}$ [18]. This

yields a long-time asymptotic scaling law $E_{tot} \simeq E_{v_x} \sim t^{-2/3}$. At this stage, E_{tot} is dominated by the kinetic energy of the clusters. The energy decay stops when an ultimate steady state of the system is reached: a single "super-cluster", moving with a small constant speed (which can be determined from the initial data, by employing the momentum conservation in the x-direction and assuming that *all N* particles are absorbed by this super-cluster).

Summary and discussion. – Our MD simulations fully support the hydrodynamic flow-by-inertia scenario [12]. The attempted singularities of this flow are suppressed when almost perfect hexagonally packed clusters are formed. At still later times the dynamics are describable by the Burgers equation with vanishing viscosity, in a striking analogy with the purely 1D results by Ben-Naim *et al.* [9]. Therefore, clustering instability in a quasi-1D setting is now well understood. What about a fully multi-dimensional geometry? It has been conjectured that, prior to the first attempted singularity, the system should be describable by a *multi-dimensional* flow-by-inertia model [12]. One can expect that an interplay between vorticity, produced during the early stage of the instability, and jamming provides a saturation mechanism for the multi-dimensional singularities. Unfortunately, the multi-dimensional Burgers model [16,17] assumes a potential velocity field and misses the important physics, caused by the presence of vorticity. The formulation of a continuum model free of this flaw should be the next step of theory.

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