RAPID COMMUNICATIONS

PHYSICAL REVIEW E VOLUME 50, NUMBER 3 SEPTEMBER 1994

Onset of convection in molecular dynamics simulations of grains

S. Luding,[1] E. Clément,[2] A. Blumen,[1] J. Rajchenbach,[2] and J. Duran[2]

[1]*Theoretische Polymerphysik, Universität Freiburg, Rheinstraße 12, D-79104 Freiburg, Germany*

[2]*Laboratoire d'Acoustique et d'Optique de la Matière Condensée, URA 800, Université Pierre et Marie Curie 4, place Jussieu, 75005 Paris, France*

(Received 28 March 1994)

We investigate granular materials undergoing vibrations, using a molecular dynamics (MD) algorithm, and we display limitations of the numerical method. We show that previously reported convection patterns obtained through MD may be due to the microscopic interactions. MD calculations often use parameters which lead to unphysically large contact times between beads and to large density fluctuations. These in turn enhance the appearance of convection rolls, a numerical finding without experimental counterpart.

PACS number(s): 46.10.+z, 05.60.+w, 05.40.+j

Recently, experiments have evidenced the appearance of convection rolls in granular materials when these substances undergo vertical vibrations. Convection appears both in three-dimensional (3D) systems [1–3] and in 2D model media [4].

On the other hand, in numerical molecular dynamics (MD) simulations several groups, working independently, have found convection under vibration as well as heaping [5–11]. Most MD simulations follow closely methods developed in the study of fluid dynamics [12–15]; an alternative are event driven (ED) algorithms [16–20].

Interestingly, convection was found when besides large friction with the walls one uses microscopic interactions of viscoelastic type [5–7]. Now viscoelastic interactions were found to lead in MD simulations to anomalously small energy dissipation in 1D and 2D [21,22]; this effect persists even when the pair interactions are strongly dissipative and also when the number of particles gets to be large. The main feature of the observed effect (called "detachment effect" in Ref. [22]) is the appearance of large density fluctuations.

In this work we focus on linear microscopic interactions, i.e., a linear spring with a linear dashpot, and determine the magnitude of the convection as a function of the parameters of the model. We show that in the simulations the convection patterns may disappear when the contact time t_c between colliding particles is close to its physical value. Thus the convection rolls reported previously may be due to the unphysically large t_c values, which also lead to the detachment effect. In the MD simulations presented here we follow the dynamics of a system of N spherical particles, all having the same diameter d_0. The particles are put in a container of width $L=13d_0$ and infinite height. The container carries out a sinusoidal motion, $z_0(t)=A_0\sin(\omega t)$. In the MD calculation a fifth order predictor-corrector algorithm is used [7,12]. Two particles (or a particle and a wall) interact when their relative distance $r_{ij}=|\mathbf{r}_{ij}|$ (where $\mathbf{r}_{ij}$ points from the center of i to the center of j) is smaller than the sum of their radii (the radius of the particle). In this regime ($r_{ij}<d_0$) three forces are considered. First, an elastic restoration force:

$$\mathbf{f}_{\rm el}^{(i)}=-K[d_0-r_{ij}]\mathbf{n}_{ij}, \tag{1}$$

where $\mathbf{n}_{ij}=\mathbf{r}_{ij}/r_{ij}$ is the normal direction of contact and K is the spring constant. Second, a force in the normal direction:

$$\mathbf{f}_{n}^{(i)}=-D_n m_0[\mathbf{v}_{ij}\cdot\mathbf{n}_{ij}]\mathbf{n}_{ij}, \tag{2}$$

where m_0 is the mass of the particles, $\mathbf{v}_{ij}$ is the relative velocity of particles i and j, and D_n is the normal dissipation parameter. Third, a force in the tangential direction:

$$\mathbf{f}_{t}^{(i)}=-D_t m_0[\mathbf{v}_{ij}\cdot\mathbf{t}_{ij}]\mathbf{t}_{ij}, \tag{3}$$

where $\mathbf{t}_{ij}=(-n_{ij}^{y},n_{ij}^{x})$ is the vector $\mathbf{n}_{ij}$ rotated by 90° and D_t is the tangential dissipation parameter. In the MD simulations reported here we neglect the rotations of the grains.

Note that the forces in Eqs. (2) and (3) are of viscous type (they depend on the velocity) and hence Eq. (3) does not follow the solid friction behavior (the Coulomb law), for which proportionality to the force normal to the surface of contact is found.

Now following the procedure of Refs. [5,7] we show that the convection stems mostly from the excessive density fluctuations which occur under the interactions described by Eqs. (1)–(3). For a central collision, from Eqs. (1) and (2) the positive penetration $x=d_0-r_{ij}$ along the line connecting the centers of the particles obeys the *linear* differential equation:

$$\ddot{x}+2\mu\dot{x}+\omega_0^2 x=0, \tag{4}$$

where in terms of the reduced mass $m=m_0/2$, of the dashpot constant D_n and of the spring constant K, one has $\omega_0=\sqrt{K/m}$, and $\mu=D_n$ ($\mu=D_n/2$ for the perpendicular collision of one particle with a wall). For two colliding particles, the contact time is

$$t_c=\pi/\sqrt{\omega_0^2-\mu^2}, \tag{5}$$

a quantity independent of the initial relative velocity v_0 [5,23,24]. From t_c one obtains the coefficient of restitution ε as being

$$\varepsilon=-\dot{x}(t_c)/v_0=e^{-\mu t_c}=e^{-\mu\pi/(\omega_0^2-\mu^2)^{1/2}}, \tag{6}$$

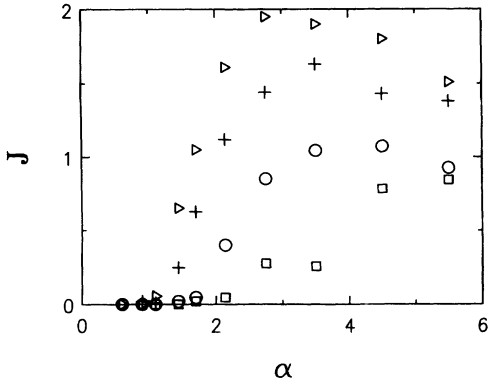

FIG. 1. The convection strength J, Eq. (8), as a function of α. The parameters used are $g=10\ \mathrm{m\,s^{-2}}$, $N=100$, $\varepsilon=0.9$, $d_0=2$ mm, $L=13d_0$, and $A_0=1.1d_0$. The contact times t_c are 0.141 cs (triangles), 0.1 cs (crosses), 0.0316 cs (circles), and 0.003 16 cs (squares).

where v_0 is the relative velocity before collision. Note that here ε is also independent of v_0.

We focus on the role of t_c, especially since it turns out to be fundamental for the onset of convection. Note that for two steel beads ($\varepsilon=0.9$, $d_0=2$ mm) colliding with a relative velocity of $v_0=0.1\ \mathrm{m\,s^{-1}}$ the contact time is roughly $t_c=10^{-5}$ s [22]. A major finding in the results [5,7], which displayed convection rolls based on MD simulations, was that rolls are created due to the large friction between the beads and the lateral boundaries. An important parameter of the problem is the dimensionless acceleration $\alpha=A_0\omega^2/g$. Here A_0, ω, and g are the amplitude, the angular frequency, and the gravitational acceleration, respectively. Thus Taguchi finds in his MD simulations as a threshold for the onset of convection α between 0.9 and 1.2 [5]; this compares rather well with the experimental finding of $\alpha=1.2\pm0.1$ [1]. In his analysis of convection Taguchi stresses the importance of the viscoelastic properties, exemplified by Eqs. (2) and (3). Here we follow this idea, and show that convection is related to large contact times t_c (for ε constant).

In the following we present results of MD simulations; the system consists of $N=100$ particles with restitution coefficient $\varepsilon=0.9$. To facilitate the connection to Ref. [5] we use the same units: the length is then given in units of 1 mm and the time in units of 0.01 s=1 cs. We set $g=10\ \mathrm{m\,s^{-2}}=1\ \mathrm{mm/(cs)^2}$, $d_0=2$ mm and $A_0=0.55d_0=1.1$ mm. We vary t_c between 0.003 16 and 0.316 cs (i.e., from a realistic value to a value two orders of magnitude larger). With these ε and t_c, K/m_0 in Eq. (1) obeys $49.35\ (\mathrm{cs})^{-2} < K/m_0 < 493\,500\ (\mathrm{cs})^{-2}$; furthermore, one also has in Eqs. (2) and (3) $0.333\ (\mathrm{cs})^{-1} < \tilde{D}_n = \tilde{D}_t < 33.3\ (\mathrm{cs})^{-1}$. We take as dissipation parameters $\tilde{D}_n$ and $\tilde{D}_t$ for the interactions between the particles and the lateral walls $\tilde{D}_n=20\tilde{D}_n$ and $\tilde{D}_t=20\tilde{D}_t$.

To monitor the onset of convection we use the order parameter J introduced by Taguchi [5]. For this the container is divided into squares of sidelength 2 mm (this corresponds to the spheres' diameter). Now one counts the number of particles coming into (or going out of) the cell centered at $\vec{r}$, and averages with respect to time:

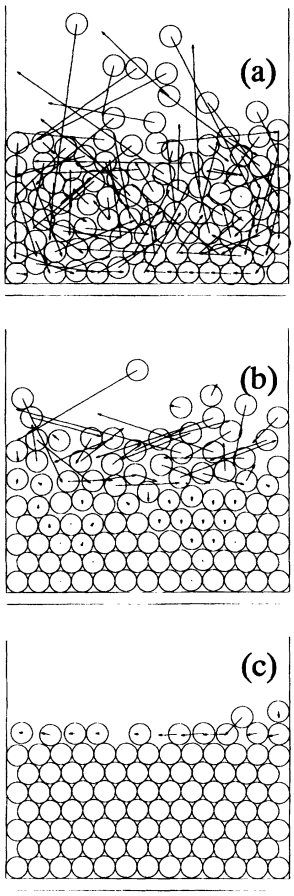

FIG. 2. (a) Plot of the particle distribution and the displacements for $g=10\ \mathrm{m\,s^{-2}}$, $N=100$, $\varepsilon=0.9$, $d_0=2$ mm, $L=13d_0$, $A_0=1.1d_0$, and $\alpha=2$. Here $t_c=0.222$ cs. (b) Parameters as in (a). Here $t_c=0.1$ cs. (c) Parameters as in (a). Here $t_c=0.01$ cs.

$$\langle \vec{J}(\vec{r})\rangle = \left\langle \sum_{i=1}^{N} \tfrac{1}{2}\left|\delta(\vec{x}_i(t)-\vec{r})-\delta(\vec{x}_i(t-\Delta t)-\vec{r})\right| \times\{\vec{x}_i(t)-\vec{x}_i(t-\Delta t)\}\right\rangle_t . \tag{7}$$

Here $\vec{r}$ denotes the (integer) coordinates of the cell considered; $\vec{x}_i(t)$ is the (integer) coordinate of the cell which contains the center of particle i at time t. Thus $\delta(\vec{x}_i(t)-\vec{r})$ equals 1, if particle i is at time t in cell $\vec{r}$, and 0 otherwise. In Eq. (7) the term between absolute value signs equals zero for the particles which during Δt did not change their cells; it equals unity for the particles which have changed their cell between times $t-\Delta t$ and t. The brackets indexed with t denote the temporal averaging. We now define J, the overall strength of convection, through

$$J=\left(\sum_{\vec{r}} \vec{J}(\vec{r})^2\right)^{1/2} . \tag{8}$$

A plot of J vs α is given in Fig. 1 for different t_c. Here we

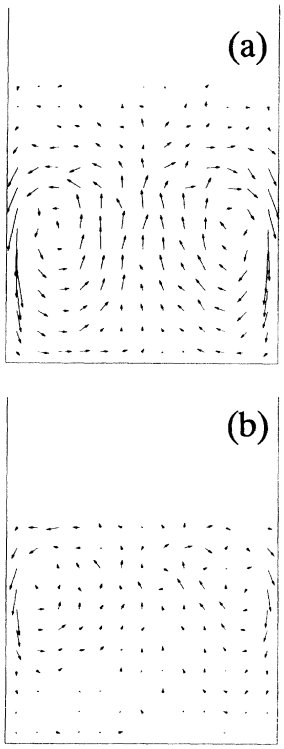

FIG. 3. (a) Plot of $\vec{J}(\vec{r})$, Eq. (7), for the simulations shown in Fig. 2(a). (b) Plot of $\vec{J}(\vec{r})$, Eq. (7), for the simulations shown in Fig. 2(b).

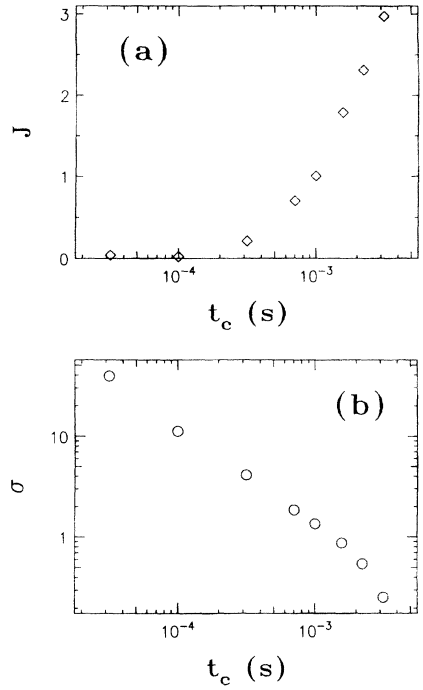

FIG. 4. (a) The convection strength J as a function of t_c for $g=10\ \mathrm{m\,s^{-2}}$, $N=100$, $\varepsilon=0.9$, $d_0=2$ mm, $L=13d_0$, $A_0=1.1d_0$, and $\alpha=2$. Here t_c varies between 0.003 16 cs and 0.316 cs. (b) Plot of σ as a function of t_c for the same parameters as in (a).

average over 180 vibration periods and the error bar on J is of the order of a symbol size. Note that J is in general an increasing function of α. For quite large α J decreases again, a fact due to the decrease in the particles' density. We focus on the onset of convection. Of interest are here moderate values of α. We find that for large t_c convection starts for α around unity (as found by Taguchi [5,25]) whereas for small t_c, i.e., closer to the physical situation, the onset of convection is above $\alpha=2$. Furthermore, the strength of the convection decreases with decreasing t_c. To visualize this statement we present in Figs. 2(a)–2(c) simulations performed at constant α and ε ($\alpha=2$, $\varepsilon=0.9$), while t_c varies: we use $t_c=0.222$ cs (a), 0.1 cs (b), and 0.01 cs (c). We display by arrows the displacements of the particles after 10 vibration periods (at phase 0); the initial positions are given by circles. Figure 2(a) shows convection in the whole volume, Fig. 2(b) only in the upper half, and Fig. 2(c) only some motion in the uppermost layer. Paralleling Figs. 2(a) and 2(b) we plot in Figs. 3(a) and 3(b) the field $\vec{J}(\vec{r})$. The average is taken over 180 vibration periods; for convenience of presentation the length of the arrows was increased by a factor of 4. Again, for decreasing t_c we find decreasing convection. An analogous figure to 2(c) shows no convection; we restrain from presenting it here.

An explanation for the dependence of J on t_c may be found in terms of the detachment effect. When the mean separation between the beads is very small, there is the possibility of multiple collisions and/or contacts between more than two beads within time intervals of the order of t_c. An indicator for this possibility is the ratio σ between the typical free-flight time and t_c:

$$\sigma=s_0/(v_0 t_c). \tag{9}$$

Here s_0 is the mean separation between the beads. The main result of Ref. [22] was that when $\sigma\gg 1$ the simulation results (MD and event driven, ED) agree quite well with each other and with experiments in 1D. For $\sigma\ll 1$, on the other hand, MD simulations show spurious effects, not found otherwise: one observes weak dissipation and large separations (detachment) between the grains.

In Eq. (9) s_0 may be approximated through the mean free path $s_0\approx(h_{\mathrm{c.m.}}-h_{\mathrm{c.m.0}})L/(Nd_0)$ [here $2(h_{\mathrm{c.m.}}-h_{\mathrm{c.m.0}})L$ is the average free volume and $2d_0$ is the cross section of hard spheres in 2D]; v_0 is a typical relative velocity, say $v_0=\sqrt{\langle v^2\rangle}$. Thus σ is determined using

$$\sigma=\frac{(h_{\mathrm{c.m.}}-h_{\mathrm{c.m.0}})L}{Nd_0v_0t_c}, \tag{10}$$

where $h_{\mathrm{c.m.}}$ is the height of the center of mass and $h_{\mathrm{c.m.0}}$ is the height of the center of mass at rest.

We argue that the observed convection is related to high t_c values (and small σ values). To justify this we give in Fig. 4 results obtained for $N=100$, $\varepsilon=0.9$, $\alpha=2$, and $A_0=0.55d_0=1.1$ mm. In Figs. 4(a) and 4(b) J and σ are plotted as a function of t_c. We observe that the sharp increase of the convection strength J correlates with the decrease of σ to values below unity and hence with the onset of the detachment effect in MD simulations.

We conclude that lowering t_c reduces the detachment, i.e., increases the density; thus convection is rendered more difficult. Moreover, the time scales are different: MD simula-

tions may show convection already when monitoring a few vibration periods, whereas convections in experiments have waiting times much larger than the period of excitation [4].

In this work we have presented situations encountered in MD simulations of densely packed grains. We have shown that taking realistic contact times t_c (while keeping the restitution coefficient ε constant) leads to quite small values for the convection strength J. On the other hand, when t_c gets to be large, convection rolls form readily. This is the domain of the so-called detachment effect, where the interparticle distances fluctuate very much; then, due to the large friction of the particles with the boundaries, convection is enhanced [5]. Of course, we based the discussion on a linear model (albeit of widespread use), so that further studies are required when other interactions are put forward, possibly involving nonlinearities, hysteresis [15], static friction [11], and even the rotation of the particles.

We close this paper on a cautionary note about taking computer-generated patterns as a valid explanation for experimental findings: a careful comparison of the macroscopic outcome with experimental benchmarks, as well as an in-depth analysis of the parameters used in the simulations, are always required.

LAOMC is an URA of the CNRS and this work was supported by a special grant A. T. P. "Matière en grain." The support of the Deutsche Forschungsgemeinschaft (SFB 60), of the Fonds der Chemischen Industrie and of the PROCOPE scientific collaboration programme administrated by the DAAD and the APAPE, is acknowledged.

[1] P. Evesque and J. Rajchenbach, Phys. Rev. Lett. **61**, 44 (1989).
[2] S. Douady, S. Fauve, and C. Laroche, Europhys. Lett. **8**, 621 (1989).
[3] J. B. Knight, H. M. Jaeger, and S. R. Nagel, Phys. Rev. Lett. **70**, 3728 (1993).
[4] E. Clément, J. Duran, and J. Rajchenbach, Phys. Rev. Lett. **69**, 1189 (1992).
[5] Y-h. Taguchi, Phys. Rev. Lett. **69**, 1367 (1992).
[6] Y-h. Taguchi, Int. J. Mod. Phys. B **7**, 1839 (1993); Y-h. Taguchi, in *Pattern Formation in Complex Dissipative Systems*, edited by S. Kai (World Scientific, 1991), p. 341.
[7] J. A. C. Gallas, H. J. Herrmann, and S. Sokolowski, Phys. Rev. Lett. **69**, 1371 (1992).
[8] J. J. Moreau, in *Powders & Grains 93*, edited by C. Thornton (Balkema, Rotterdam, 1993), p. 227.
[9] J. Lee and H. J. Herrmann, J. Phys. A: Math. Gen. **26**, 373 (1993).
[10] J. Lee, J. Phys. (France) I **3**, 2017 (1993).
[11] J. Lee, J. Phys. A **27**, L257 (1994).
[12] M. P. Allen and D. J. Tildesley, *Computer Simulation of Liquids* (Oxford University Press, Oxford, 1987).
[13] P. A. Cundall and O. D. L. Strack, Geotechnique **29**, 47 (1979).
[14] H. J. Herrmann, Physica A **191**, 263 (1992).
[15] O. R. Walton and R. L. Braun, Acta Mech. **63**, 73 (1993).
[16] B. Bernu and R. Mazighi, J. Phys. A **23**, 5745 (1990).
[17] B. Bernu, F. Delyon, and R. Mazighi, Phys. Rev. E (to be published).
[18] B. D. Lubachevsky, J. Comput. Phys. **94**, 255 (1991).
[19] E. Clément, S. Luding, A. Blumen, J. Rajchenbach, and J. Duran, Int. J. Mod. Phys. B **7**, 1807 (1993).
[20] S. Luding, E. Clément, A. Blumen, J. Rajchenbach, and J. Duran, Phys. Rev. E **49**, 1634 (1994).
[21] M. H. Sadd, Q. Tai, A. Shukla, Int. J. Non-Linear Mech. **28**, 251 (1993).
[22] S. Luding, E. Clément, A. Blumen, J. Rajchenbach, and J. Duran, Phys. Rev. E (to be published).
[23] P. A. Thompson and G. S. Grest, Phys. Rev. Lett. **67**, 1751 (1990).
[24] Yi Zhang and C. S. Campbell, J. Fluid Mech. **237**, 541 (1992).
[25] Y-h. Taguchi has informed us that the vertical axis of Fig. 4 in Ref. [5] has to be scaled (private communication).