Size Segregation in the Brazil Nut Effect

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Abstract. Granular materials are ubiquitous in nature and in our daily lives, and used in many industrial processes. Depending on the physical conditions that they are subjected, granular materials may present unusual behavior, combining properties of solids, liquids or gases, and displaying interesting and diversified phenomena. In this work we numerically simulated a granular system in order to investigate the phenomena of size segregation in the Brazil Nut Effect. Our simulations indicate that the phenomenon of size segregation results from the combined effect of two different mechanisms: buoyancy and convection. Increasing the vibration amplitude, the behavior of the system becomes less periodic and more turbulent, with evidence of deterministic chaos in the dynamics of the large particle.

Keywords: granular material, size segregation, Brazil Nut Effect, numerical simulation, molecular dynamics

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INTRODUCTION

A granular material is a collection of distinct macroscopic particles. Examples include coal, sand, rice, coffee, corn flakes, fertilizer and nuts. Depending on the physical conditions to which they are subjected, granular materials may present unusual behavior, combining properties of solids, liquids or gases, and displaying interesting and diversified phenomena. Granular convection is a phenomenon where a granular material subjected to shaking or vibration exhibits circulation patterns similar to the ones observed in fluid convection [1]. It is sometimes described as the Brazil Nut Effect (BNE) when the largest particles end up on the surface of a granular material containing a mixture of variously sized objects [2]. In this work we numerically simulated a granular system in order to investigate the phenomena of size segregation in the BNE. To this end, we used the software LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator), a classical molecular dynamics code distributed as an open source code by Sandia National Laboratories [3].

PROBLEM DESCRIPTION

Molecular dynamics simulations are a common way to simulate granular materials. LAMMPS uses the spring-dashpot model with static friction. Considering two contacting particles \( \{i,j\} \) at positions \( \{r_i, r_j\} \), with velocities \( \{v_i, v_j\} \) and angular velocities \( \{\omega_i, \omega_j\} \) (see Fig. 1), the normal compression \( \delta_{ij} \), the relative normal velocity \( v_{nj} \), and the relative tangential velocity \( v_{tij} \) are given by [4]:

\[
\delta_{ij} = d - r_{ij},
\]

\[
v_{nj} = (v_i - v_j) \cdot n_{ij},
\]

\[
v_{tij} = (v_i - v_j) - \frac{1}{2} (\omega_i + \omega_j) \times r_{ij},
\]

where \( r_{ij} = r_i - r_j, n_{ij} = r_{ij}/|r_{ij}| \), and \( v_{tij} = v_i - v_j \). The change rate of the elastic tangential displacement \( u_{tij} \) is given by

\[
\frac{du_{tij}}{dt} = v_{tij} - \frac{(u_{tij} \cdot v_{tij}) r_{ij}}{r_{ij}^2}.
\]

The normal and tangential forces acting on a particle \( i \) are [4]:

\[
F_{nj} = f(\delta_{ij}/d)(k_n \delta_{ij} n_{ij} - \gamma_e m_{eff} v_{nj})
\]

\[
(5)
\]
where $k_{n,t}$ and $\gamma_{n,t}$ are elastic and viscoelastic constants, respectively; $m_{\text{eff}} = m_i m_j / (m_i + m_j)$ is the effective mass of spheres with masses $\{m_i, m_j\}$; and $\mathbf{n}$ is the unit vector in the normal direction. For linear contacts $f(\delta_{ij}) = 1$. As soon as the contact force is calculated, Newton’s equations of motion can be numerically integrated to get the particle trajectories. The results of simulations are given in non-dimensional quantities and measured in units of $d$ for distance, $t_o = \sqrt{d/g}$ for time, $v_o = \sqrt{gd}$ for velocities, $F_o = mg$ for forces, $k_o = mg/d$ for elastic constants, and $\sigma_o = mg/d^2$ for stresses. The basic set of parameters used in our simulation was $\mu_w = 0.5$ (friction coefficient in the walls), $\mu_p = 0.5$ (friction coefficient between particles), $k_o = 2 \times 10^3 k_0$ (elastic constant), $\gamma_o = 40 / t_o$ (viscoelastic constant) and $\Delta t = 1 \times 10^{-3}$ (time step).

Here, in order to reproduce the BNE on LAMMPS, we considered a granular system with $N = 8,000$ small monodisperse spheres (or particles) of diameter $d$, mass $m$ and density $\rho = 1 m/d^3$, and a large particle of diameter $D = \alpha d$, with $\alpha > 1$, and density $\rho = 3 m/d^3$. The particles are inside a box of base side $L = 12d$ subjected to vertically sinusoidally vibration with frequency $f = 0.125/t_o$ and amplitude $A = 5d$. Figure 2 illustrates the BNE, showing different snapshots of the numerical simulation, while the largest particle moves to the top of the vibrating container.

**NUMERICAL SIMULATIONS**

In the simulations described here, we analyzed the influence on the BNE of two key parameters: the diameter of the large particle (by the ratio $D/d$) and the vibration amplitude ($A$). First, we set $f = 0.125/t_o$ and $A = 5d$, and varied $D/d$. For $D/d$ equal to 1.5 and 3.0, the large particle oscillates by continuously rising to the top and falling back to the
bottom. Only for $D/d = 4.0$ the large particle is segregated from the rest of the particles, rising to the top and staying there. This behavior is evident in Fig. 3, which shows the large particle vertical position as a function of the shaking cycles, for $D/d = 1.5$ on the left and $D/d = 4.0$ on the right. As expected, this result shows that the vertical thrust that generates the BNE is directly proportional to the volume displaced by the large particle within the small ones, much like the volume displaced by a ship hull is responsible for keeping it afloat.

![Figure 3](image1)

**FIGURE 3.** The large particle vertical position as a function of shaking cycles, for $D/d = 1.5$ (left) and $D/d = 4.0$ (right).

To analyze the impact of the energy introduced by the vibration on the BNE, we kept constant the diameter ratio $(D/d = 4.0)$ and varied the amplitude $(A = 3d, 5d$ and $8d)$. Figure 4 shows the behavior of the large particle (above) and one small particle (below) for $f = 0.125/t_0$ and different values of $A$.

![Figure 4](image2)

**FIGURE 4.** The vertical position of the large particle (above) and a small particle (below), for $f = 0.125/t_0$ and different values of $A$: (a) & (d) $3d$, (b) & (e) $5d$ and (d) & (b) $8d$.

In Fig. 4a & d, we notice that, although the energy introduced into the system is too small to start and maintain a convection cell inside the container, still the large particle is segregated from the small ones. Since there is no convection, the BNE occurs by buoyancy effects alone and the collection of particles behaves as a strongly viscous fluid. As the amplitude and, thus, the energy input increase (Fig. 4b & e), we observe the onset of a convection cell within the container, with the small particles flowing up and down almost periodically, and the large particle moving to and staying at the top of the particles column. In this case, the vertical position of the large particle varies between...
50d and 60d. For larger levels of energy (Fig. 4c & f), as the behavior of both particles becomes less periodic and more turbulent-like, the BNE starts to disappear. Now, the large particle, although still on the top, displays large oscillations with the vertical position ranging from 30d to 75d.

Overall, the behavior shown in these results is reminiscent of the one displayed by real fluids, such as in Rayleigh-Bénard convection and its transition to chaos [6]. To further investigate this point, we considered the trajectories of large and small particles as time series, for different amplitudes (3d, 5d and 8d) and frequency $f = 0.125/t_0$. We then applied tools for non-linear time series analysis, such as computation of Lyapunov exponents [7] and recurrence plots [6]. Figure 5 shows the Lyapunov exponent evolution $\lambda(t)$, where the time $t$ represents the cycles, and the recurrence plot for the large particle when $A = 8d$. Our results suggest that indeed the dynamics of granular materials displays some features of deterministic chaos. First, the Lyapunov exponent converges to a positive value around 1.6. Second, the recurrence plot presents structures parallel to the main diagonal, indicating that the large particle trajectory in the phase space visits the same region at different times, another evidence of deterministic chaos.

**FIGURE 5.** Evolution of the Lyapunov exponent (left) and recurrence plot (right) for the time series of the large particle when $f = 0.125/t_0$ and $A = 8d$.

**CONCLUSIONS**

Summarizing, in this work we numerically simulated a granular system in order to investigate the BNE. We observed how parameters such as the size of the large particle and the vibration amplitude influence this phenomenon. Our results indicate that the main physical mechanisms behind the BNE are convection and buoyancy. As in fluids, convection depends crucially on the energy input but also on other factors, such as the container geometry. The buoyancy is more associated with the relative size of large and small particles. The fact that the BNE does not depend on only one physical mechanism to be generated probably explains why this phenomenon is so common in nature and in our daily lives, for example, in our morning cereal boxes.

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**REFERENCES**
