

Jamming in frictionless packings of spheres: determination of the critical volume fraction

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Abstract. The jamming transition in granular packings is characterized by a sudden change in the coordination number. In this work we investigate the evolution of coordination number as function of volume fraction for frictionless packings of spheres undergoing isotropic deformation. Using the results obtained from Discrete Element Method simulations, we confirm that the coordination number depends on volume fraction by a power law with exponent $\alpha \approx 0.5$ above the critical volume fraction and up to rather high densities. We find that the system size and loading rate do not have an important effect on the evolution of the coordination number. Polydispersity of the packing seems to cause a shift in the critical volume fraction, i.e., more heterogeneous packings jam at higher volume fractions. Finally, we propose and evaluate alternative methods to determine the critical volume fraction based on the number of rattlers, the pressure and the ratio of kinetic and potential energies. The results are all consistent with the critical volume fractions obtained from the fits of the power law to the simulation data.

Keywords: jamming, frictionless spheres, volume fraction, coordination number

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INTRODUCTION

A common property of materials like molecular liquids, colloids, foams or granular materials is that they have an amorphous structure and they behave like a solid when either temperature or applied shear force is decreased or volume fraction is increased. The transition from fluid to solid-like behavior in disordered states is generally referred to as jamming. Liu and Nagel [1] have proposed a “jamming phase diagram” to unify this concept for different materials with temperature, volume fraction and applied shear stress as control parameters. For athermal systems such as granular materials, temperature has no effect and at zero applied shear stress, there is a well defined point on the volume fraction axis at which jamming first occurs [2]. The objective of this study is to gain a better understanding of this critical volume fraction, the effect of various system parameters on it and how to best identify it.

In particular, we analyze the evolution of the coordination number as function of the volume fraction and examine the discontinuity with power law shape above the critical volume fraction [2, 3, 4]. We perform DEM simulations of isotropic compression in frictionless packings of spheres. We vary system properties such as the number of particles, polydispersity and loading rate.

SIMULATION SETUP

The Discrete Element Method [5, 6, 7] is used. Frictionless spherical particles are enclosed in a cubic vol-

ume with periodic boundary conditions. A linear viscoelastic contact model defines the particle normal contact forces. Besides the damping at the contact, an artificial background dissipation is introduced to reduce dynamical effects. Furthermore, in all simulations we neglect gravity. Typical values of the simulation parameters are: system size $N = 1000, 5000, 10000$ particles, density $\rho = 2000$ [kg/m³], elastic stiffness $k_n = 5000$ [N/m], particle damping coefficient $\gamma = 1000$ [kg/s], background dissipation $\gamma_b = 100$ [kg/s] (see Ref. [6] for a discussion of the units). The contact duration of two average particles is $t_c = 0.31$ seconds and the coefficient of restitution is $r = 0.85$. Polydispersity is measured by the width $w = r_{max}/r_{min}$ of the uniform particle radius distribution. Typical values of w are 1, 2 and 3. Note that $w = 1$ corresponds to a monodisperse packing. The (average) loading rate is defined as the ratio of relative volume change over the total simulation time. Since we are interested in relative rates for identical deformations, we use instead $D = T_{ref}/T_{sim}$ where T_{ref} is the simulation time of the fastest simulation which is 1000 seconds. Typical values of D are 0.1, 0.5 and 1.

EFFECT OF SYSTEM SIZE

Figure 1 shows the evolution of coordination number

$$C^*(v) = C_0 + A \left(\frac{v}{v_c} - 1 \right)^\alpha \quad (1)$$

with volume fraction v for polydisperse packings ($w = 3$) with different sizes. The power law is quantified by an

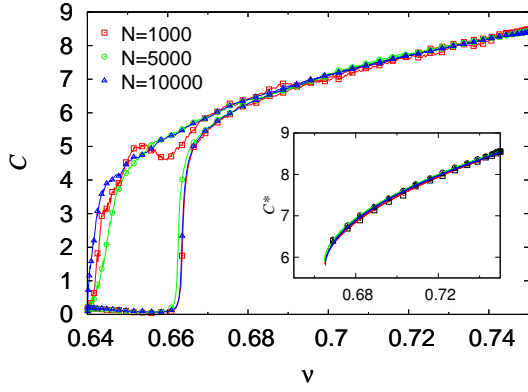


FIGURE 1. Coordination number C as function of density v for different system sizes. Inset: Fit of Eq. (1) to the corrected coordination number C^* computed from the data recorded during decompression with $D = 0.5$. The red, green and blue lines are the fits of the systems containing 1000, 5000 and 10000 particles, respectively.

algebraic behavior with power α , where v_c is the critical volume fraction and C^* is the corrected coordination number obtained by excluding the particles without contacts, i.e. the rattlers. Frictionless particles cannot be mechanically stable unless they have at least 4 contacts. Therefore we define as rattlers those particles having less than 4 contacts. C_0 corresponds to the isostatic limit [2] which is $C_0 = 6$ for 3D and $C_0 = 4$ for 2D.

The fluctuations and the finite values of the coordination number C during compression prior to jamming are due to dynamical effects caused by the moving boundaries of the simulation domain. After jamming, these effects are less visible since the ratio between the kinetic and potential energies is much smaller, i.e., $e = E_{kin}/E_{pot} \ll 1$. The strong jump in the coordination number is only clean during decompression at the transition from solid to fluid phase.

The inset of Figure 1 shows the fit of Eq. (1) to the decompression branch of the simulation data. The critical densities obtained from the fits are 0.6650 ± 0.0002 , 0.6647 ± 0.0002 and 0.6652 ± 0.0001 for $N = 1000, 5000$ and 10000 , respectively. Other parameters are reported in Table 1. It is clear that the system size has no significant effect on the critical volume fraction.

INFLUENCE OF POLYDISPERSITY

We have performed simulations using three packings of 1000 particles with respective widths of the size distribution $w = 1, 2, 3$. All of the samples were compressed from $v = 0.5$ to $v = 0.9$ and then decompressed. Figure 2 shows coordination number as function of the volume

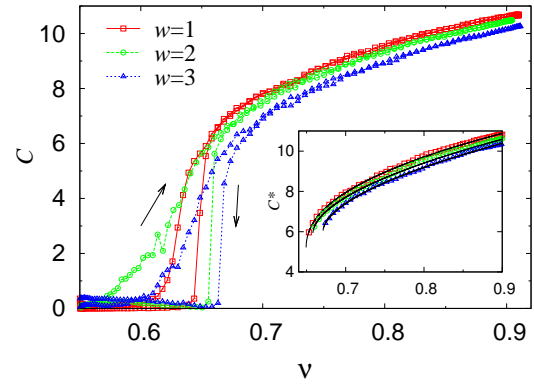


FIGURE 2. The evolution of the coordination number C with the volume fraction v for different polydispersities. The arrows indicate the compression (up) and decompression (down) directions. Inset: The solid lines are the fits according to Eq. (1).

fraction for the corresponding packings. The inset shows the fit of Eq. (1) to the decompression branch of the simulation data. The critical volume fractions obtained from the fits are 0.649 ± 0.002 , 0.658 ± 0.002 and 0.671 ± 0.002 for $w = 1, 2$ and 3 , respectively. This indicates that more heterogeneous packings jam at higher volume fractions.

EFFECT OF LOADING RATE

Figure 3 shows the coordination number as function of the volume fraction for a polydisperse packing ($w = 3$) of 10000 particles deformed at three different rates. The relative rates of loading are $D = 0.1, 0.5$ and 1 . Jamming occurs at vanishing deformation rates, which is consistent with the observation that the slower the system is deformed, the sharper the transition gets. The evolution of the corrected coordination number and the fits of Eq. (1) are shown in the inset of Figure 3. It seems that by removal of rattlers the effect of loading rate disappears in high volume fraction. The critical volume fractions obtained from the fits are 0.6648 ± 0.0002 , 0.6652 ± 0.0001 and 0.6654 ± 0.0001 for $D = 0.1, 0.5$ and 1 , respectively. However, these values are questionable since the derivative of Eq. (1) has a singularity at v_c which makes the results very sensitive to the fit range. Consequently, the exponent $\alpha \approx 0.5$ which is reported in 2D experiments and simulations [3, 4] cannot always be recovered (see Table 1). Furthermore, knowing that the rate effects are important close to v_c , using the fit of Eq. (1) to analyze the effect of the compression rate might be unreliable. Therefore we propose and evaluate different alternatives.

TABLE 1. Critical volume fractions and fit parameters for polydisperse ($w = 3$) packings obtained from the fits of Eq. (1) and alternative methods for different system sizes and loading rates.

		C_0	A	α	v_c	v_c^*	v_c^\dagger	v_c^{**}
$N = 1000$	$D = 0.5$	5.8221	8.4875	0.5572	0.6650	0.6641	0.6644	0.6705
	$D = 1$	5.0256	7.5938	0.3904	0.6650	0.6634	0.6652	0.6669
$N = 5000$	$D = 0.5$	5.8838	8.1661	0.5431	0.6647	0.6622	0.6620	0.6658
	$D = 1$	5.7645	8.2019	0.5279	0.6654	0.6623	0.6624	0.6685
$N = 10000$	$D = 0.1$	6.0643	8.4204	0.5909	0.6648	0.6636	0.6624	0.6647
	$D = 0.5$	5.7887	7.9915	0.5199	0.6652	0.6624	0.6632	0.6665
	$D = 1$	5.7645	8.2019	0.5279	0.6654	0.6634	0.6627	0.6675

* Obtained from the peaks in the evolution of fraction of rattlers.

† Obtained from the fits of Eq. (3).

** Obtained from the intersection points in the $e-v$ graphs.

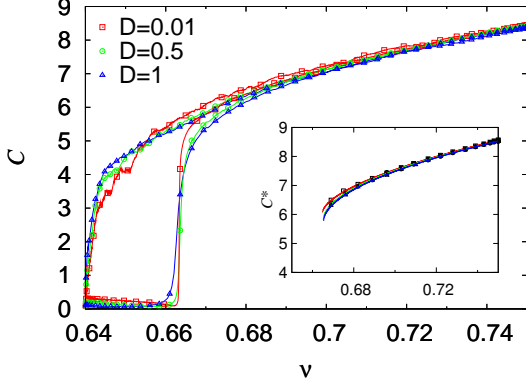


FIGURE 3. Coordination number C as function of density v for different loading rates. Inset: The fits of Eq. (1).

THE FRACTIONS OF RATTLERS

An alternative way to determine the critical density v_c at which the jamming transition occurs is to examine the number of rattlers, i.e. particles with fewer than 4 contacts. Typically, it has a reverse behavior to the coordination number, i.e. when C decreases it increases and vice versa. However the number of particles with less than four but more than zero contacts increases or decreases only during the transition. Figure 4 shows the evolution of the fraction of particles having different number of contacts during decompression. The critical volume fractions are determined by taking the average of the volume fractions at which the peaks occur in the $v-\phi$ graphs for the fractions of particles with $0 < C < 4$. The v_c obtained using this method are 0.6634, 0.6623 and 0.6634 for packings with $N = 1000, 5000$ and 10000 , respectively. These values are close to those obtained from the fits of Eq. (1). The advantage of this method is that it can be given a physical explanation. During the transition from the solid to fluid phase, most of the contacts will open and as mentioned earlier the number of rattlers will quickly increase. However, after the transition the

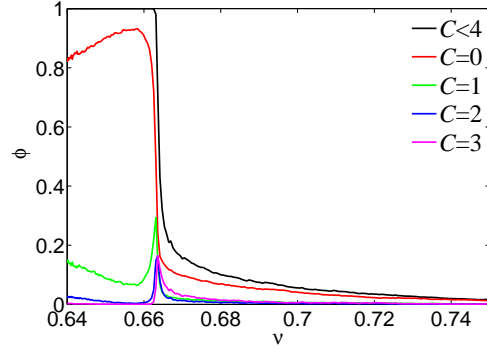


FIGURE 4. Evolution of fractions of rattlers during decompression.

coordination number is normally equal to zero. Therefore, the number of particles with less than four but more than zero contacts will first increase then decrease, which results in the peaks in their fraction.

PRESSURE

The static pressure p in a packing is obtained from the $(1/3)$ trace of the averaged micromechanical stress:

$$\bar{\sigma}_{ij} = \frac{1}{V} \sum_{c \in V} f_i^c l_j^c \quad (2)$$

where V is the total volume of the packing, l_j^c is the branch vector of contact c and f_i^c is the force associated with the contact. During decompression most of the contacts open at the jamming point and the static pressure drops to zero. Hence, an alternative definition of v_c can be given as the volume fraction at which the pressure vanishes. In order to determine numerical values of v_c we use the relation:

$$\frac{P}{CV} = P_{\text{ref}} \log \left(\frac{v}{v_c} \right) \quad (3)$$

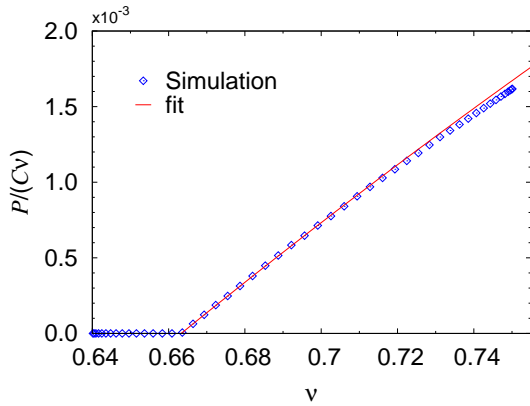


FIGURE 5. $P/(Cv)$ as a function of volume fraction for a polydisperse ($w = 3$) packing.

where $P = pa_0/k_n$ is the pressure normalized by k_n and the average particle radius a_0 . Figure 5 shows the fit of Eq. (3) to the simulation data. The critical volume fractions obtained from the fits are shown in Table 1. Note the good agreement between the values obtained from the peaks in the fraction of rattlers and the pressure.

AN ENERGY BASED CRITERION

The values of the critical density v_c and coordination number C_0 at the jamming transition can also be obtained from considerations of the ratio of the kinetic and potential energies of the system $e = E_{kin}/E_{pot}$ [8]. We identify the jammed state as the point where the compression branch of the $e-v$ curve crosses its decompression branch (Fig. 6). At this point e diverges, which implies a sudden drop in the elastic energy as a clear signature that the unjammed state is reached. This method leads to the expected coordination number $C_0 \approx 6$ which corresponds to the mechanical stability of an isostatic system [2]. The critical volume fractions found using this method are $v_c = 0.652 \pm 0.005$, 0.659 ± 0.005 and 0.6666 ± 0.0006 for polydisperse samples with $w = 1, 2$ and 3 , respectively. The accuracy of this method is limited by the spacing of the data points around the crossing point.

CONCLUSIONS

We have analyzed the effect of different system properties on the critical volume fraction in jamming and the evolution of the coordination number. We find that system size does not have a significant effect on both of these parameters. On the other hand, polydispersity causes a shift in the critical volume fraction, i.e. less homogeneous packings jam at higher volume fractions. We

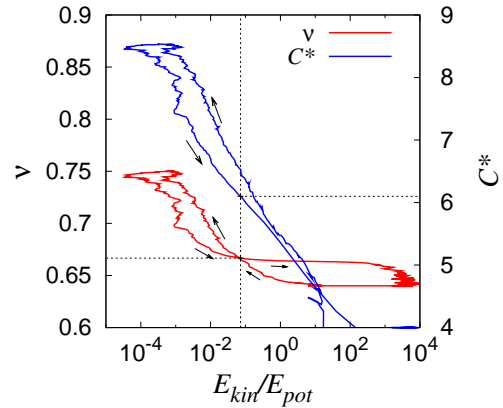


FIGURE 6. Corrected coordination number C^* and volume fraction v as functions of the energy ratio for a polydisperse ($w = 3$) packing of 10000 particles. The arrows indicate the compression (up) and decompression (down) directions.

find that the jump in the coordination number becomes sharper as the loading rate is lowered. A more detailed study of the effects of much slower loading rates on the critical volume fraction are required. However, the loading rate has no visible effect on the evolution of the coordination at high volume fractions – after the removal of the rattlers. Finally, we proposed alternative methods to identify the critical volume fraction based on (1) the fraction of rattlers, (2) the energy ratio, and (3) the pressure. A summary of the fits to the power law Eq. (1) and the v_c obtained from the proposed methods for different system sizes and compression rates is given in Table 1. In conclusion, we recommend to not rely on a single method but, e.g., use the fits to coordination number and pressure in parallel.

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