



Microstructure evolution of compressible granular systems under large deformations



Marcial Gonzalez ^{a,*}, Alberto M. Cuitiño ^b

^a School of Mechanical Engineering, Purdue University, West Lafayette, IN 47907, USA

^b Department of Mechanical and Aerospace Engineering, Rutgers University, Piscataway, NJ 08854, USA

ARTICLE INFO

Article history:

Received 30 June 2015

Received in revised form

17 March 2016

Accepted 26 March 2016

Available online 31 March 2016

Keywords:

Granular systems

Contact mechanics

Nonlocal contact formulation

Microstructure evolution

Compaction

Powders

Particle mechanics

Discrete element method

ABSTRACT

We report three-dimensional particle mechanics static calculations that predict the microstructure evolution during die-compaction of elastic spherical particles up to relative densities close to one. We employ a nonlocal contact formulation that remains predictive at high levels of confinement by removing the classical assumption that contacts between particles are formulated locally as independent pair-interactions. The approach demonstrates that the coordination number depends on the level of compressibility, i.e., on Poisson's ratio, of the particles. Results also reveal that distributions of contact forces between particles and between particles and walls, although similar at jamming onset, are very different at full compaction. Particle–wall forces are in remarkable agreement with experimental measurements reported in the literature, providing a unifying framework for bridging experimental boundary observations with bulk behavior.

© 2016 Elsevier Ltd. All rights reserved.

1. Introduction

The microstructure of confined granular media is typically inhomogeneous, anisotropic and disordered. Under external loading, these systems exhibit a non-equilibrium jamming transition from a liquid-like to a solid-like state (Liu and Nagel, 1998; Jin and Makse, 2010; Trappe et al., 2001; O'Hern et al., 2003; Song et al., 2008). Under increasing confinement, these amorphous solids support stress by spatial rearrangement and deformation of particles and by the development of inhomogeneous force networks (Majmudar and Behringer, 2005; Durian, 1995; Makse et al., 2000; Blair et al., 2001; Liu et al., 1995; Radjai et al., 1996; Chan and Ngan, 2005). Understanding and predicting the formation and evolution of such microstructure under finite macroscopic deformations and at high levels of confinement remains a fundamental goal of granular mechanics (Edwards and Oakeshott, 1989; Cates et al., 1998; Richard et al., 2005; Blumenfeld and Edwards, 2009; Ciamarra et al., 2012; Ostojic et al., 2006).

In this paper, we report three-dimensional particle mechanics static calculations that enable us to predict microstructure evolution during die-compaction of elastic spherical particles up to relative densities close to one. We employ a nonlocal contact formulation (Gonzalez and Cuitiño, 2012) that remains predictive at high levels of confinement by removing the classical assumption that contacts between particles are formulated locally as independent pair-interactions. We specifically study a noncohesive frictionless granular system composed of 40,000 weightless elastic spherical particles with radius

* Corresponding author.

E-mail addresses: marcial-gonzalez@purdue.edu (M. Gonzalez), cuitino@jove.rutgers.edu (A.M. Cuitiño).

$R=0.125$ mm, Young's modulus $E=7.0$ GPa, and Poisson's ratio ν . The granular bed, which is numerically generated by means of a ballistic deposition technique (Jullien and Meakin, 1989), is constrained by a rigid cylindrical container of diameter 10 mm. The systems are deformed under die-compaction up to a relative density ρ of 1. Assuming a sufficiently small compaction speed, we consider rate-independent material behavior and we neglect traveling waves, or any other dynamic effect (Richard et al., 2005). The deformation process is therefore described by a sequence of static equilibrium configurations. In this work we employ 125 quasi-static load steps and we consider two materials that only differ in their level of compressibility, namely $\nu=0.35$ and $\nu=0.45$.

The paper is organized as follows. The particle mechanics approach used to generate a sequence of static equilibrium configurations of granular systems at high levels of confinement is presented in Section 2. The evolution of microstructural statistical features of these equilibrium configurations is investigated in Section 3. Specifically, we study the evolution of the mechanical coordination number (number of non-zero contact forces between a particle and its neighbors) in Section 3.1, punch and die-wall pressures in Section 3.2, the network of contact forces in Section 3.3, and the network of contact radiuses in Section 3.4. Finally, a summary and concluding remarks are collected in Section 4.

2. Particle mechanics approach to granular systems at high levels of confinement

Due to the high level of confinement experienced by the particles in the system, we adopt a nonlocal contact formulation (Gonzalez and Cuitiño, 2012) that accounts for the interplay of deformations due to multiple contact forces acting on each single particle. This nonlocal formulation removes the classical assumption that contacts between particles are formulated locally as independent pair-interactions. Its predictions are in remarkable agreement with detailed finite-element simulations of a neo-Hookean solid extended to the compressible range and with experimental observations of a rubber sphere that exhibits no permanent deformations. This good agreement at moderate to large levels of confinement, however, is not obtained with Hertz theory (see Fig. 1 and Gonzalez and Cuitiño, 2012 for further details). It bears emphasis that the nonlocal contact formulation is not an extension of Hertz theory to finite deformations but rather a systematic approach for accounting the interaction between contact interfaces. In a manner analogous to interacting cracks or dislocations in elastic media, the nonlinear behavior is confined to small regions and the interaction between these regions is through an elastic field of deformations.

An equilibrium configuration is defined by the solution of two sets of coupled nonlinear equations. The first set of equations corresponds to static equilibrium of the granular system, that is sum of all elastic contact forces acting on each particle equals zero. The second set of equations accounts for the contribution to each contact interface of the nonlocal mesoscopic deformations induced by all other contact forces acting on the particles, that is for the nonlocal terms γ^{NL} (Gonzalez and Cuitiño, 2012). Thus, the nonlinear system of equations is given by

$$\sum_{j \in N_i} n_{ij}^{\text{H}} (R_i + R_j - \|\mathbf{x}_i - \mathbf{x}_j\| + \gamma_{ij}^{\text{NL}})^{3/2} \frac{\mathbf{x}_i - \mathbf{x}_j}{\|\mathbf{x}_i - \mathbf{x}_j\|} = \mathbf{0}$$

$$\gamma_{ij}^{\text{NL}} - \sum_{k \in N_i, k \neq j} \frac{n_{ik}^{\text{H}} (R_i + R_k - \|\mathbf{x}_i - \mathbf{x}_k\| + \gamma_{ik}^{\text{NL}})^{3/2}}{n_{jik}^{\text{NL}}(\mathbf{x}_j, \mathbf{x}_i, \mathbf{x}_k)} - \sum_{k \in N_j, k \neq i} \frac{n_{jk}^{\text{H}} (R_j + R_k - \|\mathbf{x}_j - \mathbf{x}_k\| + \gamma_{jk}^{\text{NL}})^{3/2}}{n_{ijk}^{\text{NL}}(\mathbf{x}_i, \mathbf{x}_j, \mathbf{x}_k)} = 0 \quad (1)$$

where \mathbf{x}_i and N_i are the position and all the neighbors of particle i , respectively, $\gamma_{ij}^{\text{NL}} = \gamma_{ji}^{\text{NL}}$ by definition, and $(\cdot)_+ = \max\{\cdot, 0\}$.

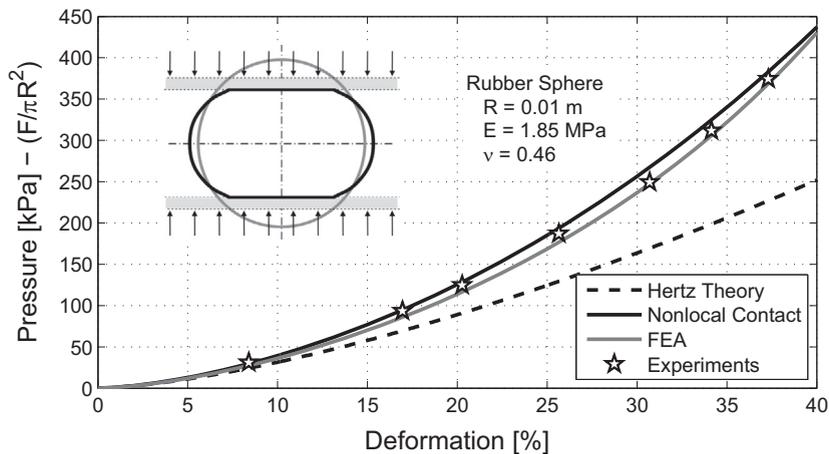


Fig. 1. Validation of the nonlocal contact formulation with experimental measurements obtained for a rubber sphere compressed between two rigid plates (Tatara, 1989) and with detailed finite-element simulations (Gonzalez and Cuitiño, 2012).

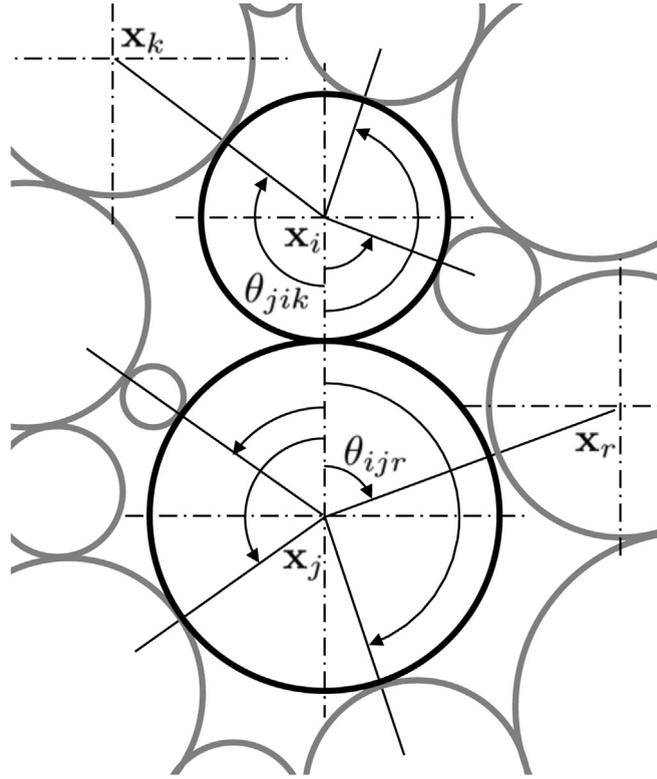


Fig. 2. Two spheres in contact under a general loading configuration composed of multiple neighbors.

In the above system of equations, n_{ij}^H and n_{jik}^{NL} correspond to Hertz theory and to the nonlocal contact formulation (Gonzalez and Cuitiño, 2012), respectively, with

$$n_{ij}^H = \frac{4}{3} \left(\frac{1 - \nu_i^2}{E_i} + \frac{1 - \nu_j^2}{E_j} \right)^{-1} \left(\frac{1}{R_i} + \frac{1}{R_j} \right)^{-1/2}$$

$$n_{jik}^{NL} = \frac{4\pi R_i E_i \sin(\theta_{jik}/2)}{(1 + \nu_i)[-2(1 - \nu_i) - 2(1 - 2\nu_i) \sin(\theta_{jik}/2) + (7 - 8\nu_i) \sin^2(\theta_{jik}/2)]} \quad (2)$$

where $\theta_{jik} = \widehat{x_j x_i x_k}$ is the angle between the coordinate points of particles j , i and k (see Fig. 2).

A sequential strategy is proposed to treat the coupled problem (see Algorithm 1). The equations of static equilibrium are solved for $\mathbf{x} = (\mathbf{x}_1^T, \dots, \mathbf{x}_N^T)^T$, assuming fixed $\boldsymbol{\gamma}^{NL} = (\gamma_{12}^{NL}, \gamma_{13}^{NL}, \dots, \gamma_{N-1,N}^{NL})^T$, by employing a trust-region method (Coleman and Li, 1996; Conn et al., 2000) that successfully overcomes the characteristic ill-posedness of the problem (e.g., due to metastability, Mehta, 2007). The basic trust-region algorithm requires the solution of a minimization problem to determine the step between iterations, namely the trust-region step. This minimization problem is of the form $\min\{\psi(\mathbf{s}) : \|\mathbf{s}\| \leq \Delta\}$, where $\mathbf{s} = {}^n\mathbf{x} - {}^n\mathbf{x}$ is the trust-region step, Δ is a trust-region radius and ψ is a quadratic function that represents a local model of the objective function about ${}^n\mathbf{x}$, that is

$$\psi(\mathbf{s}) = \frac{1}{2} \|\mathbf{}^n\mathbf{F} + \mathbf{}^n\mathbf{K}\mathbf{s}\|^2 = \frac{1}{2} \langle \mathbf{}^n\mathbf{F}, \mathbf{}^n\mathbf{F} \rangle + \langle \mathbf{}^n\mathbf{K}\mathbf{s}, \mathbf{}^n\mathbf{F} \rangle + \frac{1}{2} \langle \mathbf{}^n\mathbf{K}\mathbf{s}, \mathbf{}^n\mathbf{K}\mathbf{s} \rangle$$

with ${}^n\mathbf{F}$ and ${}^n\mathbf{K}$ being the global force vector and stiffness matrix, respectively, at ${}^n\mathbf{x}$ —the first term in the above equation is not required in the minimization problem. It is worth noting that the trust-region step is not necessarily in the direction of a quasi-Newton step and that the trust-region radius acts as a regularization term that controls the growth in the size of the least squares solution observed in most ill-posed (Vicente, 1996). Trading accuracy for performance, Byrd et al. (1988), among others, proposed to approximate the minimization problem by restricting the problem to a two-dimensional subspace. Furthermore, the two-dimensional subspace can be determined by a preconditioned conjugate gradient process and the trust-region radius can be adjusted over the iterative process (see, e.g., Moré and Sorensen, 1983). Here we adopt the implementation available in MATLAB R2014a Optimization Toolbox.

The nonlocal terms are solved by a few fixed point iterations of the second set of equations in (1), assuming a given \mathbf{x} (see Gonzalez and Cuitiño, 2012 and Algorithm 2). It is worth noting that an equilibrium configuration is not obtained by

artificially damped or cooled-down dynamic processes but rather by iterative solvers that follow the energy landscape around the solution of static equilibrium. Each iteration of the trust-region method involves the solution of γ^{NL} (subject to a given tolerance TOL2) and the evaluation of an approximate solution for \mathbf{x} . A notable feature of the nonlocal contact formulation is that, when nonlocal effects are neglected, it reduces to Hertz theory. Under such simplification, an equilibrium configuration is readily obtained from the solution of the first set of equations in (1), assuming $\gamma^{\text{NL}} = 0$.

3. Post-jamming behavior of compressible granular systems

We next study the post-jamming behavior of two granular systems that only differ in the level of compressibility of the particles (i.e., in ν). The geometric configuration of the initial granular bed is the same for both systems, and simulations are performed for both Hertz theory and the nonlocal contact formulation (each simulation takes several months of CPU time). Deformations at the particle scale are within the validated range of the nonlocal contact formulation, that is smaller than 40% (see Fig. 1), for relative densities smaller than 0.90. We investigate the evolution of statistical features of the mechanical coordination number (number of non-zero contact forces between a particle and its neighbors), punch and die-wall pressures, the network of contact forces, and the network of contact radiuses. Error bounds in tables and plots represent the 95% confidence envelope for fitted coefficients.

Algorithm 1. ParticleMechanicsApproach: sequential strategy for solving the coupled equilibrium problem.

```

Require: Initial guess for particles' coordinates  ${}^1\mathbf{x}$ , initial guess for nonlocal terms  ${}^0\gamma^{\text{NL}}$ , TOL1, TOL2, trust-region radius  $\Delta$  and the simplicial complex  $X$ 
1: Error  $\leftarrow$  TOL1
2:  $n \leftarrow 1$ 
3: while Error  $\geq$  TOL1 do
4:   /* Compute global force, global stiffness, and nonlocal terms. */
5:    $\{{}^n\mathbf{F}, {}^n\mathbf{K}, {}^n\gamma^{\text{NL}}\} \leftarrow \text{NonlocalContactFormulation}({}^n\mathbf{x}, \text{TOL2}, {}^{n-1}\gamma^{\text{NL}}, X)$ 
6:   /* Update coordinates with the trust-region step obtained by restricting the problem to a two-dimensional subspace (Byrd et al., 1988). */
7:    ${}^n\mathbf{s} \leftarrow \arg \min_{\mathbf{s}} \left( {}^n\mathbf{K}\mathbf{s}, {}^n\mathbf{F} \right) + \frac{1}{2} \left( {}^n\mathbf{K}\mathbf{s}, {}^n\mathbf{K}\mathbf{s} \right)$  subject to  $\|\mathbf{s}\| \leq \Delta$ 
8:    ${}^{n+1}\mathbf{x} \leftarrow {}^n\mathbf{x} + {}^n\mathbf{s}$ 
9:   /* Compute a measure of convergence */
10:  Error  $\leftarrow$   $\|{}^n\mathbf{s}\|$ 
11:   $n \leftarrow n + 1$ 
12: end while
13: /* Compute nonlocal terms of the converged solution. */
14:  $\{{}^n\gamma^{\text{NL}}\} \leftarrow \text{NonlocalContactFormulation}({}^n\mathbf{x}, \text{TOL2}, {}^{n-1}\gamma^{\text{NL}}, X)$ 
15: return  $\{{}^n\mathbf{x}, {}^n\gamma^{\text{NL}}\}$ 

```

3.1. Mechanical coordination number

The mean coordination number \bar{Z} evolves as a power law of the following form:

$$\bar{Z} - \bar{Z}_c = \bar{Z}_0(\rho - \rho_c)^\theta \quad (3)$$

where ρ_c is the critical relative density, \bar{Z}_c is the minimal average coordination number and θ is the critical exponent. This well-known critical-like behavior has an exponent consistent with 1/2 for different pair-interaction contact laws, polydispersity and dimensionality of the problem (O'Hern et al., 2002, 2003; Durian, 1995). Fig. 3(a) shows the results obtained from the particle contact mechanics simulations for Hertz theory and their best fit to Eq. (3). For $\nu=0.35$, jamming occurs at $\bar{Z}_c = 5.372$ and $\rho_c = 0.5878$ with $\theta=0.5009$. The fit to numerical results is excellent not only near jamming but also at large relative densities [see Fig. 3(b)]. It is worth noting that the isostatic condition for frictionless packings implies a critical coordination number equal to 6 and a critical density close to 0.64. Our initial powder bed, however, is generated such that a subset of particles is jammed, namely the backbone, while the remainder of the particles are not jammed but locally imprisoned by their neighbors, referred to as rattlers. In this work, we do not exclude rattlers from packings, when calculating packing densities, mean coordination numbers and networks of contact forces. Therefore, compaction is initially characterized by rearrangement and very small deformations of the particles, and it is followed by an early jamming transition at $\bar{Z}_c < 6$, reaching the isostatic coordination number at a relative density very close to 0.60. There exists a body of work that indicates that ρ_c depends on the protocol used for obtaining jammed configurations and that mono-disperse systems are prone to crystallization (Baranau and Tallarek, 2014; Chaudhuri et al., 2010; Schreck et al., 2011; Vågberg et al., 2011). While a detailed analysis concerning these points is a worthwhile direction of future work, specially the investigation of polydisperse packings for which some results are observed to be independent of the generation protocol, here we restrict our discussion to post-jamming behavior and to one preparation protocol. Results for $\nu=0.45$ are only marginally different.

Algorithm 2. NonlocalContactFormulation: computation of global force, global stiffness, and nonlocal terms.

Require: Particles' coordinates $\mathbf{x} = (\mathbf{x}_1^T, \dots, \mathbf{x}_N^T)^T$, TOL, initial guess for nonlocal terms ${}^0\gamma^{\text{NL}} = ({}^0\gamma_{12}^{\text{NL}}, {}^0\gamma_{13}^{\text{NL}}, \dots, {}^0\gamma_{N-1,N}^{\text{NL}})^T$ and the simplicial complex X .

```

1:  /* Compute nonlocal contributions  $\gamma^{\text{NL}}$  */
2:  Error  $\leftarrow$  TOL
3:   $n \leftarrow 0$ 
4:  while Error  $\geq$  TOL do
5:     $n+1\gamma^{\text{NL}} \leftarrow \mathbf{0}$ 
6:    /* Loop over all contact pair-interactions between vertices  $\{v_i, v_j\}$  */
7:    for  $[v_i, v_j] \in E_1(X)$  do
8:      for  $[v_i, v_{k \neq i}] \in \text{Incident}(v_i)$  do
9:        /* Update  $\gamma_{ij}^{\text{NL}}$  with the nonlocal displacement induced by contact force  $P_{ik}$  */
10:        $n+1\gamma_{ij}^{\text{NL}} \leftarrow n+1\gamma_{ij}^{\text{NL}} + \frac{n_{ik}^{\text{H}}(R_i + R_k - \|\mathbf{x}_i - \mathbf{x}_k\| + n_{ik}^{\text{NL}})^{3/2}}{n_{ijk}^{\text{NL}}(\mathbf{x}_j, \mathbf{x}_i, \mathbf{x}_k)}$ 
11:      end for
12:      for  $[v_j, v_{k \neq j}] \in \text{Incident}(v_j)$  do
13:        /* Update  $\gamma_{ij}^{\text{NL}}$  with the nonlocal displacement induced by contact force  $P_{jk}$  */
14:        $n+1\gamma_{ij}^{\text{NL}} \leftarrow n+1\gamma_{ij}^{\text{NL}} + \frac{n_{jk}^{\text{H}}(R_j + R_k - \|\mathbf{x}_j - \mathbf{x}_k\| + n_{jk}^{\text{NL}})^{3/2}}{n_{ijk}^{\text{NL}}(\mathbf{x}_i, \mathbf{x}_j, \mathbf{x}_k)}$ 
15:      end for
16:    end for
17:    /* Compute a measure of convergence */
18:    Error  $\leftarrow$   $\|n+1\gamma^{\text{NL}} - n\gamma^{\text{NL}}\|$ 
19:     $n \leftarrow n + 1$ 
20:  end while
21:  /* Assemble global force  $F$  and stiffness  $K$  using converged nonlocal terms  $n\gamma^{\text{NL}}$  */
22:  for  $[v_i, v_j] \in E_1(X)$  do
23:     $\gamma_{ij} \leftarrow R_i + R_j - \|\mathbf{x}_i - \mathbf{x}_j\|$ 
24:     $\mathbf{F} \leftarrow \text{Assemble}(v_r; n_{ij}^{\text{H}}\{\gamma_{ij} + n_{ij}^{\text{NL}}\}^{3/2} \frac{\mathbf{x}_i - \mathbf{x}_j}{\|\mathbf{x}_i - \mathbf{x}_j\|} (\delta_{ir} - \delta_{jr}))$  for all  $v_r \in E_0(X)$ 
25:     $\mathbf{K} \leftarrow \text{Assemble}(v_r, v_s; \frac{n_{ij}^{\text{H}}\{\gamma_{ij} + n_{ij}^{\text{NL}}\}^{3/2}}{\|\mathbf{x}_i - \mathbf{x}_j\|} \mathbf{I}(\delta_{ir} - \delta_{jr})(\delta_{is} - \delta_{js}) \dots$ 
       $- [\frac{3n_{ij}^{\text{H}}\{\gamma_{ij} + n_{ij}^{\text{NL}}\}^{1/2}}{2} + \frac{n_{ij}^{\text{H}}\{\gamma_{ij} + n_{ij}^{\text{NL}}\}^{3/2}}{\|\mathbf{x}_i - \mathbf{x}_j\|}] \frac{(\mathbf{x}_i - \mathbf{x}_j) \otimes (\mathbf{x}_i - \mathbf{x}_j)}{\|\mathbf{x}_i - \mathbf{x}_j\|^2} (\delta_{ir} - \delta_{jr})(\delta_{is} - \delta_{js}))$ 
      for all  $v_r \in E_0(X)$  and  $v_s \in E_0(X)$ 
26:  end for
27:  return  $\{\mathbf{F}, \mathbf{K}, n\gamma^{\text{NL}}\}$ 

```

Hertz theory, and any other contact law formulated locally as pair-interactions, does not account for the interplay of deformations due to multiple contact forces acting on a single particle. As relative density increases, these nonlocal deformations are responsible for the formation and breakage of contacts between particles which in turn manifest as a crossover in the local coordination number [see the top inset in Fig. 3(a) for two bi-dimensional examples]. This local crossover is predicted by the nonlocal contact formulation and it emerges in the evolution of the mean mechanical coordination number depicted in Fig. 3(a). For highly compressible materials ($\nu=0.35$), the evolution of \bar{Z} is below the predictions of Hertz theory, i.e., some contacts are broken as the level of confinement increases. In sharp contrast, for nearly incompressible materials ($\nu=0.45$), the evolution of \bar{Z} is above the predictions of Hertz theory, i.e., new contacts are formed due to volume conservation at the particle scale. Therefore, while Eq. (3) is valid and independent of any material property near jamming, its validity fails at high levels of confinement where \bar{Z} strongly depends on ν .

The probability distribution of the local coordination number Z is best described by the granocentric model proposed in Clusel et al. (2009) and Newhall et al. (2011). Here we restrict our attention to monodisperse systems and approximate Z by a binomially distributed variable characterized by its mean and variance, that is

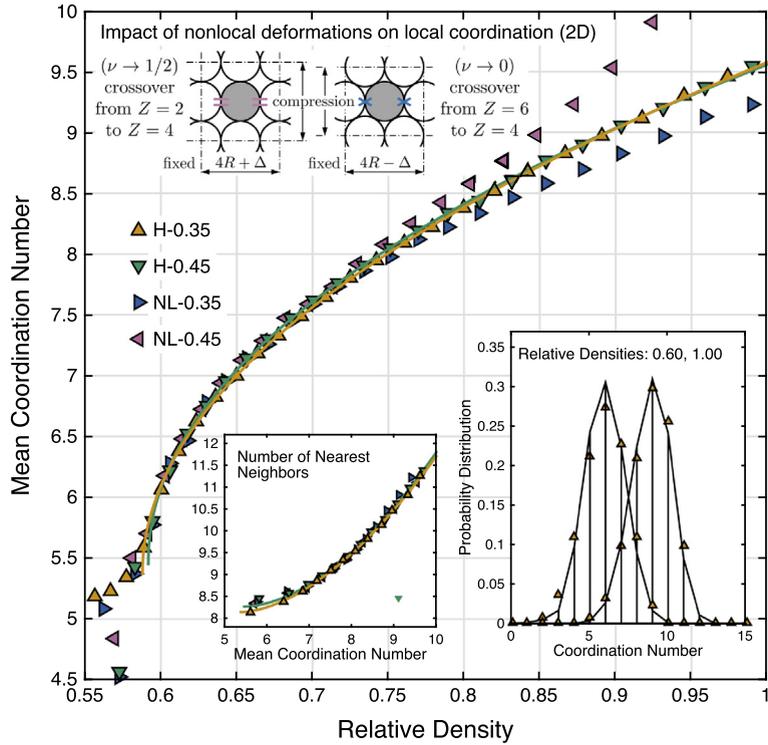
$$Z \sim B(\lceil \bar{N} \rceil, p) = B(\lceil \bar{Z} / (1 - \text{Var}(Z)/\bar{Z}) \rceil, 1 - \text{Var}(Z)/\bar{Z}) \quad (4)$$

where \bar{N} represents the mean number of (nearest) neighbors and p corresponds to the probability of finding a contact among these neighbors. The insets in Fig. 3(a) show that this is an accurate approximation for both formulations at small and large relative densities—though distributions for the nonlocal contact formulation are not shown in the figure. The numerical results also suggest the existence of a universal relationship between \bar{N} and \bar{Z} of the following form:

$$\bar{N} - \bar{N}_c = \bar{N}_0 (\bar{Z} - \bar{Z}_c)^\varepsilon \quad (5)$$

with $\bar{N}_c \approx 8$ and $\varepsilon \approx 7/4$, for both formulations and Poisson's ratios [see Fig. 3(b) for exact numerical values obtained for Hertzian interactions].

Finally, we investigate the sensitivity of these results to the numerical tolerance used to identify the non-zero contact



(a)

(b)

System	ρ_c	\bar{Z}_c	\bar{Z}_0	θ	\bar{N}_c	\bar{N}_0	ε
$\nu = 0.35$	0.5878	5.372 $\pm 0.2\%$	6.552 $\pm 0.3\%$	0.5009 $\pm 0.6\%$	8.144 $\pm 0.2\%$	0.2547 $\pm 3.1\%$	1.723 $\pm 1.2\%$
$\nu = 0.45$	0.5916	5.452 $\pm 0.3\%$	6.347 $\pm 0.6\%$	0.4863 $\pm 1.0\%$	8.270 $\pm 0.2\%$	0.2334 $\pm 4.4\%$	1.795 $\pm 1.6\%$

Fig. 3. (a) Statistical description of the coordination number as a function of relative density. Solid lines correspond to the best fit of Eq. (3) to the mean coordination number obtained from the particle contact mechanics simulation of the granular bed (symbols). The bottom-right inset depicts local coordination number probability distribution, and its binomial function approximation. The bottom-left inset depicts the evolution of number of nearest neighbors with mean coordination number. The top inset shows two-dimensional examples of coordination number crossover, due to nonlocal deformations, for different levels of compressibility and confinement. (b) Coefficients and critical exponents for best fits.

forces that contribute to the mechanical coordination number. We thus define ϵ_{tol} as the inter-particle deformation above which a contact force is identified as non-zero, i.e., if $(R_i + R_j - \|\mathbf{x}_i - \mathbf{x}_j\| + \gamma_{ij}^{NL})_+ / (R_i + R_j) > \epsilon_{tol}$ then the contact force ij contributes to the mechanical coordination number. We also investigate how the ordering effect of the container walls penetrates into the bulk of the powder bed. We thus define Gap as the distance between the boundary and the bulk region. Fig. 4(a) shows that the evolution of the mean coordination number is insensitive to the choice of ϵ_{tol} at high relative densities and barely sensitive at small densities, for values of ϵ_{tol} equal to 0.1%, 0.05%, 0.01% and 0.005% and for Gap = 4R. Fig. 4(b) indicates that the effect of the boundary on the mean coordination number only penetrates one or two particle radiuses into the bulk, for ϵ_{tol} equal to 0.005%. Therefore, the results presented in Fig. 3 correspond to $\epsilon_{tol} = 0.005\%$ and Gap = 4R.

3.2. Applied pressure

The pressures applied by the punches and the reaction at the die wall are effective macroscopic variables predicted by the particle contact mechanics simulation. These predictions are presented in Fig. 5(a) and follow a power law of the following form:

$$\sigma = K_H(\rho - \rho_c)^{\beta_H} + K_{NL}(\rho - \rho_c)^{\beta_{NL}} \quad (6)$$

where the pressure σ is evaluated at the deformed configuration, ρ_c is obtained from the evolution of \bar{Z} , the coefficients in

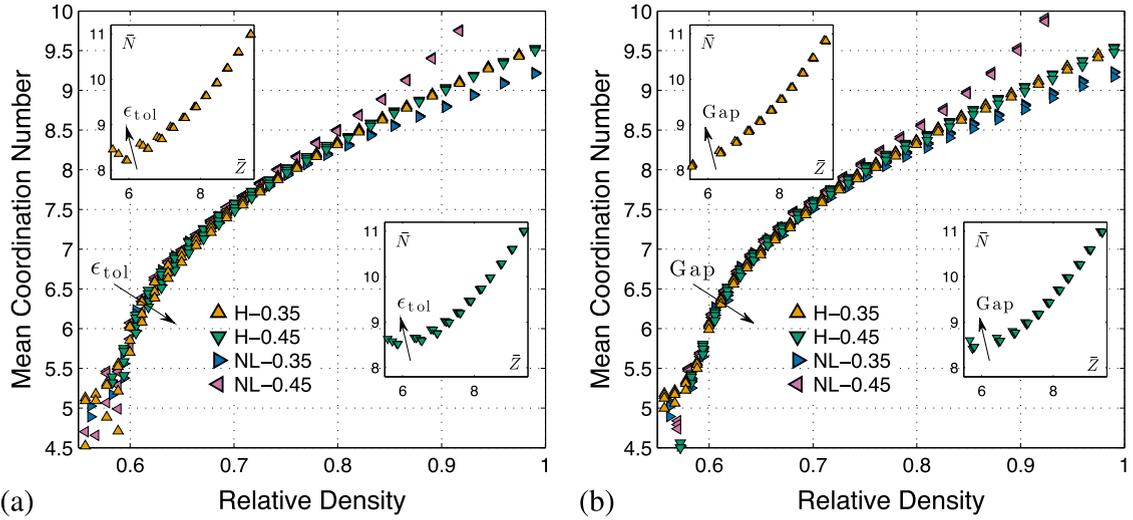
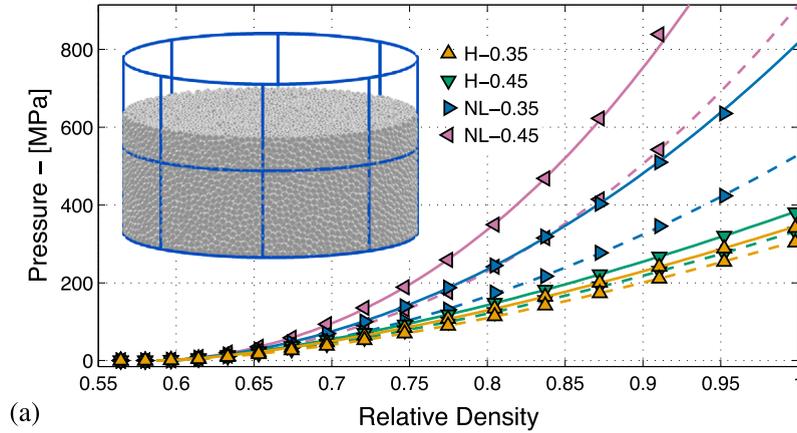


Fig. 4. (a) Sensitivity of the mean mechanical coordination number to value of the smallest contributing contact force, for $\epsilon_{tol} \in [0.1\%, 0.05\%, 0.01\%, 0.005\%]$ and $\text{Gap} = 4R$. (b) Sensitivity of the mean mechanical coordination number to boundary effects, for $\text{Gap} = [R, 2R, 3R, 4R]$ and $\epsilon_{tol} = 0.005\%$.



Pressure	K_H	β_H	eqn.(7)	K_{NL}	β_{NL}
Punch ($\nu = 0.35$)	1301 $\pm 0.3\%$	1.491 $\pm 0.2\%$	1269	3466 $\pm 1.4\%$	2.254 $\pm 0.5\%$
Wall ($\nu = 0.35$)	1237 $\pm 0.2\%$	1.565 $\pm 0.1\%$	—	1372 $\pm 3.2\%$	2.066 $\pm 1.2\%$
Punch ($\nu = 0.45$)	1454 $\pm 0.2\%$	1.498 $\pm 0.1\%$	1397	8640 $\pm 1.5\%$	2.453 $\pm 0.5\%$
Wall ($\nu = 0.45$)	1306 $\pm 0.6\%$	1.538 $\pm 0.3\%$	—	5436 $\pm 2.1\%$	2.528 $\pm 0.7\%$

Fig. 5. (a) Pressures at upper/lower punch (solid lines) and at die wall (dashed lines) as a function of relative density. Lines correspond to the best fit of Eq. (6) to results of the particle contact mechanics simulation of the granular bed (symbols). The inset depicts the compacted granular bed at $\rho = 1$. (b) Coefficients and exponents for best fits. Stiffnesses are in MPa.

the first term of the equation (i.e., K_H and β_H) are best-fitted to the numerical results for Hertz theory. The remaining coefficients (i.e., K_{NL} and β_{NL}) are best-fitted to predictions of the nonlocal contact formulation with K_H and β_H kept fixed [see Fig. 5(b) for numerical values]. It is interesting to note that stiffnesses K_H and critical exponents β_H for Hertzian systems are well approximated by

$$K_H = \frac{E}{2\pi(1-\nu^2)}; \quad \beta_H = 3/2 \quad (7)$$

near jamming (see, e.g., O'Hern et al., 2002; Durian, 1995; Makse et al., 2000; Mason et al., 1997) and at large relative densities. In fact, the form of Eq. (6) is motivated by the observation that, for Hertzian systems, pair-interactions and effective macroscopic behavior are described by powder laws with the same exponent (3/2). Thus, for non-local contact interactions, we propose a macroscopic behavior that contains the first two terms in the series expansion of the contact force of a single particle pressed between rigid plates (Fig. 1), i.e., that contains the Hertzian term and a nonlocal correction (Gonzalez and Cuitiño, 2012).

The fitting procedure described above results in $\beta_{\text{NL}} \geq 2$ which is consistent with the exponents in a series expansion of the nonlocal contact formulation (see Eq. (12) in Gonzalez and Cuitiño, 2012). An analytical derivation of K_{NL} is a worthwhile direction of future work, for which one may expect $K_{\text{NL}}/K_{\text{H}}$ to only depend on ν and thus to be in agreement with studies presented in Gonzalez and Cuitiño (2012) for granular crystals or highly packed granular lattices. In a similar manner, one may expect that the behavior observed in Fig. 3 for \bar{Z} solely depends on ν . A detailed analysis concerning this point is however beyond the scope of this work.

3.3. Network of contact forces

The probability distribution of the contact forces is assumed to have an algebraic tail with exponent α and to be translated by f_0 , that is

$$P(\bar{f}) \propto \bar{f}^{\gamma-1} \exp[-\lambda^\alpha \bar{f} - f_0]^\alpha \quad (8)$$

where $\bar{f} = f/f_{\text{av}}$ is the non-dimensional contact force and γ is a shape parameter that controls the behavior of weak forces— for $\alpha > 1$, $\int_0^{+\infty} P(\bar{f}) d\bar{f}$ is finite if $\gamma > 0$; and for $\gamma = 1$, $P(\bar{f} = 0)$ is finite. Contact forces between particles and between particles and walls are studied separately and non-dimensionalized by their own average value f_{av} . Fig. 6 shows that, as relative density increases, the tails of both probability distributions transition from exponential ($\alpha = 1$) to Gaussian ($\alpha = 2$). However, the distributions, although similar at jamming onset, are very different at full compaction. The particle–wall force distribution becomes increasingly symmetric, that is its mode approaches its mean value. In sharp contrast, the particle–particle force distribution shows a peak at small forces and a local maximum, or a plateau, whose location saturates to 3/4. These results agree with previous studies that noted a transition from exponential to Gaussian tails (Antony, 2000; Brujić et al., 2003; Brukić et al., 2003; Erikson et al., 2002; Jorjadze et al., 2013; Makse et al., 2000; Thornton, 1997; Van Eerd et al., 2007). They also extend to three-dimensional systems the observation that distributions measured at the walls do not reflect accurately distributions of the bulk in general (see, e.g., Snoeijer et al., 2004; Tighe et al., 2008 for two-dimensional studies).

A best fit of the numerical results suggests the following further simplification:

$$\text{particle – particle: } f_0 = \sqrt{\alpha - 1}; \quad \lambda = \sqrt{\alpha} - 1/2 \quad (9)$$

$$\text{particle – wall: } f_0 = \alpha - 1; \quad \gamma = 1 \quad (10)$$

Thus, after best fitting the numerical results of the particle contact mechanics simulations to (8) with (9) and (10), it is evident from Fig. 6 that two parameters fully describe each probability distribution with remarkable accuracy. Furthermore, the numerical results are in excellent agreement with experimental measurements reported in the literature for one-dimensional compaction of spherical deformable particles in cylindrical containers. These measurements are obtained at, or near, the wall using a carbon paper technique (Erikson et al., 2002; Mueth et al., 1998; Makse et al., 2000), or confocal microscopy (Zhou et al., 2006), respectively—with the remarkable exception of Brujić et al. (2003), and recently (Brodu et al., 2015), which are obtained within the bulk of monodisperse emulsions by confocal microscopy. Naturally, the statistical significance obtained for particle–wall interactions is smaller than the one obtained for particle–particle interactions—e.g., in this study, the ratio between the number of each type of interaction remains almost constant during compaction and equal to 3%.

Fig. 7 shows the evolution of $\{\alpha, \gamma\}_{\text{PP}}$ for particle–particle interactions and of $\{\alpha, \lambda\}_{\text{PW}}$ for particle–wall interactions. Interestingly, the figure suggests a critical-like behavior for the parameter α_{PP} with critical exponent 1/5 and critical density ρ_c . It also reveals that predictions of the nonlocal contact formulation depart from those obtained with Hertz theory at moderate to high levels of confinements (e.g., α_{PP} saturates at 1.8, not reaching truly Gaussian values). The systematic investigation of this critical-like behavior, and the elucidation of the material properties and microstructural features that control it, are worthwhile directions of future research. In addition, the figure reveals that γ_{PP} is larger than 0.6 and saturates at 0.80, whereas γ_{PW} is found to be 1. This is in agreement with recent theoretical and numerical calculations (see, e.g., Bo et al., 2014; Lerner et al., 2013 and references therein). It is worth noting that the probability distribution of particle–wall contact forces thus takes a finite value at zero proportional to $\exp[-\lambda^\alpha(\alpha - 1)^\alpha]$. Finite values for $P(\bar{f} = 0)$ have been reported in Bo et al. (2014) for particle–particle forces.

Finally, Fig. 8 illustrates the network of forces in the three-dimensional granular system for four different relative densities. We only visualize non-dimensional contact forces \bar{f} larger than 2.5, that is the forces that carry most of the load in the system. It is clearly observed in the figure that at low relative density or confinement the network is inhomogeneous in

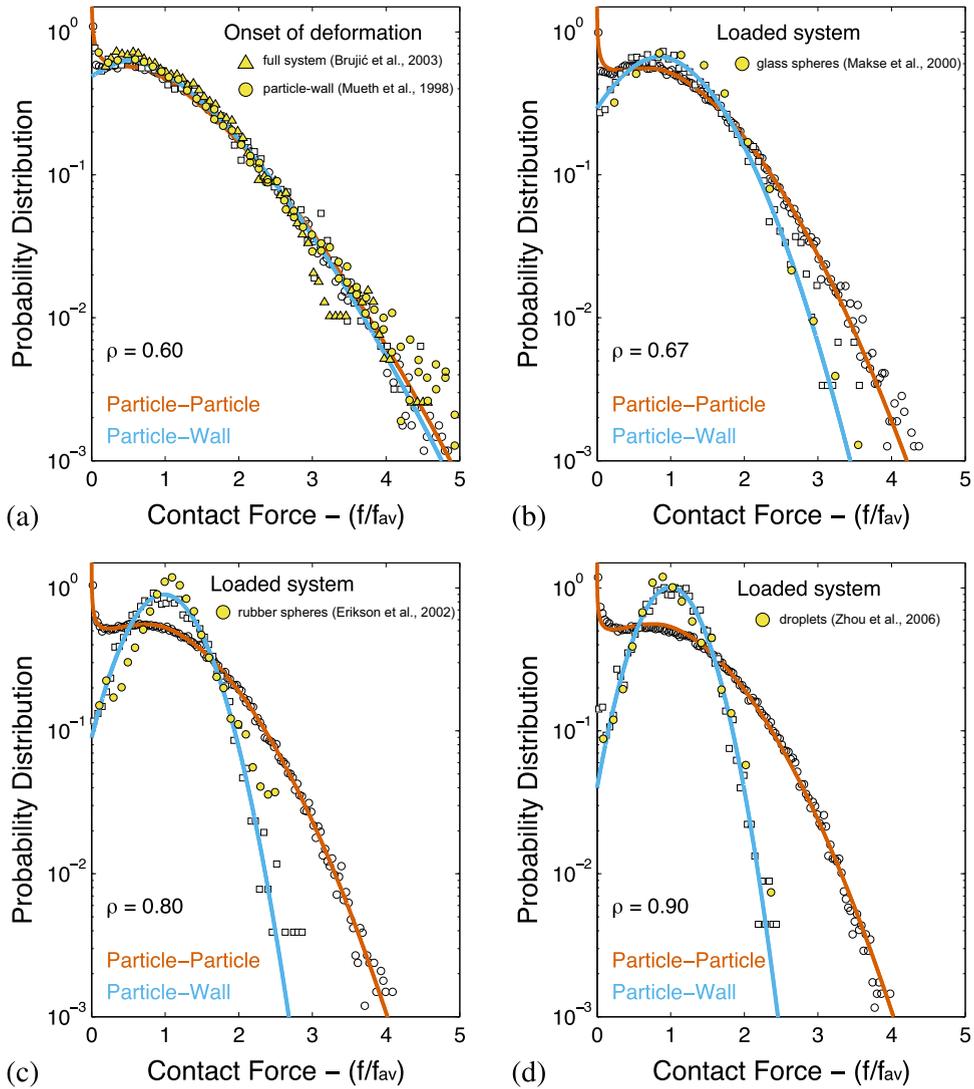


Fig. 6. Probability distribution of particle–particle (\circ) and particle–wall (\square) contact forces determined from the particle contact mechanics simulation for (a) Hertz theory with $\nu=0.45$, (b) nonlocal contact formulation with $\nu=0.35$, and (c, d) nonlocal contact formulation with $\nu=0.45$. Filled symbols correspond to die compaction experiments in cylindrical containers and solid lines correspond to the best fit of the numerical results to Eq. (8), with (9) and (10). All calculations correspond to $\epsilon_{\text{tol}} = 0.005\%$ and particle–particle calculations are for $\text{Gap} = 4R$.

space and characterize by a broad range of forces. In contrast, at high relative density or confinement the network becomes more homogeneous in space and the range of observed forces is narrower (Makse et al., 2000). These observations are consistent with the transition from exponential to Gaussian tails in the distribution of particle–particle interactions under increasing relative density.

3.4. Network of contact radiuses and areas

The probability distribution of the contact radiuses is assumed to have an algebraic tail with exponent α and to be translated by a_0 , that is

$$P(\bar{a}) \propto \bar{a}^{3\gamma-1} \exp\left[-\lambda^\alpha \left|\bar{a}^3 - a_0^3\right|^\alpha\right] \quad (11)$$

where we have changed variables in (8) using $\bar{f} \propto \bar{a}^3$. We note that the Hertzian relationship $f = Ka^3$ does not hold for the average values (i.e., $f_{\text{av}} \geq Ka_{\text{av}}^3$) and thus the non-dimensional values are related by the following inequality: $\bar{f} \leq \bar{a}^3$. The identification of tighter bounds for the inequality and how these bounds can be used to bound $P(\bar{a})$ are however beyond the scope of this work. Fig. 9 shows that, as relative density increases, the range of observed contact radiuses is narrower. This transition however occurs faster than in the case of contact forces for particle–particle interactions (cf. Fig. 6). In accordance

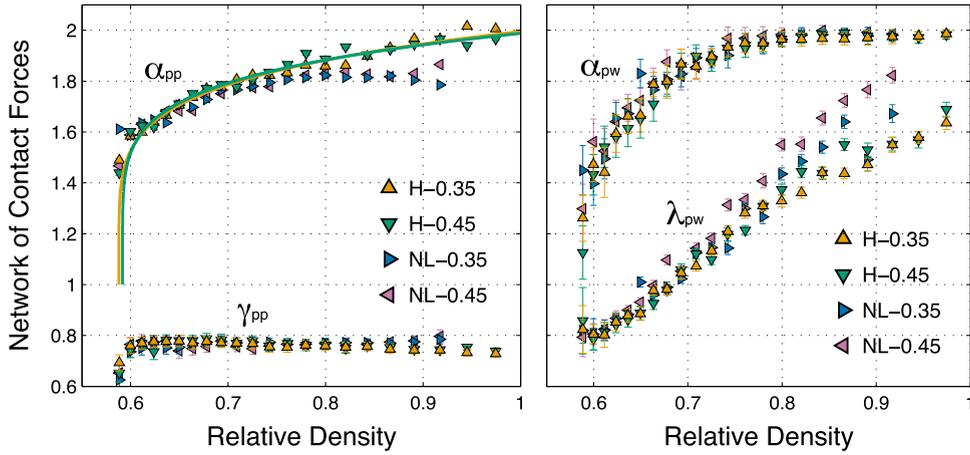


Fig. 7. Statistical description of the probability distribution of particle–particle (PP) and particle–wall (PW) contact forces, as a function of relative density. Symbols represent the parameters obtained from the best fit of numerical results to Eq. (8), with (9) and (10). All calculations correspond to $\epsilon_{\text{tol}} = 0.005\%$ and particle–particle calculations are for $\text{Gap} = 4R$.

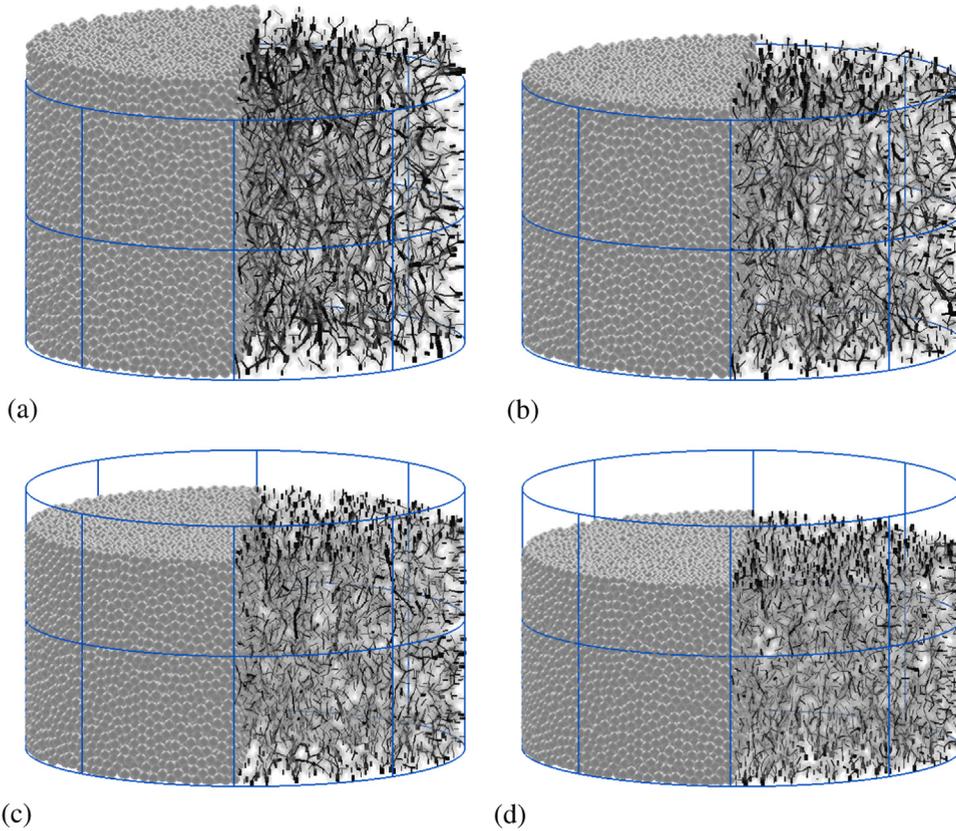


Fig. 8. Network of forces in the compacted granular bed for (a) $\rho=0.60$, (b) $\rho=0.67$, (c) $\rho=0.80$ and (d) $\rho=0.90$. Thicker lines depict larger forces. Only normalized contact forces \bar{f} larger than 2.5 are not shown and the particles involved in these pair-interactions are depicted as semi-transparent gray spheres.

with the behavior of the network of forces, the figure indicates that the distributions, though similar at jamming onset, are very different at full compaction. Fig. 9 also shows a best fit of the numerical results to Eq. (11) for reference purposes. However, the simplifications proposed for the network of forces, i.e., Eqs. (9) and (10), do not hold true for the network of contact radiuses. It is worth noting that the choice of ϵ_{tol} does influence the tail of the probability distribution at $\bar{a} = 0$ when the system is at jamming onset, see Fig. 9(a).

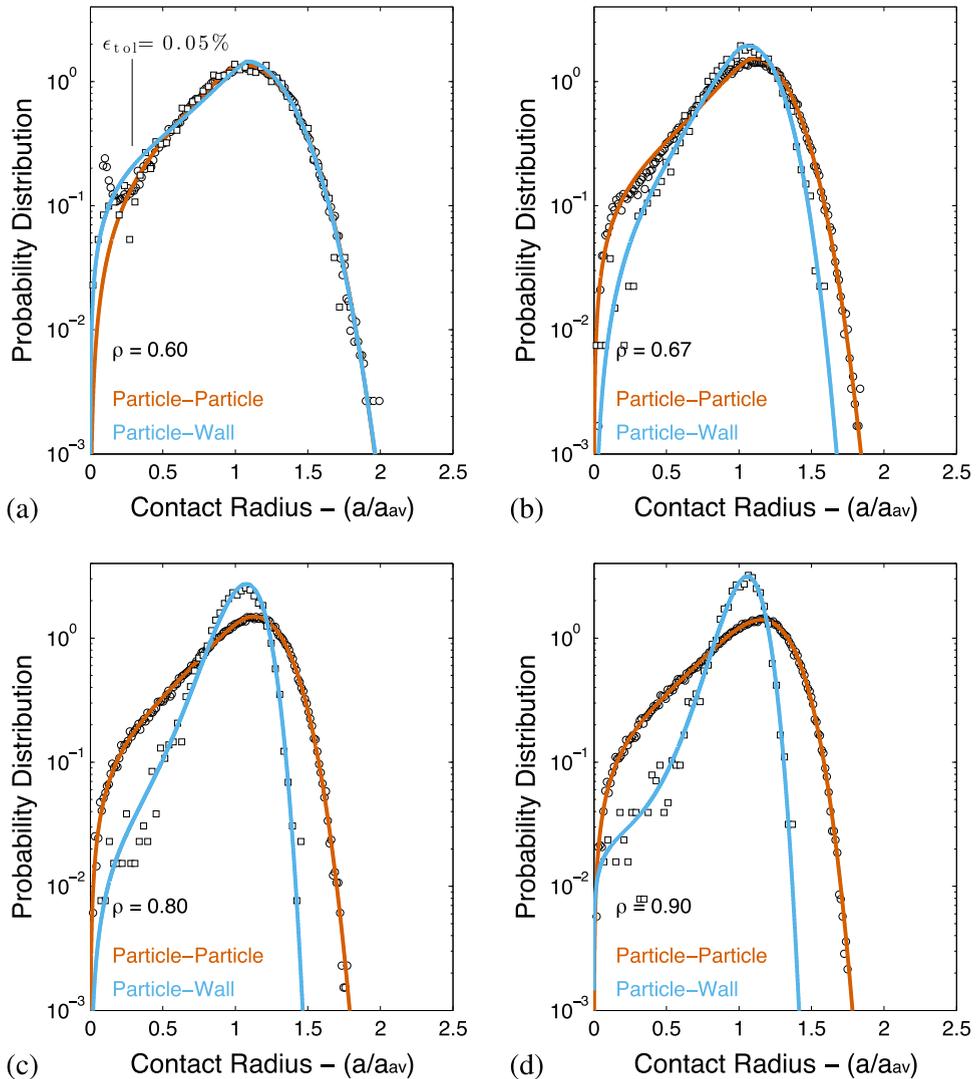


Fig. 9. Probability distribution of particle–particle (\circ) and particle–wall (\square) contact radii determined from the particle contact mechanics simulation for (a) Hertz theory with $\nu=0.45$, (b) nonlocal contact formulation with $\nu=0.35$, and (c, d) nonlocal contact formulation with $\nu=0.45$. Solid lines correspond to the best fit of the numerical results to Eq. (11). All calculations correspond to $\epsilon_{tol} = 0.005\%$ and particle–particle calculations are for $\text{Gap} = 4R$.

4. Summary and discussion

We have reported three-dimensional particle mechanics static calculations that predict the microstructure evolution of monodisperse elastic spherical particles during die-compaction up to relative densities close to one (<https://nanohub.org/resources/gscopy>). We employ a nonlocal contact formulation that remains predictive at high levels of confinement by removing the classical assumption that contacts between particles are formulated locally as independent pair-interactions. Our approach demonstrates that the coordination number depends on the level of compressibility, i.e., on Poisson's ratio, of the particles and thus its scaling behavior is not independent of material properties as previously thought. Our results also reveal that distributions of contact forces between particles and between particles and walls, although similar at jamming onset, are very different at full compaction. Both distribution tails transition from exponential to Gaussian under increasing relative density—with particle–wall forces exhibiting an earlier transition. Particle–wall forces are in remarkable agreement with experimental measurements reported in the literature, providing a unifying framework for bridging experimental boundary observations with bulk behavior. The evolution of these microstructural features is not otherwise amenable to direct experimental determination. Furthermore, prediction of such evolution is key to better design, optimize and control many manufacturing processes widely used in pharmaceutical, energy, food, ceramic and metallurgical industries.

We close by pointing out some limitations of our approach and possible avenues for extensions of the analysis.

First, we have generated the initial powder bed by means of a ballistic deposition technique and progressively moving

the upper punch until particle rearrangement and small deformations lead to a jammed configuration. This is not the only—perhaps even the best—available protocol for obtaining jammed configurations in rigid containers. A case in point consists in modeling the filling process (see, e.g., Mateo-Ortiz et al., 2014; Wu, 2008) by solving the equations of motion of the Lagrangian system of particles with a numerical time integrator (see, e.g., Gonzalez et al., 2010, 2012; Hairer et al., 2006 and references there in). However, this approach, though more realistic, may also result in a jammed backbone and a number of rattlers. The systematic investigation of the effect of the filling protocol on the formation and evolution of the microstructural features studied here at high relative densities is a worthwhile direction of future research.

Second, we have restricted attention to die-compaction of monodisperse system constrained by a rigid cylindrical container and two flat punches. The systematic extension of this analysis to dies and punches of other shapes, hydrostatic compaction conditions, polydispersity and mixtures of particles with different material properties are interesting topics to study.

Third, although our analysis has focused on coordination number, punch and die-wall pressures, and the network of contact forces and radiuses, there are other microstructural features of theoretical and practical importance. For example, it is relevant to study the evolution of material-fabric tensor, force-fabric tensor and pore size distribution during die compaction.

Acknowledgments

The authors gratefully acknowledge the support received from the NSF ERC Grant number EEC-0540855, ERC for Structured Organic Particulate Systems. M.G. also acknowledges support from Purdue University's startup funds and from the Network for Computational Nanotechnology (NCN) and nanoHUB.org.

References

- Antony, S.J., 2000. Evolution of force distribution in three-dimensional granular media. *Phys. Rev. E* 63 (1), 011302.
- Baranau, V., Tallarek, U., 2014. On the jamming phase diagram for frictionless hard-sphere packings. *Soft Matter* 10, 7838.
- Blair, D.L., Mueggenburg, N.W., Marshall, A.H., Jaeger, H.M., Nagel, S.R., 2001. Force distributions in three-dimensional granular assemblies: effects of packing order and interparticle friction. *Phys. Rev. E* 63 (4), 041304.
- Blumenfeld, R., Edwards, S.F., 2009. On granular stress statistics: compactivity, anisotropy, and some open issues. *J. Phys. Chem. B* 113, 3981–3987.
- Bo, L., Mari, R., Song, M., Makse, H.A., 2014. Cavity method for force transmission in jammed disordered packings of hard particles. *Soft Matter* 10, 7379–7392.
- Brujić, J., Edwards, S.F., Grinev, D.V., Hopkinson, I., Brujić, D., Makse, H.A., 2003. 3D bulk measurements of the force distribution in a compressed emulsion system. *Faraday Discuss.* 123, 207–220.
- Brukić, J., Edwards, S.F., Hopkinson, I., Makse, H.A., 2003. Measuring the distribution of interdroplet forces in a compressed emulsion system. *Physica A* 327, 201–212.
- Brodu, N., Dijkstra, J.A., Behringer, R.P., 2015. Spanning the scales of granular materials: microscopic force imaging. *Nat. Commun.* 6, 6361.
- Byrd, R.H., Schnabel, R.B., Shultz, G.A., 1988. Approximate solution of the trust region problem by minimization over two-dimensional subspaces. *Math. Program.* 40, 247–263.
- Cates, M.E., Wittmer, J.P., Bouchaud, J.-P., Claudin, P., 1998. Jamming, force chains, and fragile matter. *Phys. Rev. Lett.* 81 (9), 1841–1844.
- Chan, S.H., Ngan, A.H.W., 2005. Statistical distribution of contact forces in packings of deformable spheres. *Mech. Mater.* 37, 493–506.
- Chaudhuri, P., Berthier, L., Sastry, S., 2010. Jamming transitions in amorphous packings of frictionless spheres occur over a continuous range of volume fractions. *Phys. Rev. Lett.* 104, 165701.
- Ciamarra, M.P., Richard, P., Schröter, M., Tighe, B.P., 2012. Statistical mechanics for static granular media: open questions. *Soft Matter* 8, 9731–9737.
- Clusel, M., Corwin, E.L., Siemens, A.O.N., Brujić, J., 2009. A granocentric model for random packing of jammed emulsions. *Nature* 460, 611–615.
- Coleman, T.F., Li, Y., 1996. An interior trust region approach for nonlinear minimization subject to bounds. *SIAM J. Optim.* 6 (2), 418–445.
- Conn, A., Gould, N., Toint, P., 2000. Trust Region Methods. Society for Industrial and Applied Mathematics, <http://epubs.siam.org/doi/pdf/10.1137/1.9780898719857.fm>.
- Durian, D.J., 1995. Foam mechanics at the bubble scale. *Phys. Rev. Lett.* 75 (26), 4780–4783.
- Edwards, S.F., Oakeshott, R.B.S., 1989. Theory of powders. *Physica A* 157, 1080–1090.
- Erikson, J.M., Mueggenburg, N.W., Jaeger, H.M., Nagel, S.R., 2002. Force distributions in three-dimensional compressible granular packs. *Phys. Rev. E* 66, 040301(R).
- Gonzalez, M., Schmidt, B., Ortiz, M., 2010. Energy-stepping integrators in Lagrangian mechanics. *Int. J. Numer. Methods Eng.* 82 (2), 205–241.
- Gonzalez, M., Yang, J., Daraio, C., Ortiz, M., 2012. Mesoscopic approach to granular crystal dynamics. *Phys. Rev. E* 85, 016604.
- Gonzalez, M., Cuitiño, A.M., 2012. A nonlocal contact formulation for confined granular systems. *J. Mech. Phys. Solids* 60, 333–350.
- Hairer, E., Lubich, C., Wanner, G., 2006. Geometric numerical integration. In: *Structure-Preserving Algorithms for Ordinary Differential Equations*. Springer Series in Computational Mathematics, 2nd ed., vol. 31. Springer, Berlin.
- Jin, Y., Makse, H.A., 2010. A first-order phase transition defines the random close packing of hard spheres. *Physica A* 389 (23), 5362–5379.
- Jorjadze, I., Pontani, L.-L., Brujić, J., 2013. Microscopic approach to the nonlinear elasticity of compressed emulsions. *Phys. Rev. Lett.* 110 (4), 048302.
- Jullien, R., Meakin, P., 1989. Simple models for the restructuring of 3-dimensional ballistic aggregates. *J. Colloid Interface Sci.* 127 (1), 265–272.
- Lerner, E., Doring, G., Wyart, M., 2013. Low-energy non-linear excitations in sphere packings. *Soft Matter* 9, 8252–8263.
- Liu, A.J., Nagel, S.R., 1998. Nonlinear dynamics: jamming is not just cool any more. *Nature* 396 (6706), 21–22.
- Liu, C.-H., Nagel, S.R., Schecter, D.A., Coppersmith, S.N., Majumdar, S., Narayan, O., Witten, T.A., 1995. Force fluctuations in bead packs. *Science* 269, 513.
- Majumdar, T.S., Behringer, R.P., 2005. Contact force measurements and stress-induced anisotropy in granular materials. *Nature* 435, 1079–1082.
- Mateo-Ortiz, D., Muzzio, F.J., Méndez, R., 2014. Particle size segregation promoted by powder flow in confined space: the die filling process case. *Powder Technol.* 262, 215–222.
- Makse, H.A., Johnson, D.L., Schwartz, L.M., 2000. Packing of compressible granular materials. *Phys. Rev. Lett.* 84 (18), 4160–4163.
- Mason, T.G., Lacasse, M.-D., Grest, G.S., Levine, D., Bibette, J., Weitz, D.A., 1997. Osmotic pressure and viscoelastic shear moduli of concentrated emulsions. *Phys. Rev. E* 56 (3), 3150–3166.
- Mehta, A., 2007. *Granular Physics*. Cambridge University Press, Cambridge.

- Moré, J.J., Sorensen, D.C., 1983. Computing a trust region step. *SIAM J. Sci. Stat. Comput.* 4 (3), 553–572.
- Mueth, D.M., Jaeger, H.M., Nagel, S.R., 1998. Force distribution in a granular medium. *Phys. Rev. E* 57 (3), 3164–3169.
- Newhall, K.A., Jorjadze, I., Vanden-Eijnden, E., Bruijic, J., 2011. A statistical mechanics framework captures the packing of monodisperse particles. *Soft Matter* 7, 11518.
- O'Hern, C.S., Langer, S.A., Liu, A.J., Nagel, S.R., 2002. Random packings of frictionless particles. *Phys. Rev. Lett.* 88 (7), 075507.
- O'Hern, C.S., Silbert, L.E., Liu, A.J., Nagel, S.R., 2003. Jamming at zero temperature and zero applied stress: the epitome of disorder. *Phys. Rev. E* 68 (1), 011306.
- Ostojic, S., Somfai, E., Nienhuis, B., 2006. Scale invariance and universality of force networks in static granular matter. *Nature* 439, 828–830.
- Radjai, F., Jean, M., Moreau, J.-J., Roux, S., 1996. Force distributions in dense two-dimensional granular systems. *Phys. Rev. Lett.* 77 (2), 274–277.
- Richard, P., Nicodemi, M., Delannay, R., Ribiere, P., Bideau, D., 2005. Slow relaxation and compaction of granular systems. *Nat. Mater.* 4 (2), 121–128.
- Schreck, C.F., O'Hern, C.S., Silbert, L.E., 2011. Tuning jammed frictionless disk packings from isostatic to hyperstatic. *Phys. Rev. E* 84, 011305.
- Snoeijer, J.H., van Hecke, M., Somfai, E., van Saarloos, W., 2004. Packing geometry and statistics of force networks in granular media. *Phys. Rev. E* 70 (15), 011301.
- Song, C., Wang, P., Makse, H.A., 2008. A phase diagram for jammed matter. *Nature* 453, 629–632.
- Tatara, Y., 1989. Extensive theory of force-approach relations of elastic spheres in compression and in impact. *J. Eng. Mater. Technol.* 111, 163–168.
- Thornton, C., 1997. Force transmission in granular media. *KONA Powder Part.* 15, 81–90.
- Tighe, B.P., van Eerd, A.R.T., Vlugt, T.J.H., 2008. Entropy maximization in the force network ensemble for granular solids. *Phys. Rev. Lett.* 100 (23), 238001.
- Trappe, V., Prasad, V., Cipelletti, L., Segre, P.N., Weitz, D.A., 2001. Jamming phase diagram for attractive particles. *Nature* 411, 772–775.
- Van Eerd, A.R.T., Ellenbroek, W.G., van Hecke, M., Snoeijer, J.H., Vlugt, T.J.H., 2007. Tail of the contact force distribution in static granular materials. *Phys. Rev. E* 75 (6), 060302. R.
- Vågberg, D., Olsson, P., Teitel, S., 2011. Glassiness, rigidity, and jamming of frictionless soft core disks. *Phys. Rev. E* 83, 031307.
- Vicente, L.N., 1996. A comparison between line searches and trust regions for nonlinear optimization. *Invest. Oper.* 16, 173–179.
- Wu, C.-Y., 2008. DEM simulations of die filling during pharmaceutical tableting. *Particuology* 6 (6), 412–418.
- Zhou, J., Long, S., Wang, Q., Dinsmore, A.D., 2006. Measurement of forces inside a three-dimensional pile of frictionless droplets. *Science* 312, 1631–1633.
- Similar results for smaller granular systems can be obtained using the “Powder Compaction” tool available in nanoHUB.org, (<https://nanohub.org/resources/gscopy>), <http://dx.doi.org/10.4231/D33N20F7K>.