A Monte Carlo packing algorithm for poly-ellipsoids and its comparison with packing generation using Discrete Element Model

Boning Zhang, Eric B. Herbold, Richard A. Regueiro

Department of Civil, Environmental, and Architectural Engineering

University of Colorado, Boulder

Boulder, CO 80309

February 5, 2023

Abstract

Granular material is showing very often in geotechnical engineering, petroleum engineering, material science and physics. The packings of the granular material play a very important role in their mechanical behaviors, such as stress-strain response, stability, permeability and so on. Although packing is such an important research topic that its generation has been attracted lots of attentions for a long time in theoretical, experimental, and numerical aspects, packing of granular material is still a difficult and active research topic, especially the generation of random packing of non-spherical particles. To this end, we will generate packings of same particles with same shapes, numbers, and same size distribution using *geometry* method and *dynamic* method, separately. Specifically, we will extend one of Monte Carlo models for spheres to ellipsoids and poly-ellipsoids.

keywords: Discrete Element Method, Numerical Simulation, Numerical Method

1 Introduction

Granular material is showing very often in geotechnical engineering, petroleum engineering, material science and physics [Buchalter and Bradley, 1994, Jaeger et al., 1996, Regueiro et al., 2014b, Senseney et al., 2017, Zhang, 2016]. The packings of the granular material play a very important role in their mechanical behaviors, such as stress-strain response, stability, permeability and so on [Troadec et al., 1991, Maggi et al., 2008, Zhang and Regueiro, 2015, Amirrahmat et al., 2018, Regueiro et al., 2014a, Luo et al., 2022]. For example, Troadec et al. [1991] studied experimentally the effects of different packings on the stress-strain relation during compression of packed cylinders and found that the coordination number of the packing govern the stress-strain paths during compression. Bassett et al. [2012], Sadd et al. [2000] then further concluded experimentally and numerically, respectively, that force chain of packed granular materials plays significant effects on sound propagation in granular materials. And our previous researches [Zhang et al., 2015] show that different packed sand grains behave differently in the simulations of Split Hopkinson Pressure Bar experiments.

Although packing is such an important research topic that its generation has been attracted lots of attentions for a long time in theoretical [Furnas, 1929, Melissen and Schuur, 1995, Brouwers, 2006, Torquato and Jiao, 2009], experimental [Furnas, 1929, Bideau and Hansen, 1993], and numerical [He et al., 1999, Jia and Williams, 2001, Jiang et al., 2003, Dong et al., 2006, Zhou et al., 2011] aspects, packing of granular material is still a difficult and active research topic, especially the generation of random packing of non-spherical particles. There are two kinds of numerical generation methods of random packing based on *geometry* and *dynamic*, respectively. *Geometry* method is moving and rotating particles in a packing by geometry constraints to reduce overlap between particles. After overlap is decreased to a small tolerance, the packing is viewed as a stable system and packing generation is finished. The *geometry* method is efficient and has been applied successfully to generate random packings of monodisperse spheres, polydisperse spheres, ellipsoids, super-ellipsoids, and spherocylinders [Buchalter and Bradley, 1994, Yang et al., 1996, He et al., 1999, Jia and

Williams, 2001, Kansal et al., 2002, Fu and Dekelbab, 2003, Abreu et al., 2003, Donev et al., 2007, Maggi et al., 2008, Stafford and Jackson, 2010, Delaney and Cleary, 2010]. Among so many *geometry* packing generation algorithms, Monte Carlo model is very famous and extended to many different variables. The *dynamic* method is simulating the physical inter-actions between particles during packing process [Cheng et al., 2000, Jiang et al., 2003, Zhou et al., 2011] based on Discrete Element Method (DEM). DEM [Cundall and Strack, 1979] is used to simulate the motion of individual particles/grains within an overall deformation and/or flow of a granular medium, which is borrowed to simulate the dynamic process during packing generation. For example, Cheng et al. [2000] randomly generated circular particles inside a box without any overlaps by removing the overlapped particles, then these random particles are settled down by gravity force to generate random packings. Jiang et al. [2003] generated particles randomly in a container without any overlaps, and then compress these particles to reach specific packing fraction. Zhou et al. [2011] generated packings by pouring ellipsoidal particles from a certain height into a container, which is more physically related to the generation of packings in experiments. These descriptions of the two methods suggest that *geometry* methods are much more faster than *dynamic* methods, since it takes a lot of time for the particles in the latter to come to rest. While *dynamic* methods considered the interactions between particles mechanically, and the pouring method is more similar phys-ically to the generation of packings in experiments. Although both *geometry* methods and *dynamic* methods can generate packings with similar fractions as in experiments, there are worries about what it will influence on the packings if *geometry* methods do not consider packing as a dynamic process involving forces between particles [Jia and Williams, 2001, Dong et al., 2006, An et al., 2008, Zhou et al., 2011]. The motivation of this paper is then to explore the influence and to answer if we can take advantages of the efficiency of *geometry* methods without introducing much difference to the final packings of particles compared with *dynamic* generating methods. To this end, we will generate packings of same particles with same shapes, numbers, and same size distribution using *geometry* method and *dynamic*

method, separately. Specifically, we will extend one of Monte Carlo models proposed by He et al. [1999] for spheres to ellipsoids and poly-ellipsoids [Peters et al., 2009]. To simulate the dynamic process during packings, we will adopt gravitational deposition [Yan et al., 2010] of particle assembly which is similar as the pouring method described in [Zhou et al., 2011]. After packings are generated by the two methods separately, the corresponding packings will be analyzed and compared with respect to packing metrics, such as packing fraction, Coordination Number (CN), Radia Distribution Function (RDF) [Konakawa and Ishizaki, 1990, He et al., 1999, Zhou et al., 2011], fabric tensor [Yimsiri and Soga, 2010, 2011], and also force chain [Sadd et al., 2000, Bassett et al., 2012].

Currently, most of packings are generated for spheres and ellipsoids. Some researchers studied and concluded that particle shape plays a crucial role in packings of ellipsoids [Bezrukov and Stoyan, 2006], super-ellipsoids [Delaney and Cleary, 2010], hyperspheres [Skoge et al., 2006], and sphereocylinders [Abreu et al., 2003]. Thus this paper also considered packings of different shapes generated by the two methods, such as spheres, ellipsoids (prolate and oblate) [Bezrukov and Stoyan, 2006], and poly-ellipsoids (carrot and half-dome) [Peters et al., 2009]. With poly-ellipsoids, we can create many unsymmetrically shaped particles, it is very important since most of geotechnical material are not regular or symmetric, and no one else has studied packings of unsymmetric particles.

2 Algorithms

This paper considered two packing generation methods, an extended Monte Carlo Model and DEM simulation of gravitational deposition, which are belonging to the two major packing generation methods in community, respectively. The two methods will be used to generate packings of same particle assemblies, and then the packings will be analyzed and compared to study the effects caused by not considering dynamic interactions between particles in Monte Carlo packing algorithm.

2.1 Extended Monte Carlo Model

He et al. [1999] presented a variable of Monte Carlo model to generate random packings of unequal spherical particles obeying any specified distributions. He et al. [1999] first generated a certain number (n) of spherical particles following a specified size distribution, and these particles are uniformly randomly placed within a cubic domain with the initial size as L_0, which is determined as [He et al., 1999]

$$L_0 = \left[\frac{1}{\Phi_0} \sum_{i=1}^{n} v_i \right]^{1/3} \tag{1}$$

where Φ_0 is an arbitrary initial packing density which can be unphysically higher than random close packing fraction, in this paper Φ_0 is taken as 0.86 following He et al. [1999]'s suggestion, and v_i is the volume of particle p_i. The meaning of Eqn.1 is generating a cubic domain containing the initial particle assembly with a packing fraction as Φ_0.

There will be lots of overlaps between particles in this initial packing. During each step, He et al. [1999] moved an overlapped particle by the sum vector considering all overlaps of this particle. For example, the new position of particle p_i with n_i overlapped particles is given by [He et al., 1999]

$$\mathbf{p}'_i = \mathbf{p}_i + \frac{1}{n_i} \sum_{j=1}^{n_i} \mathbf{t}_{ij} \tag{2}$$

where $\mathbf{t}_{ij}$ is the translation vector of particle p_i caused by the overlapping with particle p_j, which is shown in Fig.1. After a certain number of iterations, the mean of the relative overlap will eventually drop to a very small preset tolerance, such that the packing is regarded as a stable packing.

To extend this Monte Carlo model for ellipsoids and poly-ellipsoids, the major changes are the contact detection and rotations of overlapped particles. The contact detection algorithm is to find contacts between particles and their overlaps. For spheres, the contact detection
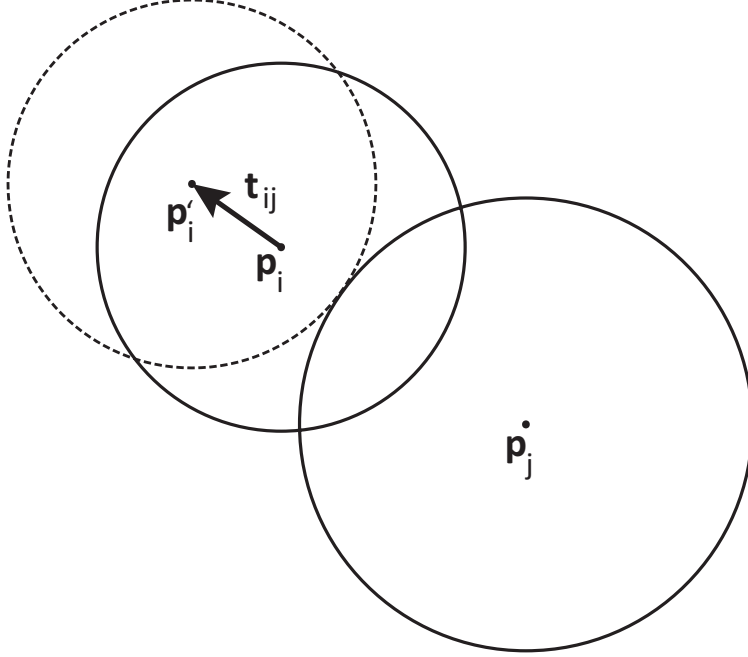
Figure 1. Push outward particle p_i in the direction of branch vector connecting the centroids of particle p_i and p_j by translation vector $\mathbf{t}_{ij}$ in order to eliminate the overlap between particle p_i and p_j, motivated by He et al. [1999].

algorithm is trivial, however it is not straightforward for ellipsoids and poly-ellipsoids, the contact detection algorithms for which are described in Yan et al. [2010] and Zhang et al. [in review], respectively. The other change is to add rotations of overlapped particles for ellipsoids and poly-ellipsoids. Suppose we have two overlapping particles (p_i and p_j) as in Fig.2, then the translation and rotation of particle p_i caused by particle p_j in our model are, respectively

$$\mathbf{t}_{ij} = \frac{m_i}{m_i + m_j} \boldsymbol{\Delta} \tag{3}$$

$$\mathbf{r}_{ij} = \mathbf{d}_i \times \mathbf{t}_{ij} \tag{4}$$

where m_i, m_j are the mass for particles p_i and p_j, and $\boldsymbol{\Delta}$, $\mathbf{d}_i$ are shown in Fig.2. $\boldsymbol{\Delta}$ is the overlap vector pointing from point i to point j, which are contact points on the surface of particle p_i and p_j, respectively. $\mathbf{d}_i$ is a vector pointing from centroid p_i to point i. Similarly,

if particle p_i has n_i overlapped particles, then the overall translation vector and rotation vector are

$$\mathbf{T}_{ij} = \sum_{j=1}^{n_i} t_{ij} \tag{5}$$

$$\mathbf{R}_{ij} = \sum_{j=1}^{n_i} r_{ij} \tag{6}$$

Then after a certain number of steps, the mean of relative overlap will drop below a tolerance and the packing generation is finished. In this research, 1×10^{-4} is accepted as the tolerance for the mean of relative overlap.
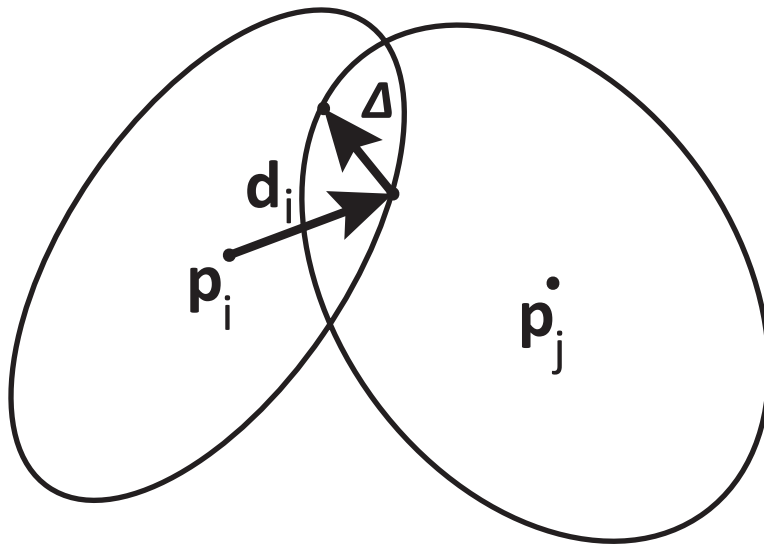

Figure 2. 2D illustration of overlapped particles. $\mathbf{\Delta}$ is the overlap vector connecting two contact points i and j, which are on the surface of particle p_i and p_j. $\mathbf{d}_i$ is pointing from centroid p_i to point i.

2.2 DEM simulation of gravitational deposition

DEM [Cundall and Strack, 1979] is often used in geotechnical engineering to simulate the motion of individual particles/grains within a deforming/flowing granular medium[Horner et al., 2001, Hopkins, 2004, Zhu et al., 2008, Yan et al., 2010, O'Sullivan, 2011, Knuth et al.,

2012]. According to Cundall and Strack [1979], Yan et al. [2010], the governing equation for the translation and rotation of DEM particle i in an assembly are

$$m_i \ddot{\mathbf{u}}_i = \mathbf{F}_i$$
$$I_i \ddot{\boldsymbol{\theta}}_i = \mathbf{M}_i$$

(7)

where $\mathbf{u}$ is the particle displacement; $\boldsymbol{\theta}$, the orientational vector of the particle; m, the particle mass; I, the moment of inertia of the particle; $\mathbf{F}$, the resultant force, which includes body force and contact forces by its overlapping particles; and $\mathbf{M}$, the resultant moment about the principal axes of inertial frame. In this DEM model, Hertz-Mindlin contact theory [Mindlin, 1949] is applied which includes nonlinear elasticity and slip, with addition of Coulomb friction model to evaluate tangential stick-slip conditions. Central difference time integration method is used to solve Eqn.7.

To generate packings of granular material, a gravitational deposition of particle assembly is simulated dynamically using DEM. The particles will be positioned inside a container with open top boundary. The particles are positioned initially without any overlaps with other particles and boundaries. Then these particles will be dropped by the gravity forces at zero initial velocities. After all the particles come to rest, the packing generation is completed.

2.3   Initial particle size distribution

Similar as He et al. [1999], sizes of particles obey truncated log-normal distribution, the probability density function of particle with radius r is

$$f(r) = \frac{1}{\sqrt{(2\pi)}\sigma r} e^{-(lnr - lnr_0)^2/(2\sigma^2)}$$

(8)

In this research, the mean radius is chosen as $r_0 = 1\,\mathrm{m}$, and the standard deviation $\sigma = 0.25\,\mathrm{m}$, and we only allow particle radius between $0.2\,\mathrm{m}$ and $2.5\,\mathrm{m}$. The particle size distribution generated in numerical sample is compared with analytical log-normal distribution
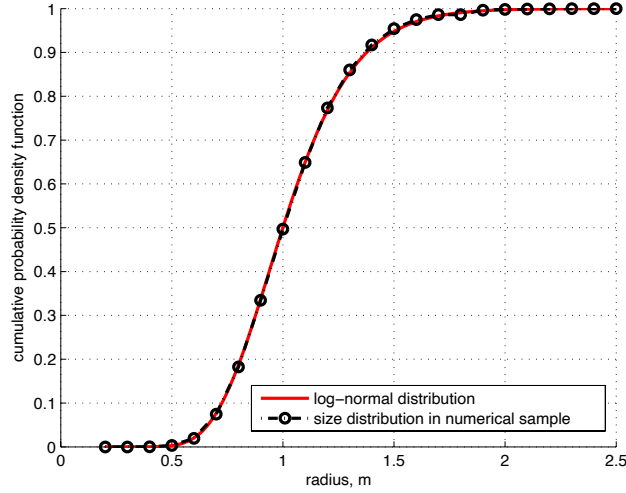
as shown in Fig.3.

Figure 3. Particle size distribution in numerical sample is compared well with the analytical log-normal distribution.

There are five types of shaped particles in this research, i.e. sphere, prolate, oblate, carrot, and half-dome. Prolate and oblate are ellipsoids, while carrot and half-dome are poly-ellipsoids. For spheres, their radii are determined by Eqn.8. For ellipsoids and poly-ellipsoids, we make their major semi-lengths equal to r determined by Eqn.8. Particle assembly with each shaped particle will be only generated once and then the same assembly will be used in the extended Monte Carlo model and DEM gravitational deposition.

References

Charlles RA Abreu, Frederico W Tavares, and Marcelo Castier. Influence of particle shape on the packing and on the segregation of spherocylinders via monte carlo simulations. *Powder Technology*, 134(1):167–180, 2003.

S Amirrahmat, KA Alshibli, MF Jarrar, B Zhang, and RA Regueiro. Equivalent continuum strain calculations based on 3d particle kinematic measurements of sand. *International Journal for Numerical and Analytical Methods in Geomechanics*, 42:999–1015, 2018.

XZ An, RY Yang, RP Zou, and AB Yu. Effect of vibration condition and inter-particle frictions on the packing of uniform spheres. *Powder Technology*, 188(2):102–109, 2008.

Danielle S Bassett, Eli T Owens, Karen E Daniels, and Mason A Porter. Influence of network topology on sound propagation in granular materials. *Physical Review E*, 86(4):041306, 2012.

Alexander Bezrukov and Dietrich Stoyan. Simulation and statistical analysis of random packings of ellipsoids. *Particle & Particle Systems Characterization*, 23(5):388–398, 2006.

Daniel Bideau and Alex Hansen. *Disorder and granular media*, volume 3. North Holland, 1993.

HJH Brouwers. Particle-size distribution and packing fraction of geometric random packings. *Physical review E*, 74(3):031309, 2006.

BJ Buchalter and RM Bradley. Orientational order in amorphous packings of ellipsoids. *EPL (Europhysics Letters)*, 26(3):159, 1994.

YF Cheng, SJ Guo, and HY Lai. Dynamic simulation of random packing of spherical particles. *Powder Technology*, 107(1):123–130, 2000.

P. A. Cundall and O. D. L. Strack. A discrete numerical model for granular assemblies. *Géotechnique*, 29:47–65, 1979.

Gary W Delaney and Paul W Cleary. The packing properties of superellipsoids. *EPL (Europhysics Letters)*, 89(3):34002, 2010.

Aleksandar Donev, Robert Connelly, Frank H Stillinger, and Salvatore Torquato. Underconstrained jammed packings of nonspherical hard particles: Ellipses and ellipsoids. *Physical Review E*, 75(5):051304, 2007.

KJ Dong, RY Yang, RP Zou, and AB Yu. Role of interparticle forces in the formation of random loose packing. *Physical review letters*, 96(14):145505, 2006.

G Fu and W Dekelbab. 3-d random packing of polydisperse particles and concrete aggregate grading. *Powder Technology*, 133(1):147–155, 2003.

Clifford Cook Furnas. *Flow of gases through beds of broken solids*. US Government Printing Office, 1929.

D. He, N.N. Ekere, and L. Cai. Computer simulation of random packing of unequal particles. *Physical Review. E*, 60(6):7098, December 1999.

M.A. Hopkins. Discrete element modeling with dilated particles. *Eng. Comp.*, 21:422–430, 2004.

David A Horner, John F Peters, and Alex Carrillo. Large scale discrete element modeling of vehicle-soil interaction. *Journal of engineering mechanics*, 127(10):1027–1032, 2001.

Heinrich M Jaeger, Sidney R Nagel, and Robert P Behringer. Granular solids, liquids, and gases. *Reviews of Modern Physics*, 68(4):1259, 1996.

X Jia and RA Williams. A packing algorithm for particles of arbitrary shapes. *Powder Technology*, 120(3):175–186, 2001.

MJ Jiang, JM Konrad, and S Leroueil. An efficient technique for generating homogeneous specimens for dem studies. *Computers and geotechnics*, 30(7):579–597, 2003.

Anuraag R Kansal, Salvatore Torquato, and Frank H Stillinger. Computer generation of dense polydisperse sphere packings. *The Journal of chemical physics*, 117(18):8212–8218, 2002.

M.A. Knuth, J.B. Johnson, M.A. Hopkins, R.J. Sullivan, and J.M. Moore. Discrete element modeling of a Mars Exploration Rover wheel in granular material. *Journal of Terramechanics*, 49:27–36, 2012.

Yasuhiro Konakawa and Kozo Ishizaki. The particle size distribution for the highest relative density in a compacted body. *Powder technology*, 63(3):241–246, 1990.

Huiyang Luo, Huiluo Chen, Runyu Zhang, Yao Ren, Boning Zhang, Richard A Regueiro, Khalid Alshibli, and Hongbing Lu. *Constitutive behavior of granular materials under high rate of uniaxial strain loading.* Elsevier, 2022.

F Maggi, S Stafford, TL Jackson, and J Buckmaster. Nature of packs used in propellant modeling. *Physical Review E*, 77(4):046107, 2008.

Jan BM Melissen and PC Schuur. Packing 16, 17 or 18 circles in an equilateral triangle. *Discrete Mathematics*, 145(1):333–342, 1995.

RD Mindlin. Compliance of elastic bodies in contact. *Journal of applied mechanics*, 16(3): 259–268, 1949.

C. O'Sullivan. Particle-based discrete element modeling: geomechanics perspective. *International Journal of Geomechanics*, 11(6):449–464, 2011.

J.F. Peters, M.A. Hopkins, R. Kala, and R.E. Wahl. A poly-ellipsoid particle for non-shperical discrete element method. *Eng. Comp.*, 26:645–657, 2009.

R.A. Regueiro, B. Zhang, and F. Shahabi. Micromorphic continuum stress measures calculated from three-dimensional ellipsoidal discrete element simulations on granular media.

In K. Soga, editor, *International Symposium on Geomechanics from Micro to Macro: IS-Cambridge 2014, Cambridge, UK*, 2014a.

RA Regueiro, B Zhang, and SL Wozniak. Large deformation dynamic three-dimensional coupled finite element analysis of soft biological tissues treated as biphasic porous media. *COLORADO UNIV AT BOULDER*, 2014b.

Martin H Sadd, Gautam Adhikari, and Francisco Cardoso. Dem simulation of wave propagation in granular materials. *Powder Technology*, 109(1):222–233, 2000.

Christopher T Senseney, Zheng Duan, Boning Zhang, and Richard A Regueiro. Combined spheropolyhedral discrete element (de)?finite element (fe) computational modeling of vertical plate loading on cohesionless soil. *Acta Geotechnica*, 12:593–603, 2017.

Monica Skoge, Aleksandar Donev, Frank H Stillinger, and Salvatore Torquato. Packing hyperspheres in high-dimensional euclidean spaces. *Physical Review E*, 74(4):041127, 2006.

D Shane Stafford and Thomas L Jackson. Using level sets for creating virtual random packs of non-spherical convex shapes. *Journal of Computational Physics*, 229(9):3295–3315, 2010.

S Torquato and Y Jiao. Dense packings of polyhedra: Platonic and archimedean solids. *arXiv preprint arXiv:0909.0940*, 2009.

JP Troadec, D Bideau, and JA Dodds. Compression of two-dimensional packings of cylinders made of rubber and plexiglas. *Powder Technology*, 65(1):147–151, 1991.

B. Yan, R.A. Regueiro, and S. Sture. Three-dimensional ellipsoidal discrete element modeling of granular materials and its coupling with finite element facets. *Eng. Comp.*, 27(4):519–550, 2010.

A Yang, CT Miller, and LD Turcoliver. Simulation of correlated and uncorrelated packing of random size spheres. *Physical review E*, 53(2):1516, 1996.

S Yimsiri and K Soga. Dem analysis of soil fabric effects on behaviour of sand. *Géotechnique*, 60(6):483–495, 2010.

S. Yimsiri and K. Soga. Effects of soil fabric on behaviors of granular soils: Microscopic modeling. *Comput. Geotech.*, 38:861–874, 2011.

Boning Zhang. Grain-scale computational modeling of quasi-static and dynamic loading on natural soils. *COLORADO UNIV AT BOULDER*, 2016.

Boning Zhang and Richard A Regueiro. On large deformation granular strain measures for generating stress–strain relations based upon three-dimensional discrete element simulations. *International Journal of Solids and Structures*, 2015.

Boning Zhang, Eric B. Herbold, Michael A. Homel, and Richard A. Regueiro. DEM Particle Fracture Model. Technical report, University of Colorado Boulder, Lawrence Livermore National Laboratory, 12 2015.

Boning Zhang, Richard A. Regueiro, Andrew M. Druckrey, and Khalid Alshibli. Construction of poly-ellipsoidal grain shapes from smt imaging on sand, and the development of a new dem contact detection algorithm. *Engineering Computations*, in review.

Zong-Yan Zhou, Rui-Ping Zou, David Pinson, and Ai-Bing Yu. Dynamic simulation of the packing of ellipsoidal particles. *Industrial & Engineering Chemistry Research*, 50(16): 9787–9798, 2011.

HP Zhu, ZY Zhou, RY Yang, and AB Yu. Discrete particle simulation of particulate systems: a review of major applications and findings. *Chemical Engineering Science*, 63(23):5728–5770, 2008.