Geophysical Research Abstracts
Vol. 14, EGU2012-7943-1, 2012
EGU General Assembly 2012

Generation of Random Particle Packings for Discrete Element Models

S. Abe (1), D. Weatherley (2), and T. Ayton (2)

(1) RWTH Aachen, Geologie-Endogene Dynamik, Aachen, Germany (s.abe@ged.rwth-aachen.de), (2) The University of Queensland, Sustainable Minerals Institute, W.H. Bryan Mining and Geology Research Centre, Brisbane, Australia, 4072 (d.weatherley@uq.edu.au, tzara.ayton@uqconnect.edu.au)

An important step in the setup process of Discrete Element Model (DEM) simulations is the generation of a suitable particle packing. There are quite a number of properties such a granular material specimen should ideally have, such as high coordination number, isotropy, the ability to fill arbitrary bounding volumes and the absence of locked-in stresses. An algorithm which is able to produce specimens fulfilling these requirements is the insertion based sphere packing algorithm originally proposed by Place and Mora, 2001 [2] and extended in this work.

The algorithm works in two stages. First a number of "seed" spheres are inserted into the bounding volume. In the second stage the gaps between the "seed" spheres are filled by inserting new spheres in a way so they have D+1 (i.e. 3 in 2D, 4 in 3D) touching contacts with either other spheres or the boundaries of the enclosing volume.

Here we present an implementation of the algorithm and a systematic statistical analysis of the generated sphere packings. The analysis of the particle radius distribution shows that they follow a power-law with an exponent $\approx$ D (i.e. $\approx$3 for a 3D packing and $\approx$2 for 2D). Although the algorithm intrinsically guarantees coordination numbers of at least 4 in 3D and 3 in 2D, the coordination numbers realized in the generated packings can be significantly higher, reaching beyond 50 if the range of particle radii is sufficiently large. Even for relatively small ranges of particle sizes (e.g. $R_{\min} = 0.5R_{\max}$) the maximum coordination number may exceed 10.

The degree of isotropy of the generated sphere packing is also analysed in both 2D and 3D, by measuring the distribution of orientations of vectors joining the centres of adjacent particles. If the range of particle sizes is small, the packing algorithm yields moderate anisotropy approaching that expected for a face-centred cubic packing of equal-sized particles. However, once $R_{\min} < 0.3R_{\max}$ a very high degree of isotropy is demonstrated in both 2D and 3D.

The analysis demonstrates that this space-filling packing algorithm fulfills many of the requirements required to produce granular material specimens for DEM simulations. These include a high coordination number, isotropy and the absence of lock-in stresses. The algorithm has been implemented as a module (called gengeo[1]) for the Python[3] scripting language and provides the capacity to fill arbitrary bounding volumes or combinations of bounding volumes. The main disadvantage of this space-filling packing approach is the inability to specify *a priori* the particle size distribution of the final specimen.

References

[1] The gengeo source code is available via the ESyS-Particle software repository, `https://launchpad.net/esys-particle`.

[2] Place, D., and P. Mora (2001), A random lattice solid model for simulation of fault zone dynamics and fracture process, in *Bifurcation and Localisation Theory for Soils and Rocks 99*, edited by D. A. Mühlhaus H-B. and E. Pasternak, AA Balkema Rotterdam/Brookfield.

[3] The Python Language website is `http://www.python.org`.