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Characterising Particle Packings by Principal Component Analysis

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Abstract

Particle packings play an important role in the discrete element modelling of particulate systems as different packings can lead to different physical behaviour, and therefore need to be properly characterised and controlled. Apart from a few conventional approaches, there is still a lack of more general, comprehensive and quantitative approaches that can reveal some fundamental features of packings. The current work attempts to develop a novel packing characterising system based on two techniques: digitalised image representation of a packing and subsequent application of Principal Component Analysis to the resulting image. It will prove that the principal components or variances of a packing image can indeed qualify as the signature of the packing, and therefore can be utilised to characterise the packing. Furthermore, a dissimilarity coefficient or a similarity index will be defined which provides a single valued metric to quantitatively compare two packings. Comprehensive investigations for two sets of purposefully generated random packings are conducted to fully understand relationships of their principal variances with packing features. Various issues, including effects of grid resolutions and packing density on principal variances are discussed. Methods of how to apply principal variances to assess spatial homogeneity and isotropy of packings are proposed. The relationship between scaled packings and their principal variances is also considered.

KEYWORDS: particle packing, digitalised image, Principal component analysis, principal variance, spatial homogeneity and isotropy

1 Introduction

Particle packings play an important role in the discrete element method [1] for modelling particulate systems as different packings can lead to different physical behaviour of the system, and therefore need to be properly characterised and controlled before being used for subsequent modelling. This is especially true for packings that are generated in a geometric fashion, see [2, 3, 4, 5, 6, 7, 8], for instance, for packing algorithms belonging to this category. Also in some critical applications, such as pebble bed reactors, detailed packing structures have an important impact on the system performance [9].

Conventional means to characterise a particle packing are limited to: particle size distribution, packing density or porosity. A more computationally expensive method involves the use of a radial correlation function to exploit the spatial distribution of a packing, but it is less effective. It is also possible to check the coordinate number distribution, and spatial isotropy via pairs of particle contacts, or their fabric tensor, when the packing is subject to

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