Available online at www.sciencedirect.com
ScienceDirect
Physica A 378 (2007) 465–474
PHYSICA A
www.elsevier.com/locate/physa

Dynamically tessellating algorithm for analysis of pore size distribution in particle agglomerates

Mark Benedict*, Meenakshi Dutt, James Elliott

Department of Materials Science and Metallurgy, University of Cambridge, Pembroke Street, Cambridge CB2 3QZ, UK

Received 19 July 2006; received in revised form 2 November 2006
Available online 4 January 2007

Abstract

We describe a novel physical application of the OctTree data structure [P. Meagher, Comput. Graphics Image Process 19(2) (1982) 129–147] in a dynamically tessellating algorithm, in conjunction with an object-oriented, constructive solid geometry library (DOC), to efficiently determine pore size distributions in large multi-particle systems. We apply the DOC library to investigate the evolving dynamics of pore formation in multi-particle systems, such as a mixture of smooth hard cubes and spheres and a collection of frictional soft spheres. We demonstrate that the algorithm is able to provide insight into the effect of structural changes on the porosity network; for example, during the uniaxial compaction of soft spheres, we find the number density of pores increases while the mean volume of the pores decreases. This trend is responsible for a shift in the distribution of the pore volumes to favour smaller volumes. We anticipate that the DOC method will have wider applications in the area of granular materials for studying the changes in pore structure in both experimental and numerical systems as a complement to the analysis of particle packing.

PACS: 81.05.Rm; 61.43.Gt; 02.70.−c

Keywords: Particle packing; Porosity; Object-oriented algorithm; Granular materials; Compaction

1. Introduction

Several different experimental imaging techniques, such as X-ray microtomography ($X\mu T$) [1,2], functional magnetic resonance imaging (fMRI) and confocal microscopy [3] are commonly used to allow the investigation of pores in material systems such as composites, powder compacts, filter media, bioactive scaffolds and geological rocks. Characterization of the pore structure in these samples, both in terms of the bulk volume and the pore size distribution, is important from the perspective of predicting material properties that are strongly dependent on the porosity [4]. For example, some of the material properties influenced by porosity are: the elastic modulus [5] in porous particulate composites [6,7], the fracture toughness [8,9] in porous metals and ceramics, and the microscopic flow characteristics in bioactive scaffolds [10,11]. It is known

*Corresponding author.
E-mail address: mb532@cam.ac.uk (M. Benedict).

0378-4371/$ - see front matter © 2007 Published by Elsevier B.V.
doi:10.1016/j.physa.2006.11.092

that when a heterogeneous pore structure exists, a potentially small number of flow channels can completely dominate the fluid transport properties within the sample [12]. Hence, there exists a sizeable body of work which has focused on methods for quantitatively characterizing the porosity in multi-particle assemblies. In addition, there has been much effort in attempting to quantitatively characterize the behaviour of these dissipative multi-particle systems via the determination of their void structure [13–17].

During the analysis of experimental reconstructions or mesoscale computer simulations of porous media, the determination and characterization of void volume can be an exceedingly difficult and computationally expensive task. Established approaches, such as Connolly surfaces [18,19], Lee–Richards surfaces [20], sectioning [21] and various other volume visualization techniques [22], are typically employed to investigate the void volume generated numerically but involve an increasingly large computational overhead as the pore volume bounding surface becomes highly convoluted. The methods do not generally scale well with the size and complexity of the system.

Utilization of experimental data characterizing porosity for analysis, and as a basis for further computer simulation [23,24] can be highly challenging. Typically, those models that deal with systems potentially containing porosity focus on simulating the occupied volume within the system rather than the void volume. The inclusion of explicit consideration of porosity can be problematic for such simulations. For instance, the inclusion of porosity in finite element models [25] can increase the required mesh resolution to the point where memory requirements can rise the order of gigabytes [26], rendering such computations highly impractical. Another example is in granular systems where the porosity generated via the topological arrangement of particles can only be measured *a posteriori*. It becomes very difficult to include any experimentally derived mapping of porosity in such simulations as the focus lies on the interactions between the constituent particles and the history of the system, and the fact that the porosity arises from these interactions rather than the other way around. In addition, the application of experimental porosity mappings to simulations can typically result in an enormous amount of data of the order of gigabytes per sample [27] because of the inefficient data format of the volumetric imaging [28] in a sample. This can overburden most analytic and computational techniques, and therefore, a more efficient algorithm for detection of porous structure in a system is required.

In this paper, we present a dynamic coarse-graining method that describes pore structures resulting from simulations in a more efficient format. In order to minimize the computational and memory requirements, we implement a dynamically tessellating, object-oriented, constructive solid geometry library (DOC) which has the ability to determine the pore size distribution. Here, we apply the DOC method to particle packing configurations from both rigid body molecular dynamics simulation of spherical and cubic particles, and granular dynamics simulations of soft elastic spheres, where the particles are first settled under gravity and then uniaxially compacted at a constant strain rate [29]. The resulting data structures are analysed to describe the changes in the pore volume distribution as both of these systems evolve under the influence of external reduction in bulk volume, therefore demonstrating the utility of this method in investigating the dynamics of pore formation in multi-particle systems. To our knowledge, this work is the first application of the OctTree data structure [30] in a dynamically tessellating algorithm to determine the porous structures in physical systems.

This paper is structured as follows: we present an overview of the numerical algorithm followed by the results from the two systems mentioned above. Finally, we summarize and discuss our findings in the conclusion section.

2. Numerical algorithm

We have developed a custom code library which can identify the pore volume and structure for an agglomerate comprised of arbitrarily shaped particulate objects which, for the purpose of the following analysis, are considered to be space-filling rigid bodies, which could possibly overlap. The positions (i.e., x, y, z coordinates), dimensions (diameter, or length, breadth and height) and orientations of all particles comprising the system should be viewed as the essential inputs to the porosity detection algorithm. The format of the input files remains unchanged for bodies which can interact with one another via soft potentials or contact deformations. The first step in the algorithm is to translate each particle in the system, based upon their shape, into an instance of a geometric class from the DOC library. These translated objects are then able to respond