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Effect of rectangular container's sides on porosity for equal-sized sphere packing

Mohammad Mahdi Roozbahani *, Bujang B.K. Huat, Afshin Asadi

Department of Civil Engineering, Universiti Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia

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ABSTRACT

Containers have a crucial role in determining the porosity of packed spheres. The new gravitational sphere packing method is applied for loose packed particles based on Monte-Carlo simulation. The model is simulated in a cylindrical container by considering the effect of the wall. A new method is employed to examine the porosity of spheres in the inner part of the cylinder without the effect of boundaries, where spheres can be packed in different rectangular containers to show the structure of packing within sides of different sizes.

1. Introduction

Sphere packing is used in many fields such as engineering, geology, physics, and chemistry [1–27]. Equal-sized sphere packing is still a major concern in terms of finding different parameters which cause changes in the characteristics of packing. A wide variety of studies have been done to identify the best method of packing spheres loosely, called gravitational sphere packing [3,5,6,8,19,25,27]. Different methods have been applied to simulate this type of packing.

In a large longitudinal study, fixed triangular lattice sites is employed inside of the container in order to control the behavior of spheres in different incidents such as collision, rotating, and stability conditions [3,5,6]. Other studies have considered fixed cubical lattice system to pack spheres loosely [8,25,27]. However, Dynamic Cubical Lattice, DCL, sites are used in this study to control the processes of packing.

Jodrey and Tory [25] successfully simulated equal-sized spheres packing through statistical geometric method with a void fraction of 42%, which is the maximum result in the experimental work. The majority of studies have been done for square containers, which indeed provide the best packing for equal spheres, while variations in the sides of rectangular containers can be interesting in terms of changes in the porosity of packed spheres. Partial ordering of spheres near the wall contributes to more porous parts in these regions [8], and it can be solved by using the periodic boundary condition, pbc, method to remove the effects of walls [8,25,27].

Mueller and Suzuki have used virtual cylindrical containers inside of the main cylindrical one to examine the effects of wall on packing [28–32]. In those articles, they proved that by moving away from container wall, the order of packing will decrease subsequently. Spheres tend to be well-ordered when they are touching the wall leading to the porous regions near the wall. In their methodologies, the wall effects have been shown by applying radial porosity distribution, in which they divided main cylindrical container into large number of radial annular layers. In such a way that elliptic integrals are commonly used to calculate volume intersection between sphere and cylinder.

The aims of this study are to present an innovative method to cope with the porous regions near the wall and to examine porosity values for different sizes of rectangular containers. It is hoped that this study will help other researchers to deal with the process of packing more efficiently.

2. Computational method

The method of gravitational sphere packing is started by randomly generating initial (x–y) coordinates of every sphere, which are chosen based on a normal distribution. The randomly chosen sphere is released from the highest height of a previously settled sphere with determined steps. Methods of rolling, collision, and stability conditions are applied for every sphere [25]. Stability conditions for each incoming sphere are as follows:

1. Hitting sphere with floor.
2. Being Placed on the top of the three spheres. This condition is accomplished by examining whether the center of the incoming sphere is located inside of the triangle generated by the centers of the three spheres, or not.
3. Examining the stability condition of incoming sphere with wall, in which stability condition is defined same as previous step.

* Corresponding author. Tel.: +1 404 452 1094.
E-mail address: mahdir@gatech.edu (M.M. Roozbahani).

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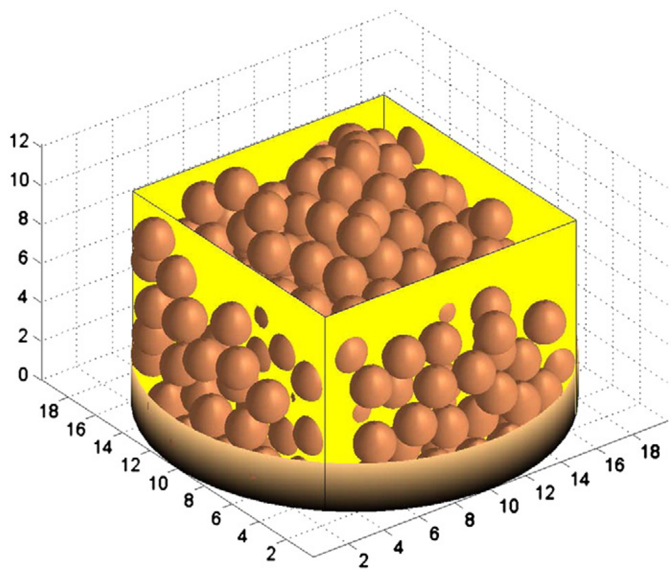

Fig. 1. Geometrical placing of one rectangular container within the main cylindrical one.

However, instead of three spheres, two spheres and wall are considered to form the triangular shape.

In fact, hard spheres are considered as mass-less and stress-free in statistical geometric method of sphere packing simulation, and the mathematical and geometrical characteristics of spheres are examined to pack them. The expression of "hard spheres" has been numerously used by literature for statistical geometric approach of sphere packing simulation [20,21,33–36].

Using this method, partial ordering caused by wall effects is removed by putting the rectangular container into the main cylindrical one, where the outer volume of every sphere intersecting with the walls of the rectangular container is not taken into account in the computations. Fig. 1 shows geometrical placing of one rectangular container, square container, within the main cylindrical one. In the recent study by Roozbahani et al. [37], it is shown that the rectangular container touching the main cylindrical one is a good choice for elimination of boundary effects.

All spheres just have interaction with themselves and main cylindrical container. Thus, rectangular container is considered as a virtual container in order to satisfy two conditions:

1. To find the porosity values without wall effects.
2. To compute the porosity values in the different sizes of rectangular container.

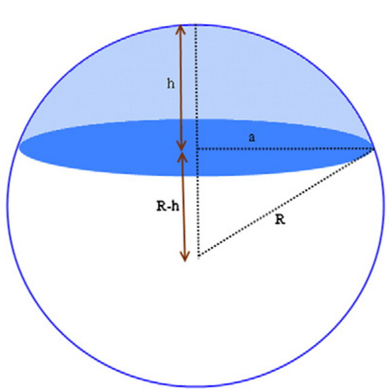

Fig. 2. Spherical cap.

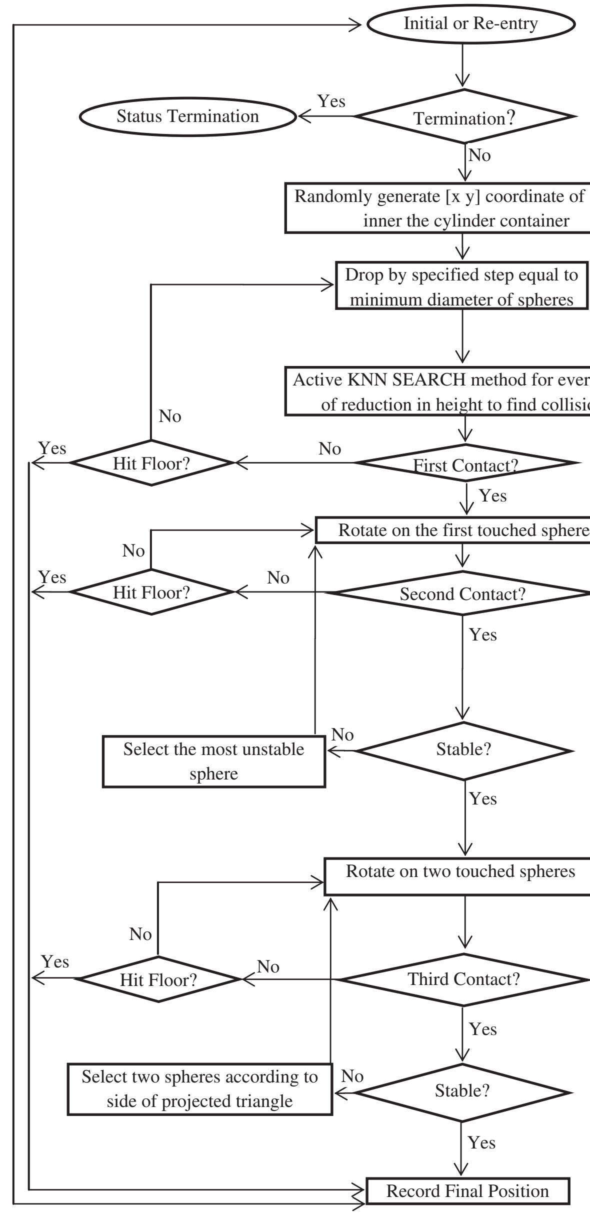

Fig. 3. Program flow chart.

It should be noted that after the packing of all spheres in cylindrical container, the virtual rectangular containers are employed to geometrically subdivide occupied spaced by packed sphere. The generated geometrical figure of intersection between the plane of the rectangular container and the sphere is well known as the spherical cap (Fig. 2) [38]. Eq. (1) gives the volume of the spherical cap:

$$V_{cap} = {}^{1}\!/_{6}\pi h\left(3a^{2} + h^{2}\right) \quad (1)$$

A K-Nearest Neighbor, KNN, method [39] is applied to find the nearest neighbors of every sphere, but it should be mentioned that before running the KNN search, the spheres' coordinates are put in DCL sites, and the volume of each cube is changed in correspondence with the nearest neighbors of the incoming sphere in order to hinder any additional calculations. As a result, the search for a sphere's collision involves in a cube of previously specific dimensions to increase the speed of implementation of the code.