Optimization of A Computer Simulation Model
for
Packing of Concrete Aggregates

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ABSTRACT

A simulation algorithm was developed for modeling the dense packing of large assemblies of particulate materials (in the order of millions). These assemblies represent the real aggregate systems of portland cement concrete. Two variations of the algorithm are proposed: Sequential Packing Model and Particles Suspension Model. A developed multi-cell packing procedure as well as fine adjustment of the algorithm's parameters were useful to optimize the computational resources (i.e., to realize the trade-off between the memory and packing time). Some options to speed up the algorithm and to pack very large volumes of spherical entities (up to 10 millions) are discussed. The described procedure resulted in a quick method for packing of large assemblies of particulate materials.

The influence of model variables on the degree of packing and the corresponding distribution of particles was analyzed. Based on the simulation results, different particle size distributions of particulate materials are correlated to their packing degree. The developed algorithm generates and visualizes dense packings corresponding to concrete aggregates. These packings show a good agreement with the standard requirements and available research data. The results of the research can be applied to the optimal proportioning of concrete mixtures.

Keywords: packing density; packing algorithm; simulation model; aggregates; particle size distribution; concrete mixture proportioning

INTRODUCTION

The properties and behavior of particulate composite materials, such as portland cement and asphalt concrete mixtures, depend to a large extent on the properties of their main constituent – the aggregates [1-5]. Among the most important parameters affecting performance of concrete are packing density and corresponding particle size distribution (PSD) of aggregates. Better packing of aggregates improves the main engineering properties of concrete: strength, modulus of elasticity, creep, and shrinkage. Further, it brings major savings due to a reduction in the volume of binder. Very early reports on concrete technology have already emphasized the important effect of aggregate grading on properties of concrete [1, 4, 5]. Since that time the problem of the best possible proportioning of aggregates and their contribution to optimal concrete mix has been the subject of many experimental and theoretical investigations [1-13]. Nevertheless, better understanding of the problem of the dense packing of large assemblies of particulate materials of non-uniform sizes needs further attention.

Several reports discuss the important contribution of the shape of the particle on packing [4, 8, 12]; however, it is considered adequate to model and represent natural or artificial aggregates (which are mainly irregular in shape) by using groups of spheres of different diameters. This assumption partially reflects the existing methods of particle size analysis and helps to simplify packing calculations [4, 6, 13]. The maximum packing value of randomly packed equally-sized spheres was found to be 0.64 [14]. An increase in density could be achieved only if spheres of different sizes are used. In this case, smaller spheres must fit into the cavities between the already packed bigger neighbors - a similar procedure to the arrangement of small spheres in the Apollonian problem [5, 15]. By using a wide range and a large number of particles, the packing density can theoretically approach very close to unity.

The first attempts to provide the "best" optimal particle size distribution were based on trials with balls of different diameters [4, 5, 16-19]. These experiments resulted in aggregate's distribution curves that are currently accepted as standards. One of the early examples presented by Fuller [5] is a series of curves that are widely used for the optimization of concrete and asphalt aggregates:

$$P_i = 100 \left(d_i \Big/ D_{\max} \right)^{\psi}$$

where:

P_i	total percent of particle passing through (or finer than) sieve;
D_{max}	maximal size of aggregate;
d_i	diameter of the current sieve; and
ψ	exponent of the equation (0.45-0.7).

Because it is relatively simple to achieve the "target" distribution with a minimum deviation using a few (at least two) sets of particulate materials [7, 20], this optimal distribution method is extensively used. Yet, in spite of its usefulness, this method cannot predict the packing degree and spatial arrangement of particles of the resultant mixture.

Due to its practical importance, the packing problem of real systems still remains a challenging subject attracting attention of many scientists. A model developed by Aim and Toufar has provided a useful tool for explaining the packing mechanism [19, 21]. Their model deals with packing of two groups of equally sized spheres. Each group of spheres is represented by its characteristic diameter and its eigenpacking degree. After minor adjustments this model gives quite a good explanation of the experimental results related to concrete aggregates [2]. However, to apply this model, it is necessary to measure or estimate the eigenpacking degree of the individual group of particles. Moreover, the real particulate systems are usually better represented by the particle size distributions rather than by the characteristic diameter. These two constraints limit the applicability of this model.

With the development of computers the packing problems of real particulate systems became a challenging subject for engineers [4, 6, 13-15, 22-27]. Advanced algorithms are usually based on the modeling of the movement of particles (represented as spheres or ellipsoids) due to rolling or sliding under the compaction gradient. Based on this strategy, the particles in a rigid container are forced to occupy the best vacant positions within the neighborhood. Modern modeling approaches include better insight into the natural packing process and even full-scale modeling of the particulate systems [23-27]. The contribution of additional factors (such as friction and deformation) acting at the contact points was found to be essential for the modeling of the dynamic processes, involving the particulate materials [26, 27]. To realize such algorithms, each movement of a particle requires the solution of the corresponding differential equations. A comprehensive survey of packing algorithms was recently presented by Jia and Williams [22].

An interesting approach to dense packing was suggested by Anishchik and Medvedev [15]. It involves the solution of the three-dimensional Apollonian problem using the Voronoi - Delaunay method extended to deal with non-equal spheres. Based on this method, a new sphere is packed into the Voronoi S-region (the region of a volume all points of which are closer to the surface of a given sphere than to the surfaces of other spheres in the packing). Using this approach, a very high packing degree of 90% was achieved using a relatively small number of particles (about 40,000) [15].

It is believed that optimal particle size distribution (PSD) corresponds to the "best" or the densest packing of the constituent particles. However, modeling of packing of large particulate assemblies had demonstrated that the densest arrangements (PSD) of particles are actually not realized in concrete technology [13]. As was shown, only "gap-gradings" could be considered to some extent as a sort of dense arrangement of particles. The majority of "practical" concrete aggregates gradings lying between the 0.45-0.7 power curves (i.e., Fuller curves with ψ = 0.45 - 0.7) are actually "Loose - Initially – Packed," LIP systems [13]. The fundamental characteristic of such systems is related to a wide range of particle sizes required to achieve the high packing degree at a limited number of largely-sized particles. These are opposed to "perfect" geometric, regular arrangements of high density, realized with a relatively narrow size range.

In spite of recent progress in the development of packing algorithms, it is evident that a new approach is needed to model the packing of large assemblies of particulate materials (up to 10 million particles) representing the aggregate structure of portland cement concrete. On the one hand, the computer simulation algorithm must imitate the natural packing processes; on the other hand, the developed approach must be easily applicable to solve practical problems. Moreover, the packing process must be accomplished in a reasonable period of time and, preferably, using conventionally available computational resources.

DESCRIPTION OF THE PACKING MODEL

It was found that a good approximation of particulate systems of elementary volume within a container with a rigid or periodic boundary can be achieved when the center of the particle is randomly located at the grid of a cubic lattice [13]. In this case, a thick 3D mesh with an opening size of less than 1/100 of the minimal diameter of the particle must be used to minimize any possible error. The particle is considered as a discrete element that is represented by a sphere.

In this work, the packing into a container with periodic boundaries was used; this considered to represent the elementary volume of particulate assemblies and also to eliminate the wall effect. The simulation takes place in a cube C(1), where 1 is a length of side and at a size of the lattice grid of 1/32767.
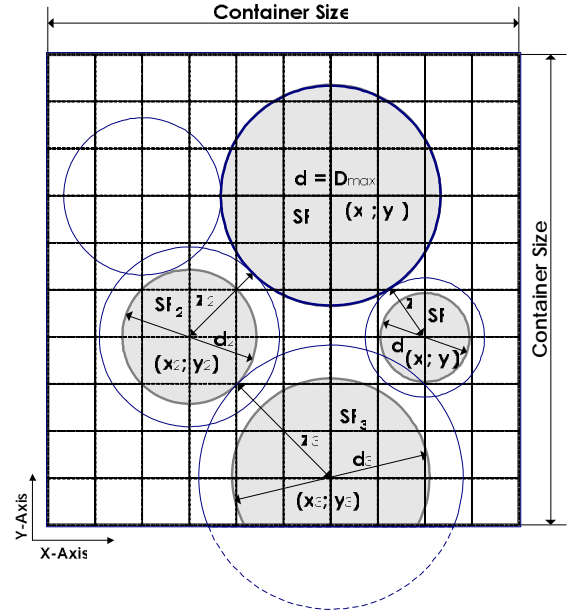
Sequential Packing Model

A two-dimensional representation of Sequential Packing Model (SPM) is shown in Fig. 1a. New spherical particles are sequentially placed into the cube with the center glued to the node of a lattice grid and with a radius in the range of $r_{min} < r \leq r_{max}$. The radius r_{max} is fixed experimentally, but r_{min} is decreased gradually, thus allowing larger spheres to be placed in a cube prior to the placement of smaller ones. The formula for calculating r_{min} is as follows:

$$r_{min(n)} = \left. r_{max} \middle/ (k_{red})^n \right. \tag{1}$$

where $k_{red} = 1+10^K$ is a constant for reduction the r_{min}, K is the reduction coefficient and n is a number of the packing attempts (steps) required to gradually reduce r_{min}.
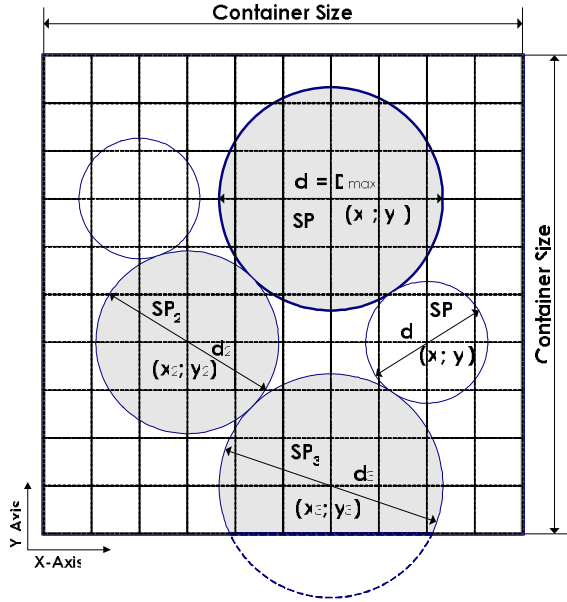
a) Sequential Packing Model (after [13])   b) Particles Suspension Model (after [28])

Fig. 1.   2D Representation of the Packing Models

Initially, the cube is prepacked with an initial sphere (or spheres). Fig. 1a shows randomly prepacked sphere SP1. Then the center of a new sphere is randomly generated within the cube lattice. Before locating the sphere with radius r, the various conditions are examined:
- the center of the new sphere can not be located inside of any already packed spheres;
- the new sphere can not cross any already packed sphere (no overlapping of spheres is permitted);
- the minimum distance to the surface of any already packed sphere should be greater than r_{min}.

The described SPM procedure results in a very dense packing arrangement [13]. Fig. 1a shows the spheres SP_2, SP_3 and SP_i are placed in the case if the d_2, d_3 and d_i, respectively, satisfy the conditions above.

Particles Suspension Model

The Particles Suspension Model assumes that the particles are located at a specified minimal distance from each other, imitating the perfect mixing process. Subsequently, all spheres are separated by a certain distance δ (varying depending on the particle size and also the packing step) and the radius of a new sphere is calculated as follows:

$$r = \frac{z}{(1 + \frac{k_{del}}{s^m})} \qquad (2)$$

where z is a minimum distance to the surface of any already packed spheres, k_{del} is an initial coefficient to provide the separation between spheres, $s = 1 + 10^{Sr}$ is a constant to reduce the separation distance, S_r is the separation reduction coefficient and m is the number of the packing attempts (cycles) required to gradually reduce this coefficient.

In Fig. 1b the spheres SP_2, SP_3 and SP_i are located with separation and the corresponding radii are calculated according to the expression (2). This arrangement allows particles to be located at the specified minimal distance from each other and avoid the formation of congested zones (clusters) or conglomerates; this also imitates the "perfect" mixing process. Finally, the radius of any new sphere should satisfy the following conditions that are calculated by combining the expressions (1) and (2):

$$\begin{cases} r \geq \dfrac{r_{max}}{(k_{red})^n * (1 + \frac{k_{del}}{s^m})} \\ r \leq r_{max} \end{cases} \qquad (3)$$

If the sphere does not meet the requirements (3), this sphere is discarded and the center of a new sphere is randomly generated. This process continues until the amount of packing attempts (N) is spent. At this point, the variables m and n are incremented by 1 and the process of placing the spheres is continued for the subsequent spheres of smaller radii. However, the incrementing procedure is limited by the following conditions:

$$(k_{red})^n \leq 256 \quad \text{and} \quad \frac{k_{del}}{s^m} \leq 10^{-6} \qquad (4)$$

The packing of a cube is terminated as all predetermined spheres are packed. Commencing the packing process of each sphere the volume fraction of solid particles, V is calculated:

$$V = \sum_{i=1}^{N_{total}} V_i \qquad (5)$$

where V_i is a volume of a particular sphere and N_{total} is the number of the spheres packed. Based on the individual volumes of newly packed spheres, the particle size distribution of particles and packing degree are updated.

It can be seen that the Sequential Packing Model (SPM) can be considered as a particular case of the Particle Suspension Model (PSM) at k_{del} = 0; this research reports on the performance of PSM (i.e., deals with the general case).

COMPUTER IMPLEMENTATION OF THE ALGORITHM

Description of the Program Modules

A schematic overview of packing algorithm is represented in Fig. 2a. The algorithm defines the variables for processing (Module 1), opens the input file and reads the initial set of packing parameters such as r_{max}, k_{red} (or K), k_{del}, s (or S_r), N, N_{total} (Module 2) and locates the initial sphere(s) to the cube (Module 3). Modules 4 to 11 perform the calculations according to the steps of SPM. Module 10 calculates the volume fraction and the size distribution of the spheres.

This model is designed to pack with separation of up to 10 million of spherical particles in order to achieve the high density; this process desired to be accomplished in a reasonable period of time. However, the described model must spend much time to pack any additional sphere because further comparison is needed to evaluate the least distance from a new sphere to all already packed entities (Module 5, Fig. 2a).
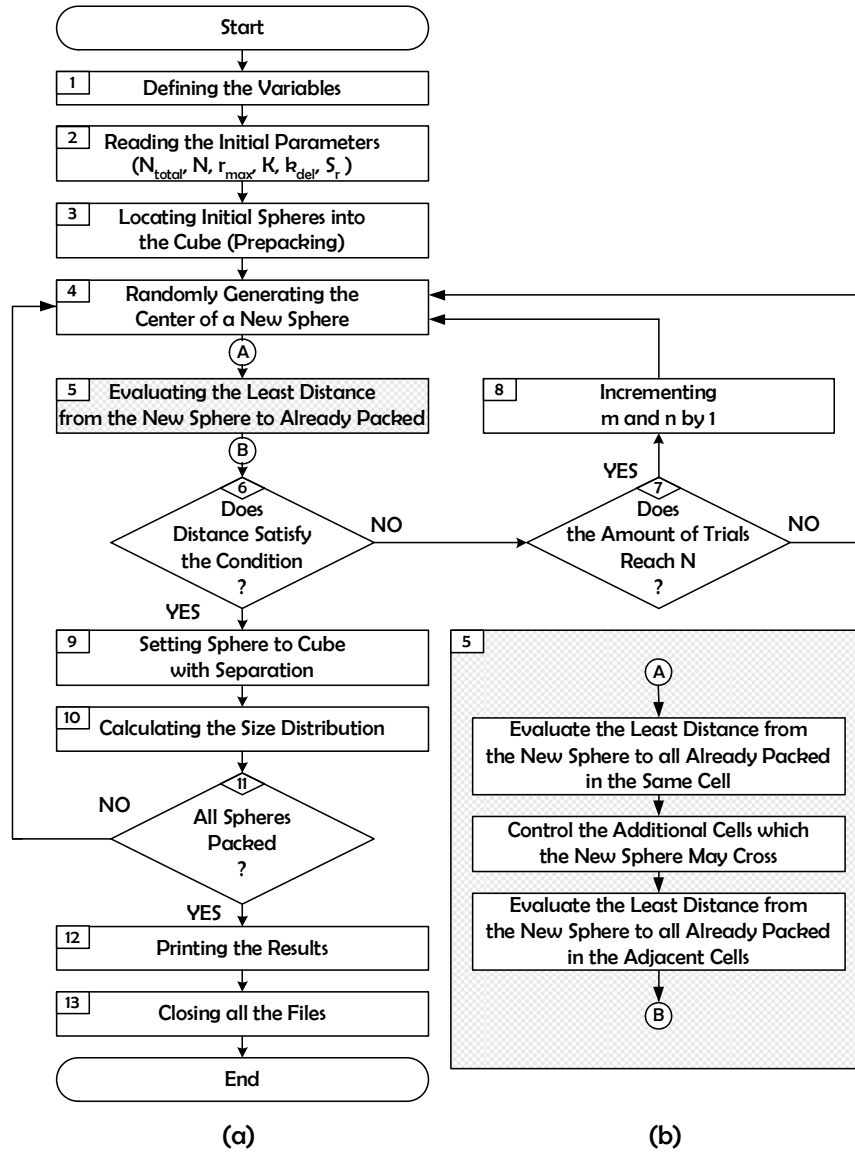
Start

1 Defining the Variables

2 Reading the Initial Parameters (N_{total}, N, r_{max}, K, k_{del}, S_r)

3 Locating Initial Spheres into the Cube (Prepacking)

4 Randomly Generating the Center of a New Sphere

(A)

5 Evaluating the Least Distance from the New Sphere to Already Packed

(B)

6 Does Distance Satisfy the Condition ? — NO

8 Incrementing m and n by 1

YES

7 Does the Amount of Trials Reach N ? — NO

YES → 8

NO →

9 Setting Sphere to Cube with Separation

10 Calculating the Size Distribution

11 All Spheres Packed ? — NO

YES

12 Printing the Results

13 Closing all the Files

End

(a)

5

(A)

Evaluate the Least Distance from the New Sphere to all Already Packed in the Same Cell

Control the Additional Cells which the New Sphere May Cross

Evaluate the Least Distance from the New Sphere to all Already Packed in the Adjacent Cells

(B)

(b)

Fig. 2.   Schematic Overview of Packing Algorithm:
(a) basic packing algorithm and (b) implementation of multiple cells mode (extension of Module #5)

Computer Simulation Algorithm with Multiple Cells

The computer simulation algorithm with multiple cells was implemented to reduce the comparison time. According to the developed approach, the main container (cube) is divided by equal cells (smaller cubes). The two-dimensional representation of the model is shown in Fig. 3.

The least distance from a new sphere to all already packed entities is performed only for the cell where the center of the new sphere was randomly generated. For example, the spheres SP_1 and SP_2 are placed into the Cell #22 and, after generating a new sphere SP_7, the least distance from this sphere to all other available (i.e., SP_1, SP_2) will be evaluated for the same Cell #22. Then, the least distance Z_{7-2} is established as a radius of SP_7. This radius is used to check if there is any additional cell crossed by the sphere SP_7. If there is no any additional cell involved, the radius of SP_7 is calculated according to the expression (3), the overlap conditions are checked and also the expression (4) is controlled.
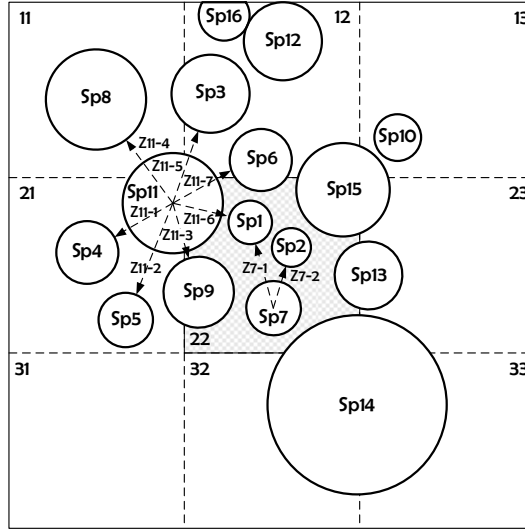
Fig. 3.   2D Representation of the Algorithm with Multiple Cells

In the case when the radius of a new sphere does not satisfy the expression (4) or overlap condition, the model follows the same procedure as PSM running in single cell mode. Otherwise, the sphere SP_7 will be placed within Cell #22 and all the parameters of the sphere (the coordinates of the center and the radius of the sphere) will be recorded in an array of this particular cell (Cell #22). Fig. 3 also demonstrates another case of locating a new sphere. Again, when the center of a new sphere SP_{11} is generated within the Cell #21, the minimal distance from this sphere to all already packed entities of the same cell (SP_4, SP_5, SP_9 located within the Cell #21) is evaluated and this distance is assigned as a radius of SP_{11} (Fig. 3 shows the minimal distance Z_{11-1}). Then the distance Z_{11-1} is used to estimate if there are any additional cells crossed by the sphere SP_{11}. Since SP_{11} crosses the Cells #11, #12 and #22, the minimal distances are evaluated from the sphere SP_{11} to all already packed spheres in these cells. That is the least distance must be evaluated from SP_{11} to SP_3, SP_6, SP_1, SP_2, and SP_7 and will be used to calculate the radius of the sphere SP_{11} according to the expression (3). In the case when the new sphere satisfies all the conditions mentioned above, the parameters of this new sphere (i.e., the coordinates of the center and the radius of the sphere) are recorded into the arrays corresponding to all the cells this sphere have crossed (i.e., the parameters of the sphere SP_{11} are recorded into the arrays of Cells #21, #11, #12 and #22).

Therefore, to represent the updates corresponding to the multiple cell mode, the Modules 5 and 9 (Fig. 2a) need to be modified. The Fig. 2b represents the schematic overview of the Module 5, which follows the PSM in multiple cell mode. The Module 9 records the parameters of new sphere in the arrays corresponding to all cells that the new sphere crosses.

Assessment of Computational Cost

A division of a cube on the cells significantly reduces the time necessary for the packing of spheres, but *a priori* increases the memory needed to keep the data on already packed spheres. The packing time consists of two parts: the first part (T_s) is required to save the sphere in an array and the second (T_d) is necessary to calculate the distance to already packed spheres. The T_s and T_d would depend on the amounts of packed spheres and also on a computational complexity of the algorithm. Generally, the packing time (for the case without division on the cells) can be represented by the formula:

$$T = T_s + T_d \approx \Omega(N_{total}) + \Omega(N_{total}^2) \qquad (6)$$

A division of a cube on the cells increases a number of spheres reported to the arrays, but reduces the computational cost to calculate the distance to already packed spheres (since only the spheres of the same cell participate in the evaluation). The formula (6) can be modified for multiple cells mode as follows:

$$T \approx \Omega(N_{total} + \Delta N_{total}) + \Omega\left(\frac{(N_{total} + \Delta N_{total})^2}{\Phi}\right) \qquad (7)$$

where ΔN_{total} is an additional number of spheres reported in an array of spheres, Φ is a number of cells the cube is divided; Φ equals to ξ^3, and ξ is an integer number that represent the division of the side of the cube on equal parts.

6

EXPERIMENTAL RESULTS AND DISCUSSION

Fine-Tuning of the Algorithm: Packing Time vs. Memory

Evaluation of the algorithm parameters (such as packing time, T and memory) in multiple cells mode was performed for different numbers of cells. The experiment involved the packing of 1 million equal spheres of a small radius (r = 0.005) into the cube with various numbers of cells. A relatively small radius was selected to avoid the increase in time due to additional trials when the sphere is rejected and a new sphere is generated. The following parameters were set for the experiment: k_{red} =1, k_{del} =0, s = 1.

The packing time and the memory units needed per sphere versus a number of cells are presented in Fig. 4 and Fig. 5, respectively.
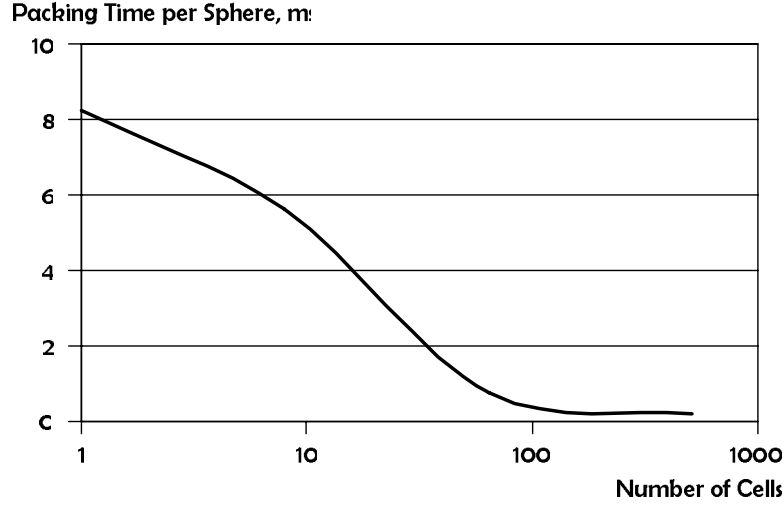
Packing Time per Sphere, ms

Fig. 4. Packing Time vs. Number of Cells

As predicted, the packing time is significantly reduced by incrementing the number of cells in a cube (Fig. 4); however, more memory units are needed to accommodate the additional spheres generated in multiple cells mode (Fig. 5). Thus, a trade-off between the speed of program execution and the memory needed can be determined by the degree of division of a cube on the cells Φ.
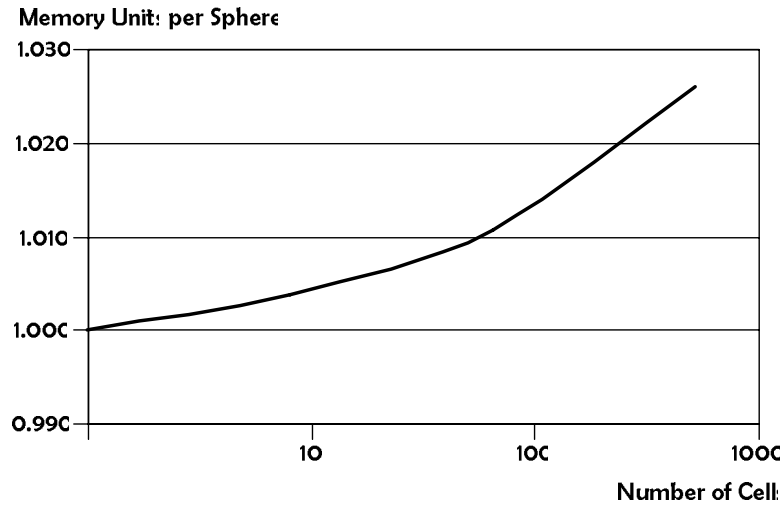
Memory Units per Sphere

Fig. 5. Memory Units vs. Number of Cells

Fine-Tuning of the Algorithm: the Effect of Particle Size

The division of a cube Φ depends on the total number of spheres, N_{total}, which, in turn, depends on the r_{min} (minimal radius) of the sphere. To evaluate the trade-off between the speed of the program execution and the memory needed, as well as

to establish the rule for cube subdivision, an additional simulation experiment involving 5 million spheres was performed using the following parameters: r_{max}=0.18, K = -1, k_{del} =0, s = 1, N= 1,000,000.

The packing time and memory units vs. the radius of the sphere at various cube division rates Φ are represented in Figs. 6 and 7, respectively. It can be observed that the division of a cube in 8 cells requires less time and less memory units for the packing of spheres within the range of r/r_{max} = 1 ... 0.1. The division of a cube in 64 cells becomes attractive for packing the range of spheres with r/r_{max} = 1 ... 0.01. However, for spheres of wider range of r/r_{max} = 1 ... 0.001, the division of the cube in 512 cells would be the best choice (Fig. 6).
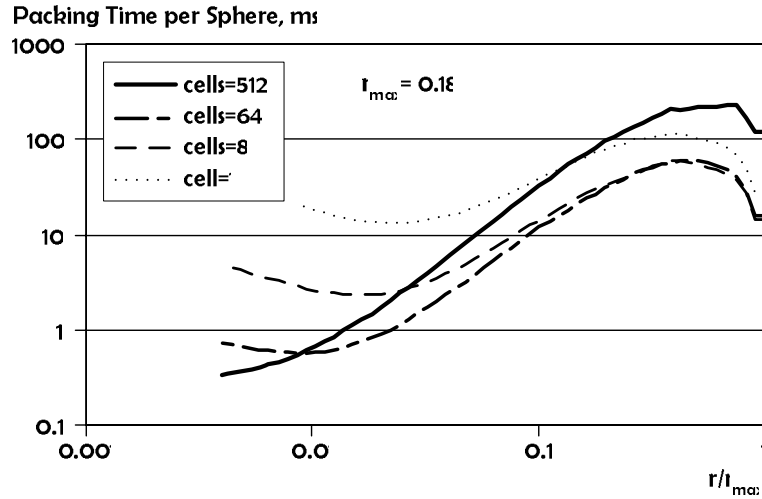
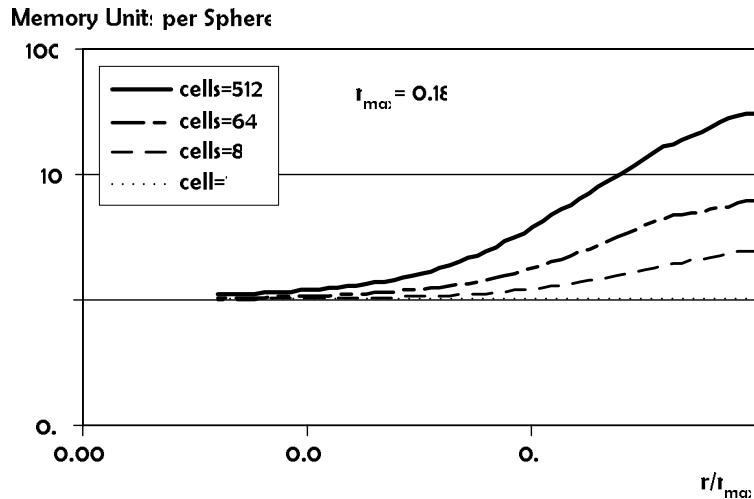Fig. 6. Packing Time vs. Radius of the Sphere

Fig. 7. Memory Units vs. Radius of the Sphere

The selection of a number of cells in a cube also depends on the value of r_{max}. Fig. 8 represents the packing time per sphere for various values of r_{max}. The decrease of a maximal radius (r_{max}) reduces the packing time per sphere until $r/r_{max} \approx 0.01$ because the spheres of smaller radius cross fewer neighboring cells and, subsequently, would require fewer comparisons to evaluate the minimum distance from a new sphere to all packed entities (i.e., the time T_d is decreased).
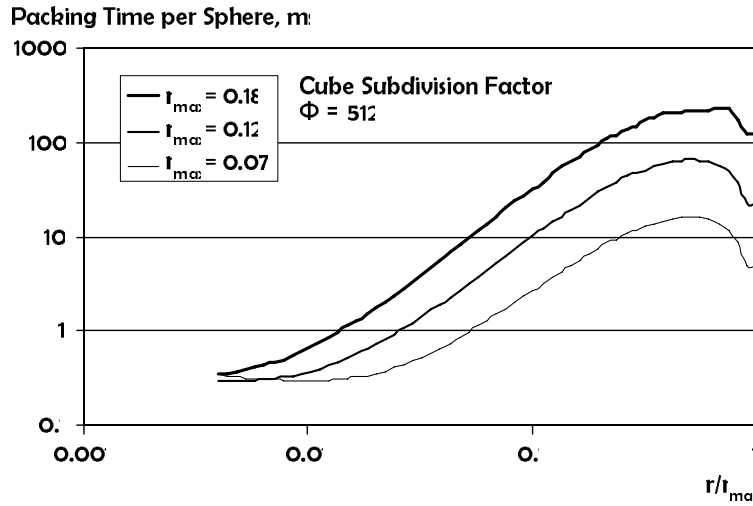
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Fig. 8. Packing Time vs. Radius of the Sphere for Various Values of r_{max}

Consequently, the division of a cube on cells can be realized based on the Figs. 6-8 to reduce the packing time and to satisfy the memory size limitation.

The suggested empirical rule is to use the division of the cube on the cells corresponding to the side length comparable to r_{max}. This rule guarantees that at the beginning of the packing process, when large spheres (close to r_{max}) are packed, in the worst case these spheres are recorded into all 8 cells. However, the spheres of smaller radii are rarely recorded in more than one cell. Since such large spheres represent a very small fraction of the sphere's pool, this approach can save the memory required for multiple cell mode (i.e., in this case it requires the resources comparable to the run in a single cell mode).

Algorithm Implementation for Large Particulate Assemblies

To simulate the "real" particle size distributions based on the PSM running in multiple cell mode, the ratio of the container size to the maximum diameter of the sphere was fixed at 3.3 (i.e. r_{max} = 0.15); this represents a common assumption related to the density measurements when the wall effect is eliminated. The total number of spheres used in the packing trials (N_{total}) was 10 million and a cube subdivision factor Φ equal to 512 (which is 8^3 for 8-cell model). The initial separation coefficient k_{del} was used as a variable parameter at the levels of 0.1, 1, 1.5 and other parameters of the model were selected to realize a relatively quick packing process: K = -1, S_r = -1, N= 10,000.

The results of the simulation algorithm are presented in Figs. 9-10 and Table 1 (the specific sizes that are standard for the sieve analysis are marked with vertical dashed lines; these are determined using the formula: $d_i = D_{max}/2^{\beta}$, where β is integer). The major interest of the model is seen in the distribution curves (Fig. 9). The 3-D representation of two limited cases with small (k_{del} = 0.1) and relatively high (k_{del} = 1.5) separations is provided in Fig. 10.

The analysis of the packing time and memory required for the process (Table 1) shows that the memory size does not depend on the separation coefficient k_{del}, because the same number of particles N_{total} is packed. However, the packing time is increased as k_{del} is reduced. This feature can be explained considering that the small value of the separation coefficient k_{del} improves the packing degree and also results in an increase in the number of packing attempts to allocate the new sphere within already packed entities; these processes correspond to the increase of packing time.

The particle size distribution curves show three characteristic zones (Fig. 9):
1st zone - almost vertical line corresponding to initial pre-packing of spheres of the size close to D_{max};
2nd zone - "structure-forming" range corresponding to spheres of the size from D_{max} to $0.5-0.85*D_{max}$;
3rd zone - "void filling" range corresponding to spheres of the size less than $0.5-0.85*D_{max}$.

It can be observed, that the best (i.e., the most dense) gradings with ~86% packing are obtained at a relatively low k_{del} = 0.1 (Figs. 9 and 10a). The particle size distribution curve representing this case is close to gap-grading and can be considered as Initially Pre-Packed (IPP) condition - with a predominant volume (~50%) of the largest particles ranging from D_{max} to $0.85*D_{max}$. The arrangement of these relatively large particles results in more than 40% of packing. The relatively narrow range of particle sizes (from D_{max} to $0.5*D_{max}$) provides about 55% of packing (Fig. 9).

For IPP condition, the group of largest particles is arranged in a manner similar to the "ideal" regular close-packed lattices (Fig. 10a) that approach the condition of maximum possible value for randomly packed systems (jammed state) [13, 14].

To achieve a similar packing degree at a less arranged initial structure, a much wider range of sizes is necessary (Fig. 9). In practice, when conventional compaction methods are used and due to friction between the particles and their irregularity, the achievement of well-arranged Initially Pre-Packed structures is quite difficult. As a result, many particulate assemblies could be described by those models with $k_{del} \geq 1$. This condition corresponds to the case of a "Loose Initial Packing" (LIP) arrangement, when the largest particles (from D_{max} to $0.5*D_{max}$) occupy only 25-35% of volume and provide 25-30% of packing (Fig. 9). At $k_{del} > 1$, the particle size distribution functions are represented by the continuous distributions involving a wide range of particles that are very close to practically applied Fuller curves.
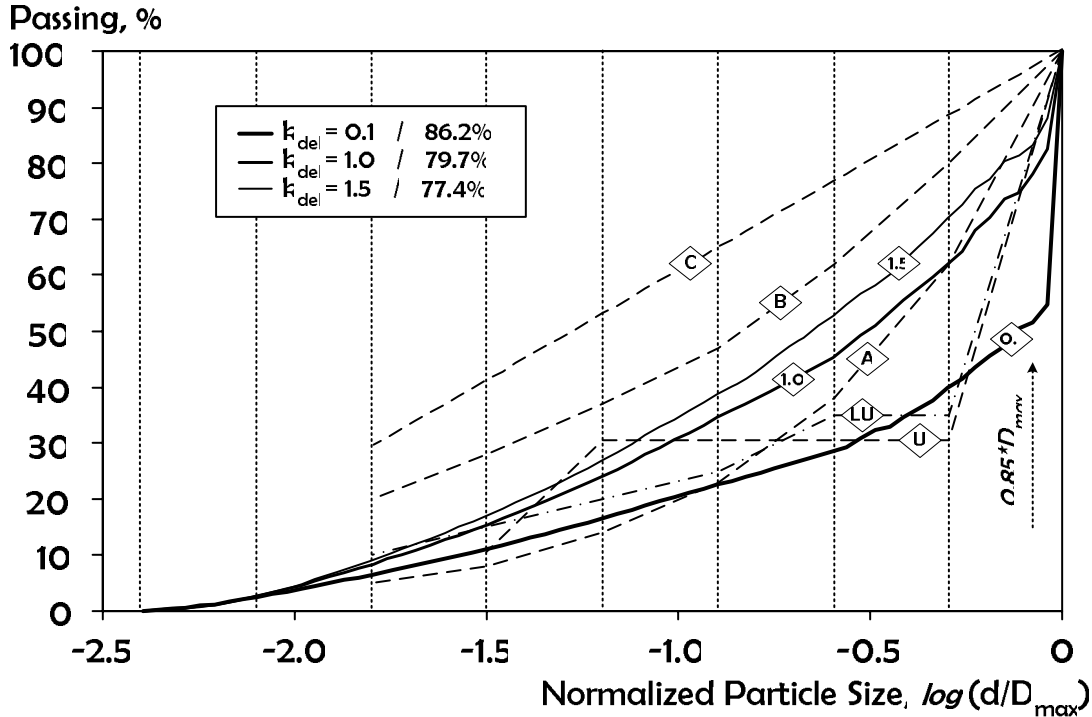

Fig. 9. Size Distribution Curves Corresponding to Packing of 10 Millions Particles

Packing of Aggregates and Concrete Mix Proportioning

As was emphasized in the case of high performance concrete (HPC) [3, 7], three fundamental relationships are important for concrete mixture proportioning: w/c – concrete strength; rheological behavior (viscosity or shear stress) of cement paste – slump of concrete mixture; and the optimal aggregate proportioning – workability of concrete. Being quantified with corresponding models, these criteria completely define the mixture proportioning and properties of HPC. On the other hand, comprehensive modeling of concrete workability and rheological behavior is not possible without the detailed knowledge of the arrangement of aggregate's particles, packing degree, and characteristics of porosity.

Similar behavior can be also attributed to common concrete [1, 4-6]. It is mutually accepted that better packing provided by the optimization of aggregates is an essential step of concrete mixture proportioning. The common tool currently used to accomplish this task is represented by the Fuller curves. Based on Fuller curves, DIN 1045 specifies the area on the particle size distribution field that includes the preferable gradings (Fig. 9). This area is limited by the grading curves A and B (in Fig. 9 the family of curves with different D_{max} are normalized to the same relative origin using the formula log(d/D_{max})). The area between the curves B and C is also allowed, but not advised. There is also curve U representing the case of "Gap-Grading." Based on the geometrical calculations, a revised version of "Gap-Grading" (curve LU) was proposed by Kessler [11]. Generally, concrete mixtures with high workability (required for self-compacting and pumped concretes) can be produced with the aggregates adjusted to grading curve B. Conventional vibro-compacted concrete with slump values from 50 to 200 mm can be effectively produced with the aggregates particle size distribution taken as a midline between A and B; and highly-dense low-slump concrete is produced preferably with A or U gradings.

Table 1. The Performance of Simulation Algorithm Corresponding to Packing of 10 Million Particles

Separation Coefficient, k_{del}	Particle Range, fraction of D_{max}	Packing Degree, %	Packing Time, hours	Memory Used (RAM), MB
0.1	0.006 − 1.0	86.2	10.2	166.87
1.0	0.006 − 1.0	79.7	8.7	166.85
1.5	0.006 − 1.0	77.4	7.3	166.86

It can be observed that the majority of "real" aggregate packings used in concrete technology (i.e., located between the curves A and B) are looser and less arranged than predicted by the "best packing curves" (these are usually located under the curve A [13, 28]). To achieve a higher packing degree, a wider range of particle sizes commonly used in concrete technology.

The model curves acquired with $k_{del} \geq 1$ lay between the curves A and B as specified by DIN 1045. The difference is that the model curves require somehow larger amounts of coarse aggregate fraction from D_{max} to $0.85*D_{max}$. However, in practice, such narrow separation of particles is not realized and real-life grading would use a somewhat wider size band (from D_{max} to $0.5*D_{max}$), eliminating this difference. Another model curve (obtained with $k_{del} = 0.1$) is very close to the dense packing LU- curve suggested by Kessler [11].

69. 07 % Packing
1000 Spheres
N = 100k
K = -1
K_{del} = 0.1
S_r = -3

28.63 % Packing
1000 Spheres
N = 100k
K = -1
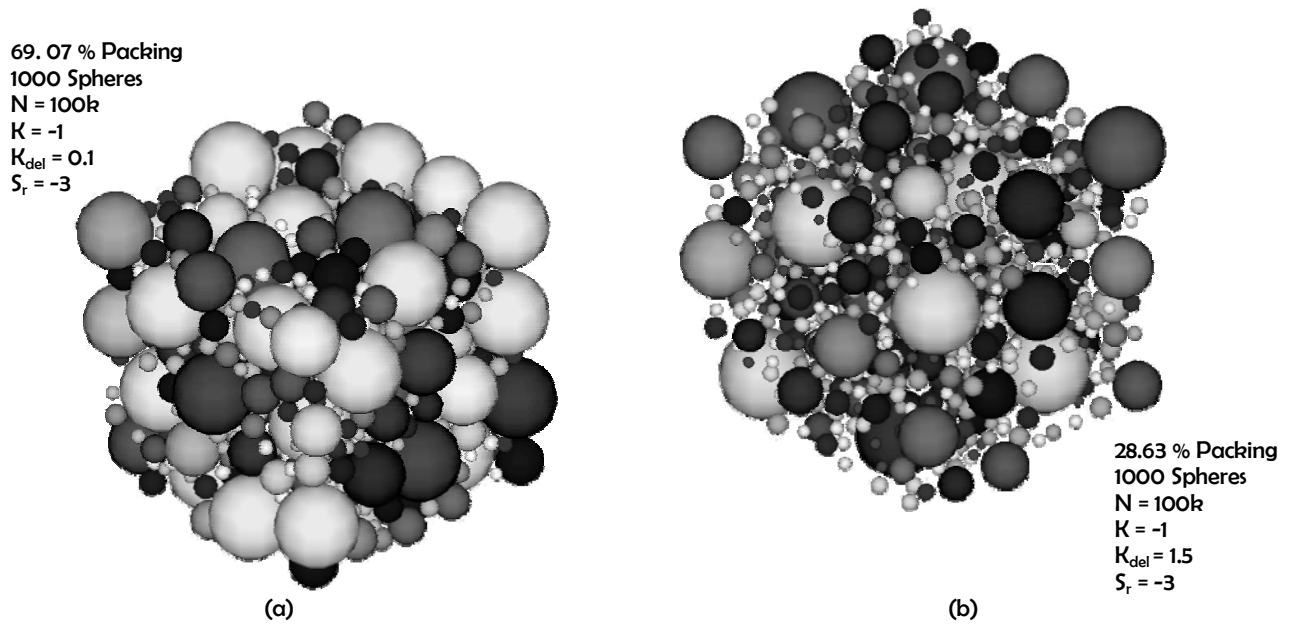K_{del} = 1.5
S_r = -3

(a)   (b)

Fig. 10. 3D Particle Arrangements Corresponding to (a) Initially Pre-Packed (IPP) Dense Packings at $k_{del} \leq 1$ and (b) Continuous Distribution (Fuller) Suspension Packings at $k_{del} \geq 1$

CONCLUDING REMARKS

1. Implementation of a multiple cell mode for the Particles Suspension Model resulted in significant improvement of the speed of sphere processing and overall enhancement of computational algorithm. The developed algorithm is capable of simulating the real-life particulate systems composed of up to 10 million entities, such as aggregates of portland cement concrete.

2. It was demonstrated that there is a trade-off between the speed of program execution and the memory required to realize the process. These parameters are controlled by the degree of division of a cube on the cells Φ. The division of the cube on the cells with a side length near to r_{max} is proposed as an empirical rule to speed up the algorithm.

3. The developed algorithm allows the modeling of real particulate systems used in concrete technology composed of up to 10 million particles that differ in size of up to 160 times. The model's particle size distribution curves acquired with $k_{del} \geq 1$ lay within the limits set by the standards. The developed algorithm and obtained patterns of particulate systems composed of up to 10 million entities can be used to visualize and model the "real life" arrangements of concrete aggregates, as well as the behavior of concrete in fresh and hardened states.

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