Packing Equal Spheres by Means of the Block Coordinate Descent Method

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Abstract. The paper deals with the problem of packing a large number of equal spheres into a container of spherocylindrical shape with a cylindrical prohibition area which arises in chemical industry. The problem is presented as a mathematical programming problem on the ground of the Stoyan's phi-functions method. Solving the problem is reduced to solving a sequence of non-linear programming problems making use of the block coordinate descent method and analysis of Lagrange multipliers to realize sequential addition of spheres. Numerical examples for up to two millions of spheres are given.

Keywords: packing, sphere, spherocylinder, catalyst, optimization

1 Introduction

Packing spheres consists to arrange equal or non-equal non-overlapping spheres within a containing space or into a larger three-dimensional domain (container). A typical objective is to fill as much of the space (container) as possible. The optimization sphere packing problem is studied in discrete and computational geometry.

C.F. Gauss proved in 1831 [1] that the hexagonal lattice sphere-packing configuration has the highest density amongst all possible lattice packings with the asymptotic value $\pi/(3\sqrt{2})$. Given a bounded container, the maximum packing density decreases depending on the ratio of the sphere diameter to the container sizes.

The sphere packing problems are of interest in studying structure of crystals [2], liquids [3], glassy materials [4], catalysts and fuel elements [5-8], etc. The packing density of equal spheres is a significant factor in the study of processes in thermal heat exchangers, chemical and nuclear reactors [9]. Well-known are applications of packing spheres in medicine and engineering.

The aim of the paper is to develop a method of dense random packing a large number of equal spheres into a composed container being a geometric model of a chemical reactor.

2 Problem Statement

Let there be spheres S_i, $i \in I_N = \{1,2,..,N\}$ with radius r and a container C which is a specific composition of cylinders C_1, C_2 and a spherical segment S_0 (Fig. 1):

$$C = (C_1 \cup S_0) \setminus \operatorname{int} C_2$$

where $c(C_2)$ is the compliment of C_2, $\operatorname{int}(\cdot)$ is the interior of the set,

$$C_1 = \{(x, y, z) \in \mathrm{R}^3 \mid x^2 + y^2 \le R^2, 0 \le z \le H\},$$

$$C_2 = \{(x, y, z) \in \mathrm{R}^3 \mid x^2 + y^2 \le r_c^2, -R \le z \le -R + h\},$$

$$S_0 = \{(x, y, z) \in \mathrm{R}^3 \mid x^2 + y^2 + z^2 \le R^2, -R \le z \le \min\{0, H\}\},$$

$R > 0$ is radius of S_0 and of base of C_1, H is height of C_1, $h > 0$ is height of C_2 and $r_c > 0$ is radius of its base, $-R + h < H$.

The bottom of C is of spherocylindrical shape and the top of C is bounded above by the plane $z = H$. In general, H can be negative. In this case $C_1 = \varnothing$.

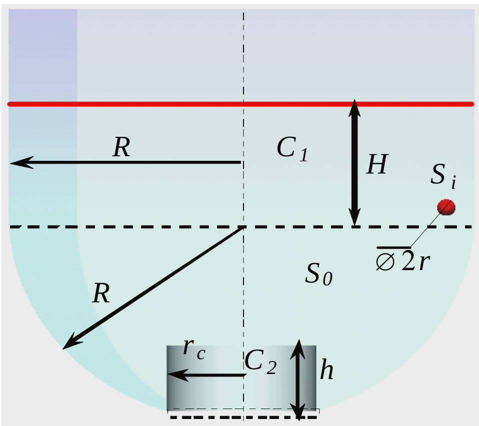

Fig. 1. Container and a sphere (catalyst) to be packed

The problem is formulated as follows: pack the maximal number n^* of spheres from the set S_i, $i \in I_N$ into the container C without overlappings and calculate their center coordinates $v_i^* = (x_i^*, y_i^*, z_i^*)$, $i = 1,2,..,n^*$.

3 Literature review

A review of numerical simulation methods to solve sphere packing problems is presented in [8]. A major part of investigations make use of the Monte-Carlo method [9,10], Discrete Element Models [11] and sequential addition techniques [6,12,13]. The papers consider as a rule cylindrical or rectangular containers.

Mueller [13] applies a sequential addition technique to pack equal spheres into a right circular cylinder and develops the packing algorithm based on a dimensionless packing parameter. The algorithm yields a layerwise structure of the desired number of spheres. The spheres are packed in stable positions under gravity with the maximum dimensionless packing parameter.

Catalytic reactors (packed bed reactors) are used in chemical industry [14]. Reactors with a single adiabatic bed are traditionally used in either exothermic or endothermic reactions. Catalyst pellets have the shape of sphere or cylinder. Packed beds of catalysts should avoid unstable and inefficient arrangements. The packing density of catalysts influences on chemical reactions.

The concept of phi-functions and quasi phi-functions is known to be an efficient tool for mathematical modeling of 3D packing problems for geometrical objects [15-17]. Powerful tools to solve problems of packing geometric objects of various spatial shapes are proposed in [18-24].

Paper [19] proposes a method of solving the sphere packing problem based on homothetic transformations of spheres. The radii of the spheres are assumed to be variable and the auxiliary problems are solved, the sum of the sphere volumes being maximized. The optimization process continues until the sphere radii reach their original values. The method allows to jump from one local extremum to another.

In this paper we consider a method to obtain a dense random packing of a large number of equal spheres into a composed container being a geometric model of the catalytic reactor with a single adiabatic bed. The Stoyan's phi-function method [15,16] is applied to describe packing constraints. Solving the problem is reduced to solving a sequence of nonlinear programming problems making use of the block coordinate descent method [25] and analysis of Lagrange multipliers [26]. We realize sequential addition of spheres. Groups of variables are formed by center coordinates of spheres to be packed. A local minimum point is calculated for each group of variables.

4 Mathematical model

A mathematical model of the problem is presented as follows:

$$n^* = \max \sum_{i=1}^{N} \psi_i(v_i) \text{ s.t. } v \in G \tag{1}$$

where $v = (v_1, v_2, ..., v_N) \in \mathrm{R}^{3N}$, $v_i = (x_i, y_i, z_i) \in \mathrm{R}^3$, $i \in I_N$;

$$\psi_i(v_i) = \begin{cases} 1 \text{ if } \Phi_i(v_i) \geq 0, \\ 0 \text{ otherwise;} \end{cases}$$

$$G = \{v \in \mathrm{R}^{3N} : \Phi_{ij}(v_i, v_j) \geq 0, i, j \in I_N, i < j\};$$

$$\Phi_{ij}(v_i, v_j) = (x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2 - 4r^2;$$

$\Phi_i(v_i)$ is a phi-function of S_i and $c(\operatorname{int} C)$, $c(\circ)$ and $\operatorname{int}(\circ)$ are the compliment and the interior of the set $(\circ)$ respectively; $\Phi_{ij}(v_i, v_j)$ is a phi-function of S_i and S_j, $i, j \in I_N$, $i < j$.

The inequality $\Phi_i(v_i) \geq 0$ provides the sphere S_i, $i \in I_N$, being within the container and the inequality $\Phi_{ij}(v_i, v_j) \geq 0$ specifies non-overlapping the spheres S_i and S_j, $i, j \in I_N$, $i < j$.

The phi-function $\Phi_i(v_i)$ can be constructed according to [15]:

$$\Phi_i(0, v_i) = \min\{\Phi_{1i}(v_i), \Phi_{2i}(v_i)\},$$

where

$$\Phi_{1i}(v_i) = \max\{\alpha_{1i}(v_i), \alpha_{2i}(v_i)\}, \ \Phi_{2i}(v_i) = \max\{\beta_{1i}(v_i), \beta_{2i}(v_i)\},$$

$$\alpha_{1i}(v_i) = \max\{\chi_{1i}(v_i), \chi_{2i}(v_i), \varphi_i(v_i)\},$$

$$\chi_{1i}(v_i) = H - z_i, \ \chi_{2i}(v_i) = z_i, \ \varphi_i(v_i) = R - r - \sqrt{x_i^2 + y_i^2},$$

$$\beta_{1i}(v_i) = \sqrt{\left(\sqrt{x_i^2 + y_i^2} - r_c\right)^2 + (z_i + R - h)^2} - r,$$

$$\beta_{2i}(v_i) = \sqrt{\left(\sqrt{x_i^2 + y_i^2} - r_c\right)^2 + (z_i + R)^2} - r.$$

The objective function $\psi_i(v_i)$ is piecewise constant. The problem (1) is multiextremum, all local maxima being non-strict due to the axial symmetry. The number of non-linear inequalities is $n(n+1)/2$.

5 Solution Method

The number of spheres that can be packed into the container C is not defined in advance. It is can be only evaluated making use of the maximum packing ratio $\pi/(3\sqrt{2}) \approx 0.74$ [1] as an upper bound. If the number of spheres is up to 100, one can adopt the method for packing spheres into a cylinder proposed in [19]. However, if the dimension of the problem is large, then the sequential addition scheme is most suitable to obtain a dense sphere packing.

According to the scheme solving the problem (1) is reduced to solving a sequence of problems. On the first step the sphere S_1 from the set S_i, $i \in I_N$ is packed into C being located at a position with the minimum value of z-coordinate. Then, the sphere S_2, $i \in I_N$ is packed into C, the sphere S_1 being immovable, and so on. The number of the last sphere S_{n*} from the set S_i, $i \in I_N$ which can be packed into C gives an evaluation of the maximum $n*$ of the problem (1). The sequential addition scheme can be realized by applying the block coordinate descent method [25].

Let the spheres $S_1, S_2, ..., S_{k-1}$ be packed at the previous $k-1$ steps, the center coordinates being $v_k^* = \left(x_k^*, y_k^*, z_k^*\right)$, $i = 1,2,...,k-1$ respectively. Coordinates of the sphere S_k form a group of variables at the step k:

$$v_k^* = \arg\min\ \kappa_k\left(v_k\right), \text{ s.t. } v^k \in G^k \subset \mathrm{R}^3,\ k = 1,2,...,N\ , \tag{2}$$

where $\kappa_k\left(v_k\right) = z_k$;

$$G_k = \{v_k \in \mathrm{R}^3 : \Phi_k\left(v_k\right) \geq 0, \Phi_{jk}\left(v_j^*, v_k\right) \geq 0,\ j = 1,2,...,k-1\}\ . \tag{3}$$

We search for a local minimum point of the problem (2)–(3). If a feasible point of the problem (2)–(3) for $k = n*+1$ cannot be found, then the solution of the previous problem ($k = n*$) solved is a solution $N = n_0$ of the problem (1).

We indicate some peculiarities of the problem (2)–(3): the objective function $\kappa_k\left(v_k\right) = z_k$ is linear and minima are reached at extreme points of the feasible region G_k.

The frontier of the feasible region G_k ($fr\left(G_k\right)$) consists of points satisfying the equations $\Phi_{jk}\left(v_j^*, v_k\right) = 0$, $j = 1,2,...,k-1$, or $\Phi_k\left(v_k\right) = 0$:

$$fr\left(G_k\right) = \left\{v = \left(x, y, z\right) \in \mathrm{R}^3 : v \in \left(T \cap G_k\right)\right\},\ k = 1,2,...,N\ ,$$

where

$$T = T_0 \cup T_1 \cup T_2 \cup ... \cup T_{k-1}\ ,$$

$$T_j = \left\{ v \in \mathrm{R}^3 : \Phi_{jk}\left(v_j^*, v\right) = 0 \right\},\ \ j = 1, 2, ..., k-1,$$

$$T_0 = T_{01} \cup T_{02} \cup T_{03} \cup T_{04} \cup T_{05} \cup T_{06} \text{ (Fig. 2).}$$

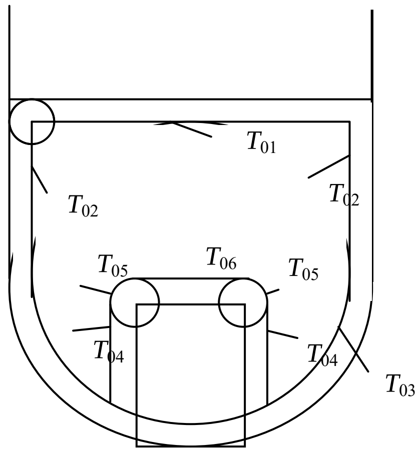

Fig. 2. Illustration of T_0

T_{02} and T_{04} lie on planes:

$$T_{01} = \begin{cases} \left\{ v \in \mathrm{R}^3 : z = H - r,\, x^2 + y^2 \le (R-r)^2 \right\} & \text{if } H \ge 0, \\ \left\{ v \in \mathrm{R}^3 : z = H - r,\, x^2 + y^2 \le (R-r)^2 - H^2 \right\} & \text{otherwise,} \end{cases}$$

$$T_{06} = \begin{cases} \varnothing & \text{if } H < -R + h + r, \\ \left\{ v \in \mathrm{R}^3 : z = -R + h + r,\, x^2 + y^2 \le (r_c)^2 \right\} & \text{otherwise.} \end{cases}$$

T_{02} and T_{04} lie on cylindrical surfaces:

$$T_{02} = \begin{cases} \left\{ v \in \mathrm{R}^3 : x^2 + y^2 = (R-r)^2,\, 0 \le z \le H - r \right\} & \text{if } H > 0, \\ \varnothing & \text{otherwise,} \end{cases}$$

$$T_{03} = \left\{ v \in \mathrm{R}^3 :\ x^2 + y^2 = (r_c + r)^2, \right.$$
$$\left. \sqrt{(R-r)^2 - (r_c + r)^2} \le z \le \min\{(-R+h), (H-r)\} \right\}.$$

T_{03} lies on spherical surface

$$T_{03}=\Big\{v\in \mathrm{R}^3:\ x^2+y^2+z^2=(R-r)^2,$$
$$\sqrt{(R-r)^2-(r_c+r)^2}\le z\le \min\{0,(H-r)\}\Big\}.$$

T_{05} lies on torus surface

$$T_{05}=\begin{cases}\varnothing \text{ if } H\le -R+h,\\ \Big\{v\in \mathrm{R}^3:\left(\sqrt{x^2+y^2}-r_c\right)^2+(z+R-h)^2=r^2,\\ \quad x^2+y^2\ge r_c^2, -R+h\le z\le \min\{(-R+h+r),(H-r)\}\Big\}\\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{otherwise.}\end{cases}$$

The set of extreme points can be presented as

$$E_k=T_{02}\cup T_{03}\cup \bigcup_{\substack{i,j,l=0\\ i<j<l}}^{k-1}\left(T_i\cap T_j\cap T_l\right)\cap frG_k\ ,\ k=1,2,...,N\ .$$

The set of local minima L_k , $k=1,2,...,N$, consists of points of ($fr(G_k)$ whose coordinate values are solutions either of the system:

$$\begin{cases}x^2+y^2+z^2=(R-r)^2,\\ x^2+y^2=(r_c+r)^2\end{cases}$$

or the systems:

$$\begin{cases}f_i=0,\\ f_l=0,\quad i,l,m=0,1,...,k-1,\quad i<l<m,\quad (i,l,m)\in I\ .\\ f_m=0,\end{cases}$$

where f_i, f_l, f_m are either $\Phi_k\left(v_k\right)$ or $\Phi_{jk}\left(v_j^*,v_k\right)$, $j=1,2,...,k-1$; the set I consists of triples of indices for which the condition of minimum [26] is fulfilled.

A sufficient condition of local minimum of the problem (2)–(3) is $\lambda_1>0,\ \lambda_2>0,\ \lambda_3>0$ [26] where the Lagrange multipliers $\lambda_1,\lambda_2,\lambda_3$ can be calculated by solving the following system of linear equations:

$$\begin{pmatrix} \frac{\partial f_i}{\partial x_k} & \frac{\partial f_l}{\partial x_k} & \frac{\partial f_m}{\partial x_k} \\ \frac{\partial f_i}{\partial y_k} & \frac{\partial f_l}{\partial y_k} & \frac{\partial f_m}{\partial y_k} \\ \frac{\partial f_i}{\partial z_k} & \frac{\partial f_l}{\partial z_k} & \frac{\partial f_m}{\partial z_k} \end{pmatrix} \begin{pmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

Thus, set

$$L_k = (T_{03} \cap T_{04}) \bigcup_{\substack{i,l,m=0 \\ i<l<m \\ (i,l,m)\in I}}^{k-1} (T_i \cap T_l \cap T_m) \cap frG_k \ .$$

The number of local minima not belonging to the set is less than $2n(n-1)(n-2)/6$.

The solution strategy of the problems (2)–(3) consists of the following stages.

1. Random choice of an initial point of the feasible region G_k .
2. Movement to the frontier of G_k decreasing the objective.
3. Movement on the frontier of G_k to an extreme point of G_k decreasing the objective.
4. Searching for an extreme point of G_k being a local minimum point of the problem (2)–(3).

6 Searching for a local minimum of subproblem

We consider a procedure to calculate a local minimum point of the problem (2)–(3).

1. A point $v_k^0 = \left(x_k^0, y_k^0, z_k^0\right)$ such that $(x_k^0)^2 + (y_k^0)^2 \le R^2$ and $z_k^0 = H - r_k$ is constructed.
2. If $v_k^0 \notin G_k$, then $n^* = k-1$ is an approximate solution of the problem (1).
3. Otherwise ($v_k^0 \in G_k$), a point $v_k^1 = \left(x_k^1, y_k^1, z_k^1\right) = \left(x_k^0, y_k^0, z_k^0 - \Delta z_q\right) \in frG_k$ at which S_k touches frC or S_p, $p \in \{1,2,...,k-1\}$. The value Δz_q, $q = 1,2,...,$ is defined by bisection within the segment $[0, R+H]$.
4. If point v_k^1 is a local minimum point, then set $v_k^* = v_k^1$ and go to the next k .
5. Otherwise, let point $v_k^1 \in T_i$, $i \in \{0,1,...,k-1\}$. A point $v_k^2 = \left(x_k^2, y_k^2, z_k^2\right) \in \left(T_i \cap T_j\right)$ is calculated where $i \ne j \in \{0,1,...,k-1\}$ and $z_k^2 < z_k^1$ such that S_k touches frC

and S_j, $j \in \{1,2,...,k-1\}$ or S_i and S_j. To this end we solve the following systems:

$$\begin{cases} f_i(x,y,z) = 0, \\ z = z_k^1 - \Delta z_q, \qquad q = 1,2,... \\ ax + by = c, \end{cases}$$

where the equation $f_i(x,y,z) = 0$ describes the frontier of T_i and $ax + by = c$ is an equation of a plane passing through the point $v^{k1} \in T_i$. The value Δz_q is defined by bisection within the segment $\left[0, R + H + z_k^1\right]$. If v^{k2} is a local minimum point, then set $v_k^* = v_k^2$ and go to the next k.

6. An extreme point $v_k^3 = \left(x_k^3, y_k^3, z_k^3\right) \in \left(T_i \cap T_j \cap T_l\right)$ is calculated where $i \neq j \neq l \in \{0,1,...,k-1\}$ and $z_k^3 < z_k^2$ such that S_k touches frC and two spheres or three spheres. To this end we solve the following systems:

$$\begin{cases} f_i(x,y,z) = 0, \\ f_j(x,y,z) = 0, \\ z = z_k^2 - \Delta z_q, \quad q = 1,2,..., \end{cases}$$

where the equations $f_i(x,y,z) = 0$ and $f_j(x,y,z) = 0$ describe the frontiers of T_i and T_j respectively. The value Δz_q is defined by bisection within the segment $\left[0, R + H + z_k^2\right]$. If v_k^3 is a local minimum point, then set $v_k^* = v_k^3$ and go to the step $k+1$.

7. Otherwise ($\lambda_1 < 0$ or $\lambda_2 < 0$ or $\lambda_3 < 0$) define $i_0 \in \{1,2,3\}$ such that $\lambda_{i_0} \le \lambda_1$, $\lambda_{i_0} \le \lambda_2$, $\lambda_{i_0} \le \lambda_3$.
8. If $i = i_0$, take $i = j$, $j = l$ and $v_k^2 = v_k^3$ and go to the item 6.
9. If $j = i_0$, take $j = l$ and $v_k^2 = v_k^3$ and go to the item 6.
10. If $l = i_0$, take $v_k^2 = v_k^3$ and go to the item 6.

A special strategy of verifying the feasibility during optimization process is proposed. The strategy forms a list of inactive constraints analyzing distances from the sphere to be packed to the spheres already packed. This allows to essentially decrease the computational complexity of the algorithm.

To improve the value of the objective of the problem (2)–(3) we realize the multistart method on each step and choose the best local minimum.

7 Experimental results and discussion

In order to numerically test the packing method proposed a software is developed. Several examples with up to 2 million spheres are calculated. The Open Graphics Library for visualization of the optimization process.

Example 1. The metric characteristics of the container and the spheres to be packed are $R = 250$, $r_c = 80$, $H = 0$, $h = 250$ and $r = 15$. We use 30 starting points for each sphere. The number of spheres packed is $n^* = 1017$ (Fig. 3). The runtime is 1 sec.

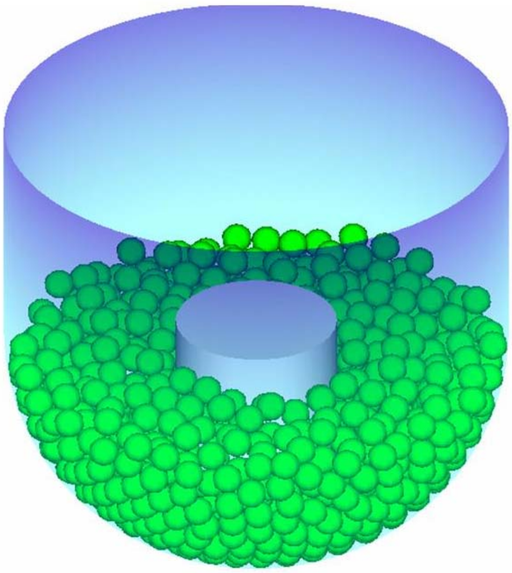

Fig. 3. Illustration of Example 1

Example 2. The metric characteristics are $R = 250$, $r_c = 80$, $H = -120$, $h = 80$ and $r = 5$. 30 starting points are chosen for each sphere. The number of spheres packed is $n^* = 9696$ (Fig. 4). The runtime is 20 sec.

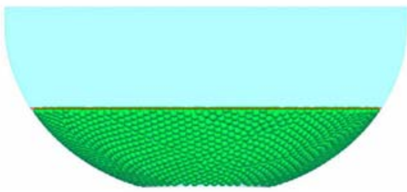

Fig. 4. Illustration of Example 2

Example 3. The metric characteristics are $R = 250$, $r_c = 50$, $H = 0$, $h = 270$ and $r = 2$. 30 starting points are chosen for each sphere. The number of spheres packed is $n^* = 539778$ (Fig. 5). The runtime is 1 h 20 min.

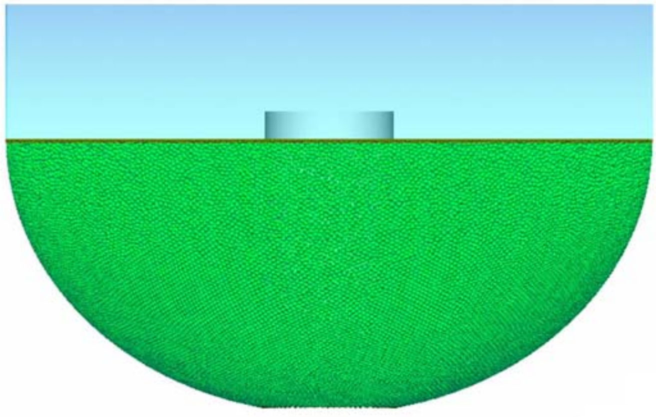

Fig. 5. Illustration of Example 3

Example 4. The metric characteristics are $R = 250$, $r_c = 80$, $H = -10$, $h = 80$ and $r = 1.25$. One local minimum is calculated for each sphere. The number of spheres packed is $n^* = 2\,063\,007$. The runtime is about 2 h.

The large-dimension problem reduces to solving a sequence of subproblems by means of the block coordinate descent method. The multistart method allows to choose a better local position for each sphere, thus increasing the total packing density.

As experimental results show (see Fig.4 and Fig.5) the spheres form regular structures along the packing domain frontier (the container wall).

It is obvious that the packings obtained in the examples do not, in general, correspond to local minimum points of the problem minimizing the height of the filled part of the container when all the spheres are moveable.

8 Conclusion

The problem of packing equal sphere into a bounded container is considered in the paper.

The method suggested allow to solve the problem of large dimension due to applying the block coordinate descent method which allow to reduce solving the problem to a sequence of non-linear programming problems.

The optimization method realizes search of a frontier point of the feasible region, an extreme point and movement to a local minimum point. Choice of descent direction is defined by analyzing Lagrange multipliers of active constraints.

Numerical examples show effectiveness of the method for up to two millions equal spheres.

The Stoyan's phi-function method allows to adopt the developed method to pack spheres into containers of arbitrary spatial shapes.

The method can be also extended to pack unequal spheres.

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