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RANDOM PACKING OF IDENTICAL SPHERES INTO A CYLINDRICAL CONTAINER

The paper proposes an algorithm for packing a great number of identical spheres into a cylindrical container.

packing, cylinder, sphere, catalyst, group of variable, greedy algorithm, local minimum

Introduction

The problem of packing of a great number of identical spheres into a container considered in this paper arises in oil-refining (catalytic cracking and reforming) and gas-processing (absorption) industries. Catalysts to be packed into the container may be of spherical form.

In this paper an algorithm to pack a great number of identical spheres is suggested. The mathematical model of the problem is constructed on the ground of Φ -functions ([1],[2]).

Mathematical model

The following mathematical model of the problem is used. Let there be a sphere S with radius r and a domain D (cylindrical container) being a specific composition of cylinders C_1, C_2 and a spherical segment S_0 (fig. 1):

$$D = (C_1 \cup S_0) \setminus C_2 = \mathrm{cl}((C_1 \cup S_0) \cap c(C_2)) = \mathrm{cl}(C_1 \cup (S_0 \cap) c(C_2))$$

where $c(C_2)$ is the compliment C_2 to R^3, $c(\cdot)$ is the closure,

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

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

$$S_0 = \{(x,y,z) \in R^3 \,|\, x^2 + y^2 + z^2 \le r_c^2, -R \le z \le H\},$$

$R > 0$ 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.

The origin of the eigen coordinate system of domain D is at point $O = v_0 = (0,0,0)$. Plane $z = H$ is a height of domain D. In general, H can be non-positive.

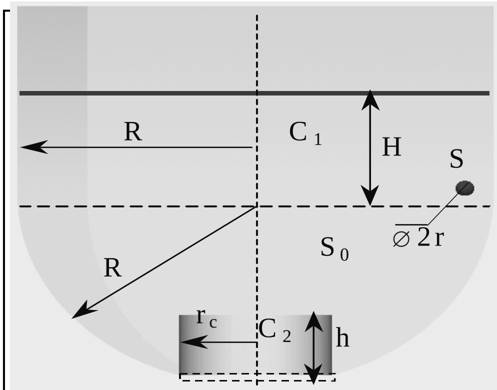

Fig. 1. Cylindrical domain D (container) and sphere S (catalyst)

Problem. It is necessary to pack a maximal number N of spheres $S_1, S_2, ..., S_N$ of the same radius r into domain D without mutual intersections and find their centre coordinates $v_i = (x_i, y_i, z_i)$, $i = 1,2,...,N$.

We consider a set of spheres S_i, $i = 1,2,...,n$. Mathematical model of the problem can be formulated as follows.

Find N and v_i, $i = 1,2,...,N$, such that

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

where $v = (v_1, v_2, ..., v_n) \in R^{3n}$,

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

$$\Phi_{ij}(v_i, v_j) \ge 0, i = 1,2,...,k-1, j = 2,3,...,k, i < j,$$

where $\Phi_i(0, v_i)$ is a Φ -function of body $\mathrm{cl}(c(D))$ and spheres S_i, $i = 1,2,...,k$, $\Phi_{ij}(v_i, v_j)$ is a Φ -function of spheres S_i and S_j, $i = 1,2,...,k-1, j = 2,3,...,k, i < j$. Inequality $\Phi_i(0, v_i) \ge 0$ ensures that spheres are located within D and inequality $\Phi_{ij}(v_i, v_j) \ge 0$ gives non-overlapping spheres.

Solution algorithm

To obtain a solution of the problem (1) a modification of the optimisation method by groups of variables (greedy algorithm) is suggested. It allows to decompose the problem (1) onto N subproblems. Each subproblem uses the packing of spheres corresponding to the previous subproblem.

We consider the problem which arises on the step k. Coordinates of spheres $S_1, S_2, ..., S_{k-1}$ packed at the previous $k-1$ steps are fixed $v_k = v_k^* = (x_k^*, y_k^*, z_k^*)$, $i = 1,2,...,k-1$. Coordinates of S_k form the k-th group of variables.

$$W(v_k^*) = \min W_k(v_k), \text{ s.t. } v_k \in G^k, \; k = 1,2,...,n_0 + 1, \quad (2)$$

where $W_k(v_k) = z_k$, $n_0 < n$; feasible region $G^k \subset R^3$ is defined by the system of inequalities:

$$\begin{cases} \Phi_k(0, v_k) \ge 0, \\ \Phi_{jk}(v_j^*, v_k) \ge 0, \; j = 1,2,..., k-1. \end{cases} \qquad (3)$$

If a solution of problem (2) for $k = n_0 + 1$ is not found, then the solution of the previous problem ($k = n_0$) is supposed to be a solution $N = n_0$ of the problem (1). The following peculiarities of subproblems can be pointed out.

1. The objective function is linear. Minima of problem are at extreme points of the feasible region.
2. The frontier of feasible region G^k. is formed by points belonging to a surface being specified by the equation $\Phi_k(0, v_k) = 0$ or surfaces being specified by the equations $\Phi_{jk}(v_j^*, v_k) = 0$, $j = 1,2,...,k-1$.

A solution strategy allows to obtain a local minimum for each subproblem. The solution strategy for the k-th subproblem 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. towards decreasing of the objective.
3. Movement along the frontier of G^k. to an extreme point of G^k. towards decreasing of the objective.
4. Searching for an extreme point of G^k. being a local minimum of problem (2).

5. Repeat of items 1 – 4 depending on number of local minima.

6. Selection of the best local minimum obtained.

We consider the steps in detail.

1. A point $v_k^0 = (x_k^0, y_k^0, z_k^0)$ is taken as an initial one where x_k^0 and y_k^0 are randomly defined within the domain D and $z_k^0 = H - r_k$. In other words, the point corresponds to the location of S_k on the top of D.

2. If $v_k^0 \notin G^k$, then take $N = k-1$ and a solution of the problem (1) is obtained. Stop the algorithm.

3. Otherwise ($v_k^0 \in G^k$), a point

$$v_k^1 = (x_k^1, y_k^1, z_k^1) = (x_k^0, y_k^0, z_k^0 - \Delta z_q) \in \mathrm{fr}G^k,$$

at which S_k touches the frontier of D ($\mathrm{fr}D$) or S_i, $i \in \{1,2,...,k-1\}$. Value Δz_q, $q = 1,2,...$, is defined by bisection within the segment $[0, R+H]$. Point $v_k^1 \in T_i$, $i \in \{0,1,...,k-1\}$ where T_i are surfaces given as

$$T_0 = \{v_k \in G^k \,|\, \Phi_k(0, v_k) = 0\},$$

$$T_i = \{v_k \in G^k \,|\, \Phi_{ik}(v_i^*, v_k) = 0\},\ i = \{1,2,...,\ k-1\}.$$

4. If point v_k^1 is a local minimum, then $v_k^* = v_k^1$ and go to the step $k+1$.

5. A point $v_k^2 = (x_k^2, y_k^2, z_k^2) \in (T_i \cap T_j)$ is found where $i \neq j \in \{1,2,...,k-1\}$ and $z_k^2 < z_k^1$. At the point sphere S_k touches $\mathrm{fr}D$ and S_j, $j \in \{1,2,...,k-1\}$ or with S_i and S_j. To this end we solve systems:

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

where $f_i(x,y,z) = 0$ describes surface T_i; $z = z_k^1 - \Delta z_q$, $q = 1,2,...$, are equations of planes to be parallel to plane XOY; $ax + by = c$ is equation of a plane to be parallel to axis of cylinders and passing through point $v_k^1 \in T_i$. Value Δz_q is defined by bisection within the segment $[0, R+H+z_k^1]$. If point v_k^2 is a local minimum, then $v^* = v_k^2$ and go to the step $k+1$.

6. An extreme point $v_k^3 \in (T_i \cap T_j \cap T_l)$ is found where $i \neq j \neq l \in \{0,1,...,k-1\}$ and $z_k^3 < z_k^2$. At the point sphere S_k touches $\mathrm{fr}D$ and two spheres or three spheres. To this end we solve systems:

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

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

7. Otherwise, some of Lagrange multipliers $\lambda_1 < 0$ or $\lambda_2 < 0$ or $\lambda_3 < 0$. We define $i_0 \in \{1,2,3\}$ such that $\lambda_{i_0} \leq \lambda_i$, $i = 1,2,3$.

8. If $i = i_0$ we take $i = j$, $j = l$ and $v_k^2 = v_k^3$ and go to item 6.

9. If $j = i_0$ we take $j = l$ and $v_k^2 = v_k^3$ and go to 6.

10. If $l = i_0$ we take $v_k^2 = v_k^3$ and go to item 6.

To decrease the algorithm runtime the following mean. In order to verify whether a point $v = (x,y,z)$ belongs to G^k a set of indices $I_L(v)$ of spheres lying close to the a point $v = (x,y,z)$ is constructed:

$$I_L(v) = \{i \in \{1,2,...,k-1\} \,|\, \|v - v_i\| \leq 2r_i\}$$

and use the system

$$\begin{cases} \Phi_k(0, v_k) \geq 0, \\ \Phi_{jk}(v_j^*, v_k) \geq 0,\ j \in I_L(v) \end{cases}$$

instead of system (3). It enables the algorithm complexity to become linear depending on the number of spheres.

Examples

Series of examples are calculated (Pentium III).

Example 1. $r = 15$, $R = 250$, $r_c = 80$, $H = 0$, $h = 250$. To improve the final result 30 attempts are made on each step. The number of spheres packed is $N = 1017$ (Fig. 2). Runtime of the problem is 12 sec.

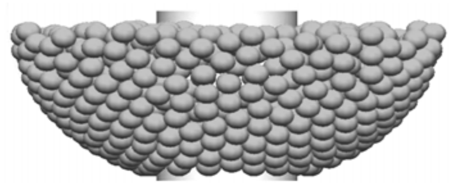

Fig. 2. Packing of 1017 spheres

Example 2. $r = 1.25$, $R = 250$, $r_c = 80$, $H = -10$, $h = 80$. Only one attempt is made on each step. The number of spheres packed is $N = 2\,063\,007$. Runtime is about 20 h.

References

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