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PACKING SPHERES INTO A PARALLELEPIPED BY MEANS OF THE DECREMENTAL NEIGHBOURHOOD METHOD

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The paper deals with the optimisation problem of packing various solid spheres into a parallelepiped with minimal height. Based on the mathematical model the peculiarities of the problem are given. Regarding these peculiarities a solution method is suggested. The method is a new modification of the decremental neighbourhood method. Numerical results are discussed.

PACKING, SPHERE, PARALLELEPIPED, OPTIMISATION, DECREMENTAL NEIGHBORHOOD METHOD

Introduction

3D packing problems are of importance in different branches of human activity, e.g., in CAD, medicine (radiosurgery treatment planning), the filtration problem, granular medium modeling, powder metallurgy packing catalysts in chemistry, etc.

Packing solid spheres into a parallelepiped is of special value in research of 3D packing problems due to simplicity of description of interactions between spheres.

T.C. Hales [1] has proved the Kepler conjecture that the packing density of identical spheres cannot exceed value $\pi/\sqrt{18} \approx 0.74$.

The problem of unequal sphere packing in a 3D polytope is analyzed in [2] as a non-convex optimization problem with quadratic constraints and a linear objective function. Algorithms which improved the existing branch-and-bound algorithm for the general non-convex quadratic program are proposed.

G.E. Mueller [3] for packing identical spheres in a cylinder uses the sequential addition technique which is based on the dimensionless packing parameter. The identical sphere packing in high Euclidean dimensions by means of their random sequential addition is considered in [4]. The technique is the optimization algorithm by groups of variables [3], i.e., as a matter of fact, it is one of greedy algorithms [5].

Paper [6] takes in a wide range of circular and spherical packing problems. Original mathematical models for these problems are offered. Local optimal solutions are calculated starting from several random initial points. The best local solution obtained is supposed to be an approximation to a global solution. A huge number of numerical examples for the range of problems are given.

Paper [7] deals with packing of different radii spheres into a parallelepiped of minimal height. A modification of the decremental neighbourhood method (DNS) in combination with local optimization based on the reduced gradient method, the Newton method and the active set strategy have been used. DNS to search for an approximation to the global minimum is adopted to the problem under consideration.

This paper is a continuation of research of DNS and suggests a new selection criterion of neighbourhoods to obtain better objective function values.

1. Mathematical model

Let there be spheres $S_i \subset R^3$ $i \in I = \{1,2,...,n\}$ with radii r_i, $i \in I = \{1,2,...,n\}$:

$$S = \left\{(x,y,z) \in R^3 : x^2 + y^2 + z^2 - r^2 \le 0\right\}$$

and a rectangular parallelepiped (cuboid)

$$P = \left\{(x,y,z) \in R^3 : 0 \le x \le a, 0 \le y \le b, 0 \le z \le h\right\}$$

where R^3 is the Euclidean 3D arithmetic space. Length a and width b of P are constant, while height h is a variable. The translation of sphere S_i by vector $v_i = (x_i, y_i, z_i)$ is denoted by $S_i(v_i)$, $i \in I$. Translation vector v_i is also called the placement parameter vector of S_i.

Problem. Find a placement parameter vector

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

so that all spheres $S_i(v_i)$ are contained completely within parallelepiped P without mutual intersections and height h of P attains a minimal value.

Thus,

$$u = (v, h) \in R^m$$

where $m = 3n+1$, is a vector of all variables of the problem.

A mathematical model of the identical sphere packing problem is represented as follows.

$$F(u^*) = \min F(u), \text{ s.t. } u \in G \tag{1}$$

where

$$G = \{u \in R^m : \varphi_k(w_k) \ge 0, k = 1,2,...,\theta = 6n + \frac{n^2 - n}{2}\} \tag{2}$$

$$\varphi_k(w_k) = \begin{cases} x_i - r,\ i = 1,2,...,n \text{ if } k = 1,2,...,n, \\ y_i - r,\ i = 1,2,...,n \text{ if } k = n+1, n+2,...,2n, \\ z_i - r,\ i = 1,2,...,n \text{ if } k = 2n+1, 2n+2,...,3n, \\ a - x_i - r,\ i = 1,2,...,n \text{ if } k = 3n+1, 3n+2,...,4n, \\ b - y_i - r,\ i = 1,2,...,n \text{ if } k = 4n+1, 4n+2,...,5n, \\ h - z_i - r,\ i = 1,2,...,n \text{ if } k = 5n+1, 5n+2,...,6n, \\ (x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2 - 4r^2,\ i < j = 1,2,...,n \\ \qquad \text{if } k = 6n+1, 6n+2,...,6n + \frac{n(n-1)}{2}, \end{cases}$$

$$u = (v_1, v_2, ..., v_n, h) \in R^m, \ m = 3n+1, \ F(u) = h;$$
$$w_k \in \{x_i, y_i, z_i, (v_i, v_j), \ i \neq j, \ i, j \in \{1,2,...,n\}\}.$$

Note that the inequalities (2) give the containment of the spheres within parallelepiped P and ensure non-overlapping of spheres.

Some characteristics of problem (1-2) can be pointed out.

(i) $F(u)$ is linear, restrictions are linear and nonlinear.

(ii) The frontier of G is formed by $6n$ linear and $\frac{n(n-1)}{2}$ surfaces of the second order.

(iii) G is in general disconnected, i. e.

$$G = \bigcup_{l=1}^{\eta} G_l, \ G_i \cap G_j = \varnothing, \ i \neq j,$$

This can occur if

$$(a-2r)^2 + (b-2r)^2 < 4r^2.$$

(iv) Each connected component of G is multiply connected.

(v) The problem is multi-extremal in general and NP-hard.

(vi) Any extreme point $u \in G$ is specified by a system of $m = 3n+1$ equations of type $\varphi_k(w_k) = 0$.

(vii) To any local minimum u^* there always corresponds at least one extreme point $\tilde{u}^* \in G$ such that $F(\tilde{u}^*) = F(u^*)$.

2. Solution method

In paper [7] to find an approximation of a global minimum a computational procedure was proposed which consists of the following steps:

(i) According to randomly generated sequences of the spheres a number of extreme points $u^i \in G$, $i = 1,2,...,\lambda$ is computed.

(ii) Among these λ extreme points a best one, say $\bar{u}^1$, is chosen which determines the centre point of a neighbourhood.

(iii) According to a modification of DNS a number of better solutions (extreme points) $\bar{u}^j$, $j = 1,2,...,\tau$ are computed iteratively where $\bar{u}^j$ denotes the best solution found within the current neighbourhood U_j. It is used as centre of the next neighbourhood.

(iv) Then, taking several of the best extreme points found in the last neighbourhood U_j, say $\tilde{u}^j$, $j = 1,2,...,\kappa$, as starting points, local minima u^{*j}, $j = 1,2,...,\kappa$, of the problem (1-2) are calculated.

(v) Finally, the point

$$u^* = \arg\ \min\{F(u^{*j}) : j = 1,2,...,\kappa\}$$

is chosen as an approximation of a global minimum.

In this paper a new modification of DNS is proposed.

Let

$$\pi_j = \{S_{j_1}, S_{j_2}, ..., S_{j_n}\}$$

be some random sequence of spheres. It means, the sequence may be considered as some permutation consisting of spheres S_j, $j = 1,2,...,n$. If all spheres are different then the number of all sequences is equal to $n!$. Thus, all sequences of kind

$$\pi_j = \{S_{j_1}, S_{j_2}, ..., S_{j_n}\}$$

form a discrete set Π.

The definition of a neighbourhood within the permutation set Π is realized by a one-to-one correspondence of a sequences

$$\pi_j = \{S_{j_1}, S_{j_2}, ..., S_{j_n}\} \in \Pi$$

of spheres and a points

$$(r_{j_1}, r_{j_2}, ..., r_{j_n}) \in \Pi_R$$

of the Euclidean space R^n, i. e. a one-to-one correspondence between sets Π and Π_R is established. By means of neighbourhood in Π_R a corresponding subset of sphere permutations in Π is determined which can be viewed also as a neighbourhood in Π, i.e. sequence

$$\rho_j = \{r_{j_1}, r_{j_2}, ..., r_{j_n}\}$$

is considered as a point in the Euclidean space R^n.

Let

$$B = \{(r_{j_1}, r_{j_2}, ..., r_{j_n})^T \in R^n : (j_1, j_2, ..., j_n) : \Pi(1,...,n)\}$$

denote the (finite) image of the set Π_R within R^n ($\Pi(1,...,n)$ is a set of permutations of $1,...,n$). As is known, the set B consists of vertices of a convex hyper-polytope inscribed into a $(n-1)$-dimensional hyper-sphere i.e. the set B is contained in an $(n-1)$-dimensional hyper-sphere. The diameter of this hyper-sphere is equal to

$$\beta = d(X^1, X^{n!}) = \sqrt{(r_1 - r_n)^2 + (r_2 - r_{n-1})^2 + ... + (r_n - r_1)^2}$$

where

$$X^1 = (r_1, r_2, ..., r_n), \ X^{n!} = (r_n, r_{n-1}, ..., r_1)$$

and $r_1 \le r_2 \le ... \le r_n$, i.e. the distance between any two points of B is equal to or smaller than β.

The approach proposed in this paper is desired to packing problems with various different radii. In case of only identical radii β becomes zero, and therefore the approach is not appropriate.

First, a set $\Pi_1 \subset \Pi$ with λ elements ($50 \le \lambda \le 100$ was defined empirically) is chosen randomly of set Π. For any $\pi^q \in \Pi_1$ an extreme point of G is computed according to the permutation which corresponds to sequence π^q. Thus, one can obtain a set $U_1 \subset G$ of extreme points $u^{1\xi}$ $\xi = 1,2,...,\lambda$, that are generated by set Π_1. After that, taking extreme points of set U_1 as starting points, appropriate set U_1^* consisting of λ local minima is found. Then three points $u^{*1\xi_1}, u^{*1\xi_2}$, $u^{*1\xi_3} \in U_1^*$ such that

$$F(u^{*1\xi_1}) < F(u^{*1\xi_2}) < F(u^{*1\xi_3}) \le F(u^{*1\xi}),$$

$\xi = 1,2,...,\lambda$, are selected. To these local minima there correspond starting points $u^{1\xi_1}, u^{1\xi_2}, u^{1\xi_3}$. To points $u^{1\xi_1}, u^{1\xi_2}, u^{1\xi_3}$ there correspond points $\pi^{1\xi_1}, \pi^{1\xi_2}, \pi^{1\xi_3} \in \Pi_1$ in turn. Whence, to points $u^{*1\xi_1}, u^{*1\xi_2}$, $u^{*1\xi_3} \in U_1^*$, there correspond points $\pi^{1\xi_1}, \pi^{1\xi_2}, \pi^{1\xi_3} \in \Pi_1$. which are taken as centres of neighbourhoods:

$$N_j\left(\pi^{\xi_j}\right)=\left\{\pi\in\Pi:\rho\left(\pi^{\xi_j},\pi\right)=\left\|\pi^{\xi_j}-\pi\right\|\le\alpha\mu\right\},\ j=1,2,3,$$

where $0<\mu<1$ is suitable chosen (see below).

Then, samples

$$\Pi_{2j}\subset N_j\left(\pi^{2\xi_j}\right)\subset\Pi$$

with λ points are chosen in the same manner as above, and appropriate sets $U_{1j}\subset G$ of extreme points $u^{2j\xi}$ and sets $U^*_{1j}\subset G$ consisting of λ local minima, $j=1,2,3$, $\xi=1,2,...,\lambda$, are constructed. From each sample of Π_{2j} points

$$\pi^{2j\xi_1},\pi^{2j\xi_2},\ \pi^{2j\xi_3}\in\Pi_{2j},\ \ j=1,2,3,$$

corresponding to local minima $u^{*2\xi_1},u^{*2\xi_2},\ u^{*2\xi_3}$ such that

$$F\left(u^{*2j\xi_1}\right)<F\left(u^{*2j\xi_2}\right)<F\left(u^{*2j\xi_3}\right)\le F\left(u^{*2j\xi}\right),$$

$j=1,2,3,\ \ \xi=1,2,...,\lambda,$ are extracted.

Since a promising criterion is the probability of obtaining better objective function values, it is evident that the criterion depends both on mathematical expectation m_{2j} and dispersion σ_{2j} of a random sample of Π_{2j}. For example, for different neighbourhoods with equal mathematical expectations and with normal, logarithmically normal or Weibul-Gnidenko probability distributions, a better value of F will be obtained for a neighbourhood with a larger dispersion [8] and [9]. In this investigation, the criterion is a quantity $\chi_{2j}=m_{2j}-\tau\sigma_{2j}$, where parameter $\tau=1.5$ is defined empirically.

The next neighbourhood centres are chosen as follows:

1. π^{21} is a point that corresponds to starting point u^{21} from which the best local minimum u^{2*} among all local minima is obtained.

2. $\pi^{22}\in\{\pi^{2j\xi_1},\pi^{2j\xi_2},\pi^{2j\xi_3}\}$ is a point that corresponds to the centre of the sample having $\chi_2=\min\{\chi_{21},\chi_{22},\chi_{23}\}$.

3. π^{23} is a point that corresponds to a starting point from which the best local minimum among all local minima of the sample with factor χ_2 is obtained.

Points π^{2j}, $j=1,2,3$, define the next promising neighbourhoods

$$N_j\left(\pi^{2j}\right)=\left\{\pi\in\Pi:\rho\left(\pi^{2j},\pi\right)\le\alpha\mu^2\right\},\ j=1,2,3,$$

and so on.

If a current local minimum u^* is obtained such that $F(u^*)<F(u^{t*})$, then radius $\alpha\mu^t$ of neighbourhoods on the next iterations is multiplied by $1/\mu$.

Since due to a large number of inconsistent systems of low levels of the search tree when forming samples in neighbourhoods of little radii, the probability of repetitions of identical starting points increases dramatically, then the solution process is repeated until either the radius of neighbourhoods becomes less than β or the number of identical points in a neighbourhood becomes greater than 20. The best local minimum obtained is an approximation of the global minimum.

The value of parameter μ influences the convergence of the process. A too small value of μ yields a bad solution. Computational experience has shown that $\mu\in[0.9,0.95]$ is most suitable to take into account both the runtime and the quality of solutions.

If computational capacities do not allow to search for local minima for each starting point, the following modification of the DNS is offered. The solution process is the same as above but searching for the local minima is realized only for two extreme points $u^{1\xi j},u^{2\xi j}\in U_{\xi j}$, $\xi=1,2,3,\ \ j=1,2,...,$ such that

$$F\left(u^{1\xi j}\right)<F\left(u^{2\xi j}\right)$$

and

$$F\left(u^{1\xi j}\right)=\min F(u),\ \text{s.t.}\ u\in U_{\xi j};$$

$$F\left(u^{2\xi j}\right)=\min F(u),\ \text{s.t.}\ u\in U_{\xi j}\setminus\left\{u^{1\xi j}\right\}$$

for each new neighbourhood.

The best local minimum is taken as some approximation of the global minimum.

8 numerical instances are computed [7]. Using approximately the same amount of computer time in comparison to the proposed algorithm, the modification of DNS proposed in [7] is carried out. Percentage of improvement of the proposed algorithm against the modification from [7] was about 1%.

Conclusions

A modification of DNS is proposed to solve three-dimensional problem of packing various sized spheres into a parallelepiped of minimal height.

Some details remain open, namely, refining parameters individually for each neighbourhood.

It is obvious that set U does not contain all extreme points of G in general, so that the approach cannot find a proved global minimum.

The calculation of proved local minima can also be applied in combination with other heuristics or metaheuristic approaches.

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