The subject matter of the paper is the problem of optimal packing of spheres of different dimension into a container of arbitrary geometric shape. The goal is to construct a mathematical model which associates different statements of the variable metric characteristic used are: the phi-um of the objective maximum packing factor (KP or ODP). Here, we propose adaptations of the efficient jump function technique, increasing the problem dimension, homothetic transformations. KP is formulated as mixed discrete-continuous programming problem. A new approach which reduces solving KP to solving ODP for packing unequal and equal spheres into a container with the variable coefficient of homothety and allows adopt the jump algorithm for KP is suggested. To this end, for a given set of spheres KP is stated as a nonlinear programming problem in which the coefficient of homothety is an independent variable bounded below. The unit value of the coefficient corresponds to the original size of the container. A graphical illustration of the optimization process is presented. Conclusions. The approach suggested is a methodological basis for solving SPP. The generality of the approach lies in the fact that solving SPP does not depend on its formulation (KP or ODP). The approach is suitable for packing unequal and equal spheres into containers of arbitrary spatial shapes for which phi-functions can be constructed.

Keywords: sphere; hypersphere; sphere packing; knapsack problem; open dimension problem; nonlinear optimization.

Introduction

Sphere packing problems (SPP) are known to be NP-hard combinatorial optimization problems. These problems relate to the field of cutting and packing. SPP consists in placement of a given set of spheres with known radii into a container of regular or irregular geometric shape. In the general case, spheres can be of different dimension (2D – circles, 3D – hard spheres, nD – hard hyperspheres).

SPP have a wide spectrum of scientific and practical applications. In two and three dimensions there are real-world applications in a range of industries, for example, the textile, apparel, automobile, aerospace and chemical industries [1], in particular, in additive manufacturing for optimization of product's topology [2] and in medicine for automated radio-surgical treatment planning [3]. In higher dimensions packing hard hyperspheres is used to model geometrical frustration and the geometry of the crystalline state [4]. Packing hyperspheres may be used in the numerical evaluation of integrals, either on the surface of a sphere or in its interior [5]. The problems also arise in coding theory, digital communications and storage, for example, CD, cell phones, and the Internet [5, 6].

Waescher et al. [7] introduce the classification of cutting and packing problems. According to the classification two classes of packing problems KP and ODP are considered depending on characteristics of dimensions (sizes) of a container (fixed dimensions or at least one variable dimension) and the form of objective function (maximum packing factor or minimum size). KP consists in packing of spheres with given radii from a collection into a container of fixed sizes with maximum packing factor. In ODP all spheres from the collection should be packed into the container with several fixed sizes and a variable metric characteristic that has to be minimized.

Some researchers (for example, [8, 9]) use the KP formulation. If it is necessary to solve the ODP, a dichotomous search for the variable size is used, i.e. ODP solution is reduced to solving a KP sequence, which leads to an increase in counting time.

In [10] the SPP is formulated as ODP. As the minimum container size, the radius, length, height, perimeter, area, volume, surface area are used. A nonlinear twice-differentiable mathematical model is proposed, which allows to obtain a local minimum of the problem.

In [11, 12] mathematical models based on increasing the problem dimension are used to solve KP for equal spheres. Radii of the spheres are temporary assumed to be variable and the sum of the sphere volumes is maximized until the radii reach their starting values. Such an optimization procedure provides growing microcopies of the spheres to its original sizes. The multistart strategy is applied to obtain a better solution of KP. If the global maximum of the objective can not be obtained, then the number of spheres to be packed into container is reduced until a feasible packing is calculated.

The idea of additional variable metric characteristics was extended for unequal spheres. Papers [13, 14] propose adaptations of the efficient jump algorithm [15] for different dimension. The jump algorithm realizes a directed transition from one local minimum of ODP to another to yield an improvement of the objective.

This paper continues to investigate mathematical models of KP and ODP. A new approach which reduces solving KP to solving ODP for packing spheres into a container with the variable coefficient of homothety and
allows adopt the jump algorithm for KP is suggested. The approach is a methodological basis for solving SPP which does not depend on the problem statement (KP or ODP).

Mathematical Models of KP and ODP

KP is stated as follows. Let there be given a container $C \subseteq \mathbb{R}^d$ of fixed sizes and a collection of spheres $S_i(u_t), i \in I_N$, with known radii. The problem consists in packing a subset spheres from the collection $S_i(u_t), i \in I_N$ without overlapping inside $C$ yielding the maximum packing factor. Here $u_t$ is a motion vector of $S_i, i \in I_N, d \geq 2$ is space dimension.

Let $K$ types of spheres from the collection $S_i(u_t), i \in I_N$ with radii $r_k$, be considered, $k \in I_K = \{1, 2, ..., K\}$. We denote the number of spheres of the $k$-th type that can be fully arranged inside $C$ by $n_k, k \in I_K$, and generate a tuple $t = (n_1, n_2, ..., n_K)$. Each tuple $t$ has to involve at least one nonzero element $n_k, k \in I_K$. We denote a set of possible tuples $t$ by $T$. The cardinality of $T$ is $\prod_{k=1}^{K} (n_k + 1)$. We form a subset $S'$ of spheres $S_j(u_t), j \in J = \{1, 2, ..., n\}$ from the collection $S_i(u_t), i \in I_N$ with respect to the tuple $t = (n_1, n_2, ..., n_K)$, where $n = \sum_{k=1}^{K} n_k.$

A subset $S'$ taking into account translation is denoted by $S' = \{E_j(v_j), j \in J\}$, where $v = (v_1, v_2, ..., v_J) \in \mathbb{R}^{dn}$ is a vector of placement parameters of spheres $S_j(u_t), j \in J,$ $v_j = (x_{ji}, x_{ji}, ..., x_{ji})$ is a translation vector of $S_j(v_j)$.

Thus, KP can be formulated as to find such subset of spheres $S'$ that can be fully arranged within the container $C$ with the maximum packing factor:

$$F^* = F(v^*, t^*) = \max_{t \in T} \sum_{j=1}^{d} (r_j)^{d} \quad \text{s.t.} \quad \text{v, t} \in W \subset \mathbb{R}^{dn} \times T$$  \quad (1)

where $W = \{(v, t): \Phi_\mu_\text{y} (v_i, v_j) \geq 0, i, j \in J, i \neq j, \Phi_1 (v_i) \geq 0, i \in J\}$,

$$\Phi_\mu_\text{y} (v_i, v_j) = \sum_{k=1}^{d} (x_{ki} - x_{kj})^2 - (r_i + r_j)^2 \geq 0.$$  \quad (2)

To solve problem (1)-(2) one should realise an exhaustive search of all elements of the set $T$ and try to find a packing of spheres according to each tuple $t \in T$.

ODP has another formulation. A collection of spheres $S_i(u_t), i \in I_N$, have to be packed into the container $C$ of a variable size (area, volume, or a metric characteristic) that has to be minimized.

A mathematical model of ODP can be presented as to find

$$\mu^* = \min_{\mu} \quad \text{s.t.} \quad Y = (u, \mu) \in \tilde{W} \subset \mathbb{R}^{dn+1},$$  \quad (3)

where $\mu$ is a metric characteristic to be optimized,

$$\tilde{W} = \{Y : \Phi_\mu(u_i, u_j) \geq 0, 0 < i < j \in I_N, \Phi_1 (u_i, \mu) \geq 0, i \in I_N\}.$$  \quad (4)

Inequality

$$\Phi_\mu(u_i, u_j) = \sum_{k=1}^{d} (x_{ki} - x_{kj})^2 - (r_i + r_j)^2 \geq 0$$

guarantees non-overlapping spheres $S_i$ and $S_j$. Inequality $\Phi_1(u_i, \mu) \geq 0$ provides a placement of $S_i(u_t)$ within $C$.

Transformation of knapsack problem to open dimension problem

The increase in the dimension of the problem due to the introduction of variable metric characteristics of the objects to be placed was successful in solving the problems of packing equal and unequal spheres [11, 14]. In this regard, this approach is distributed to the metric characteristics of the container. Taking into account the ODP peculiarities, it is convenient to choose a coefficient homothety of the container as such a characteristic. With the ability to proportionally resize the container, one can solve KP (1)-(2) for a tuple as ODP (3)-(4). The homothety coefficient $\lambda$ is associated as the open dimension parameter which is the metric characteristic to be minimized.

Let $C(\lambda) = \{x \in \mathbb{R}^d : x \in C\}$, where $\lambda$ is a scaling parameter.

To describe placement (non-overlapping and containment) constraints the phi-function technique [16, 17] is employed. A mathematical model of KP for a given tuple can be formulated as the following nonlinear programming problem:

$$\min_{\lambda} \quad \text{s.t.} \quad Y = (\lambda, u_1, u_2, ..., u_N) \in \tilde{W} \subset \mathbb{R}^{dn+1},$$  \quad (5)

$$\tilde{W} = \{Y : \Phi_\mu(u_i, u_j) \geq 0, i, j \in I_N, j > i, \Phi_1 (Y) \geq 0, i \in I_N, \lambda \geq 1\},$$  \quad (6)

where $u_1, u_2, ..., u_N$ are motion vectors for spheres $S_i(u_t), i \in I_N$, function $\Phi_\mu(Y), i, j \in I_N, j > i$, is a phi-function to ensure the non-overlapping constraint, function $\Phi_1(v), i \in I_N$, is a phi-function for the containment constraints. Variable $\lambda$ occurs in all inequalities $\Phi_1 (Y) \geq 0, i \in I_N$, describing interaction of spheres and container $C(\lambda)$ and bounded from below by inequality $\lambda \geq 1$. To this end, $C \subset C(\lambda).$
Thus, problem (5)-(6) can be considered as ODP with open parameter $\lambda$. To solve the problem the jump algorithm can be efficiently applied.

A global minimum point $v^* = (\lambda^*_1, \mu^*_1, \mu^*_2, \ldots, \mu^*_n)$ for problem (5)-(6) provides packing spheres $S_i(\mu^*_i)$, $i \in N$, into container $C(\lambda^*_i)=C_i$, $\lambda^*_i = 1$, and corresponds to a solution of problem (1)-(2) for the given tuple. If at the point $v^*$ value $\lambda^*_i > 1$, then $C \subset C(\lambda)$, i.e. we do not have original container and hence there is no a feasible packing corresponding to a solution of problem (1) – (2). The multistart strategy should be exploited to obtain the required size of the container.

A starting point to solve problem (5) – (6) can be calculated by solving the problem for container $C(\lambda^0)$ where $\lambda^0 > 1$ should provide a packing of the spheres according to the tuple $t$. In Fig. 1 a starting point for the packing circles into the rectangle $C(\lambda^0)$, $\lambda^0 = 1.1$ is shown. Solving problem by means of the jump algorithm leads to the packing illustrated in Fig. 2.

**Fig. 1. Illustration of a packing of circles into the rectangle $C(1,1)$**

Although, solving problem (5)-(6) does not save from an exhaustive search of tuples from the set $T$ such approach improve significantly quality of solution obtained due to high performance of the jump algorithm. The jump algorithm is suitable for packing unequal spheres. So, in order to pack equal spheres, another solution method of problem (5)-(6) is required. Any optimization procedure which gives a global solution of problem (5)-(6) can be applied.

**Conclusions**

The approach suggested in the paper allows to reduce KP to ODP and apply the known jump algorithm to solve KP for a given tuple. Such a transition was made possible by introducing a variable container size using the homothety coefficient. The approach is suitable for packing unequal and equal spheres into containers of arbitrary spatial shapes for which phi-functions can be constructed. The more complicated the spatial shape of the container, the harder to solve the problem.

Mathematical models constructed contribute to the field of cutting and packing to describe a common methodology to solve SPP. Further study of the properties of SPP and the development of effective solution methods is a priority for advance research.

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Предметом статті є задача оптимальної упаковки куль різної розмірності в контейнер довільної геометричної форми. Мета полягає в тому, щоб побудувати математичну модель, в якій з'являються різні формування задачі. Задача упаковки куль (SPP) є задачею комбінаторної оптимізації, відомою як задача упаковки шарів в контейнер. Задача формулюється як змішана задача дискретно-неперервного програмування. Універсальний підхід полягає в тому, що розв'язання задачі нелінійного програмування, в якій коекфіцієнт гомотетії розглядається в якості незалежної змінної, обмежено знизу. Коефіцієнт гомотетії, який дорівнює одиниці, відповідає початковому розміру контейнера. У цій статті наведені результати перетворення задачі про рюкзак у задачу зі змінним розміром.

Ключові слова: куля, гіперкуля; упаковка куль; задача про рюкзак; задача с переменным размером; нелінійна оптимізація.

Методологічні основи розв'язання задачі упаковки шарів: преобразование задачи о рюкзаке в задачу с переменным размером

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Предметом статті є задача оптимальної упаковки шарів різної розмірності в контейнер, формулювання якої полягає в тому, щоб побудувати математичну модель, в якій з'являються різні формування задачі. Задача упаковки шарів (SPP) є задачею комбінаторної оптимізації, відомою як задача упаковки шарів в контейнер. Задача формулюється як змішана задача дискретно-неперервного програмування. Універсальний підхід полягає в тому, що розв'язання задачі нелінійного програмування, в якій коекфіцієнт гомотетії розглядається в якості незалежної змінної, обмежено знизу. Коефіцієнт гомотетії, який дорівнює одиниці, відповідає початковому розміру контейнера. У цій статті наведені результати перетворення задачі про рюкзак у задачу зі змінним розміром.

Ключові слова: шар; гіпершар; упаковка шарів; задача о рюкзаке; задача с переменным размером; нелінійна оптимізація.