CLUSTER PACKING
OF CONCAVE NON-ORIENTED POLYHEDRA IN A CUBOID

The subject matter of the article is the solution of the problem of optimal packing of concave polyhedra in a cuboid of minimal volume. The goal is to construct a mathematical model of the problem under consideration and to develop a solution method. The task to be solved are: to develop tools for mathematical modeling of the interaction of two concave non-oriented polyhedra; to construct a mathematical model of the problem of packing concave non-oriented polyhedra in a cuboid of minimal volume; to investigate the peculiarities of the mathematical model; to develop an effective method of solution and implement its software. The methods used are: the phi-function technique, the internal point method. The following results are obtained. Using the phi-function for two convex non-oriented polyhedra, a phi-function for two concave non-oriented polyhedra is constructed. On the basis of the phi-function, an exact mathematical model of the packing problem for concave polyhedra that allow simultaneous continuous translations and rotations is constructed. The mathematical model is represented as a nonlinear programming problem. The properties of the constructed mathematical model are analyzed and a multi-stage approach based on them is proposed, which makes it possible to obtain a good locally optimal solution of the problem posed. Since working with polyhedra is an important to determine the optimal clustering of two objects, one of the stages of the proposed approach is to solve the problem of pairwise clustering of polyhedra. A numerical example demonstrating the effectiveness of the proposed approach is given. Conclusions. The scientific novelty of the obtained results consists in the following: an exact mathematical model of the packing problem of concave non-oriented polyhedra is constructed in the form of a nonlinear optimization problem and a multi-stage approach is proposed that allows obtain a good locally optimal solution of the problem.

Keywords: cluster packing; concave polyhedra; continuous rotation; nonlinear optimization.

Introduction

The 3D packing problems of concave polyhedra have extensive engineering applications. For example, as actual applications of the problems we can note the following problems: the optimization of the 3D-printing process in SLS technologies of additive production [1]; 3D simulation of microstructures of different materials (including nanomaterial’s) [2]. Also it has a wide spectrum of applications in powder metallurgy, modern biology, mineralogy, materials science, nanotechnology, robotics, pattern recognition systems, control systems, space apparatus control systems, aircraft construction, civil engineering, etc.

It is well known that the 3D objects packing problem is NP complex. Because of its NP complexity, it is hard to be solved satisfactorily. So, to find their approximate solution many research works use a wide variety of techniques, including heuristics, traditional optimization methods and different mixed approaches which utilize heuristics and methods of non-linear mathematical programming. The review of this methods is given in [3].

In most works, orientation changes of 3D objects either are not allowed or only discrete changes in the orientation for given angles (45 or 90 degrees) are permitted. In [4] authors propose HAPE3D algorithm which can deal with arbitrarily shaped polyhedral which may be rotated around each coordinate axis at four different angles only.

Due to the difficulty of construction of adequate mathematical models at present there are few works that solve the 3D packing problems of concave provided that continuous rotations of geometric objects are allowed.

The solutions of such problems are considered in works [5-6].

This work is devoted to solving of the packing problem of concave polytopes with continuous angles rotations. Our approach is based on mathematical modeling of relations between geometric objects reducing the problem to a nonlinear programming one. To this end we use the phi-function technique for analytic description of objects interactions and objects placements into a container taking into account continuous rotations and translations.

Problem statement and its mathematical model

Let there be concave polyhedra \( P_i \), \( i \in I = \{1, 2, ..., n\} \), and a cuboid

\[
C = \{X \in \mathbb{R}^3, w_1 \leq x \leq w_2, l_1 \leq y \leq l_2, \eta_1 \leq z \leq \eta_2\},
\]

where \( w_1, w_2, l_1, l_2, \eta_1 \) and \( \eta_2 \) are variables, i.e. a vector \( \zeta = (w_1, w_2, l_1, l_2, \eta_1, \eta_2) \) defines sizes of \( C \).

The polyhedra \( P_i \) are a union of convex polyhedra

\[
P_i = \bigcup_{k=1}^{e_i} P_{ik}, i \in I,
\]

where polyhedra \( P_{ik} \) are given by vertices

\[
P_{ik} = (p_{ik1}^1, p_{ik2}^2, p_{ik3}^3), \quad i \in I, \quad k \in K_i = \{1, 2, ..., e_i\},
\]

\[
t \in T_{ik} = \{1, 2, ..., \rho_{ik}\}.
\]

A location of polyhedra \( P_i \) in the Euclidean 3D arithmetic space \( \mathbb{R}^3 \) is defined by a translation vector \( v_i = (x_i, y_i, z_i) \) and rotation angles

\[
\theta_i = (\phi_i, \psi_i, \omega_i), \quad i \in I.
\]
Thus, a motion vector
\[ u_i = (v_i, 0) = (x_i, y_i, z_i, \phi_i, \psi_i, \omega_i) \]
gives the location of \( P_i \) in \( R^3 \).

Whence, a vector \( u = (u_1, u_2, \ldots, u_n) \in R^{mn} \) defines the location of \( P_i, \ i \in I \), in \( R^3 \) and, consequently, a complete set of variables makes up a vector \( u (\zeta) = (u_1, u_2, \ldots, u_n, \zeta) \in R^{m+2} \), where \( m = 6n + 6 \).

In what follows, polyhedra \( P_i \) translated by vector \( v_i \) and rotated by angles \( \phi_i, \psi_i \) and \( \omega_i \) is denoted by \( P_i (u_i) \) and a cuboid \( C \) with variable sizes \( s \) is designated as \( C (\zeta) \).

Let \( V_{ir} = (V_{1ir}, V_{2ir}, V_{3ir}), \ r \in J_i = \{1, 2, \ldots, g_i\} \), be vertex coordinates of convex hull of \( P_i \). Then a location of \( V_{ir} \) and \( p_{id} \) in \( R^3 \) are defined by the relations
\[ V_{ir} (u_i) = (V_{1ir} (u_i), V_{2ir} (u_i), V_{3ir} (u_i)) = R^{T} V_{ir} + v_i, \]
\[ p_{id} (u_i) = R^{T} p_{id} + v_i, \ i, j \in I, \ k \in K_i, t \in T_{ik}, \]
where \( R_i \) is a rotation operator.

Then the following packing problem arises.

**Basic problem.** Find a vector \( u \in R^m \) which insures the arrangement \( P_i (u_i) \), \( i \in I \), without mutual overlapping’s into a cuboid \( C (\zeta) \) so that the cuboid volume \( H (\zeta) \) will attain the minimal value.

Based on phi-functions (see [3, 7]) a mathematical model of the problem takes the form
\[
H (\zeta^*) = \min H (\zeta) \ s.t. (u, \zeta) \in \Lambda \subset R^m, \tag{1}
\]
where
\[
\Lambda = \{(u, \zeta) \in R^m : \Phi_j (u_i, u_j) \geq 0, i < j \in I, \Phi_j (u_i, \zeta) \geq 0, i \in I, F (\zeta) \geq 0\};
\]
\[
H (\zeta) = (w_2 - w_1) (l_2 - l_1) (\eta_2 - \eta_1),
\]
\[
F (\zeta) = \min \{w_2 - w_1, l_2 - l_1, \eta_2 - \eta_1\},
\]
\[
\Phi_j (u_i, \zeta) = \min \{\phi^{j_1}_{ij} (u_i, \zeta), \alpha \in O_2 = \{1, 2, \ldots, 6\}, r \in J_i\},
\]
\[
\phi^{j_1}_{ij} (u_i, \zeta) = V_{1ir} (u_i) - w_1 \phi^{j_2}_{ij} (u_i, \zeta) = w_2 - V_{1ir} (u_i),
\]
\[
\phi^{j_3}_{ij} (u_i, \zeta) = V_{2ir} (u_i) - l_1 \phi^{j_4}_{ij} (u_i, \zeta) = l_2 - V_{2ir} (u_i),
\]
\[
\phi^{j_5}_{ij} (u_i, \zeta) = V_{3ir} (u_i) - \eta_1 \phi^{j_6}_{ij} (u_i, \zeta) = \eta_2 - V_{3ir} (u_i).
\]

Here the inequality \( \Phi_j (u_i, u_j) \geq 0 \) insures non-overlapping \( P_i \) and \( P_j \), the inequality \( \Phi_j (u_i, \zeta) \geq 0 \) provides a containment of \( P_i \) into \( C (\zeta) \) i.e. \( \Phi_j (u_i, \zeta) \) is the phi-function for \( P_i \) and

\[ B (\zeta) = R^3 \setminus \text{int} C (\zeta) \]

where int \( C (\zeta) \) is the interior of \( C \).

Since \( P_i = \bigcup_{s=1}^k P_{is} \) and \( P_j = \bigcup_{p=1}^k P_{jp} \) then
\[ P_i \cap P_j = \emptyset \]  
\[ P_{is} \cap P_{jp} = \emptyset, \ s \in K_i, p \in K_j. \]

This means that
\[ \Phi_j (u_i, u_j) = \min \{\Phi_{ij}^{sp} (u_i, u_j), s \in K_i, p \in K_j\}, \]
where \( \Phi_{ij}^{sp} (u_i, u_j) \) is the phi-function for \( P_{is} \) and \( P_{jp} \) [7]. Hence, \( \Phi_j (u_i, u_j) \geq 0 \) if the following condition if fulfilled

\[ \min \{\Phi_{ij}^{sp} (u_i, u_j), s \in K_i, p \in K_j\} \geq 0. \]

**Clustering of polyhedra**

In order to obtain starting point for the problem (1)-(2) the following step by steps procedure is offered. Firstly polyhedra are in pair packed into clusters to be cuboids and spheres of the minimal volumes. Next the cuboids and spheres are placed into a cuboid of the minimal volume. Then having taken the polyhedra instead of cuboids and spheres packed into the cuboid we pack the polyhedra into a cuboid of the minimal volume.

Let \( P_i, \ i \in I \), consists of \( k \) groups each from which contains \( l_i \) identical polyhedra. We cluster in pairs \( P_i, \ i \in I \), into cuboids \( Q_{ij} \) of the minimal volumes \( D^C_{ij} \), \( i < j \in K = \{1, 2, \ldots, k\} \). To this end we solve the problems
\[
D^C_{ij} = H_{ij} (\zeta^*) = \min H (\zeta), \s.t. (u_i, u_j, \zeta) \in \Omega_{ij} \subset R^{16}, i < j \in I, \tag{3}
\]
where
\[
\Omega_{ij} = \{(u_i, u_j, \zeta) \in R^{16} : \Phi_j (u_i, u_j) \geq 0, \Phi_j (u_i, \zeta) \geq 0, F (\zeta) \geq 0\}. \tag{4}
\]

The inequality
\[ \Phi_j (u_i, u_j) \geq 0 \]
insures int\( P_i \cap \text{int} P_j = \emptyset \) and \( \Phi_j (u_i, \zeta) \geq 0 \) guarantees placement of \( P_i \) within \( C_{ij} (\zeta) \).

After that we cluster in pairs \( P_i, \ i \in I \), into spheres \( S_{ij} \) of the minimal volumes \( D^S_{ij} \), \( i < j \in K = \{1, 2, \ldots, k\} \). Then we solve the problems
\[
D^S_{ij} = \frac{4}{3} \pi \min R^3, \s.t. (u_i, u_j, R_i) \in \Omega_{ij} \subset R^{16}, i < j \in I, \tag{5}
\]
where
\[ \Omega_y = \{(u_i,u_j,R_{iy}) \in \mathbb{R}^3 : \Phi_j(u_i,u_j) \geq 0, \Phi_i(u_i,R_{iy}) \geq 0, \}\]
\[ \Phi_j(u_i,u_j) = (V_{1}(u_i)^2 + (V_{2}(u_i))^2 + (V_{3}(u_i))^2 - R_{iy}^2 \geq 0, \]

The inequality
\[ \Phi_j(u_i,u_j) \geq 0 \]
insures
\[ \text{int}P_i \cap \text{int}P_j = \emptyset \]

and
\[ \Phi_i(u_i,\zeta) = \]

 guarantees placement of \( P \) within \( S_j(R_y) \) (10).

Note that local extrema of the problems (3)-(4) and (5)-(6) are calculated in the same way as a local minimum point of the problem (1)-(2). For local optimization we used the IPOPT code (https://projects.coin-or.org/Ipopt).

Let \( P_i \), \( i \in I \), consists of \( k \) groups each from which contains \( l_k \) identical polyhedra. We construct clusters pack in pairs \( P_i \), \( i \in I \), into cuboids \( Q_j \) of the minimal volumes \( D_j \), \( i < j \in K = \{1,2,...k\} \).

Now we compute
\[ \delta_{ij}^C = (D_i + D_j) / D_{ij}^C \]
and
\[ \delta_{ij}^S = (D_i + D_j) / D_{ij}^S, \]

and find
\[ \delta_{ij} = \max(\delta_{ij}^C, \delta_{ij}^S, i < j \in K). \]

If \( \delta_{ij} = \delta_{ij}^C \) then we generate identical cuboids
\[ Q_i = Q_j, \quad i = 1,2,...,k_{sp} = \min\{l,s,l_p\}. \]

In addition, if \( k_{sp} = l_i \) \( (k_{sp} = l_p) \) then we exclude \( s \) \( (p) \) from \( K \).

If \( k_{sp} = l_i = l_p \) then we omit \( s \) and \( p \) from \( K \). If
\[ \delta_{ij} = \delta_{ij}^S \] then we generate identical spheres
\[ S_j = S_j, \quad i = 1,2,...,k_{sp} = \min\{l,s,l_p\}. \]

In addition, if \( k_{sp} = l_i \) \( (k_{sp} = l_p) \) then we exclude \( s \) \( (p) \) from \( K \).

If \( k_{sp} = l_i = l_p \) then we omit \( s \) and \( p \) from \( K \).

After that we define
\[ \delta_{rt} = \max\{\delta_{ij}^C, \delta_{ij}^S, i < j \in K \}. \]

where either \( \lambda_{sp} = s \) or \( \lambda_{sp} = p \) or \( \lambda_{sp} = \{s,p\} \) and so on until \( K \) is exhausted.

As a result sets of cuboids \( C_j, \quad i = 1,2,...,\mu_1 \), and spheres \( S_j, \quad i = 1 + \mu_1,2 + \mu_1,..,\mu = \mu_1 + \mu_2 \) are formed. For the sake of convenience we rename
\[ C_j, \quad i = 1,2,...,\mu_1, \]
and spheres
\[ S_j, \quad i = 1 + \mu_1,2 + \mu_1,..,\mu = \mu_1 + \mu_2, \]
as \( Q_i, \quad i \in M = \{1,2,...,\mu\} \).

Thus each cluster \( Q_i \) contains pair of polyhedra \( P_i \) and \( P_i \) with placement parameters \( u_{ki}^C \) and \( u_{ki}^S \) with respect to the local coordinate system of \( Q_i \). Next we solve a packing problem of \( Q_i \), \( i \in M \), into a cuboid \( C \) of the minimal volume. We suppose that a location of cluster \( Q_j \) in \( R^3 \) is defined by a vector
\[ \gamma_j = (u_j,\xi_j) = (x_{1j},y_{1j},z_{1j},\xi_{1j},\xi_{1j},\xi_{1j}) \in R^6, \quad j \in M. \]

Then a mathematical model of the packing problem has the form
\[ H(\zeta) = \min H(\zeta), \quad s.t. (\gamma,\zeta) \in \Omega \subset R^{6(n+1)}, \]
where
\[ \Omega = \{(u,\zeta) \in R^{6(n+1)} : \Phi_j(\gamma_k,\gamma_j) \geq 0, i < j \in M, \]
\[ \Phi_i(\gamma_j,\zeta) \geq 0, i \in T, F(\zeta) \geq 0. \]

The inequality
\[ \Phi_j(\gamma_i,\gamma_j) \geq 0 \]
insures
\[ \text{int}Q_i \cap \text{int}Q_j = \emptyset \]
and \( \Phi_j(\gamma_i,\zeta) \geq 0 \)
guarantees placement of \( Q_i \) within \( C(\zeta) \).

Searching for an approximation to a global minimum point of the problem is realized by methods which are presented in the papers [8, 9].

Let \( (\gamma^0,\zeta^0) \in R^{6(n+1)} \) be an approximation to a global minimum point of the problem (7)-(8). To the point \( (\gamma^0,\zeta^0) \) there corresponds the arrangement of clusters \( Q_i(\gamma_i^0) \), \( i \in M \) into the cuboid \( C(\zeta^0) \) and each cluster contains a pair of polyhedra \( P_i \) and \( P_i \) with placement parameters \( u_{ki}^C \) and \( u_{ki}^S \). It permits to take appropriate polyhedra \( P_i \), \( i \in I \), instead of clusters \( Q_i \), \( i \in M \), and form a starting point \( (u^0,\zeta^0) = (u^0,\zeta^0) \) for the problem (1)-(2).
Construction of the point is executed by the special problem that called “inverse rotation”.

**Multistage solution approach**

A solution strategy (3D MultiStage Approach (3D-MSA)) can be described by the following stages.

1. Pack in pair polyhedra $P_i$, $i \in I$, into cuboids $C_i$, $i = \{1, 2, ..., \mu_1\}$, and spheres $S_i$, $i = 1 + \mu_1, 2 + \mu_1, ..., \mu = \mu_1 + \mu_2$, of minimum volumes. For optimal clustering of two polyhedrons also we can apply quasi phi-function technique. This approach presented in [10].

2. Cover polyhedra $P_i$ by spheres $S_i$ with centers $v_i$, $i \in I$; cover convex polyhedra $P_k$ by spheres $S_{ik}$ of minimal radius $\rho^0$ and centers $v_{ik}^0 = (x_{ik}, y_{ik}, z_{ik})$, $i \in I$, $k \in K_i$.

3. Solve the packing problem of cluster $Q_i$, $i \in M = \{1, 2, ..., \mu\}$. Wherein, if $Q_i$, $i \in M = \{1, 2, ..., \mu\}$ is set of cuboids $C_i$ then we solve packing problem of parallelepipeds with the feasibility of changing their orthogonal orientation [8]. And if $Q_i$, $i \in M = \{1, 2, ..., \mu\}$ is set of cuboids $C_i$ and spheres $S_i$ then we solve packing problem of cuboids and spheres using approach proposed in [9]. As a result we obtain local minimum point $(\gamma^0, \zeta^0) \in R^{6(n+1)}$.

4. Replace clusters $Q_i$, $i \in M$, with corresponding polyhedra $P_i$, $i \in I$. In order to form a starting point $(u^0, \zeta^0)$ for the problem (1)-(2) we solve $n$ auxiliary non-linear optimization problems (“inverse rotation”) to define vector $u^0$ based on $\gamma^0$. As a result we derive a point $(u^0, \zeta^0) \in R^{6(n+1)}$ on the ground of the point $(\gamma^0, \zeta^0) \in R^{6(n+1)}$.

5. Fix $0^0$ and find a local minimum point $X^*$ of the problem

$$H(\zeta^*) = \min H(\zeta) \quad s.t. \quad X \in Q \subset R^{3n+6} \quad (9)$$

where

$$Q = \{X = (v, \zeta) \in R^{3n+6} : \Phi_{ij}(v, \zeta) \geq 0, i < j \in I, \Phi_i(v, \zeta) \geq 0, i \in I, F(\zeta) \geq 0\} \quad (10)$$

As a starting point of problem (9)-(10) we take point $(v^0, \zeta^0)$. Since rotation angles are fixed then inequality system (10) is linear.

6. Form a starting point $(u^0, \zeta^0) = (v^*, 0^0, \zeta^*)$, and calculate a local minimum point $(u^{0*}, \zeta^{0*})$ of the problem (1)-(2).

**Numerical results**

Here presented an example that demonstrates the efficiency of proposed methodology.

We have run our experiments on an Intel Core i5 750 computer and for local optimisation we used the IPOPT code (https://projects.coin-or.org/Ipopt).

We consider the collection of polytopes of example 1 given in [4]. In fig. 1 depicted five types of polyhedrons that need to pack.

![Fig. 1. Five types of polyhedrons](image1.png)

Figure 2 presents clusters $Q_i$ used for solving problem (7)-(8).

![Fig. 2. Clusters $Q_i$](image2.png)

Fig. 3 shows the results obtained on each stage of 3D-MSA of optimal placement of 36 polyhedrons. The container has volume $H^* = 10720$.

![Fig. 3. Solution stages of 3D-MSA](image3.png)
As shown in table 1, the 3D-MSA allows us to significantly improve the solution time by 60%.

Table 1. Comparison of HAPE3D and 3D-MSA

|          | HAPE3D | 3D-MSA |
|----------|--------|--------|
| H*      | 12480  | 10720  |
| Time(s) | 9637   | 3789   |

Conclusions

The paper presents an exact mathematical model of packing optimization problem of concave polyhedra which are allowed both translations and continuous rotations. The phi-functions enable us to apply state-of-the-art methods of nonlinear optimization on all solution stages of the problem (1)-(2) including the construction of starting points, the calculation of local extrema and searching for of "approximations" to global extrema.

Iterative processes being used to solve the problem can be easily parallelized.

Numerical results above have shown effectively of solution approach offered when tackling optimization 3D packing problems.

Optimization approaches worked out in the paper can be used for solving other packing optimization problems.

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Кластерная упаковка неоциклических багатогранников в кубоид

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Предметом изучения в статье является решение задачи оптимального поиска многогранников в прямой параллелепипед минимального объема. Целью является построение математической модели рассматриваемой задачи и разработка метода решения. Задачи: разработать средства математического моделирования взаимодействия двух многогранников, построить математическую модель задачи упаковки неоциклических многогранников в кубоид минимального объема; исследовать особенности математической модели; разработать эффективный метод решения и выполнить его программную реализацию. Используя методы программирования, были получены следующие результаты. Используя функцию для двух выпуклых неориентированных многогранников, построена функция для двух выпуклых неориентированных многогранников. На основании этой функции построена точная математическая модель задачи упаковки многогранников, допускающих непрерывное вращение.

Ключевые слова: кластерная упаковка; неоциклические багатогранники; безперерывное вращение; нелинейная оптимизация.