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TWO APPROACHES TO MODELING AND SOLVING THE PACKING PROBLEM FOR CONVEX POLYTOPES

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Abstract. *We consider the problem of packing convex polytopes in a cuboid of minimum volume. To describe analytically the non-overlapping constraints for convex polytopes that allow continuous translations and rotations, we use phi-functions and quasi-phi-functions. We provide an exact mathematical model in the form of an NLP-problem and analyze its characteristics. Based on the general solution strategy, we propose two approaches that take into account peculiarities of phi-functions and quasi-phi-functions. Computational results to compare the efficiency of our approaches are given with respect to both the value of the objective function and runtime.*

Keywords: *packing, convex polytopes, phi-function, quasi-phi-function, mathematical model, nonlinear optimization.*

INTRODUCTION

Optimization problems of packing 3D-objects are a part of the theory of operations research and have a wide range of practical application, for example, in solving modern problems in biology, mineralogy, medicine, materials technology, nanotechnologies, robotics, and pattern recognition.

Solving such problems is important since they allow replacing full-scale expensive experiments with computer simulation of real processes and structures of materials. This considerably saves time and financial resources.

For example, three-dimensional modeling of microstructures of various materials (including nanomaterials) is an innovative application of polytope allocation problems. The latest advances in this field are related to development of the computer technology of 3D tomographic analysis of mineral particles [1]. The paper [2] describes application of the polytope packing problem to powder metallurgy. These problems are also used to efficiently solve the problem of disposal of dangerous waste and automation of the process of crucible packing in manufacturing semiconductor plates.

Problems of packing 3D-objects are NP-hard and various heuristics are usually used to solve them.

The available approaches to solving three-dimensional packing problems can be divided into the following groups:

— heuristic methods (heuristics based on relaxation of information about the form of objects [3], as well as algorithms, namely, genetic ones [4], based on the idea of simulated annealing [5], ant algorithms [6], and those using pattern search [7]);

— traditional methods of linear and nonlinear optimization [8];

— combined approaches, which use heuristics and mathematical programming methods [9].

In [10], the conclusion is made that solving packing problems for complex three-dimensional objects reduces to cyclic execution of the following steps: generating the sequence of objects being allocated; formalizing the conditions of non-intersection of the objects with regard for their translation (parallel displacement) and rotation, placement at a prescribed distance; and calculating the objective function.

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In the majority of studies in three-dimensional packing, continuous rotations of objects are not admitted. For example, transformation of translation is only used in [11]. In [12], the HAPE3D algorithm is proposed, which allows rotation of polytopes about each coordinate axis discretely by angles multiple of 45°.

In the present study, we will compare two approaches to the solution of the problem of packing convex polytopes (taking into account their continuous translations and rotations) in a parallelepiped of minimum volume depending on the form of functions (either *phi*-functions or quasi-*phi*-functions [13]) used to model the constraints of non-intersection of polytopes.

PROBLEM STATEMENT

Given a set of convex polytopes K_i, $i \in \{1, 2, \dots, n\} = I_n$, and a direct parallelepiped $\Omega = \{(x, y, z) \in R^3 : 0 \le x \le l, 0 \le y \le w, 0 \le z \le h\}$ with variable dimensions l, w, and h. Each polytope K_i is defined by the coordinates of its vertices $p_{ij} = (x_{ij}, y_{ij}, z_{ij})$, $j = 1, \dots, m_i$, in the intrinsic frame.

Let us introduce the following notation for the polytope K_i: G_i is the set of edges g_{ij} that belong to planes $\{(x, y, z) : A_{ij} x + B_{ij} y + C_{ij} z + D_{ij} = 0\}$, $j \in I_{G_i}$; P_i is the set of vertices $p_{ik} = (x_{ik}, y_{ik}, z_{ik})$, $k \in I_{P_i}$; T_i is the set of edges t_{il} specified by pairs of vertices (p_{il_1}, p_{il_2}), $l \in I_{T_i}$. Note that $A_{ij} = A_{ij}(u_i)$, $B_{ij} = B_{ij}(u_i)$, $C_{ij} = C_{ij}(u_i)$, $D_{ij} = D_{ij}(u_i)$, $x_{ik} = x_{ik}(u_i)$, $y_{ik} = y_{ik}(u_i)$, and $z_{ik} = z_{ik}(u_i)$.

Let $K_i = \{X = (x, y, z) \in R^3 : f_{ij}(X) = A_{ij} x + B_{ij} y + C_{ij} z + D_{ij} \le 0,\ j \in I_{G_i}\}$.

Without loss of generality, we assume that the center of the intrinsic frame of the polytope K_i coincides with the center of circumscribed sphere S_i of radius r_i.

The position and orientation of the polytope K_i are defined by the vector of its allocation parameters (υ_i, θ_i), where $\upsilon_i = (x_i, y_i, z_i)$ is the translation vector, $\theta_i = (\theta_i^1, \theta_i^2, \theta_i^3)$ is the vector of rotation parameters, θ_i^1, θ_i^2, and θ_i^3 are respective angles of rotation from axis OX to OY, from axis OY to OZ, and from axis OX to OZ in the local frame of the polytope K_i, respectively.

Simultaneous translation of polytope K_i by vector υ_i and its rotation by vector θ_i is defined as

$$K_i(u_i) = \{p \in R^3 : p = \upsilon_i + M(\theta_i) \cdot p^0 \ \forall p^0 \in K_i^0\},$$

where K_i^0 is non-translated and non-rotated polytope K_i, $M(\theta_i) = M_1(\theta_i^1) \cdot M_2(\theta_i^2) \cdot M_3(\theta_i^3)$ is the rotation matrix,

$$M_1(\theta_i^1) = \begin{pmatrix} \cos\theta_i^1 & -\sin\theta_i^1 & 0 \\ \sin\theta_i^1 & \cos\theta_i^1 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

$$M_2(\theta_i^2) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta_i^2 & -\sin\theta_i^2 \\ 0 & \sin\theta_i^2 & \cos\theta_i^2 \end{pmatrix}, \quad M_3(\theta_i^3) = \begin{pmatrix} \cos\theta_i^3 & 0 & \sin\theta_i^3 \\ 0 & 1 & 0 \\ -\sin\theta_i^3 & 0 & \cos\theta_i^3 \end{pmatrix}.$$

The problem of packing convex polytopes is to allocate a given set of disjoint convex polytopes $K_i(u_i)$, $i \in I_n$, in a parallelepiped Ω of minimum volume $F = l \cdot w \cdot h$.

MATHEMATICAL MODELING OF THE ALLOCATION CONSTRAINTS

To generate the mathematical model in the form of a nonlinear programming problem, it is necessary to describe analytically the constraints of non-intersection of polytopes K_1 and K_2, $\operatorname{int} K_1 \cap \operatorname{int} K_2 = \varnothing$, and membership of polytope K_1 in the allocation domain Ω, $K_1 \subset \Omega \Leftrightarrow \operatorname{int} K_1 \cap \Omega^* = \varnothing$, where $\Omega^* = R^3 \setminus \operatorname{int} \Omega$. To this end, two types of continuous functions are used: *phi*-functions and quasi-*phi*-functions. Their definitions and properties are described in [14–18].

Constructing *phi*-functions (normalized) for 3D-objects is generally a challenge. Currently, *phi*-functions are constructed for some regular 3D-objects [14, 19], including full-spheres, parallelepipeds, and convex polytopes.

For the polytopes $K_1(u_1)$ and $K_2(u_2)$, which admit continuous translations and rotations, *phi*-function can be defined as follows:

$$\Phi^{K_1K_2}(u_1, u_2) = \max\{\psi_i(u_1, u_2), i = 1, 2, 3\},$$

where function $\psi_1(u_1, u_2) = \max_{j \in I_{G_1}} \min_{k \in I_{P_2}} (A_{1j}x_{2k} + B_{1j}y_{2k} + C_{1j}z_{2k} + D_{1j})$ describes interaction of vertices of the polytope $K_2(u_2)$ with edges of the polytope $K_1(u_1)$, function $\psi_2(u_1, u_2) = \max_{j \in I_{G_2}} \min_{k \in I_{P_1}} (A_{2j}x_{1k} + B_{2j}y_{1k} + C_{2j}z_{1k} + D_{2j})$ describes interaction of vertices of the polytope $K_1(u_1)$ with edges of the polytope $K_2(u_2)$, and function $\psi_3(u_1, u_2) = \max\{\Psi^{ab}(u_1, u_2), a \in I_{T_1}, b \in I_{T_2}\}$ describes interaction of edges of the polytope $K_1(u_1)$ with edges of the polytope $K_2(u_2)$. Here,

$$\Psi^{ab}(u_i, u_j) = \min\{F_{12}^{ab}(p_{1o}(u_1), u_1, u_2), F_{12}^{ab}(p_{1k}(u_1), u_1, u_2),$$

$$F_{21}^{ba}(p_{2s}(u_2), u_1, u_2), F_{21}^{ba}(p_{2v}(u_2), u_1, u_2)\},$$

$$F_{12}^{ab}(x, y, z, u_1, u_2) = (x - x_{1o}(u_1))(x - x_{1k}(u_1))(x - x_{12}^{ab}(u_1, u_2))$$

$$+ (y - y_{1o}(u_1))(y - y_{1k}(u_1))(y - y_{12}^{ab}(u_1, u_2)) + (z - z_{1o}(u_1))(z - z_{1k}(u_1))(z - z_{12}^{ab}(u_1, u_2)),$$

$$F_{21}^{ba}(x, y, z, u_1, u_2) = (x - x_{2s}(u_2))(x - x_{2v}(u_2))(x - x_{12}^{ba}(u_1, u_2))$$

$$+ (y - y_{2s}(u_2))(y - y_{2v}(u_2))(y - y_{12}^{ba}(u_1, u_2)) + (z - z_{2s}(u_2))(z - z_{2v}(u_2))(z - z_{12}^{ba}(u_1, u_2)),$$

$p_{1o}(u_1)$ and $p_{1k}(u_1)$ are vertices of the edge a of the polytope K_1; $p_{2s}(u_2)$ and $p_{2v}(u_2)$ are vertices of the edge b of the polytope $K_2(u_2)$; $a_{12}^{ab}(u_1, u_2) = p_{1o}(u_1) - p_{2s}(u_2) + p_{2k}(u_2)$, and $a_{12}^{ba}(u_1, u_2) = p_{2s}(u_2) - p_{1o}(u_1) + p_{1k}(u_1)$.

In order to expand the class of 3D-objects for which it is possible to construct the mathematical model of the packing problem in the form of a nonlinear programming problem (for example, for ellipsoids, cones, and cylinders), the concept of quasi-*phi*-function is introduced in [14].

For some types of 3D-objects (for example, convex polytopes), the form of quasi-*phi*-functions is much simpler than the form of respective *phi*-functions.

However, unlike *phi*-function, quasi-*phi*-function depends not only on the vector of parameters of allocation of the polytopes but also on additional variables.

Qausi-*phi*-function for polytopes $K_1(u_1)$ and $K_2(u_2)$, which admit continuous translations and rotations, can be defined as follows [18]:

$$\Phi'^{K_1K_2}(u_1, u_2, u_P) = \min\{\Phi^{K_1P}(u_1, u_P), \Phi^{K_2P^*}(u_2, u_P)\},$$

where $u_P = (\theta_{xP}, \theta_{yP}, \mu_P)$ is the vector of additional variables, which defines parameters of half-plane of the form $P(u_P) = \{(x, y, z): \psi_P = \alpha \cdot x + \beta \cdot y + \gamma \cdot z + \mu_P \leq 0\}$, $\alpha = \sin\theta_{yP}$, $\beta = -\sin\theta_{xP} \cdot \cos\theta_{yP}$, $\gamma = \cos\theta_{xP} \cdot \cos\theta_{yP}$; $\Phi^{K_1P}(u_1, u_P) = \min_{1 \leq i \leq m_1} \psi_P(p_{1i})$ is a *phi*-function for $K_1(u_1)$ and $P(u_P)$; $\Phi^{K_2P^*}(u_2, u_P) = \min_{1 \leq j \leq m_2} (-\psi_P(p_{2j}))$ is a *phi*-function for $K_2(u_2)$ and $P^*(u_P) = R^3 \setminus \operatorname{int} P(u_P)$. Note that $\max_{u_P} \Phi'^{K_1K_2}(u_1, u_2, u_P)$ is a *phi*-function for the polytopes $K_1(u_1)$ and $K_2(u_2)$.

MATHEMATICAL MODEL OF THE PROBLEM OF PACKING CONVEX POLYTOPES

Generally, it is possible to present the mathematical model of the problem of packing convex polytopes into a cuboid of minimum volume as follows:

$$\min_{u \in W \subset R^{\sigma}} F(u), \tag{1}$$

$$W = \{u \in R^{\sigma} : f_{ij} \geq 0,\ f_i \geq 0,\ i = 1, 2, \ldots, n,\ j = 1, 2, \ldots, n,\ j > i\}, \tag{2}$$

where $F(u) = l \cdot w \cdot h$, f_{ij} is either a quasi-*phi*-function or *phi*-function for polytopes K_i and K_j (which describes the conditions of non-intersection of the polytopes K_i and K_j), f_i is a *phi*-function for the polytope K_i and object Ω^* (which describes the conditions of allocation of the polytope K_i inside the parallelepiped Ω).

The dimension of vector $u \in R^{\sigma}$ of variables of problem (1), (2) depends on the approach used to generate the mathematical model. In case of quasi-*phi*-functions, the vector of variables of the problem is defined as follows: $u = (l, w, h, u_1, u_2, \ldots, u_n, \tau) \in R^{\sigma}$, where (l, w, h) are variable dimensions (length, width, and height) of the parallelepiped Ω; $u_i = (\upsilon_i, \theta_i) = (x_i, y_i, z_i, \theta_i^1, \theta_i^2, \theta_i^3)$ is the vector of parameters of allocation of the polytope K_i, $i \in I_n$; $\tau = (u_P^1, \ldots, u_P^m)$ is the vector of additional variables; $u_P^k = (\theta_{xP}^k, \theta_{yP}^k, \mu_P^k)$ is additional variables for the kth pair of polytopes, $k = 1, \ldots, m$, $m = 0.5(n-1)n$. Thus, the number of variables in the problem (1), (2) if quasi-*phi*-functions are used is $\sigma = 3 + 6n + 3m$, and if *phi*-functions are used, it is $\sigma = 3 + 6n$.

SPECIAL FEATURES OF TWO IMPLEMENTATIONS OF THE MATHEMATICAL MODEL (1), (2)

Let us mention some distinctive features of the mathematical model (1), (2) that influence the choice of the method of problem solution with the use of the above-mentioned tools of mathematical modeling.

1. Problem (1), (2) is an exact mathematical model of the formulated problem of optimal packing of convex polytopes and contains all its global solutions.

2. The domain of feasible solutions W of the form (2) can be described by n inequalities of the form $f_i \geq 0$ and by $\frac{1}{2}n(n-1)$ inequalities of the form $f_{ij} \geq 0$. Function f_i is the minimum out of $6m_i$ differentiable functions, and f_{ij} is the maximin function when f_{ij} is a *phi*-function. Each inequality $f_{ij} \geq 0$ can be represented as a set of systems of inequalities with differentiable functions, including g_i systems of m_j inequalities, g_j systems of m_i inequalities, and $t_i \cdot t_j$ systems consisting of one inequality. If f_{ij} is a quasi-*phi*-function, then $f_{ij} \geq 0$ can be described by a system of $m_i + m_j$ inequalities with differentiable functions.

3. Using the *phi*-function method allows representing the problem as a nonsmooth optimization problem. The domain of feasible solutions can be described by the system of inequalities with maximin functions and has the property $W = \bigcup_{q=1}^{\varsigma} W_q$, where each of the subdomains W_q is defined by the system of inequalities with differentiable functions. Thus, problem (1), (2) can be represented as

$$F(u^*) = \min\{F(u^{*q}),\ q = 1, 2, \ldots, \varsigma\}, \tag{3}$$

where

$$F(u^{*q}) = \min_{u \in W_q} F(u). \tag{4}$$

In the model (3), (4), each subproblem (4) is a multiextremum nonlinear programming problem.

4. The domain of feasible solutions of problem (1), (2), generated with the use of quasi-*phi*-functions, can be described by a system of inequalities with differentiable functions. In this case, we have a nonconvex nonlinear programming problem, which can be immediately solved by modern solvers for global and local optimization.

For example, for two three-dimensional simplexes, i.e., $m_1 = m_2 = m = 4$, depending on the form of functions f_{ij} in (2), problem (1), (2) can be reduced to the following:

— a problem of dimension $\sigma = 18$ with the domain of feasible solutions W, which is described by a system of $6m + 6m + 2m = 56$ inequalities if quasi-*phi*-functions are used;

— a sequence of subproblems of dimension $\sigma = 15$, in each of which the domain of feasible solutions W_q is defined either by $6m + 6m + m = 52$ or by $6m + 6m + 5 = 54$ inequalities if *phi*-functions are used.

THE PROBLEM SOLUTION STRATEGY

Taking into account the properties of the mathematical model (1), (2), two solution techniques are proposed to solve the problem. They are based on the multistart strategy, which consists of the following stages.

Stage 1. Finding Feasible Starting Points of Problem (1), (2). This stage is common for the both approaches. First of all, the convex polytopes K_i are covered with full-spheres S_i of minimum radii r_i^*, $i \in I$. To this end, the optimization problem is solved:

$$r_i^* = \min_{(v_i, r_i) \in D_i \subset R^4} r_i, \tag{5}$$

where $D_i = \{(v_i, r_i) \in R^4 : r_i^2 - (x_{ij} - x_i)^2 - (y_{ij} - y_i)^2 - (z_{ij} - z_i)^2 \geq 0, r_i \geq 0, j \in 1, 2, \dots, m_i\}$. As a result of solution of problem (5), vector $r = (r_1, r_2, \dots, r_n) \in R^n$ is generated.

Then sufficiently large dimensions (l^0, w^0, h^0) of container Ω are selected so as to certainly guarantee the allocation of all disjoint full-spheres S_i, $i \in I$, inside this container. The dimensions of the container Ω are fixed, and radii r_i of the full-spheres S_i, $i \in I$, are assumed to be variable.

At the next step, the nonlinear programming problem is solved:

$$\max \kappa(v, r) = \max_{(v, r) \in G} \sum_{i=1}^{n} r_i, \tag{6}$$

where

$$G = \{(v, r) \in R^{4n}, \Phi_{ij}^{SS}(v_i, v_j, r_i, r_j) \geq 0, \ i < j \in I, \Phi_i^S(v_i, r_i) \geq 0, r_i^* - r_i \geq 0, i \in I\}, \tag{7}$$

$$\Phi_{ij}^{SS}(v_i, v_j, r_i, r_j) = (x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2 - (r_i + r_j)^2,$$

$$\Phi_i^S(v_i, r_i) = \min\{x_i - r_i, y_i - r_i, z_i - r_i, l^0 - x_i - r_i, w^0 - y_i - r_i, h^0 - z_i + r_i\}.$$

Specifying randomly point (v^0, r^0), $v^0 = (v_1^0, \dots, v_n^0)$, $v_i^0 \in \Omega^0 = \Omega(l^0, w^0, h^0)$, $r^0 = (r_1^0, \dots, r_n^0)$, $r_i^0 = 0$, $i \in I$, we can find the point of global maximum (v^*, r^*) of problem (6), (7). Note that the global maximum always exists since the dimensions of the domain are selected sufficiently large.

Stage 2. Finding the Local Minima of Problem (1), (2). Generate the point $u^s = (v^s, \theta^s)$, where $v^s = v^*$, and randomly generate the vector θ^s of angular parameters. Find a local minimum of problem (1), (2), starting with the point u^s.

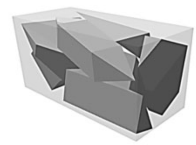
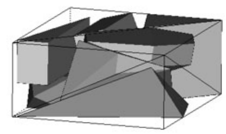
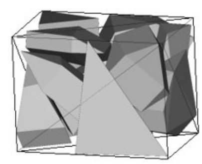
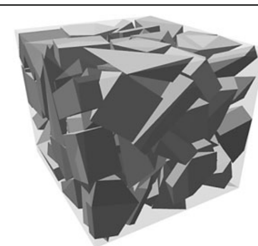
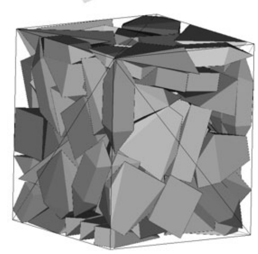
If quasi-*phi*-functions are used, then the Local Optimization Feasible Region Transformation (LOFRT) procedure described in [18] is immediately applied to problem (1), (2). The proposed local optimization procedure substantially reduces computing costs (time and memory) at the expense of decomposition of problem (1), (2) into a sequence of nonlinear programming subproblems with a smaller number of inequalities and (in case of application of quasi-*phi*-functions) of smaller dimension as well. Go to Stage 4.

If *phi*-functions are used, then for each feasible starting point u^s, a subregion $W^s \subset W$, $u^s \in W^s$ is formed. The LOFRT procedure is applied to solve subproblems (4) on subregion $W^s = W_q(u^s)$. Passage from one subregion to another is carried out by means of the algorithm described in [19].

Stage 3. Finding the Approximation to the Global Minimum of Problem (1), (2). If *phi*-functions are used, then the procedure of incomplete directional search of local minima with application of the Jump algorithm [19] is executed.

Stage 4. Search of Local Minima. The best local minimum obtained at the previous stages is taken as the approximate solution of problem (1), (2).

TABLE 1. Results of Solving the Polytope Packing Problem

Approaches to the Solution	Value of the Objective Function	Time	Locally Optimal Allocation of the Polytopes
$n = 7$			
Phi-function	1837	370 sec	
Quasi-*phi*-function	1699	323 sec	
$n = 12$			
Phi-function	3150	450 sec	
Quasi-*phi*-function	3131	410 sec	
$n = 98$			
Phi-function	22623	7 hours	
Quasi-*phi*-function	23113	41 hours	

RESULTS OF THE COMPUTING EXPERIMENTS

The computing experiments were carried out using an AMD Athlon 64 X2 5200 + computer. Solver IPOPT [20] was used to find local minima in the nonlinear programming problems. Let us consider an example.

Example 1. There are sets of polytopes for $n = 7$, $n = 12$, and $n = 98$ (n is the number of polytopes) from the study [18, Examples 1, 2, and 4, respectively]. The results of solving the polytope packing problem by two approaches are presented in Table 1.

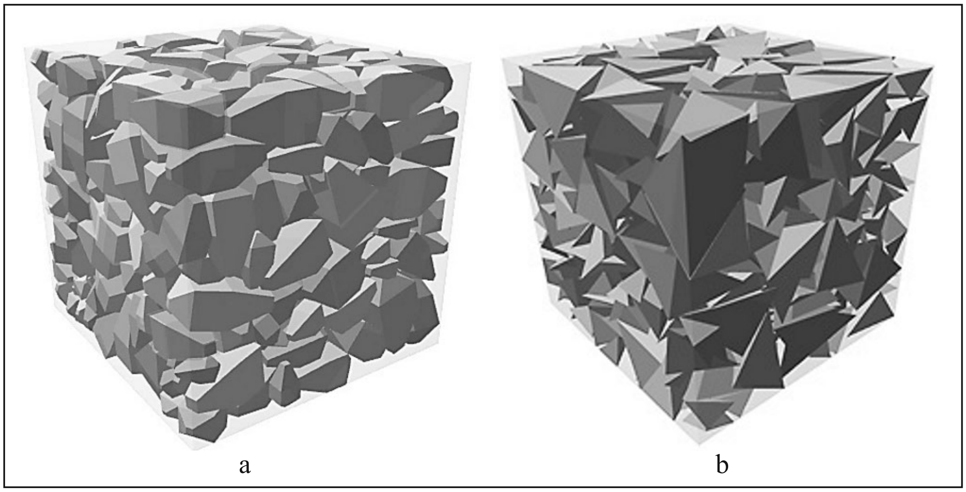


Fig. 1. Locally optimal allocations of 400 convex polytopes with 16 vertices (a) and of 500 convex polytopes with three vertices (b).

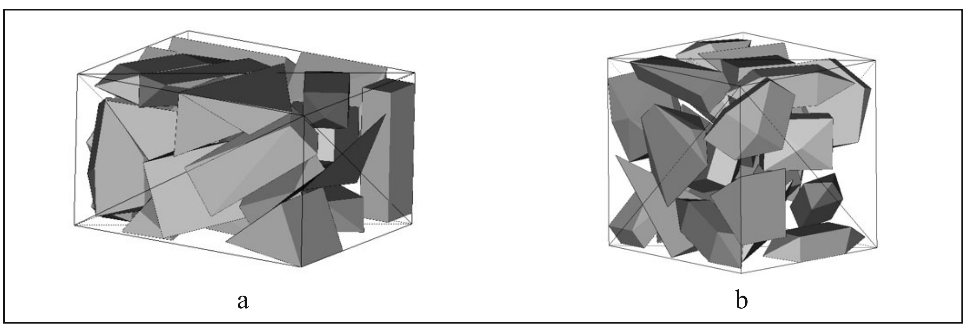


Fig. 2. Locally optimal allocations of 25 convex polytopes without regard for minimum feasible distances (a) and with regard for minimum feasible distances (b).

The results of the computing experiments allow making the following conclusions.

1. For $n \leq 50$, the obtained results slightly differ in the value of the objective function and solution time.

2. For problems of greater dimension ($n > 50$), the time of problem solution by means of the approach based on *phi*-functions is much less. This result follows from the fact that in the mathematical model (1), (2) constructed by means of *phi*-functions, there is no vector of additional variables, which reduces the problem dimension by $3m$.

3. An advantage of the approach based on *phi*-functions is that it possible to solve problems for a considerable quantity of objects in a reasonable time. Figures 1a and 1b show the results of allocation of 400 and 500 convex polytopes, respectively. The runtime for the problem of allocation of 400 convex polytopes with the use of *phi*-functions is 30 hours. If the approach based on quasi-*phi*-functions is applied, a 48-hour constraint (during which the solution has not been obtained) was established for the problem solution.

4. An advantage of the approach based on quasi-*phi*-functions is that it is possible to obtain a locally optimal allocation of convex polytopes with regard for the given minimum feasible distances [18, 21, 22]. Figure 2 gives an example of allocation of 25 polytopes with regard for the given minimum feasible distances. Moreover, to solve nonlinear programming problems, it is possible to use modern NLP-solvers to find local and global extrema.

CONCLUSIONS

Using quasi-*phi*-functions instead of *phi*-functions substantially simplifies the analytical description of the conditions of non-intersection of convex polytopes and allows formalizing the constraints on minimum feasible distances. Quasi-*phi*-functions can also be used to model allocation constraints in problems of packing various three-dimensional objects that admit continuous rotations for which *phi*-functions are too complicated (for example, nonconvex polytopes) or have not been constructed (for example, ellipsoids, cylinders, cones, and spherocylinders). However, using quasi-*phi*-functions has disadvantages related to introducing additional variables, which considerably increases problem dimension. To find efficient solutions to problems of packing convex polytopes, separating their combinatorial structure is also promising [23, 24].

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