У даній роботі розглядається задача оптимальної упаковки заданого набору еліпсоїдів у опуклому контейнері мінімального об'єму. Еліпсоїди задані розмірами напівосей і параметрами розміщення у локальній системі координат та допускають неперервні обертання і трансляції. У якості контейнера може виступати кубоїд (прямокутний паралелепіпед), циліндр, куля, еліпсоїд або опуклий багатогранник. Для аналітичного опису відношень неперетену еліпсоїдів застосовуються квазі-phi-функції. Для моделювання відношень включення використовуються квазі-phi-функції або phi-функції залежно від форми контейнеру. Використовуючи відповідні засоби моделювання будується математична модель у вигляді задачі нелінійного програмування.

Розроблено стратегію розв'язання, в основі якої лежить метод мультистарту. Пропонується швидкий алгоритм генерації початкових точок з області допустимих розв'язків та спеціальна оптимізаційна процедура, що зводить початкову задачу великої розмірності $O(n^2)$ зі великою кількістю нелінійних нерівностей до послідовності підзадач нелінійного програмування з меншою розмірністю $O(n)$ та з меншою кількістю нелінійних нерівностей.

Оптимізаційна процедура дозволяє значно зменшити (від 10 % до 90 % в залежності від розмірності задачі) обчислювальні ресурси, такі як час та пам'ять. В залежності від форми контейнера, обмежень на орієнтацію еліпсоїдів (можливість безперервних поворотів, фіксована орієнтація) та особливостей метричних характеристик еліпсоїдів в результаті розв'язання задачі отримані локально-оптимальні або гарні допустимі розв'язки. В роботі проведені чисельні експерименти для різних форм контейнерів (включаючи циліндр, кубоїд, кулю, еліпсоїд)

Ключові слова: оптимальна упаковка, еліпсоїди, опуклий контейнер, метод phi-функції, моделювання відношень розміщення, нелінійна оптимізація

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DEVELOPMENT OF THE MATHEMATICAL MODEL AND THE METHOD TO SOLVE A PROBLEM ON THE OPTIMIZATION OF PACKING THE ELLIPSOIDS INTO A CONVEX CONTAINER

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1. Introduction

The problems that belong to the class of NP-hard [1] have a wide range of scientific and practical applications. For example, in modern biology, medicine, materials science, in thermodynamics when fluids pass into a crystalline form, in nanotechnologies, chemical industry, mechanical engineering, etc. As well as in molecular dynamics for growing crystals, when modeling the structure of liquids, crystals and glass, while modeling the motion and pressing of loose substances. At present, interest in the search for effective solutions for placement problems of ellipsoids is growing rapidly. This is due to a large number of practical applications and the extraordinary complexity of the methods used to solve many of them. Here are several examples of practical applications.

3D modeling of granulated structures and substances whose particles have a shape of ellipsoids: the family of software products to enable visual and quantitative analysis of structural characteristics, such as spatial density, spatial porosity, spatial distribution, grain grade, and porosity of structure.

Robotics: an arm and other elements of the robot are approximated by ellipsoids, so there is a task to formalize the relation between the overlapping of ellipsoids and the overlapping of free-form objects.

The task that is associated with the arrangement of chromosomes in the nuclei of human cells also requires solving the problems on packing the ellipsoids.

Nuclear medicine: in the production of medical preparations that are used during cancer therapy, the optimization problem is solved on packing the two kinds of nanoparticles for the efficient use of power of the accelerator's beam. One of the types of nanoparticles could be approximated by ellipsoids.

In each of the above applications, different forms of containers are considered while ellipsoids have an arbitrary orientation. Given the practical importance of the optimization problem on packing the ellipsoids, it appears relevant to develop effective methods to solve it by using the modern NLP solvers. Employing them will make it possible to obtain the feasible and local optimal solutions within a reasonable time. The development of such methods is impossible without the construction of mathematical models in the form of nonlinear programming problems. In turn, construction of the models is based on the further development of constructive means to model the non-overlapping of ellipsoids and the belonging of ellipsoids to the convex container of an arbitrary special shape with respect to translations and rotations of ellipsoids.

2. Literature review and problem statement

Paper [2] reported a precise and efficient algorithm to detect continuous collisions between two movable ellipsoids. First, the authors conducted a highly optimized research into collision of two stationary ellipsoids, the base of which is the algebraic condition that is described in terms of the signs of roots of the characteristic equation of two ellipsoids. Next, the work describes obtaining a time-dependent characteristic equation for two movable ellipsoids, which makes it possible to construct a real-time algorithm for computing the time intervals in which the two movable ellipsoids collide. Several practical examples demonstrate the effectiveness of the proposed approach. This study gave impetus to the development of the modeling of arranging the ellipsoids, thereby showing that it is possible to analytically investigate the collision of ellipsoids. However, the work considers the model that makes it possible to examine the interaction between two ellipsoids only.

Paper [3] addresses the problem on packing the ellipsoids of various sizes and types into an elliptical container. The problem implies the minimization of the measure of the total overlap of ellipsoids from a given set, located inside the preset elliptic container. A special feature of this work is that the optimization problem is solved for a container that has the shape of an ellipsoid. However, the problem did not consider the means that would provide for an analytical description of the non-overlapping between ellipsoids.

The density of a three-dimensional packing of ellipsoids is analyzed in [4]. Experimentally, and using the new simulation algorithm, the authors showed that the random packing of ellipsoids can be quite dense up to packing fraction from $\varphi=0.68$ to 0.71 to spheroids with a ratio of sides close to the M&M's candies, and even approach $\varphi\approx 0.74$ for ellipsoids with a different ratio of sides. The authors suggest that the higher density is directly connected to the larger number of degrees of freedom and, accordingly, to more contacts between particles required for the mechanical stabilization of packing. However, when modeling, ellipsoids were not confined to a container, which is why the optimization procedure was not used in the work. In addition to [4], the density of packing the ellipsoids is analyzed in many studies, example [5, 6] which makes it a relevant task to develop constructive means of mathematical and computer modelling of the ratio of the non-overlapping of ellipsoids.

Paper [7] addresses the problem of packing ellipsoids in a rectangular container of minimum volume. The author proposes a non-convex NLP model, based only on mathematical approaches to describe the rotation and motion of ellipsoids. An assumption is made on that the elements of the rotation matrix are variable. In order to make sure that the ellipsoids do not overlap with each other, the separating hyperplanes are constructed. Using the global solvers available in GAMS, the authors obtained feasible solutions for packing the ellipsoids. However, only one type of container was considered. The problematic part of a given work is the fact that the number of additional variables in the model is quadratic in relation to the number of ellipsoids.

Study [8] reports continuous and differentiated models of nonlinear programming and algorithms for packing the ellipsoids in n-dimensional space. Two different models were proposed to constraint the non-overlapping of ellipsoids, as well as models for the inclusion of ellipsoids into half-spaces. The strategy of a multistart is combined with software tools to find the local solutions to nonlinear programming problems for two kinds of containers.

However, the issue on the development of means of mathematical and computer modeling to optimize the packing of ellipsoids that allow continuous rotations in arbitrary convex containers over feasible time remains open. Thus, it is a relevant task to construct NLP models and to develop optimization algorithms, linear relative to the number of ellipsoids that needs to be arranged.

The problem on packing the ellipsoids is considered in the following statement.

Let $\Omega=\Omega(p)$ be a convex container with variable dimensions p,

$$\Omega=\{(x,y,z,p)\in R^3:\Psi(x,y,z,p)\geq 0\},$$

assigned in the global coordinate system $OXYZ$ where $\Psi_s(x,y,z,p)$ is the differentiable function $s=1,...,n_\Omega$. Particularly, the following types of containers (Fig. 1) are considered:

– cuboid:

$$\mathbf{B}=\left\{\begin{matrix}(x,y,z,l,w,h)\in R^3\middle|\min\{x+l,-x+l,\\ y+w,-y+w,z+h,-z+h\}\geq 0\end{matrix}\right\}$$

of variable dimensions l, w and h, $p=(l, w, h)$;

– sphere:

$$\mathbf{S}=\left\{(x,y,z,r)\in\mathbb{R}^3\middle|r^2-x^2-y^2-z^2\geq 0\right\}$$

with a variable radius r, $p=(r)$;

– cylinder:

$$\mathbf{C}=\left\{\begin{matrix}(x,y,z,\lambda)\in\mathbb{R}^3\middle|\min\{(\lambda r)^2-x^2-y^2,\\ -z+\lambda h,z+\lambda h\}\geq 0\end{matrix}\right\}$$

with a radius of λr and a height of λh where λ is the variable coefficient of homothety, $p=(\lambda)$, subject to for original container $\lambda=1$;

– ellipsoid:

$$\mathbf{E}=\left\{(x,y,z,\lambda)\in\mathbb{R}^3\middle|\lambda^2-\frac{x^2}{a^2}-\frac{y^2}{b^2}-\frac{z^2}{c^2}\geq 0\right\}$$

with variable sizes of semi-axes λa, λb, λc, $p=(\lambda)$, subject to for original container $\lambda=1$;

– convex polyhedron with a variable coefficient of homothety λ:

$$\mathbf{K}=\left\{(x,y,z,\lambda)\in\mathbb{R}^3\middle|\min\left\{\begin{matrix}\alpha_s\cdot x+\beta_s\cdot y+\gamma_s\cdot z+\lambda\cdot\mu_s,\\ s=1,...,n_K\end{matrix}\right\}\geq 0\right\}.$$

Remark. Each metrical characteristic Ω can be variable by itself, that is, r and h for a cylinder, or a, b, c – for an ellipsoid.

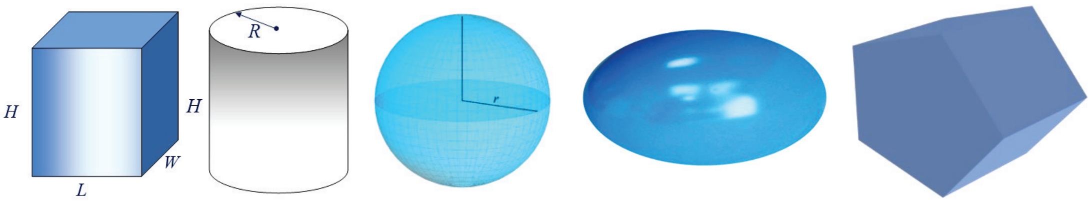


Fig. 1. Types of containers

Container Ω has fixed pacement parameters $(0,0,0)$ in the global coordinate system.

Each ellipsoid E_i, $i \in I_n = \{1,...,n\}$, assigned by its semi-axes a_i, b_i, c_i and the variable vector of pacement parameters $u_i = (v_i, \theta_i)$ in the local coordinate system, where $v_i = (x_i, y_i, z_i)$ is the vector of translation, $M(\theta)$ is the matrix of rotation, takes the form:

$$\begin{pmatrix} \cos\theta^1\cos\theta^3 - \sin\theta^1\cos\theta^2\sin\theta^3 & -\cos\theta^1\sin\theta^3 - \sin\theta^1\cos\theta^2\cos\theta^3 & \sin\theta^1\sin\theta^2 \\ \sin\theta^1\cos\theta^3 + \cos\theta^1\cos\theta^2\sin\theta^3 & -\sin\theta^1\sin\theta^3 + \cos\theta^1\cos\theta^2\cos\theta^3 & -\cos\theta^1\sin\theta^2 \\ \sin\theta^2\sin\theta^3 & \sin\theta^2\cos\theta^3 & \cos\theta^2 \end{pmatrix},$$

and $\theta_i = (\theta_i^1, \theta_i^2, \theta_i^3)$ is the vector of rotation parameters where θ_i^1, θ_i^2, θ_i^3 are the Euler's angles.

3. The aim and objectives of the study

The aim of this study is to construct a mathematical model and develop an effective method for solving the problem on packing the ellipsoids into a convex container of minimum volume. That would make it possible to build precise models when modeling the arrangement of ellipsoids, to obtain locally optimal or good feasible solutions over a reasonable time.

To accomplish the aim, the following tasks have been set:

– to develop constructive means of mathematical modeling and computer simulation for the analytical description of containment constraint and non-overlapping that occur between objects in the problems on packing the ellipsoids into a convex container;

– to construct a mathematical model in the form of a nonlinear programming problem;

– to develop a method for optimizing the packing of ellipsoids using the procedure of decomposition, which makes it possible to significantly reduce the cost of computing resources required to search for feasible and locally optimal solutions.

4. Analytical description of the constraints for arrangement

This chapter describes the procedure of mathematical modeling of arrangement constraints, which are found in the problem on packing the ellipsoids:

– constraints for non-overlapping:

$$\operatorname{int} E_i(u_i) \cap \operatorname{int} E_j(u_j) = \varnothing, \quad i < j \in I_n,$$

– containment constraints:

$$E_i(u_i) \subset \Omega \Leftrightarrow \operatorname{int} E_i(u_i) \cap \Omega^* = \varnothing, \quad i \in I_n.$$

In order to describe pacement constraints in analytical form, we used the method of phi-functions [9]. We introduce the phi-functions to model the containment constraints, and quasi-phi-functions [10] to model constraints for non-overlapping.

4. 1. Modeling the containment constraints

In this paper, in order to describe a constraint for inclusion:

$$E_i(u_i) \subset \Omega \Leftrightarrow \operatorname{int} E_i(u_i) \cap \Omega^* = \varnothing,$$

we propose an approach related to the construction of the phi-function for the object that approximates an ellipsoid with the predefined precision. We have used two types of approximations:

– approximation of each ellipsoid E_i by a convex polyhedron K_i, assigned by its vertices p_j^i, $j = 1,....,m_i$, whose values are unchanged in the local coordinate system of ellipsoid E_i;

– approximation of each ellipsoid E_i by spheres S_{ki} [11],

$$\widehat{E}_i(u_i) = \bigcup_{k=1}^{n_i} S_i^k\left(u_i + u_i^k\right),$$

assigned by translation vectors v_{si} and radii r_i, whose values are fixed in the local coordinate system of ellipsoid E_i.

We denote the ellipsoid approximated by spheres as $\widehat{E}_i(u_i)$, and the one approximated by a convex polyhedron as $\dot{E}_i(u_i)$.

Phi-function $\widehat{E}_i(u_i)$ and $\Omega^* = R^3 \setminus \operatorname{int}\Omega$ can be represented in the form

$$\Phi(u_i, p) = \min\left\{\Phi_1(u_i, p), ..., \Phi_{n_i}(u_i, p)\right\},$$

where $\Phi_k(u_i, p)$ is the phi-function for S_{ki} and Ω^*.

Specifically, we employ the following phi-functions for the constraints on inclusion.

Under condition of applying the approximation of each ellipsoid E_i by a convex polyhedron, depending on the shape of a container, we use such phi-functions as:

Phi-function for a convex polyhedron $K_i(u_i)$ and object $\mathbf{S}^* = \mathbb{R}^3 / \operatorname{int}\mathbf{S}$:

$$\Phi^{K_i \mathbf{S}^*}(u_i, r) = \Psi(u_i, r) = \min\left\{\varphi(p_k^i(u_i), r), k = 1, ..., m_i\right\},$$

$$\varphi(p_k^i(u_i), r) = (r)^2 - \left(p_{kx}^i(u_i)\right)^2 - \left(p_{ky}^i(u_i)\right)^2 - \left(p_{kz}^i(u_i)\right)^2.$$

Phi-function for a convex polyhedron $K_i(u_i)$ and object $\mathbf{C}^* = \mathbb{R}^3 / \operatorname{int}\mathbf{C}$:

$$\Phi^{K_i \mathbf{C}^*}(u_i, \lambda) = \min\left\{\Psi_s(u_i, \lambda), s = 1,2,3\right\},$$

$$\Psi_s(u_i, \lambda) = \min\left\{\varphi_s(p_k^i(u_i), r), k = 1, ..., m_i\right\},$$

$$\varphi_1(p_k^i(u_i),\lambda)=(\lambda r)^2-\left(p_{xk}^i(u_i)\right)^2-\left(p_{yk}^i(u_i)\right)^2,$$

$$\varphi_2(p_k^i(u_i),\lambda)=-p_{zk}^i(u_i)+\lambda h,$$

$$\varphi_3(p_k^i(u_i),\lambda)=p_{zk}^i(u_i)+\lambda h.$$

Phi-function for a convex polyhedron $K_i(u_i)$ and object $\mathbf{B}^*=\mathbb{R}^3/\operatorname{int}\mathbf{B}$:

$$\Phi^{K_i\mathbf{B}^*}(u_i,l,h,w)=\min\left\{\Psi_s(u_i,l,h,w),s=1,...,6\right\},$$

$$\Psi_s(u_i,l,h,w)=\min\left\{\varphi_{ks}^i(u_i,l,h,w),k=1,...,m_i\right\},$$

$$\varphi_{k1}^i(ui,l,h,w)=p_{xk}^i(u_i)+l,$$

$$\varphi_{k2}^i(u_i)=-p_{xk}^i(u_i)+l,$$

$$\varphi_{k3}^i(u_i,l,h,w)=p_{yk}^i(u_i)+w,$$

$$\varphi_{k4}^i(u_i,l,h,w)=-p_{yk}^i(u_i)+w,$$

$$\varphi_{k5}^i(u_i,l,h,w)=p_{zk}^i(u_i)+h,$$

$$\varphi_{k6}^i(u_i,l,h,w)=-p_{zk}^i(u_i)+h.$$

Phi-function for a convex polyhedron $K_i(u_i)$ and object $\mathbf{E}^*=\mathbb{R}^3/\operatorname{int}\mathbf{E}$:

$$\Phi^{K_i\mathbf{E}^*}(u_i,\lambda)=\Psi(u_i,\lambda)=\min\left\{\varphi\left(p_k^i(u_i),\lambda\right),k=1,...,m_i\right\},$$

$$\varphi(p_k^i(u_i),\lambda)=(\lambda)^2-\frac{\left(p_{kx}^i(u_i)\right)^2}{a^2}-\frac{\left(p_{ky}^i(u_i)\right)^2}{b^2}-\frac{\left(p_{kz}^i(u_i)\right)^2}{c^2}.$$

Under condition of applying the approximation of each ellipsoid E_i by spheres, depending on the shape of a container, we use such the following phi-functions.

$$\Phi^{\hat{E}_i\Omega}(u_i,\lambda)=\min\left\{\Phi_s^{\hat{E}_i}(u_i,\lambda),s=1,...,n_\Omega\right\},$$

$$\Phi_s^{\hat{E}_i}(u_i,\lambda)=\min\left\{\varphi_{si}^k(u_i,\lambda),k=1,...,n_i\right\}.$$

Phi-function for object $\hat{E}_i(u_i)$ and object $\mathbf{S}^*=\mathbb{R}^3/\operatorname{int}\mathbf{S}$:

$$\Phi^{\hat{E}_i\mathbf{S}^*}(u_i,r)=\min\left\{\Psi_s^{\hat{E}_i}(u_i,r),s=1\right\}=$$
$$=\min\left\{\varphi_i^k(u_i,r),k=1,...,n_i\right\},$$

$$\varphi_i^k(u_i,r)=\left(r+r^k\right)^2-\left(x-x^k\right)^2-\left(y-y^k\right)^2-\left(z-z^k\right)^2.$$

Phi-function for ellipsoid $E_i(u_i)$ and object $\mathbf{C}^*=\mathbb{R}^3/\operatorname{int}\mathbf{C}$:

$$\Phi^{E_iC^*}(u_i,r,h)=\min\left\{\psi_1(u_i),\psi_2(u_i)\right\},$$

$$\psi_1(u_i)=\min\left\{z_i-a_{i1},h-z_i-a_{i1}\right\},$$

$$\psi_2(u_i)=\Phi^{E_{i2}\Omega_2^*}(u_i),$$

$$\Phi^{E_{i2}\Omega_2^*}(u_i)=\Phi^{CE_\Omega^*}(u_i),$$

$$\Phi^{CE_\Omega^*}(u_i(s,\varphi))=\Lambda_i(s,\varphi),$$

$$u_i(s,\varphi)=(x_i(s,\varphi),y_i(s,\varphi),\theta_i^1,\theta_i^2),$$

$$\Lambda_i(s,\varphi)=\left(b_i^*-s\right)\sqrt{\frac{b_i^{*2}}{a_i^{*2}}\cos^2\varphi+\sin^2\varphi}-b_i,$$

$$a_i^*=R,\quad b_i^*=R\cdot\frac{b_i}{a_i},$$

$$a_{i1}=\sqrt{b_i^2+\left(a_i^2-b_i^2\right)\sin^2\left(\theta_i^2\right)},\quad b_{i1}=b_i,$$

$$a_{i2}=\sqrt{b_i^2+\left(a_i^2-b_i^2\right)\cos^2\left(\theta_i^2\right)},\quad b_{i2}=b_i,$$

where ellipse E_{i1} with semi-axes (a_{i1},b_{i1}) can be obtained as a projection of ellipsoid E_i onto rectangle $\mathbf{\Omega}_1$, which belong to the plane parallel to OZ; ellipse E_{i2} with semi-axes (a_{i2},b_{i2}) can be obtained as a projection of ellipsoid E_i onto XOY (Fig. 2). To determine phi-function $\mathbf{\Phi}^{E_2\Omega_2^*}(u)$ we apply affine transforms.

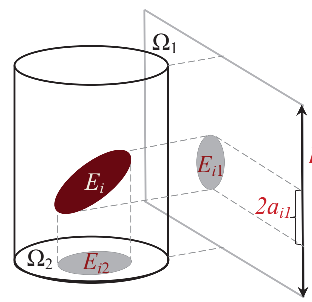


Fig. 2. Ellipses E_{i1} and E_{i2}

Phi-function for object $\hat{E}_i(u_i)$ and object $\mathbf{C}^*=\mathbb{R}^3/\operatorname{int}\mathbf{C}$:

$$\Phi^{\hat{E}_iC^*}(u_i,r,h)=\min\left\{\Phi_s^{\hat{E}_i}(u_i,r,h),s=1,2,3\right\},$$

$$\Phi_s^{\hat{E}_i}(u_i,r,h)=\min\left\{\varphi_{si}^k(u_i,r,h),k=1,...,n_i\right\},$$

$$\varphi_{1i}^k(u_i,r,h)=\left(r-r^k\right)-\sqrt{x^2+y^2},$$

$$\varphi_{2i}^k(u_i,r,h)=-z_k^i(u_i)+h,$$

$$\varphi_{3i}^k(u_i,r,h)=z_k^i(u_i)+h.$$

Phi-function for ellipsoid $E_i(u_i)$ and object $\mathbf{B}^*=\mathbb{R}^3/\operatorname{int}\mathbf{B}$:

$$\Phi^{E_i\mathbf{B}^*}(u_i,l,h,w)=\min\left\{\varphi_1(u_i),\varphi_2(u_i)\right\},$$

$$\varphi_1(u_i)=\min\left\{z_i-a_{i1},h-z_i-a_{i1}\right\},$$

$$\varphi_2(u_i)=\Phi^{E_{i2}R^*}(x_i,y_i,\theta_i^1,\theta_i^2)$$

$$E_{i1}(a_{i1},b_{i1}):a_{i1}=\sqrt{b_i^2+\left(a_i^2-b_i^2\right)\sin^2\left(\theta_i^1\right)},\quad b_{i1}=b_i,$$

$$E_{i2}(a_{i2},b_{i2}):a_{i2}=\sqrt{b_i^2+\left(a_i^2-b_i^2\right)\cos^2\left(\theta_i^1\right)},$$

where ellipse E_{i1} with semi-axes (a_{i1},b_{i1}) can be obtained as a projection of ellipsoid E_i onto rectangle $\mathbf{\Omega}_1$, which belong to the plane parallel to OZ; ellipse E_{i2} with semi-axes (a_2, b_2) can be obtained as a projection of ellipsoid E_i onto XOY, $\Phi^{E_{i2}R^*}$ is the phi-function for ellipse E_{i2} with location parameters (x, y, θ_2) and $\Omega_2^* = \mathbb{R}^2 \setminus \operatorname{int}\Omega_2$, where Ω_2 is a rectangle (Fig. 3).

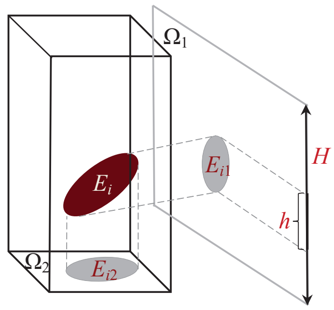


Fig. 3. Phi-function for ellipsoid and cuboid

Phi-function for object $\hat{E}_i(u_i)$ *and object* $\mathbf{B}^* = \mathbb{R}^3 / \operatorname{int}\mathbf{B}$:

$$\Phi^{\hat{E}_i\mathbf{B}^*}(u_i, l, h, w) = \min\left\{\Phi_s^{\hat{E}_i}(u_i, l, h, w), s = 1, \ldots, 6\right\},$$

$$\Phi_s^{\hat{E}_i}(u_i, l, h, w) = \min\left\{\varphi_{ks}^i(u_i, l, h, w), k = 1, \ldots, n_i\right\},$$

$$\varphi_{k1}^i(u_i, l, h, w) = r_k + l, \quad \varphi_{k2}^i(u_i, l, h, w) = -r_k + l,$$

$$\varphi_{k3}^i(u_i, l, h, w) = r_k + w, \quad \varphi_{k4}^i(u_i, l, h, w) = -r_k + w,$$

$$\varphi_{k5}^i(u_i, l, h, w) = r_k + h, \quad \varphi_{k6}^i(u_i, l, h, w) = -r_k + h.$$

Phi-function for object $\hat{E}_i(u_i)$ *and object* $K^* = \mathbb{R}^3 / \operatorname{int} K$:

$$\Phi^{\hat{E}_i K^*}(u_i, \lambda) = \min\left\{\Phi_s^{\hat{E}_i}(u_i, \lambda), s = 1, \ldots, n_\Omega\right\},$$

$$\Phi_s^{\hat{E}_i}(u_i, \lambda) = \min\left\{\varphi_{ks}^i(u_i, \lambda), k = 1, \ldots, n_i\right\},$$

$$\varphi(u_i, \lambda) = -\alpha x - \beta y - \gamma z - \lambda\mu - r_k.$$

4. 2. Modeling the constraints for non-overlapping

First, we shall consider a quasi-phi-function for a pair of ellipsoids.

To describe constraints for non-overlapping, that is,

$$\operatorname{int} E_i(u_i) \cap \operatorname{int} E_j(u_j) = \varnothing,$$

we shall use a quasi-phi-function.

Let $E_i(u_i)$ and $E_j(u_j)$ be two spheroids (ellipsoids of revolution).

A quasi-phi-function for $E_i(u_i)$ and $E_j(u_j)$ can be represented in the following form:

$$\Phi'_{ij}(u_i, u_j, u'_{ij}) = \min\left\{\begin{array}{l} \psi(\theta_i, \theta_j, u'_{ij}), \psi_1^+(u_i, u_j, u'_{ij}), \\ \psi_1^-(u_i, u_j, u'_{ij}), \psi_2^+(u_i, u_j, u'_{ij}), \\ \psi_2^-(u_i, u_j, u'_{ij}) \end{array}\right\}, \quad (1)$$

where

$$u'_{ij} = (t_i, g_i, t_j, g_j), \quad \psi = -\alpha'_i\alpha'_j - \beta'_i\beta'_j - \gamma'_i\gamma'_j, \quad \theta_i = (\theta_i^1, \theta_i^2),$$

$$(\alpha'_i, \beta'_i, \gamma'_i) = M(\theta_i) \cdot (\alpha_i, \beta_i, \gamma_i)^{\mathrm{T}},$$

$$\alpha_i = \frac{\cos t_i}{a_i}, \quad \beta_i = \frac{\sin t_i \cos g_i}{b_i}, \quad \gamma_i = \frac{\sin t_i \sin g_i}{b_i},$$

$$\theta_j = (\theta_j^1, \theta_j^2), \quad (\alpha'_j, \beta'_j, \gamma'_j) = M(\theta_j) \cdot \left(\alpha_j, \beta_j, \gamma_j\right)^{\mathrm{T}},$$

$$\alpha_j = \frac{\cos t_j}{a_j}, \quad \beta_j = \frac{\sin t_j \cos g_j}{b_j}, \quad \gamma_j = \frac{\sin t_j \sin g_j}{b_j},$$

$$\psi_k^+ = \alpha'_i\left(x_{jk}^+ - x_i\right) + \beta'_i\left(y_{jk}^+ - y_i\right) + \gamma'_i\left(z_{jk}^+ - z_i\right) - 1,$$

$$\psi_k^- = \alpha'_i\left(x_{jk}^- - x_i\right) + \beta'_i\left(y_{jk}^- - y_i\right) + \gamma'_i\left(z_{jk}^- - z_i\right) - 1,$$

$$(x_{j2}^+, y_{j2}^+, z_{j2}^+) = v_j + M(\theta_j)M_2(g_j)\left(a_j \cos t_j, b_j \sin t_j, \sqrt{2}a_j\right)^{\mathrm{T}},$$

$$(x_{j2}^-, y_{j2}^-, z_{j2}^-) = v_j + M(\theta_j)M_2(g_j)\left(a_j \cos t_j, b_j \sin t_j, -\sqrt{2}a_j\right)^{\mathrm{T}},$$

$$(x_{j1}^+, y_{j1}^+, z_{j1}^+) = v_j + M(\theta_j)M_2(g_j)\left(x_j^+, y_j^+, 0\right)^{\mathrm{T}},$$

$$(x_{j1}^-, y_{j1}^-, z_{j1}^-) = v_j + M(\theta_j)M_2(g_j)\left(x_j^-, y_j^-, 0\right)^{\mathrm{T}},$$

$$(x_j^+, y_j^+) = \left(\alpha_j^t, \beta_j^t\right) + \eta\left(-\beta_j^t, \alpha_j^t\right),$$

$$(x_j^-, y_j^-) = \left(\alpha_j^t, \beta_j^t\right) - \eta\left(-\beta_j^t, \alpha_j^t\right),$$

$$(\alpha_j^t, \beta_j^t) = M_1(t_j)\left(a_j, 0\right)^{\mathrm{T}}, \quad \eta = \sqrt{2}\left(a_j\right)^2.$$

Thus, the constraint for non-overlapping takes the form $\Phi'_{ij}(u_i, u_j, u'_{ij}) \geq 0$, where Φ'_{ij} is the quasi-phi-function for spheroids (ellipsoids of revolution) $E_i(u_i)$ and $E_j(u_j)$, represented in (1). Here we use the important property of a quasi-phi-function: if $\Phi'_{ij}(u_i, u_j, u'_{ij}) \geq 0$ for some u'_{ij}, then:

$$\operatorname{int} E_i(u_i) \cap \operatorname{int} E_j(u_j) = \varnothing$$

(more detailed information is provided in paper [10]).

5. Mathematical model of the problem on the optimal packing of ellipsoids

The vector of all variables $u \in R^\sigma$ can be described in the following way:

$$u = (p, u_1, u_2, \ldots, u_n, \tau),$$

where p is the vector of variable metric characteristics of convex container Ω, and $u_i = (v_i, \theta_i)$ is the vector of placement parameters of ellipsoid E_i, $i \in I_n$, where $v_i = (x_i, y_i, z_i)$, $\theta_i = (\theta_i^1, \theta_i^2, \theta_i^3)$. Vector $\tau = (u'_{ij}, i < j \in I_n)$ is the vector of additional variables (for our quasi-phi-function), where u'_{ij} is defined in (1).

The mathematical model of the basic problem on packing can now be represented in the following form:

$$\min_{u \in W \subset R^\sigma} F(u), \quad (2)$$

$$W = \left\{u \in R^\sigma : \Phi'_{ij}(u_i, u_j, u'_{ij}) \geq 0, \Phi_i(u_i) \geq 0, i < j \in I_n\right\}, \quad (3)$$

where $F(u)$ is the volume Ω or one of the metric characteristics of Ω, $\Phi'^{E_iE_j}$ is the quasi-phi-function (1), determined for a pair of ellipsoids E_i and E_j, which ensures that the constraint for the non-overlapping is met, Φ_i is the phi-function for objects $\dot{E}_i$ $(\widehat{E}_i)$ and Ω^*, which is used for meeting the containment constraint.

6. A solving algorithm

The strategy of a multistart includes the following stages:

Stage 1. Generate a set $\{\varsigma^0\}$ of vectors $\varsigma^0=(p^0,u_1^0,...,u_n^0)$ with the feasible placement parameters $(u_1^0,...,u_n^0)$ of ellipsoids, arranged in container Ω^0 with dimensions (p^0) for problem (2), (3). To derive a feasible solution, there are different methods. We use an intuitive and fast algorithm.

Stage 2. Starting at each point of the set $\{\varsigma^0\}$, obtained at stage 1, we search for the local extrema for the objective function $F(u)$ and problem (2), (3). To derive a local extremum to problem (2), (3), there is a compaction algorithm for the ellipsoids that allow rotation.

Stage 3. We choose the best local extremum from those derived at stage 2 as a solution to problem (2), (3).

6. 1. Search algorithm for feasible placement parameters (FPPA_E)

To find the vector of feasible parameters for arranging the ellipsoids, we used a modification of the FPPA algorithm, described in [12] for the problem on packing the polyhedra and based on the homothetic transformations of objects. The algorithm includes the following stages (Fig. 4).

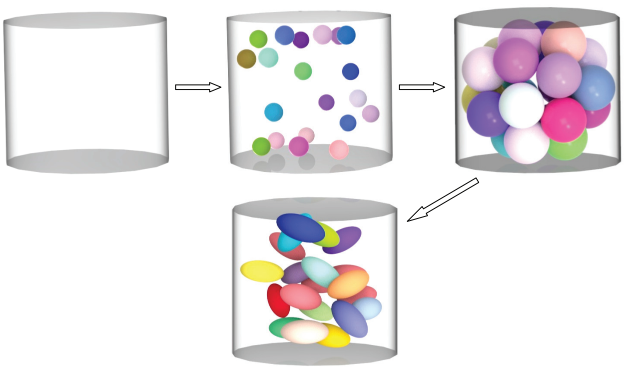


Fig. 4. Illustration of the optimization procedure FPPA_E to search for feasible parameters of arranging the ellipsoids inside spheres using the homothetic transformations

Stage 1. Choose large enough initial size for container $\Omega^0=\Omega(p^0)$, to ensure the arrangement of all spheres S_i of radius r_i, $i\in I_n$, inside container Ω^0.

Stage 2. Generate in the container Ω^0 a set of n randomly selected centers (x_i^0,y_i^0,z_i^0) of spheres S_i.

Stage 3. Increase spheres S_i of radius βr_i, $i\in I_n$, starting from $\beta=0$ to full size $(\beta=1)$, in this case, centers S_i and coefficient of homothety β are the variables, $0\le\beta\le 1$. To perform this stage, fix $p=p^0$ and, starting at point:

$$v^0=(x_1^0,y_1^0,z_1^0,...,x_n^0,y_n^0,z_n^0,\beta^0=0),$$

we solve the following NLP subproblem:

$$\max_{v\in W_\beta}\beta, \tag{4}$$

$$W_\beta=\left\{\begin{matrix} v\in R^{3n+1}:\Phi^{S_iS_j}(v)\ge 0,\Phi^{S_i\Omega^*}(v)\ge 0,\\ j>i\in I_n, 1-\beta\ge 0,\beta\ge 0\end{matrix}\right\}, \tag{5}$$

where

$$v=(x_1,y_1,z_1,...,x_n,y_n,z_n,\beta),$$

$$\Phi^{S_iS_j}(v)=\left(x_i-x_j\right)^2+\left(y_i-y_j\right)^2+\left(z_i-z_j\right)^2-\beta^2(r_i+r_j)^2, \tag{6}$$

where $\widehat{\Phi}^{S_i\Omega^*}(v)$ is the phi-function function for sphere S_i of radius βr_i and object Ω^*.

Denote the point of a global maximum in problem (4), (5):

$$v^*=(x_1^*,y_1^*,z_1^*,...,x_n^*,y_n^*,z_n^*,\beta^*=1).$$

Stage 4. Form the vector of feasible parameters:

$$\varsigma^0=(p^0,u_1^0,...,...,u_n^0),$$

assuming

$$u_i^0=(x_i^0,y_i^0,z_i^0,\theta_i^0),\ \ (x_i^0,y_i^0,z_i^0)=(x_i^*,y_i^*,z_i^*),$$

where θ_i^0 is the vector of randomly-generated rotation parameters of ellipsoids E_i, $i\in I_n$. Note that the global solution to problem (4), (5) can always be found (under condition of selecting sufficiently large initial dimensions p^0 at the first stage).

Stage 5. To search for a local minimum to problem (2), (3), we build, based on vector ς^0, a starting point $u^0=(\varsigma^0,\tau^0)$. To obtain vector τ^0, we apply a specialized optimization procedure named the Feasible Auxiliary Parameters Algorithm (FAPA_E).

6. 2. Compaction algorithm (COMPOLY)

The proposed algorithm transforms problem (2), (3) with a large number of inequalities and dimensionality $O(n^2)$ of the region of feasible values W, specified in (3), into a sequence of nonlinear programming subproblems, which have a smaller number of linear inequalities $(O(n))$ and dimensionality $O(n)$. The basic idea of the algorithm implies performing the following stages.

Stage 1. We build for each vector of feasible arrangements of ellipsoids a fixed individual cubic container around the sphere produced by the respective ellipsoid (Fig. 5).

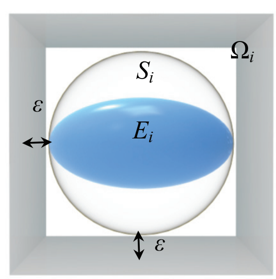


Fig. 5. Ellipsoid and its individual container Ω_i

Stage 2. Move each sphere inside the corresponding individual container. The motion of each sphere is described by the system of additional inequalities.

Stage 3. Form a subset of feasible solutions W as follows: add $O(n)$ inequalities (for all spheres) to the system of inequalities (3), which makes it possible for us to discard $O(n^2)$ of phi-inequalities for those pairs of ellipsoids whose individual containers do not intersect, and to exclude some redundant constraints for the condition for inclusion.

Stage 4. Search for a local minimum at the subset of dimensionality $O(n)$. The subset is described by $O(n)$ nonlinear inequalities. Next, we employ the resulting local minimum as a starting point for the next iteration. At the last iteration of the algorithm, find a local minimum to problem (2), (3).

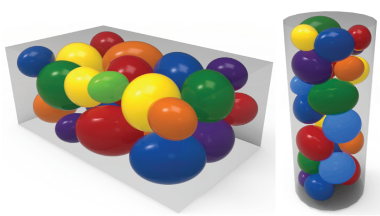
7. Numerical results

In this chapter, we report results of computational experiments that demonstrate the effectiveness of the proposed specialized optimization procedure for the problem on packing the ellipsoids.

Examples 1, 2, 6 are based on numerical experiments using the computer AMD Athlon 64 X2 5200+. The search for local extrema employed IPOPT, available from an open non-profit software repository [13]. Examples 3, 4, 5 are based on numerical experiments using the computer Intel(R) Core(TM) i7-3630QM. To search for local extrema, we applied the method InteriorPoint from the solver FindArgMin in the software package Wolfram Mathematica 9 [14].

Example 1. Locally optimal arrangement = 24 ellipsoids in a cuboid is shown in Fig. 6, *a*. Volume of the container is $F^*=25546.353$, dimensions are $(l^*, w^*, h^*)=(28.618, 46.172, 19.33)$. Application of the specialized optimization procedure made it possible, for a given example, to reduce the mean time for finding a local minimum from 17,801 to 6,983 seconds.

Example 2. Locally optimal arrangement $N=24$ ellipsoids in a cylinder is shown in Fig. 6, *b*. Volume of the container has a value of $F^*=11768.260385$, and the dimensions are $(h^*, r^*)=(60.491, 11.542)$. Application of the specialized optimization procedure made it possible, for a given example, to reduce the mean time for finding a local minimum from 19.317 to 8.791 seconds.



a *b*

Fig. 6. Examples of the locally optimal arrangement of ellipsoids: *a* – in a cuboid; *b* – in a cylinder

Example 3. Locally optimal arrangement $N=50$ homothetic ellipsoids in a cuboid. The container has a volume of $F^*=33874.5$ and dimensions $(l^*, w^*, h^*)=(84.6863, 20, 20)$. Application of the specialized optimization procedure made it possible, for a given example, to reduce the mean time for finding a local minimum from 4,680 to 1,800 seconds; the number of iterations of the solver's optimization method is 1,000.

Example 4. Locally optimal arrangement $N=30$ of the directed homothetic ellipsoids in an elliptical container is shown in Fig. 7. The container has dimensions $(a^*, b^*, c^*)=(21.3155, 7.10516, 7.10516)$. of the Application of the specialized optimization procedure made it possible, for a given example, to reduce the mean time for finding a local minimum from 6,480 to 2,880 seconds; the number of iterations of the solver's optimization method is 1,000.

Example 5. Locally optimal arrangement $N=640$ of the directed homothetic ellipsoids in a cuboid. Volume of the container is $F^*=33874.5$, dimensions are $(l^*, w^*, h^*)=(84.6863, 20, 20)$. The mean time for finding a local minimum is 836.70 seconds: the number of iterations of the solver's optimization method is 500. Calculations without the specialized optimization procedure were not carried out due to the large dimensionality of the problem.

Fig. 7. Locally optimal arrangement of ellipsoids for example 4

Example 6. The feasible arrangement of $N=40$ ellipsoids in a sphere is shown in Fig. 8. The container's dimensions are $(r^*)=2.919435$. The mean time to find a local minimum is 34,182.59 seconds. Without the use of the specialized optimization procedure, the result was not obtained over three days.

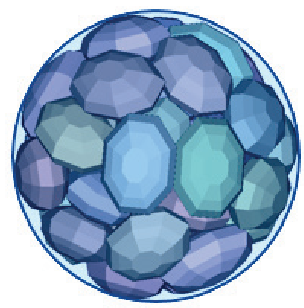


Fig. 8. Feasible arrangement of ellipsoids using the approximation

Fig. 8 shows a locally optimal solution to the problem on packing the polyhedra that approximate ellipsoids, which corresponds to the feasible arrangement of true ellipsoids.

8. Discussion of results of studying the problem on the optimal packing of ellipsoids

Owing to the developed means of modeling, we constructed a mathematical model in the form of a linear non-convex programming task.

It should be noted that by using the proposed means of modeling the constraints for arrangement, one can consider the problems on packing the ellipsoids in which a container is the convex containers, which are the combinations of containers that were considered in this work.

The benefits of our work include the construction of a precise mathematical model of the problem, and the development of a procedure of decomposition for the method of optimization of packing the ellipsoids, which makes it possible to significantly reduce the cost of computing resources while searching for a local extremum in the problem. We should also note that many types of containers were considered, some of which (for example, a cylinder) were not examined in studies by other researchers.

The disadvantage is the fact that for some containers, to construct a mathematical model, we used approximations, which is why for such a case the result of solving the problem is a feasible solution, rather than the locally optimal one.

Limitations of this study for the time being are the lack of a means to model the required constraints for ellipsoids and certain types of containers; however, their construction might be continuation of our study.

9. Conclusions

1. We have developed the tools for the mathematical modeling and computer simulation of constraints that occur between objects in problems on packing the ellipsoids into a convex container. To describe the constraints for non-overlapping, we used the quasi-phi-functions, and to analytically describe the containment constraint – we applied the phi-functions. The container considered took the shape of a cuboid, a cylinder, a sphere, an ellipsoid, and a convex polyhedron.

2. By using the proposed phi-functions and quasi-phi-functions, we constructed a precise mathematical model in the form of a non-linear non-convex programming task. The objective function for the constructed problem might be the volume of a container or one of its metric characteristics, while the region of feasible solutions is described by phi-inequalities and quasi phi- inequalities, which ensure that the constraints for arrangement are met. The model could be directly realized by means of modern local or global solvers and, depending on the shape of a container, makes it possible to obtain locally optimal or feasible solutions.

3. To solve the problem, the algorithm is proposed, based on the method of a multistart and the specialized optimization procedure of decomposition. The paper describes a fast algorithm for constructing the starting points from the region of feasible values. We have developed a decomposition procedure for the method to optimize the packing of ellipsoids, which makes it possible to reduce the problem of large dimensionality to a sequence of tasks with smaller dimensionality. The procedure makes it possible to significantly reduce the cost of computing resources while searching for a local extremum in the problem. The effectiveness of the proposed solution algorithm and the decomposition procedure is confirmed by the results of numerical experiments, which were conducted for containers of different shapes.

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