On the densest packing of equal spheres into a three - dimensional convex set

Nguyen Huy Liem[1], Phung The Bao[2,*], Ta Trung Thanh[3], Vuong Anh Tuan[1], Pham Thi Tuyet[4]
[1]Le Quy Don University, [2]Tran Dai Nghia University
[3]Irkutsk National Research Technical University, Irkutsk, Russia
[4]Academy of Air Defense and Air Force, Vietnam

ABSTRACT

Packing problems are classic problem of mathematical optimization and are very interesting NP - hard optimization problems with a wide variety of applications. That is, no procedure is able to exactly solve them in deterministic polynomial time. In this paper, we focus on problems dealing with circular objects, being three - dimensional. A special algorithm based on the optical - geometric approach for solving the problem is suggested. We also present illustrative numerical results using our algorithm both in three - dimensional Euclidean and non - Euclidean spaces.

Keywords: *packing equal spheres, three - dimensional space, optimal packing of spheres, optical - geometric approach, billiard simulation*

1. INTRODUCTION

The circle packing problem is one of the most popular problems among mathematicians in the last years. It has arisen for a long time, but still, it remains relevant, due to its wide applications in various fields of industry, such as production, logistics, circular cutting, communication networks, facility location and materials science [1 - 3]. For example, in materials science, the problem of packing balls is used to model certain models of absorption of molecules [4], in radio - surgery, packing of unequal balls is used in planning automated radio - surgical treatment [5]. In practical life, for example, when designing a city, this problem is used to plant trees in a given region in order to maximize forest density [6]. Or in logistics it is used for a facility location problem or a segmentation of logistics service areas [7 - 8].

The packing problem, as defined in [9], consist in packing a set of geometric objects of fixed shapes into an area of a predetermined shape. The packing identifies the arrangement and positions of the geometric objects that determine the dimensions of the containing shape and reach the extremum of a specific objective function [9]. In this paper, we focus on special objects having a fixed form of a ball with the same radii, an area of arbitrary three - dimensional convex shape and the objective function is to maximize the radius of packed objects.

Most published materials deal with the problem of packing circles in two - dimensional space. Many packaging results for various containers (such as a triangle, a semicircle, a circular quadrant ...) were published in [10] and they are regularly updated. Some of them were proved optimal, for example, for the problem of packing equal circles into square, optimal results were proved with the number of circles up to 36 [11 - 12], and into circle up to 19 [13 - 16].

Corresponding author: Dr. Phung The Bao
Email: phungthebao2003@gmail.com

In particular, Szabo and Specht proposed the result of packing circles into unit square up to 200 circles [17]. For the circular container many results are proposed in [16, 18 - 19].

For circle packing into a rectangle with given length and minimal width, Hifi and M'Hallah [20] propose the constructive heuristic and the genetic algorithm. Galiev and Lisafina in their work [21] proposed linear models for determining the maximum number of congruent circles of the given radius that can be packed into a given connected closed bounded domain.

In three - dimensional space, most work considers the problem of packing spheres into a popular container such as a cube, rectangular box, sphere, and cylinder. In [22] and [23] the authors consider the problem of packing identical spheres into a rectangular parallelepiped and a cylinder of minimal height.

In the case where the container is a cube or a sphere, many works are published. Gensane, in his work [24], used the billiard simulation method to solve the problem of packing equal spheres into a unit cube. Tatarevic proposed an algorithm to determine the smallest size of a cube that contains all spheres of unit radius [25]. In [26] authors used a variable neighborhood search for solving the problem of packing unit radius spheres into the smallest cube.

The vast majority of books and articles devoted to the study of the problem of packing in Euclidean space. In the case of non - Euclidean metrics, this problem is weakly studied.

In this paper, we propose an algorithm, which can solve the sphere packing problem in various cases. We consider the packing problem in both three - dimensional Euclidean and non - Euclidean spaces. In the case of non - Euclidean space, we use a special non - Euclidean metric, which means not the distance between points, but the time that is required to pass this way.

2. FORMULATION

Let X is three - dimensional metric space, let P is closed convex set in X. The distance between the points of the space X is defined as follows:

$$\rho(a,b) = \min_{G \in G(a,b)} \int_G \frac{dG}{f(x,y,z)}, \qquad (1)$$

where $G(a,b)$ is the set of all continuous curves, which belong X and connect the points a and b, and $0 < \alpha \le \beta f(x,y,z) \le$ is a continuous function, which specifies the instantaneous speed of movement at any point $T(x,y,z) X \in$.
Let $S_i, i = \overline{1,n}$ be congruent balls with centers $s_i(x_i, y_i, z_i)$ and radii R. We need to find vector, $s = (s_1, s_2, \ldots, {}_n) \in R^{3n}$ which ensures that the radius of the given number of balls reached maximum, and all balls are inside P.
The problem of packing spheres in our article is rewritten as follows.

$$R \rightarrow max \qquad (2)$$

$$\rho(s_i, s_j) \ge 2R, \forall i, j = \overline{1,n}, i \ne j \qquad (3)$$

$$\rho(s_i, \partial P) \ge R, \forall i = \overline{1,n} \qquad (4)$$

$$s_i \in P, \forall i = \overline{1,n} \qquad (5)$$

Here ∂P is the boundary of the set P, $\rho(s_i, \partial P)$ is the distance from a point to the closed surface. The objective function (2) maximizes the radius of the packed spheres. Inequality (3) ensures that no circles overlap each other. Inequalities (4) - (5) are the constraints which ensure that every circle is fully inside the container.

3. SOLUTION METHOD

When one considers the packing problem in three - dimensional space, it is important to be able to measure the distance from the point to the surface (as well as the distance between two points) with respect to the given metric. To solve this problem, the authors proposed an algorithm based on the fundamental principles of Fermat and Huygens. A more detailed description of the algorithm can be found in [27] and for the three - dimensional case, it is presented in [28].

Here we extend our method for the two -dimensional problem (see [29]) to the three - dimensional case. The main idea of the algorithm is to partition the set P into Dirichlet cells P_i with respect to the known vector S of centers of packed spheres [30]. Then, for each Dirichlet cell the billiard simulation algorithm is used to find a new center $s_i^* \in P_i$ and radius R_i of the inscribed ball, where:

$$R_i = \rho(s_i^*, \partial P_i) = \max_{p \in P_i} \rho(p, \partial P_i).$$

We will describe these steps in more detail below.

3.1. The algorithm for constructing Dirichlet cells

This algorithm is based on the fundamental principles of Fermat and Huygens [28]. Let a set P and n points $s_i, i = \overline{1,n}$ be given. It is necessary to split the set into n_i subsets P_i so that, the distance from each point of the subset P_i to the corresponding point s is less than the distance to any other point.

- *Step 1:* A light wave is emitted from each given point $s_i, i = \overline{1,n}$
- *Step 2:* For each point $\alpha \in P$, the time to reach the light wave from each source is calculated. An array $t_\alpha = \{t_\alpha^1, t_\alpha^2, \ldots, t_\alpha^n\}$ is used to keep track of the time it takes light from all sources to reach point α.
- *Step 3:* The minimum value $t_{\min} = \min\{t_\alpha^1, t_\alpha^2, \ldots, t_\alpha^n\}$ is calculated. If $t_{\min} = t_\alpha^i$ then point α belongs to the subset P_i.

3.2. The algorithm for packing n spheres into a closed set

In this subsection, we describe the algorithm for packing n spheres into a closed set. Note that this algorithm does not provide a global solution.

- *Step 1:* Approximate the surface function by the grid function using a uniform grid with a step h.
- *Step 2:* Specify the maximum number of iterations, set the value of the iteration number counter $Iter = 1$.
- *Step 3:* Randomly generate an initial vector $s = (s_1, s_2, ..., s_n)$, which satisfies the constraint (5). The radius R is assumed to be zero.
- Step 4: The set P is divided into subsets by $P_i, i = \overline{1,n}$ Algorithm for constructing Dirichlet cells.
- *Step 5:* For each $P_i, i = \overline{1,n}$ we find the coordinates of the packed sphere center O_i and its maximum radius R_i by the billiard simulation algorithm below.
- *Step 6:* Calculate $R = \min R_i, i = \overline{1,n}$

Steps 4 - 6 are repeated as long as R increases.

- *Step 7:* The counter of an initial solution generations Iter is incremented. If it becomes equal a pre-assigned value, then the algorithm is terminated. Otherwise, go to Step 4.

3.3. The billiard simulation algorithm for packing a sphere into a closed set

In this subsection we propose an algorithm based on the principle of billiard modeling [18]. According to this principle, packing spheres are billiard balls that can move inside a given closed set. During the movement of the balls, its radius increases.

Assuming that there is a closed set P_i, we need to find the maximal sphere with center s_i and radii R_i that is inside P_i.

- *Step 1:* The initial coordinate of point s_i is generated randomly and the distance $\rho(s_i, \partial P_i)$ from point to the boundary of the set P_i is calculated.
- *Step 2:* Construct a ball with center and radii and find the set of tangent points M_i:

$$M_i = \{m \mid \rho(s_i, m) = R_i, m \in \partial P_i\}$$

- *Step 3:* Construct vectors whose origins are located in the center of the ball s_i, and the terminuses belong to the corresponding tangent points set M_i. If there are more than one such vectors, we find the sum vector:

$$\vec{c} = \sum_{m \in M_i} \overrightarrow{s_i m}$$

- *Step 4:* Move s_i against the direction of $\vec{c}$ the distance h. The obtained point s_i^* becomes the new center of the packed ball.

Steps 2 - 4 are carried out as long as the radius increases. The algorithm is completed if the radius of the current iteration is less than the previous one. As a result, we obtain the radius and coordinates of the centers of the packed balls.

4. COMPUTATIONAL EXPERIMENT

In this section, we present some preliminary numerical results. The experiment is carried out on a personal computer with a Itel(R) Core(TM) i5-3570K 3.4GHz processor and 8GB RAM running on 64-bit Windows 7 operating system. CPU times are given in seconds. The algorithm is implemented in C# programming language using Visual Studio 2012.

Example 1. To check the accuracy of the algorithm we will consider the Euclidean metric space $(f(x,y,z)\equiv 1)$ and the unit sphere container. **Table 1** shows the comparison of our results ($R_{\max}$) with the best known result (R_{known}) from [31]. Here and further time $t_{executed}$ is measured in seconds.

Table 1. *Comparison of packing results for the unit sphere with the Euclidean metric*

n	R_{known}	$R_{\max}$	Relative error (%)	$t_{executed}$
2	0.25000	0.25000	0	134
3	0.46410	0.46394	0.035	227
4	0.44948	0.44922	0.060	304
5	0.41421	0.41354	0.162	524
6	0.41421	0.41348	0.184	688
7	0.38591	0.38439	0.394	857
8	0.37802	0.37651	0.400	984
9	0.36603	0.36455	0.403	1,378
10	0.35305	0.35157	0.419	1,712
15	0.31830	0.31482	1.094	2,487
20	0.28789	0.28458	1.149	3,515

It should be noted that the calculation error depends on the grid step h. Here and further step of grid h = 0.001. The deviation of the radius of the packed spheres is not greater than 1.15%. The reduction of the grid step increases the computational accuracy, but calculation time increases significantly. In this example, with the number of balls n=20 , the calculation time is 3h 16min.

Example 2. In this example we pack equal balls into cylinder in the Euclidean metric space $(f(x,y,z)\equiv 1)$. A closed circular cylinder has a diameter of 1 unit and a height of 1 unit. Some of the results are shown in **Table 2** and in **Figure 1**.

***Table 2.** Packing of equal spheres in cylinder*

n	$R_{\max}$	Relative error (%)	$t_{executed}$
1	0.4982	65.95	153
2	0.2928	26.78	248
3	0.25962	28.00	323
4	0.24942	33.102	625
5	0.24348	38.491	758
6	0.23233	40.127	976
7	0.21935	39.401	1,047
8	0.21124	40.217	1,178
9	0.20280	40.035	1,632
10	0.19442	39.194	2,478

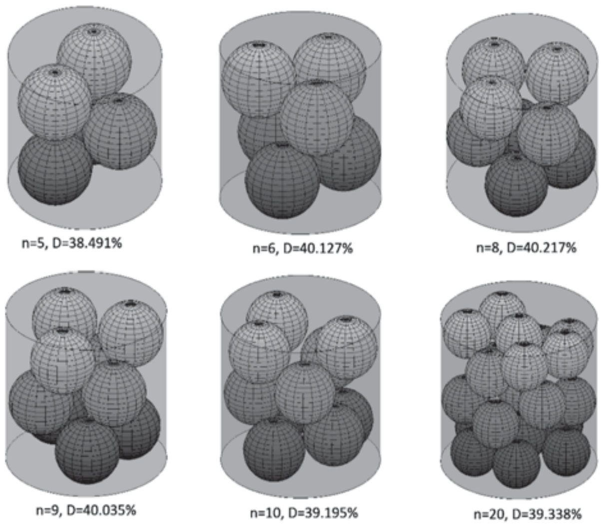

***Figure 1.** Packing of equals spheres in Cylinder*

Considering **Table 2** we can see that the highest density is achieved for $n = 1$. In this case, the radius of the ball almost reaches the optimal value ($R_{optimal} = 0.5$). When $n>1$ as the number of balls increases, the packing density also increases.

Example 3. Consider the problem of placing underwater mines in a given territory. The mines are located in such a way that the affected area of individual mines should not overlap (for example, to exclude serial triggering), and the combined area of effect of all installed mines was maximum. Let the area under consideration be a rectangular box 80 m wide, 100 m long and 60 m high. This problem is equivalent to the problem of packing equal spheres into a rectangular box. The results are shown in **Table 3** and **Figure 2**.

***Table 3.** Packing of equal spheres in a rectangular box*

n	$R_{\max}$	Relative error (%)	$t_{executed}$
1	30.00	23.56	58
2	26.83	33.69	144
3	22.92	31.52	326
4	21.75	35.94	834
5	20.00	34.91	1,214
6	18.52	33.15	1,832
7	17.84	34.45	2,418
8	17.35	36.46	2,574
9	16.82	37.24	3,018
10	16.04	39.91	3,427

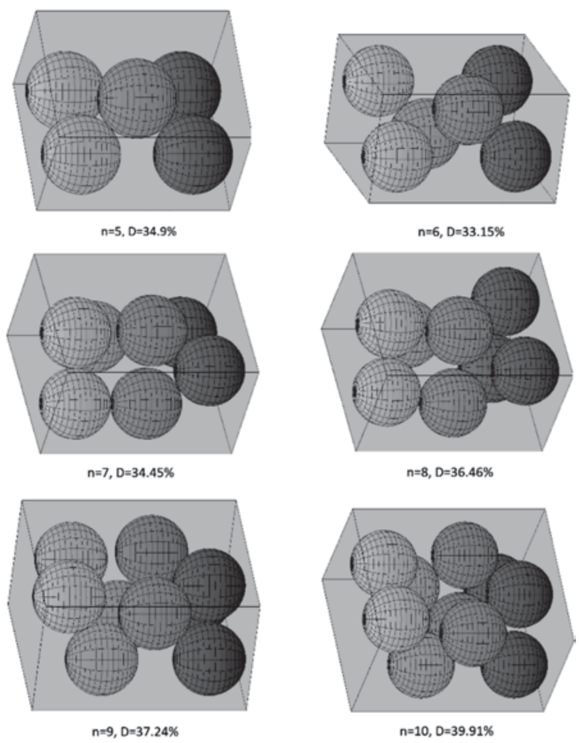

***Figure 2.** Packing of equals spheres in rectangular box*

Example 4. In this example we consider the sphere packing problem for the non - Euclidean space. The metric is given by formula (1) where $f(x,y,z)=x+y+1$.

It means that the light velocity linearly increases with respect to coordinates. In this metric space, the wave fronts have the shape of a sphere (as in Euclidean), but the center of the sphere shifts toward the origin.

The container is a part of a sphere and
$P=\{(x,y,z)\in R^3 : 0\le x,y,z\le 1, x^2+y^2+z^2\le 1\}$
The results are shown in **Table 4** and **Figure 3**. Note that in **Figure 3** balls look different, but they have the same radius in a given metric.

Table 4. *Packing of equal spheres in non - Euclidean space*

n	R_{max}	Relative error (%)
1	0.21689	38.583
2	0.16011	28.623
3	0.13913	29.153
4	0.13897	36.945
5	0.12140	28.677
6	0.11685	32.188
7	0.11609	38.329
8	0.10823	31.352
9	0.10477	35.692
10	0.10296	36.863

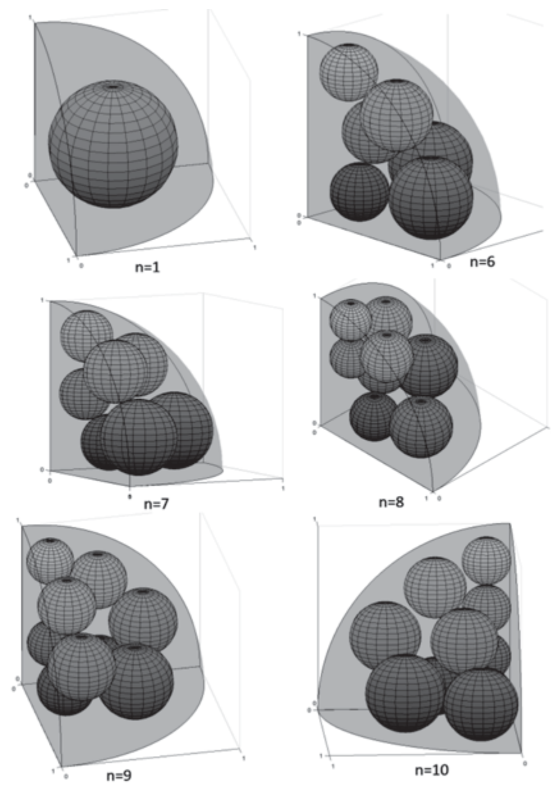

***Figure 3**. Packing in non - Euclidean metrics*

5. CONCLUSION

In this article, we consider the problem of packing equal balls into a three-dimensional convex set. The presented algorithm works on both Euclidean and non - Euclidean spaces and allows us to find good packaging results in various cases.

The results of the computational experiments make it possible to conclude that the algorithm is operable. The disadvantages of the algorithm are high computational complexity.

The proposed algorithms can be used to solve the problem of the unequal sphere packing and for the non-convex containers. The authors use a modified algorithm to solve the problem of packing two types of spheres.

REFERENCES

[1] I. Castillo, F. J. Kampas, J. D. Pinter, "Solving circle packing problems by global optimization: Numerical results and industrial applications", *uropean Journal of Operational Research*, vol. 191, iss. 3, 2008, pp. 786 – 802.

[2] J. A. George, J. M. George and B. W. Lamar, "Packing different – sized circles into a rectangular container", *European Journal of Operational Research*, vol.84, 1995, pp. 693 – 712.

[3] J. A. George, "Multiple container packing: a case study of pipe packing", *Journal of the Operational Research Society*, vol. 47, 1996, pp. 1098 – 1109.

[4] F. Harary, W. Randolph, P. G. Mezey, "A study of maximum unit-circle caterpillars — tools for the study of the shape of adsorption patterns", *Discrete Applied Mathematics*, vol. 67, iss. 1 – 3, 1996, pp. 127 – 135.

[5] J. Wang, "Packing of Unequal Spheres and Automated Radiosurgical Treatment Planning", *Journal of Combinatorial Optimization*, vol. 3, 1999, pp. 453 – 463.

[6] P. Szabo, M. Markot, T. Csendes, E. Specht, and L. Casado, "New approaches to circle packing in square with program codes," *in Springer US*, New York, 2007.

[7] A. L. Kazakov, A. A. Lempert and D. S. Bukharov, "On segmenting logistical zones for servicing continuously developed consumers", *in Automation and Remote Control*, vol. 74 (6), 2013, pp. 968 – 977.

[8] A. L. Kazakov and A. A. Lempert, "On mathematical models for optimization problem of logistics infrastructure", *in International Journal of Artificial Intelligence*, vol. 13 (1), 2015, pp. 200 – 210.

[9] Y. Stoyan, "Mathematical methods for geometric design", *in Advances in CAD/CAM//. Proceeding PROLAMAT82*. Leningrad, USSR, 1982, pp. 67 – 86. Amsterdam: North-Holland.

[10] E. Specht, "Packomania". Internet: http://www.packomania.com, 2010.

[11] K.J.Nurmela and P.R.J. Ostergard , "Packing up to 50 equal circles in a square", *in Discrete and Computational Geometry*, vol. 18, 1997, pp. 111 – 120.

[12] M.Cs. Markot and T.A. Csendes, "A new verified optimization technique for the packing circles in a unit square problems", *In SIAM Journal on Optimization*, vol. 16, 2005, pp. 193 – 219.

[13] F. Fodor, "The densest packing of 19 congruent circles in a circle", *in Contributions to Algebra and Geometry*, vol. 74 (2), 1999, pp. 139 – 145.

[14] F. Fodor, "The densest packing of 12 congruent circles in a circle", *in Contributions to Algebra and Geometry*, vol. 43, 2000, pp. 401 – 409.

[15] F. Fodor, "The densest packing of 13 congruent circles in a circle", *in Contributions to Algebra and Geometry*, vol. 40 (2), 2003, pp. 431 – 440.

[16] A. Grosso, A. R. M. J. U. Jamali and M. Locatelli, "Solving the problem of packing equal and unequal circles in a circular container", *Journal of Global Optimization*, vol. 47, 2010, pp. 63 – 81.

[17] P. Szabo and E. Specht, "Packing up to 200 equal circles in a square.models and algorithms for global optimization", *Optimization and Its Applications*, vol. 4, 2007, pp. 141 – 156.

[18] R. L. Graham, B. D. Lubachevsky, K. J. Nurmela and P. R. J. Ostergard, "Dense packings of congruent circles in a circle", *in Discrete Mathematics*, vol. 181, 1998, pp. 139 – 154.

[19] E. G. Birgin and F. N. C. Sobral, "Minimizing the object dimensions in circle and sphere packing problems", *Computers and Operations Research*, vol. 35, 2008, pp. 2357 – 2375.

[20] M. Hifi and R. M'Hallah, "Approximate algorithms for constrained circular cutting problems", *Computers and Operations Research*, vol. 31 (5), 2004, pp. 675 – 694.

[21] S. I. Galiev and M. S. Lisafina, "Linear models for the approximate solution of the problem of packing equal circles into a given domain", *European Journal of Operational Research, Elsevier*, vol. 230 (3), 2013, pp.505 – 514.

[22] Y. Stoyan and G. Yaskov, "Packing Identical Spheres into a Rectangular Parallelepiped", *in Intelligent Decision Support*, Gabler, 2008, pp.47 – 67.

[23] Y. G. Stoyan and G. Yaskov, "Packing identical spheres into a cylinder", *International Transactions in Operational Research*, vol. 17, 2009, pp. 51 – 70.

[24] T. Gensane, "Dense packing of equal spheres in a cube", *the Electronic Journal of Combinatorics*, vol. 11, 2004, pp. 1 – 17.

[25] M. Tatarevic, "On limits of dense packing of equal spheres in a cube", *CoRR, abs*/1503.07933, 2015, Internet:

http://arxiv.org/abs/1503.07933.

[26] R. M'Hallah and A. Alkandari, "Packing Unit Spheres into a Cube Using VNS", *Electronic Notes in Discrete Mathematics*, vol. 39, 2012, pp. 201 – 208.

[27] A. L. Kazakov and A. A. Lempert, "An approach to optimization in transport logistics", *in Automation and Remote Control*, vol. 72(7), 2011, pp. 50 – 57.

[28] A. L. Kazakov, A. A. Lempert and T. T. Thanh, "The sphere packing problem into bounded containers in three - dimension non - Euclidean space", *in IFAC – Papers On Line*, vol. 51(32), 2018, pp. 782 – 787.

[29] A. L. Kazakov, A. A. Lempert and N. H. Liem, "The problem of the optimal packing of the equal circles for special non - euclidean metric", *Communications in Computer and Information Science*, vol. 661, 2017, pp. 25 – 68.

[30] F. Preparata and M. Shamos, *Computational Geometry: An Introduction*. New York: Springer – Verlag, Berlin, Heidelberg, 1985.

[31] H. Pfoertner, "Densest packings of n equal spheres in a sphere of radius 1", 2008, Internet: www.randomwalk.de/sphere/insphr/spisbest.txt

Phương pháp giải bài toán sắp xếp các khối cầu giống nhau vào tập lồi trong không gian ba chiều

Nguyễn Huy Liêm[1], Phùng Thế Bảo[2,*], Tạ Trung Thanh[3], Vương Anh Tuấn[1], Phạm Thị Tuyết[4]

TÓM TẮT

Bài toán đóng gói là một trong những bài kinh điển của toán tối ưu thuộc lớp các bài toán NP khó với rất nhiều ứng dụng khác nhau trong cuộc sống cũng như trong khoa học. Điều đó có nghĩa là không tồn tại một phương pháp cụ thể để giải bài toán này trong một khoảng thời gian xác định. Trong nội dung bài báo, nhóm tác giả tập trung vào vấn đề sắp xếp các khối cầu giống nhau vào một tập lồi trong không gian ba chiều. Nhóm tác giả đề xuất một thuật toán dựa trên phương pháp quang hình học để giải quyết bài toán. Trong nội dung bài báo cũng trình bày một số kết quả minh họa trong không gian ba chiều cho các trường hợp khoảng cách Euclid và phi Euclid.

Từ khóa: *đóng gói hình cầu giống nhau, không gian ba chiều, đóng gói tối ưu hình cầu, phương pháp quang hình học, thuật toán mô phỏng bi-a*

Received: 10/11/2020
Revised:22/11/2020
Accepted for publication: 7/12/2020