Quasi-Phi-Functions in Packing Problem of Ellipsoids

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Abstract - **The paper considers the problem of packing a given collection of ellipsoids of revolution into a rectangular container of minimal volume. Our ellipsoids can be continuos rotated and translated. A class of radical-free quasi-phi-functions is used for an analytical description of non-overlapping and containment constraints. We formulate the packing problem in the form of a nonlinear programming problem and propose a solution strategy, which allow us to search for local optimal packings. The actual search for a local minimum is performed by IPOPT. We provide computational results.**

Index Terms – **packing, ellipsoids, continuous rotations, non-overlapping, containment, quasi-phi-functions, solution algorithm, nonlinear optimization**

I. Introduction

In this paper we deal with the optimal ellipsoid packing problem, which is a part of operational research and computational geometry. The problem is NP-hard [1] and has multiple applications in modern biology, mineralogy, medicine, materials science, nanotechnology, as well as in the chemical industry, power engineering etc.

Our approach is based on mathematical modeling of relations between ellipsoids and thus reducing the packing problem to a nonlinear optimization problem. To this end a class of quasi-phi-functions [2] is used for analytic description of placement of ellipsoids in a rectangular container taking into account their continuous rotations and translations.

The paper is organized as follows: In Section 2 we formulate the optimal ellipsoid packing problem and give a short review of related works. In Section 3 we define quasi-phi-functions for nonoverlapping and containment constraints. In Section 4 we propose a mathematical model as a continuous nonlinear programming problem by means of quasi-phi-functions and describe a solution strategy. In Section 5 we provide our computational results. Finally we give some conclusions in Section 6.

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II. Problem Formulation

We consider here a packing problem in the following setting**.** Let Ω denote a rectangular domain of length l, width w and height h. All of these dimensions may be variable, or one (two) may be fixed and the other variable. Suppose a set of ellipsoids of revolution, E_i, $i \in \{1, 2, \ldots, n\} = I_n$, is given to be placed in Ω without overlaps. Each ellipsoid E_i is generated by rotation of an ellipse of semi-axes a_i and b_i, $a_i > b_i$, along the axis of revolution *OX*, therefore we assume that third semi-axe is defined as $c_i = b_i$. With each ellipsoid E_i we associate its local coordinate system whose origin coincides with the center of the ellipsoid and the coordinate axes are aligned with the ellipsoid's axes. In that system the ellipsoid is described by parametric equations $x = a_i \cos t_i$, $y = b_i \sin t_i \cos g_i$, $z = b_i \sin t_i \sin g_i$, $0 \le t_i \le 2\pi, 0 \le g_i \le 2\pi$. We also use a fixed coordinate system attached to the container Ω. The location and orientation of each ellipsoid E_i is defined by a variable vector of its placement parameters (v_i, θ_i). Here $v_i = (x_i, y_i, z_i)$ is a translation vector, $\theta_i = (\theta_i^1, \theta_i^2)$ is a vector of rotation parameters, where θ_i^1, θ_i^2 are appropriate angles from axis OX to OY, from axis OY to OZ in the local coordinate system of ellipsoid E_i. The rotated by angles θ_i^1, θ_i^2 and translated by vector v_i ellipsoid E_i is defined as $E_i(u) = \{p \in R^3 : p = v_i + M(\theta_i) \cdot p^0, \forall p^0 \in E_i^0\}$, where E_i^0 denotes the non-translated and non-rotated ellipsoid E_i, $M(\theta) = M_2(\theta_i^2) \cdot M_1(\theta_i^1)$ is a rotation matrix, where

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

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

Packing problem of ellipsoids. Pack the set of ellipsoids E_i, $i \in I_n$, within a rectangular domain

$\Omega = \{(x, y, z) \in R^3 : 0 \le x \le l, 0 \le y \le w, 0 \le z \le h\}$ of minimal volume. If one of the two dimensions (l or w or h) is fixed, we need to minimize the other ones. If all are variable, it is natural to minimize the volume $F = l \cdot w \cdot h$ of the container.

At present, the interest in finding effective solutions for placement problems of ellipsoids is growing rapidly (see, e.g., [4-8]). This is due to a large number of applications and an extreme complexity of methods used to handle many of them.

The remarkable method of the problem of cutting ellipses from a rectangular plate of minimal area was developed by Josef Kallrath and Steffen Rebennack, see [10]. The paper offers a good overview of related publications. For a small number of ellipses they are able to compute a globally optimal solution subject to the finite arithmetic of global solvers at hand. However, for more than 14 ellipsoids none of the nonlinear programming (NLP) solvers available in GAMS can even compute a locally optimal solution. Therefore, the authors of [10] develop polylithic approaches, in which the ellipses are added sequentially in a strip-packing fashion to the rectangle restricted in width but unrestricted in length. The rectangle's area is minimized at each step in a greedy fashion. The sequence in which they add ellipses is random; this adds some GRASP flavor to the approach. The polylithic algorithms allow the authors to compute good solutions for up to 100 ellipses.

Paper [9] studies the problem of placing a given collection of ellipses into a rectangular container of minimal area. Radical free quasi-phi-functions are used to reduce it to a nonlinear programming problem and develop an efficient solution algorithm. The paper provides computational results with local optimal solutions for the problem (up to 120 ellipses).

The present paper proposes an approach, which is capable of handling precise ellipsoids (without approximations) and thus finding an exact local optimal solution. The approach can be considered as some extension of quasi-phi-functions for ellipses, derived in [9], to 3D case.

III. Quasi-phi-functions for Nonoverlapping and Containment Constraints

Quasi-phi-functions for nonoverlapping constraints. Let $E_i(u_i)$ and $E_j(u_j)$ be two ellipsoids of revolution with semi-axes a_i, b_i, c_i and a_j, b_j, c_j.

Then, a quasi-phi-function for $E_i(u_i)$ and $E_j(u_j)$ may be defined as follows

$$\Phi'_{ij}(u_i, u_j, u'_{ij}) = \min\{\chi(\Theta_i, \Theta_j, u'_{ij}), \chi_1^+(u_i, u_j, u'_{ij}),$$

$$\chi_1^-(u_i, u_j, u'_{ij}), \chi_2^+(u_i, u_j, u'_{ij}), \chi_2^-(u_i, u_j, u'_{ij})\}, \quad (1)$$

where $u'_{ij} = (t_i, g_i, t_j, g_j)$,

$$\chi = -\langle N'_i, N'_j \rangle = -\alpha'_i\alpha'_j - \beta'_i\beta'_j - \gamma'_i\gamma'_j, \ \Theta_i = (\theta_i^1, \theta_i^2),$$

$$(\alpha'_i, \beta'_i, \gamma'_i) = M(\Theta_i) \cdot (\alpha_i, \beta_i, \gamma_i)^T,$$

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

$$\Theta_j = (\theta_j^1, \theta_j^2), \ (\alpha'_j, \beta'_j, \gamma'_j) = M(\Theta_j) \cdot (\alpha_j, \beta_j, \gamma_j)^T,$$

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

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

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

$(x_{jk}^+, y_{jk}^+, z_{jk}^+)$ are coordinates of point q_{jk}^+ and $(x_{jk}^-, y_{jk}^-, z_{jk}^-)$ are coordinates of point q_{jk}^-, $k = 1, 2$ (see Fig.1).

We derive q_{jk}^+ and q_{jk}^- as follows:

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

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

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

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

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

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

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

Thus a nonoverlapping constraint, i.e. $\operatorname{int} E_i(u_i) \cap \operatorname{int} E_j(u_j) = \varnothing$, can be defined as $\Phi'_{ij}(u_i, u_j, u'_{ij}) \ge 0$, where Φ'_{ij} is a quasi-phi-function of ellipsoids $E_i(u_i)$ and $E_j(u_j)$ given by (1).

Quasi-phi-functions for containment constraints. Let vertices of our rectangular container $\Omega = \{(x, y, z) \in R^3 : 0 \le x \le l, 0 \le y \le w, 0 \le z \le h\}$ be given as follows: $\{v_i, i = 1, \dots, 8\} = \{(0, w, 0), (l, w, 0), (l, 0, 0), (0, 0, 0), (0, w, h), (l, w, h), (l, 0, h), (0, 0, h)\}$.

And let $E_i(u_i)$ be ellipsoid of revolution with semi-axes a_i, b_i and $c_i = b_i$, $a_i > b_i$, $i = 1, 2 \dots, n$.

Then a quasi-phi-function for $E_i(u_i)$ and object $\Omega^* = R^3 \setminus \operatorname{int} \Omega$ may be defined in the form

$$\Phi'_i(u_i, u'_i) = \min\{\varphi_{i1}(u), \varphi_{i2}(u), \varphi_{i3}(u)\}, \quad (2)$$

where $(u_i, u'_i) \in R^{11}$, $u'_i = (t'_{i1}, t'_{i2}, t'_{i3}, g'_{i1}, g'_{i2}, g'_{i3})$, $0 \le t'_{ik} \le 2\pi$, $0 \le g'_{ik} \le 2\pi$,

$$\varphi_{i1}(u) = \min\{\varphi_{11}^i(v_1), \varphi_{11}^i(v_2), \varphi_{11}^i(v_3), \varphi_{11}^i(v_4),$$

$$\varphi_{12}^i(v_5), \varphi_{12}^i(v_6), \varphi_{12}^i(v_7), \varphi_{12}^i(v_8)\},$$

$$\varphi_{i2}(u) = \min\{\varphi_{21}^i(v_1), \varphi_{21}^i(v_4), \varphi_{21}^i(v_5), \varphi_{21}^i(v_8),$$

$$\varphi_{22}^i(v_2), \varphi_{22}^i(v_3), \varphi_{22}^i(v_6), \varphi_{22}^i(v_7)\},$$

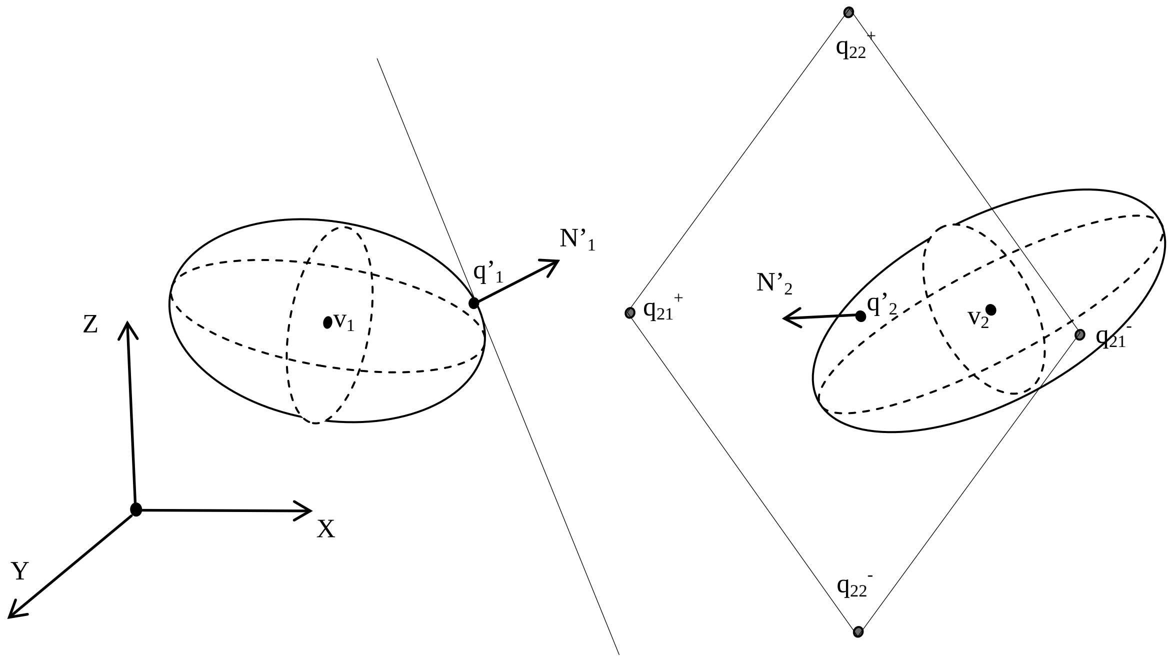


Fig. 1 Illustration to construction of a quasi-phi-function for two ellipsoids $E_1(u_1)$ and $E_2(u_2)$

$$\varphi_{i3}(u) = \min\{\varphi^{i}_{31}(v_1), \varphi^{i}_{31}(v_2), \varphi^{i}_{31}(v_5), \varphi^{i}_{31}(v_6), \varphi^{i}_{32}(v_3), \varphi^{i}_{32}(v_4), \varphi^{i}_{32}(v_7), \varphi^{i}_{32}(v_8)\},$$

$$\varphi^{i}_{k1} = A_{ik}x + B_{ik}y + C_{ik}z + D_{ik} - 1,$$

$$\varphi^{i}_{k2} = -A_{ik}x - B_{ik}y - C_{ik}z - D_{ik} - 1,$$

$$(A_{ik}, B_{ik}, C_{ik}) = M(\Theta_i)(a_i \cos t_{ik}, b_i \sin t_{ik} \cos g_{ik}, b_i \sin t_{ik} \sin g_{ik})^T,$$

$$D_{ik} = -A_{ik}x_i - B_{ik}y_i - C_{ik}z_i, \ k = 1, 2, 3.$$

Thus, a containment constraint, i.e. $E_i(u_i) \subset \Omega \Leftrightarrow \operatorname{int} E_i(u_i) \cap \Omega^* = \varnothing$, can be defined as $\Phi'_i(u_i, u'_i) \geq 0$, where Φ'_{ij} is a quasi-phi-function for $E_i(u_i)$ and Ω^* given by (2).

IV. Mathematical Model And Solution Strategy

The vector $u \in R^{\sigma}$ of all our variables can be described as follows: $u = (l, w, h, u_1, u_2, \ldots, u_n, \tau)$, where (l, w, h) denote the variable dimensions of the rectangular container Ω and $u_i = (v_i, \theta_i)$ is the vector of placement parameters for the ellipsoid E_i, $i \in I_n$, where $v_i = (x_i, y_i, z_i)$, $\theta_i = (\theta_i^1, \theta_i^2)$. The vector τ denotes the vector of extra variables (for our quasi-phi-functions), defined as follows:

$$\tau = (t^1_1, g^1_1, t^1_2, g^1_2, \ldots, t^m_1, g^m_1, t^m_2, g^m_2,$$
$$t'^1_1, g'^1_1, t'^1_2, g'^1_2, t'^1_3, g'^1_3, \ldots, t'^n_1, g'^n_1, t'^n_2, g'^n_2, t'^n_3, g'^n_3),$$

where t^k_1, g^k_1, t^k_2, g^k_2 are extra variables for the *k*-th pair of ellipsoids, $k = 1, \ldots, m$, $m = \dfrac{(n-1)n}{2}$, and t'^i_1, g'^i_1, t'^i_2, g'^i_2, t'^i_3, g'^i_3, are extra variables for each ellipsoid E_i, $i \in I_n$. Lastly, R^{σ} denotes the σ-dimensional Euclidean space, where $\sigma = 3 + 5n + 2n(n-1) + 6n = 2n^2 + 9n + 3$ is the number of the problem variables.

A mathematical model of the basic packing problem may now be stated in the following form:

$$\min_{u \in W \subset R^{\sigma}} F(u), \tag{3}$$

$$W = \{u \in R^{\sigma} : \Phi'_{ij} \geq 0, \Phi'_i \geq 0, i = 1, 2, \ldots, n, j = 1, 2, \ldots, n, j > i\}, \tag{4}$$

where $F(u) = l \cdot w \cdot h$, Φ'_{ij} is a quasi-phi-function (1) defined for the pair of ellipsoids E_i and E_j, (to hold *nonoverlapping* constraint), Φ'_i is a quasi-phi-function (2) defined for an ellipsoid E_i and the object Ω^* (to hold the *containment* constraint).

Our constrained optimization problem (3)-(4) is a continuous nonlinear programming problem.

We propose the following solution strategy for the problem, which involves three major stages:

1)First we generate a number of random starting points.

2)Then starting from each point obtained at Step 1 we search for a local minimum of the objective function *F*(u) of problem (3)-(4).

3)Lastly, we choose the best local minimum from those found at Step 2. This is our best solution of the problem (3)-(4).

V. Computational results

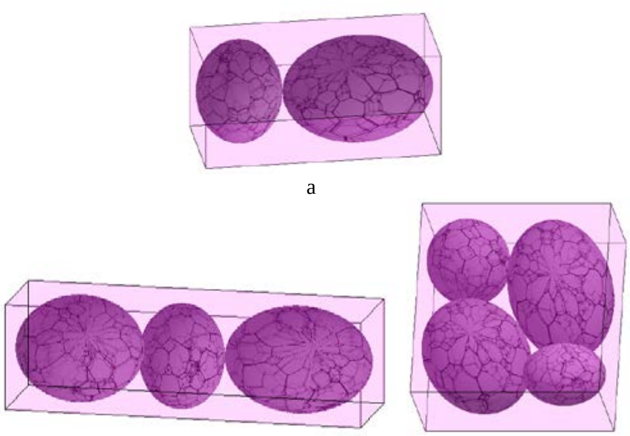
Here we present a number of Instances to demonstrate the efficiency of our quasi-phi-functions. We have run our experiments on an AMD Athlon 64 X2 5200+ computer. We search for 100 local minima to each of Instances. The actual search for a local minimum is performed by IPOPT proposed in [11], which is available at an open access noncommercial software depository (https://projects.coin-or.org/Ipopt) .

We consider a collection of ellipsoids: $\{E_i, i=1,..,12\}=\{(a_i, b_i, c_i), i=1,2,\dots,12\}=\{(5, 4, 4)$, (7, 5, 5), (6, 5, 5), (4, 3, 3), (5.5, 4.5, 4.5), (7.5, 5.5, 5.5), (6.5, 5.5, 5.5), (4.5, 3.5, 3.5), (5.3, 4.3, 4.3), (7.3, 5.3, 5.3), (6.3, 5.3, 5.3), (4.3, 3.3, 3.3)$\}$.

Instance E2. Local optimal placement of ellipsoids $\{E_i, i=1,2\}$ is shown in Figure 2,a. Container has volume $F^*=2192.513985$ and sizes $(l^*, w^*, h^*)=(10.000000,$ $10.006950,$ $21.909912)$. Average time per one local minimum is 2.09 sec.

Instance E3. Local optimal placement of ellipsoids $\{E_i, i=1,2,3\}$ is shown in Figure 2,b. Container has volume $F^*=3385.008834$ and sizes $(l^*, w^*, h^*)=(10.000000,$ $33.797139,$ $10.015667)$. Average time per one local minimum is 5.89 sec**.**

Instance E4. Local optimal placement of ellipsoids $\{E_i, i=1,\dots,4\}$ is shown in Figure 2,c. Container has volume $F^*=3539.283378$ and sizes $(l^*, w^*, h^*)=(18.273863, 10.014451, 19.340061)$. Average time per one local minimum is 22.76 sec.



a

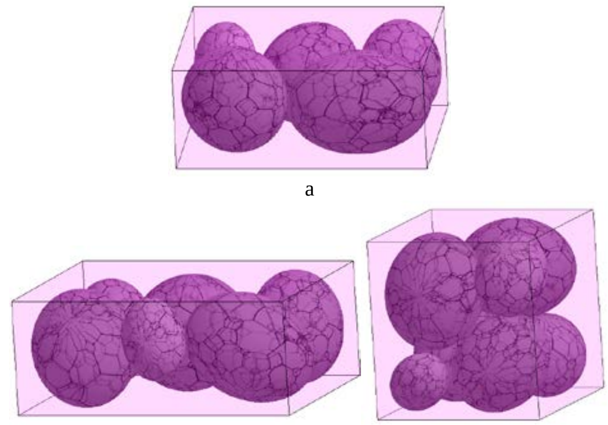
b c

Fig. 2. Local optimal placement of ellipsoids in Instances:
a − E2, b − E3, c − E4

Instance E5. Local optimal placement of ellipsoids $\{E_i, i=1,\dots,5\}$ is shown in Figure 3,a. Container has volume $F^*=4347.434370$ and sizes $(l^*, w^*, h^*)=(24.366822, 10.000252, 17.841164)$. Average time per one local minimum is 60.71 sec**.**

Instance E6. Local optimal placement of ellipsoids $\{E_i, i=1,\dots,6\}$ is shown in Figure 3,b. Container has volume $F^*=6312.236870$ and sizes $(l^*, w^*, h^*)=(27.244026, 11.000291, 21.062399)$. Average time per one local minimum is 126.02 sec**.**

Instance E7. Local optimal placement of ellipsoids $\{E_i, i=1,\dots,7\}$ is shown in Figure 3,c. Container has volume $F^*=7687.512942$ and sizes $(l^*, w^*, h^*)=(18.960443, 19.723184, 20.557029)$. Average time per one local minimum is 222.36 sec**.**

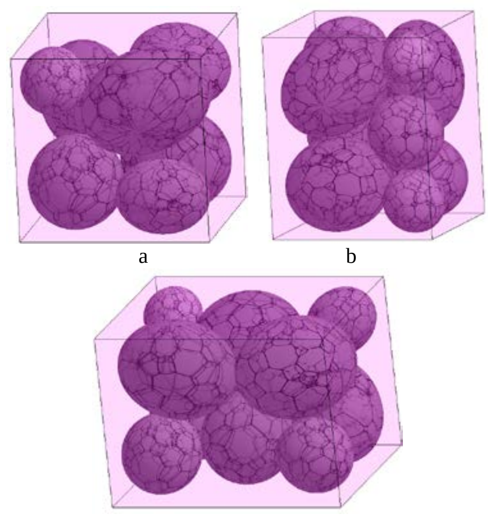


a

b c

Fig. 3. Local optimal placement of ellipsoids in Instances:
a − E5, b − E6, c − E7

Instance E8. Local optimal placement of ellipsoids $\{E_i, i=1,\dots,8\}$ is shown in Figure 4a. Container has volume $F^*=7998.224794$ and sizes $(l^*, w^*, h^*)=(20.223526, 19.919118, 19.854851)$. Average time per one local minimum is 359.88 sec**.**



a b

c

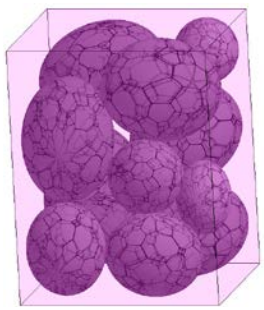
Fig. 4. Local optimal placement of ellipsoids in Instances:
a − E8, b − E9, c − E10

Instance E9. Local optimal placement of ellipsoids $\{E_i, i=1,\dots,9\}$ is shown in Figure 4b. Container has volume $F^*=8524.765214$ and $(l^*, w^*, h^*)=(19.365765,$ $18.695366,$ $23.545819)$. Average time per one local minimum is 369.42 sec**.**

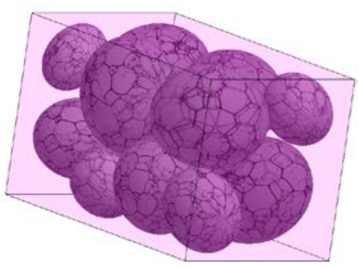
Instance E10. Local optimal placement of ellipsoids $\{E_i, i=1,\dots,10\}$ is shown in Figure 4c. Container has volume $F^* = 10263.381559$ and sizes $(l^*, w^*, h^*) = (25.780036,\ 18.893787,\ 21.071135)$. Average time per one local minimum is 371.23**.**

Instance E11. Local optimal placement of ellipsoids $\{E_i, i = 1,\ldots,11\}$ is shown in Figure 5a. Container has volume $F^* = 11860.716557$ and sizes $(l^*, w^*, h^*) = (21.945274,\ 27.902451,\ 19.369908)$. Average time per one local minimum is 445.95 sec**.**

Instance E12. Local optimal placement of ellipsoids $\{E_i, i = 1,\ldots,12\}$ is shown in Figure 5b. Container has volume $F^* = 11768.260385$ and sizes $(l^*, w^*, h^*) = (19.327419\ \ 19.558038\ \ 31.132438)$. Average time per one local minimum is 836.70 sec.



a



b

Fig. 5. Local optimal placement of ellipsoids in Instances:
a − E11, b −E12

VI. CONCLUSIONS

We developed here an *exact* continuous NLP model of the placement problem of ellipsoids, using quasi-phi-functions. The use of quasi-phi-functions allows us to handle ellipsoids which can be continuously rotated and translated, but there is a price to pay: now the optimization has to be performed over a larger set of parameters, including the extra variables, besides placement parameters of ellipsoids. The model can be realized by the current state-of-the art local or global solvers. We are working on the improvement of our algorithms to generate feasible starting points, as well as, to reduce our problem dimension in local optimisation procedures, based on the paper [9]. We expect that efficiency of our algorithms will be increased in the future.

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