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OPTIMAL CLUSTERING OF POLYHEDRA

Cutting and packing problems have a wide spectrum of applications. When dealing with polyhedra, an important problem is the identification of the optimal clustering of two objects. Within this paper we consider a containing region (cuboid, sphere, cylinder) of variable sizes and two polyhedra that can be continuously translated and rotated. In addition minimal allowable distances between objects and between each object and the frontier of a containing region may be imposed. The objects should be arranged within a containing region such that a given objective will reach its minimal value. We consider a volume or metrical characteristics of the containing region as the objective, which depends on the variable parameters associated with the objects and the containing region. The paper presents a mathematical model in the form of nonlinear optimisation problem, based on the phi-function technique. We also developed a solution algorithm and provide new benchmark instances of finding the containing region that has either minimal volume or homothetic coefficient of a given containing region.

MINIMUM CONTAINMENT, POLYHEDRA CLUSTERUNG, MATHEMATICAL MODELING, NONLINEAR OPTIMIZATION.

Ю.Е. Стоян, А.В. Панкратов, Т.Е. Романова. ОПТИМАЛЬНАЯ КЛАСТЕРИЗАЦИЯ МНОГОГРАННИКОВ. Задачи упаковки и раскроя имеют широкий спектр применения. При размещении многогранников важной задачей является поиск оптимальной кластеризации двух объектов. В качестве области размещения рассматривается контейнер (кубоид, шар, цилиндр) с переменными метрическими характеристиками и два многогранника, которые допускают непрерывные трансляции и вращения. Учитываются ограничения на минимально допустимые расстояния между объектами и между каждым объектом и границей области размещения. Объекты должны быть размещены в контейнере таким образом, чтобы заданная функция цели достигала минимального значения. В качестве функции цели рассматривается объем или метрические характеристики контейнера. Функция цели зависит от переменных параметров, зависящих от объектов размещения и вида контейнера. В статье представлена математическая модель в виде задачи нелинейной оптимизации, основанная на методе phi-функций. Предлагается алгоритм решения и приводятся новые результаты для поиска контейнера минимального объема или с минимальным коэффициентом гомотетии.

МИНИМАЛЬНОЕ ВКЛЮЧЕНИЕ, КЛАСТЕРИЗАЦИЯ МНОГОГРАННИКОВ, МАТЕМАТИЧЕСКОЕ МОДЕЛИРОВАНИЕ, НЕЛИНЕЙНАЯ ОПТИМИЗАЦИЯ

Ю. Є. Стоян, О.В. Панкратов, Т.Є. Романова. ОПТИМАЛЬНА КЛАСТЕРИЗАЦІЯ БАГАТОГРАННИКІВ. Задачі упаковки і розкрою мають широкий спектр застосування. При розміщенні багатогранників важливою задачею є знаходження оптимальної кластеризації двох об'єктів. У статті розглядається контейнер (кубоід, куля, циліндр) зі змінними метричними характеристиками та два багатогранника, які допускають безперервні трансляції та обертання. Враховуються обмеження на мінімально допустимі відстані між об'єктами і між кожним об'єктом і границею області. Об'єкти повинні бути розташовані в контейнері таким чином, щоб задана функція мети досягала мінімального значення. Як функція мети розглядається об'єм або метричні характеристики контейнера. Функція мети залежить від змінних параметрів, залежних від об'єктів і типу контейнера. У статті представлена математична модель у вигляді задачі нелінійної оптимізації яка заснована на методі phi-функцій. Запропоновано алгоритм розв'язання та наведено нові результати пошуку контейнеру мінімального об'єму або з мінімальним коефіцієнтом гомотетії.

МІНІМАЛЬНЄ ВКЛЮЧЕННЯ, КЛАСТЕРИЗАЦИЯ БАГАТОГРАННИКІВ, МАТЕМАТИЧНЕ МОДЕЛЮВАННЯ, НЕЛІНІЙНА ОПТИМІЗАЦІЯ

Introduction

Packing problems are interesting theoretically and have many important applications. Applications in industry include such problems as autonomously packing the hazardous waste into drums, which should then be melted in a plasma arc furnace, determining the placement of polycrystalline silicon nuggets during crucible packing as a key component of a robotic system to automated crucible packing process in semiconductor wafer production, creating the optimization frameworks for powder and FDM-based 3D printing that seeks to save printing time and the support material required to print 3D shapes, parts nesting for shipbuilding, glass cutting, furniture and other goods. It is well known that even the one-dimensional version of the problem of finding the optimal usage of a given resource, the classical knapsack problem, belongs to the class of NP-hard optimisation problems. For this reason, most of the work related to cutting and packing problems employ heuristic approaches. Nevertheless, the development of exact solution methods is an important task to broaden the range of optimal solvable cases.

One of the successful concepts in the case of irregular objects, which lends itselft to exact approaches, is phi-functions [1], [2].

The new functions, called quasi-phi-functions [3], can be described by analytical formulas that are substantially simpler than those used for phi-functions, for some types of objects, in particular, for polyhedra. In addition we construct an adjusted phi-function for describing distance constraints for a pair of polyhedra.

Using this approach leads, in general, to multi-extremal non-linear optimisation problems. Our tools permit the modelling of continuous object rotations, non-overlapping, containment and distance constraints. The concept allows the computation of high quality local optima, and in some cases, the global optimum.

In this paper, we address the problem of determining the minimum size containing region to house two polyhedra and use the phi-function technique to achieve this aim. In detail, we will investigate the following problem:

Optimal clustering 3D-problem. Given two polyhedra where free continuous rotations of the objects are permitted, find the minimal sizes of a given containing region (cuboid, sphere, or cylinder) according to a given objective and placement parameters of two objects such that the objects are placed completely inside the containing region without overlap and taking in to account allowable distances between objects. We consider a number of frequently occurring objectives, i.e. minimum volume and homothetic coefficient of a given containing region .

1. Related work

The containment problem is useful in the design of packing solution approaches in a number of ways. Some researchers develop approaches based on mathematical modeling and general optimisation procedures; for example see [4-9]. Egeblad et al [6] present an efficient solution method for packing polyhedra within the bounds of a polyhedron containing region. Utilization of containing region space is improved by an average of more than 14 percentage points compared to previous methods proposed in [10]. However, in the experiments the largest total volume of overlap allowed in a solution corresponds to *one* percent of the total volume of all polyhedra for the given problem.

Liu et al [11] propose a new constructive algorithm, called HAPE3D, which is a heuristic algorithm based on the principle of minimum total potential energy for the 3D irregular packing problem, involving packing a set of irregularly shaped polyhedrons into a box-shaped containing region with fixed width and length but unconstrained height. The objective is to allocate all the polyhedrons in the containing region, and thus minimize the waste or maximize profit.

The objective of A. Pasha's [12] task was to autonomously pack the hazardous waste into fifty-five gallon drums, which would then be melted in a plasma arc furnace. Central to the task was the development of a bin packing algorithm that was capable of finding near optimal packing configurations for a set of irregular shaped objects.

Vivek A. Et al [13] present an algorithm to automatically determine the placement of polycrystalline silicon nuggets during crucible packing is a key component of a robotic system to automated crucible packing process in semiconductor wafer production. To solve this problem of packing 3-D highly irregular objects with industrial constraints, an on-line model-free packing algorithm has been developed. It is based on the approach called Virtual Trial and Error.

Vanek et al [14] propose an optimization framework for 3D printing that seeks to save printing time and the support material required to print 3D shapes. Authors use the tabu search optimization [15] that has polynomial complexity to find a near to optimal solution and that has been used with success for packing problems.

Most of the approaches dealing with the interaction of two (or a few) objects are used in placement algorithms for larger instances as local decision rules. Some of the earliest approaches to irregular packing problems used the strategy of first clustering pieces within easier to handle shapes, for example [16]. However, such approaches lost popularity as computational speed and methodology improvements facilitated the direct packing of polyhedra. There are recent examples where the packing process requires the initial clustering. Further, the more sucessful placement heuristics use hole filling strategies that is the equivalent of the containment problem described here.

2. The concept of phi-functions

Packing problems involving irregular shapes require the modelling of interaction of two objects with respect to containment, overlap constraints and allowable distances. In this section we describe the core phi-function concepts including the definition of a phi-object, describing a placement objects and a containing regions, identify the interactions between objects. Finally we describe the containment and non-overlapping constraints taking into account allowable distances using phi-functions and quasi-phi-functions.

2.1. Placement objects. We assume that any placement object $\mathbb{Q}$ (an object which has to be placed into a containing region) considered here, is a three-dimensional phi-object [1], where a phi-object is a canonically closed point set $\mathbb{Q} \subset R^3$ $(\mathbb{Q} = cl^*(\mathbb{Q}) = cl(int(\mathbb{Q}))$ having the same homothopic type as its interior. As placement objects we consider, in general, non-convex polyhedra.

The location and orientation of each polyhedron $\mathbb{Q}$ is defined by a variable vector of its placement parameters (v,θ). Here $v=(x,y,z)$ is a translation vector, $\theta=(\theta^1,\theta^2,\theta^3)$ is a vector of rotation parameters, where $\theta^1,\theta^2,\theta^3$ are appropriate angles from axis *OX* to *OY*, from axis *OY* to *OZ* and from axis *OX* to *OZ* in the local coordinate system of a polyhedron $\mathbb{Q}$.

The translated by vector v and rotated by angles $\theta^1,\theta^2,\theta^3$, a polyhedron $\mathbb{Q}$ is denoted as $\mathbb{Q}(u)=\{p\in R^3: p=v+M(\theta)\cdot p^0, \forall p^0\in\mathbb{Q}^0\}$, where $\mathbb{Q}^0$ denotes the non-translated and non-rotated polyhedron $\mathbb{Q}$, $M(\theta)$ is a standart rotation matrix.

Assuming that non-convex polyhedron $\mathbb{Q}$ may be presented as a union of convex polyhedra. Various algorithms can be applied to solve the problem, for example, the algorithm proposed in [17]. For the purposes of this paper, we assume the decomposition of the polyhedra is known.

With each convex polyhedron that form a polyhedron $\mathbb{Q}$ we associate the local coordinate system which coincides with the local coordinate system of a polyhedron $\mathbb{Q}$. Note, that each convex polyhedron $K_i\subset\mathbb{Q}$ is defined by its vertices p_s^i, $s=1,....,m_i$, $i\in I_q$, in the local coordinate system of $\mathbb{Q}$.

We assume here that *placement objects* have *fixed metrical characteristics* and *variable placement parameters* $(x,y,z,\theta^1,\theta^2,\theta^3)$.

2.2. Containing regions. We consider the following containing regions: a) a cuboid: $\mathbf{B}=\{(x,y,z)\in R^3 \mid \min\{x+l,-x+l,y+w,-y+w, \; z+h, -z+h\}\geq 0\}$ where variables *l, w* and *h* are the dimensions of the cuboid respectively; b) a sphere of variable radius *r*: $\mathbf{S}=\{(x,y,z)\in\mathbb{R}^3 \mid r^2-x^2-y^2-z^2\geq 0\}$; c) a cylinder of radius λr and height λh, λ is a variable homothetic coefficient:

$$\mathbf{C}=\{(x,y,z)\in\mathbb{R}^3 \mid \min\{(\lambda r)^2-x^2-y^2,-z+\lambda h,z+\lambda h\}\geq 0\},$$

subject to for original containing region $\lambda=1$.

Containing region Ω have fixed *pacement parameters* $(0,0,0)$ and variable *metrical characteristics* p defined above. Hereinafter, we denote a *containing region* $\Omega=\Omega(p)$.

2.3. Description of relationships between objects. In order to feasibly place two objects within a containing region, we need to formalise placement constraints.

We employ the phi-function technique to describe analytically the placement constraints.

Let $A=\bigcup_{i=1}^{n_A}A_i$, and $B=\bigcup_{j=1}^{n_B}B_j$, be non-convex polyhedra, where A_i,B_j are convex polyhedra.

Containment constraints

Phi-functions allow us to distinguish the following three cases: *A* and *B* are intersecting so that *A* and *B* have common interior points; *A* and *B* do not intersect, i. e. *A* and *B* do not have common points; *A* and *B* are in contact, i. e. *A* and *B* have only common frontier points. By definition, the phi-function of *A* and *B* is everywhere defined for a continuous function that possesses the following characteristics: $\Phi_{AB}>0$ if $A\cap B=\varnothing$; $\Phi_{AB}=0$ if $\operatorname{int}A\cap\operatorname{int}B=\varnothing$ and $frA\cap frB\neq\varnothing$; $\Phi_{AB}<0$ if $\operatorname{int}A\cap\operatorname{int}B\neq\varnothing$, where $\operatorname{int}A$, frA is the interior and the frontier of object *A*. We employ phi-functions for the description of the contaiment relationship $A\subseteq B$ as follows: $\Phi_{AB^*}\geq 0$, where $B^*=R^3\setminus\operatorname{int}B$. See [1], [2] for definitions and basic features of phi-functions.

For mathematical modelling of containment constraints of form $A\subset\Omega\Leftrightarrow\operatorname{int}A\cap\Omega^*=\varnothing$

It is used a phi-function $И\Omega^*$ for non-convex polyhedron A and object $\Omega^*=R^3\setminus\operatorname{int}\Omega$, that can be represented in the following form depending on the type of the containing region

$$\Phi^{A\Omega^*}=\begin{cases}\Phi^{A\mathbf{S}^*}, \text{ if } \Omega=\mathbf{S}\\ \Phi^{A\mathbf{C}^*}, \text{ if } \Omega=\mathbf{C}\\ \Phi^{A\mathbf{B}^*}, \text{ if } \Omega=\mathbf{B}\end{cases}$$

The phi-function for non-convex polyhedron A and object Ω^* has the form

$$\Phi^{A\Omega^*}=\min\{\Phi^{A_1\Omega^*},\Phi^{A_2\Omega^*},...,\Phi^{A_{n_A}\Omega^*}\}$$

Where $\Phi^{A_i\Omega^*}$ is a phi-function for a convex polyhedron A_i and object Ω^*.

Phi-function for A_i *and object* $\mathbf{S}^*=\mathbb{R}^3/\operatorname{int}\mathbf{S}$.

$$\Phi^{A_i\mathbf{S}^*}=\min\{\varphi_s, s=1,...,\mathrm{m}_{A_i}\},$$

$$\varphi_s=(\lambda r)^2-(p_{sx}^i)^2-(p_{sy}^i)^2-(p_{sz}^i)^2$$

Phi-function for A_i *and object* $\mathbf{C}^*=\mathbb{R}^3/\operatorname{int}\mathbf{C}$.

$$\Phi^{A_i\mathbf{C}^*}=\min\{\mu,\psi,\omega\},$$

$$\mu=\min\{\mu_s,s=1,...,m_{A_i}\},\ \mu_s=r^2-(p_{sx}^i)^2-(p_{sy}^i)^2,$$

$$\psi=\min\{\psi_s,s=1,...,m_{A_i}\},\ \psi_s=p_{sz}^i+h,$$

$$\omega=\min\{\omega_s,s=1,...,m_{A_i}\},\ \omega_s=-p_{sz}^i+h,$$

Phi-function for A_i *and object* $\mathbf{B}^*=\mathbb{R}^3/\operatorname{int}\mathbf{B}$.

$$\Phi^{A_i\mathbf{B}^*}=\min\{\min_{1\leq s\leq m_{A_i}}\eta_{sj}, j=1,...,6\},$$

$$\eta_{s1}=x_1+p_{sx}^i,\ \eta_{s2}=-(x_1+p_{sx}^i)+l,\ \eta_{s3}=y_1+p_{sy}^i,$$

$$\eta_{s4}=-(y_1+p_{sy}^i)+w,\ \eta_{s5}=z_1+p_{sz}^i,\ \eta_{s6}=-(z_1+p_{sz}^i)+h.$$

Non-overlapping constraints

For mathematical modelling of non-overlapping constraint $\operatorname{int}A\cap\operatorname{int}B=\varnothing$ a quasi-phi-function for a pair of non-convex polyhedra A and B may be defined in the form

$$\Phi'_{AB}(u_A,u_B,u_{AB})=$$

$$=\min\{\Phi'_{ij}(u_A,u_B,u'_{ij}),i=1,...,n_A,j=1,...,n_B\},\qquad(1)$$

where $\Phi'_{AB}(u_A,u_B,u'_{ij})$ is a quasi-phi-function and u'_{ij} is a vector of additional variables for for a pair of convex polyhedra $A_i(u_A)$ and $B_j(u_B)$, $i=1,...,n_A$, $j=1,...,n_B$, $u_{AB}=(u'_{ij},i=1,...,n_A,j=1,...,n_B)$.

It should be noted that replacing quasi-phi-functions $\Phi'^{A_iB_j}$ in (1) by adjusted $\hat{\Phi}'^{A_iB_j}$ quasi-phi-functions for $i=1,...,n_A$, $j=1,...,n_B$, we get an adjusted quasi-phi-function $\hat{\Phi}'_{AB}(u_A,u_B,u_{AB})$ for non-convex polyhedra $A(u_A)$ and $B(u_B)$.

Let us consider two convex polyhedra $A_1(u_1)$ and $B_2(u_2)$, given by their vertices p_i^1, $i=1,....,m_1$, and p_j^2, $j=1,....,m_2$.

A radical free quasi-phi-function $\Phi'^{A_1B_2}(u_1,u_2,u_P)$ for convex polyhedra $A_1(u_1)$ and $B_2(u_2)$ may be defined by formula [3]

$$\Phi'^{A_1B_2}(u_1,u_2,u_P)=$$
$$=\min\{\Phi^{A_1P}(u_1,u_P),\Phi^{B_2P^*}(u_2,u_P)\}, \qquad (2)$$

where $\Phi^{A_1P}(u_1,u_P)$ is a phi-function for $A_1(u_1)$ and a half-space $P(u_P)$, $\Phi^{B_2P^*}(u_2,u_P)$ is a phi-function for $B_2(u_2)$ and a half-space $P^*(u_P)=R^3\setminus\operatorname{int}P(u_P)$, where $\operatorname{int}P(u_P)$ is the interior of $P(u_P)$. Here $P(u_P)=\{(x,y,z):\psi_P=\alpha\cdot x+\beta\cdot y+\gamma\cdot z+\mu_P\le 0\}$ is a half-space, where $\alpha=\sin\theta_{yP}$, $\beta=-\sin\theta_{xP}\cdot\cos\theta_{yP}$, $\gamma=\cos\theta_{xP}\cdot\cos\theta_{yP}$ (note that $\alpha^2+\beta^2+\gamma^2=1$) and $u_P=(\theta_{xP},\theta_{yP},\mu_P)$, θ_{xP} and θ_{yP} are appropriate variable angles of the half-space $P(u_P)$ from axis *OY* to *OZ* and from axis *OX* to *OZ* in the fixed coordinate system in R^3.

We follow [2] to define phi-function

$$\Phi^{A_1P}(u_1,u_P)=\min_{1\le i\le m_1}\psi_P(p_i^1)$$

and phi-function

$$\Phi^{B_2P^*}(u_2,u_P)=\min_{1\le j\le m_2}(-\psi_P(p_j^2)).$$

We note that if $\Phi'^{A_1B_2}(u_1,u_2,u_P)>0$ then a plane

$$L_P=\{(x,y,z):\psi_P(u_P)=0\}$$

is a separating plane for $A_1(u_1)$ and $B_2(u_2)$

Thus, if two convex polyhedra $A_1(u_1)$ and $B_2(u_2)$ do not have common points then there always exists additional variables $u_P=(\theta_{xP},\theta_{yP},\mu_P)$ such that $\max_{u_P}\Phi'^{A_1B_2}>0$. Therefore,

$$\max_{u_P}\Phi'^{A_1B_2}\ge 0\Leftrightarrow \operatorname{int}A_1(u_1)\cap\operatorname{int}B_2(u_2)=\varnothing.$$

Further we use the following important characteristic of a *quasi-phi-function*: if $\Phi'^{A_1B_2}\ge 0$ for some u_P, then $\operatorname{int}A_1(u_1)\cap\operatorname{int}B_2(u_2)=\varnothing$ (see [3] for details).

Distance constraints

We take into account *distance constraints* replacing quasi-phi-functions in *non-overlapping* with adjusted quasi-phi-functions and phi-functions in *containment constraints* with adjusted phi-functions.

By definition an adjusted *phi*-function of A and B is an everywhere defined continuous function $\hat{\Phi}^{AB}$, such that $\hat{\Phi}^{AB}>0$, if $\operatorname{dist}(A,B)>\rho$, $\hat{\Phi}^{AB}=0$, if $\operatorname{dist}(A,B)=\rho$, $\hat{\Phi}^{AB}<0$, if $\operatorname{dist}(A,B)<\rho$, where ρ is the minimum allowable distance between objects *A* and *B*.

Function $\hat{\Phi}'^{AB}(u_A,u_B,u')$ is called an adjusted quasi-phi-function for objects $A(u_A)$ and $B(u_B)$, if function $\max_{u'\in U}\hat{\Phi}'^{AB}(u_A,u_B,u')$ is an adjusted phi-function for the objects.

In particular, we have $\operatorname{dist}(A,B)\ge\rho \Leftrightarrow \hat{\Phi}^{AB}\ge 0$.

Let minimal allowable distance ρ_1^- between a convex polyhedron A_i and the *object* Ω^* be given. To describe distance constraint, $\operatorname{dist}(A_i,\Omega^*)\ge\rho_1$, we use adjusted radical free phi-function $\hat{\Phi}_1$ for a convex polyhedron A_i and the object Ω^* defined by

$$\hat{\Phi}^{A_i\Omega^*}=\tilde{\Phi}^{A_i\Omega^*}-\rho_1.$$

where $\tilde{\Phi}^{A_i\Omega^*}$ is a normalized phi-function for the convex polyhedron A_i and the object Ω^*.

Normalized phi-function for the convex polyhedron A_i and the object S^*:

$$\tilde{\Phi}^{A_iS^*}=\min\{\tilde{\varphi}_s,s=1,...,m_{A_i}\}, \qquad (3)$$

$$\tilde{\varphi}_s=r-\sqrt{(p_{sx}^i)^2-(p_{sy}^i)^2-(p_{sz}^i)^2}, \qquad (4)$$

Normalized phi-function for the convex polyhedron A_i and the object C^*

$$\tilde{\Phi}^{A_iC^*}=\min\{\tilde{\mu},\psi,\omega\},\ \tilde{\mu}=\min\{\tilde{\mu}_s,s=1,...,m_{A_i}\},$$
$$\tilde{\mu}_s=r-\sqrt{(p_{sx}^i)^2-(p_{sy}^i)^2}, \qquad (5)$$
$$\psi=\min\{\psi_s,s=1,...,m_{A_i}\},\ \psi_s=p_{sz}^i+h,$$
$$\omega=\min\{\omega_s,s=1,...,m_{A_i}\},\ \omega_s=-p_{sz}^i+h,$$

Normalized phi-function for the convex polyhedron A_i and the object $\mathbf{B}^*$

$$\Phi^{A_iB^*}=\min\{\min_{1\le s\le m_{A_i}}\eta_{sj},j=1,...,6\},$$
$$\eta_{s1}=x_1+p_{sx}^i,\ \eta_{s2}=-(x_1+p_{sx}^i)+l,\ \eta_{s3}=y_1+p_{sy}^i,$$
$$\eta_{s4}=-(y_1+p_{sy}^i)+w,\ \eta_{s5}=z_1+p_{sz}^i,\ \eta_{s6}=-(z_1+p_{sz}^i)+h.$$

Let minimal allowable distance ρ_{12} between two convex polyhedra $A_1(u_1)$ and $B_2(u_2)$ be given. To describe a *distance* constraint, $\operatorname{dist}(A_1,B_2)\ge\rho_{12}$, we use an adjusted radical free quasi-phi-function $\hat{\Phi}'_{12}$ for convex polyhedra $A_1(u_1)$ and $B_2(u_2)$ derived by

$$\hat{\Phi}'^{A_1B_2}(u_1,u_2,u_P)=\Phi'^{A_1B_2}(u_1,u_2,u_P)-0.5\rho_{12}. \quad (6)$$

Thus, $\max_{u'\in U}\hat{\Phi}'^{A_1B_2}\ge 0\Leftrightarrow\operatorname{dist}(A_1,B_2)\ge\rho_{12}$. It follows from (2) and (6) that

$$\Phi'^{A_1B_2}(u_1,u_2,u_P)-0.5\rho_{12}\ge 0\Rightarrow\operatorname{dist}(A_1,B_2)\ge\rho_{12}.$$

3. Mathematical model

In terms of phi-functions we can formulate *the optimal clustering problem* as a NLP problem:

$$F(u^*)=\min\{F(u):u\in W\}, \qquad (7)$$

$$W=\{u\in R^\sigma:\hat{\Phi}^{\Omega^*A}\ge 0,\hat{\Phi}^{\Omega^*B}\ge 0,\hat{\Phi}'^{AB}\ge 0\}, \qquad (8)$$

where $F(u)$ is a polynomial function, $u=(p,u_A,u_B)\in R^\sigma$ is a vector of variables, R^σ is Euclidean space of σ dimension, p is a vector of variable metrical characteristics of Ω,

$$(u_A,u_B)=(x_A,y_A,z_A,\theta_A^1,\theta_A^2,\theta_A^3,x_B,y_B,z_B,\theta_B^1,\theta_B^2,\theta_B^3)$$

is vector of variable placement parameters of objects A and B, W denotes the corresponding set of feasible solutions (the solution space), $\widehat{\Phi}'^{AB}$ is an adjusted quasi-phi-function for objects A and B taking into account a given minimal allowable distance ρ between the objects, $\widehat{\Phi}^{\Omega^* A}$ is an adjusted phi-function for objects A and Ω^*, $\widehat{\Phi}^{\Omega^* B}$ is an adjusted phi-function for objects B and Ω^* taking into account a given minimal allowable distances ρ' between each object and the frontier of Ω. It should be noted that if $\rho = 0$ and $\rho' = 0$, then we use the original phi-function and quasi-phi-functions instead of the adjusted phi-functions and adjusted quasi-phi-functions in (8).

We consider three realizations of problem (7)-(8), denoted by P1,P2, P3, with respect to the shape of the containing region Ω and the form of the objective function $F(u)$:

P1: $\Omega \equiv \mathbf{B}$, $F_1(u) = l \cdot w \cdot h$ (volume of **B**):
$u = (l, w, h, u_A, u_B) \in R^\sigma$,
$\sigma = 15$

P2: $\Omega \equiv \mathbf{S}$, $F_2(u) = r$ (radius of **S**):
$u = (r, u_A, u_B) \in R^\sigma$,
$\sigma = 13$

P3: $\Omega \equiv \mathbf{C}$, $F_3(u) = \lambda$ (homothety coefficient of **C**):
$u = (\lambda, u_A, u_B) \in R^\sigma$,
$\sigma = 13$

Each quasi-phi-function inequality in (8) is presented by a system of inequalities with infinitely differentiable functions. Our model (7)-(8) is a nonconvex and continuous nonlinear programming problem. Problem (7)-(8) is an exact formulation for the polyhedron packing problem. It contains all glospherey optimal solutions. It is possible, at least in theory, to use a global solver for the nonlinear programming problem and obtain a solution which is an optimal packing.

However in practice, we deal with a large number of variables and a huge number of inequalities in our model. As a result, finding a locally optimal solution becomes an unrealistic task for the available state of the art NLP solvers. In order to search for a "good" locally optimal polyhedron packing within a reasonable computational time we propose here a solution algorithm, which can be considered as *an extension* of the solution algorithm developed in [3] for the optimal ellipse packing problem.

4. General solution strategy

As discussed in the previous section, solving the polyhedron packing problem using an NLP solver is not practical. Instead we look to identify multiple starting solutions and search for the best of found local optimal solutions. Our multistart solution strategy involves the following steps:

1. Generate a set of vectors $\varsigma^0 = (p^0, u_1^0, u_2^0, ..., u_N^0)$ of feasible placement parameters $(u_1^0, u_2^0, ..., u_N^0)$ of our polyhedra placed into the containing region Ω^0 of starting dimension p^0 in the problem (7)-(8). Various algorithms exist for obtaining a feasible solution for example [18]. We employ here the algorithm (called FSPA-S), which is described in Subsection 5.1.

2. Form an appropriate set $\{u^0\}$ of feasible starting points $u^0 = (\varsigma^0, \tau^0)$ for problem (7)-(8), using the set $\{\varsigma^0\}$ obtained at Step 1. We use a special procedure (FAPA-S) to generate a vector τ^0 of additional variables.

3. Search for a local minimum of the objective function $F(u)$ in problem (7)-(8), starting from each point from the set $\{u^0\}$ obtained at Step 2.

4. Choose the best local minimum from those found at Step 3 as the final solution of the problem (7)-(8).

The actual search for a local minimum in all our optimisation procedures (to realise steps 1-3) is performed by IPOPT [19], which is available at an open access noncommercial software depository (https://projects.coin-or.org/Ipopt).

5. Starting Point Algorithm (FSPA-S)

In order to find a vector of starting feasible placement parameters of our polyhedra we apply an algorithm, which is based on homothetic transformation of spheres. The algorithm consists of the following steps:

1. Choose starting dimensions p^0 for our containing region . They must be sufficiently large to allow for a placement of all circumscribed spheres S_q, $q = 1, 2, ..., N$, within the containing region Ω^0.

2. Generate within the containing region Ω^0 a pair of randomly chosen center points $(x_q^{'0}, y_q^{'0}, z_q^{'0})$, $q = 1,2$, of circumbsribed spheres S_q of radius λr_q. We assume here that λ is a homothetic coefficient for all our spheres S_q and $0 \le \lambda \le 1$.

3. Assuming that $p = p^0$, and starting from the point $u'^0 = (x_1^{'0}, y_1^{'0}, z_1^{'0}, x_2^{'0}, y_2^{'0}, z_2^{'0}, \lambda'^0 = 0)$, solve the following *auxiliary* nonlinear programming problem:

$$\max_{\tilde{u} \in \tilde{W}} \lambda, \tag{9}$$

$$\tilde{W} = \{\tilde{u} \in \mathrm{R}^7 : \widehat{\Phi}^{S_1 S_2} \ge 0, \widehat{\Phi}^{S_1 \Omega^*} \ge 0, \widehat{\Phi}^{S_2 \Omega^*} \ge 0, 1 - \lambda \ge 0, \lambda \ge 0\}, \tag{10}$$

где $\tilde{u} = (x_1, y_1, z_1, x_2, y_2, z_2, \lambda)$,

$$\widehat{\Phi}^{S_1 S_2} = (x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2 - \lambda^2 (r_1 + \rho_{12}^- + r_2)^2, \tag{11}$$

is an adjusted phi-function for a sphere S_1 of radius λr_1 and a sphere S_2 of radius λr_2.

$$\widehat{\Phi}^{S_q \Omega^{0*}}(u_q) = \begin{cases} \widehat{\Phi}^{S_q \mathbf{S}^{0*}}(u_q), \text{если } \Omega = \mathbf{S} \\ \widehat{\Phi}^{S_q \mathbf{C}^{0*}}(u_q), \text{если } \Omega = \mathbf{C}, \\ \widehat{\Phi}^{S_q \mathbf{B}^{0*}}(u_q), \text{если } \Omega = \mathbf{B} \end{cases} \tag{12}$$

$$\widehat{\Phi}^{S_q \mathbf{S}^{0*}} = (r^0 - \lambda(r_q + \rho_q^-))^2 - (x_q)^2 - (y_q)^2 - (z_q)^2,$$

$$\widehat{\Phi}^{S_q \mathbf{C}^{0*}} = \min\{(\eta^0 r - \lambda(r_q + \rho_q^-))^2 - (x_q)^2 - (y_q)^2, z_q + \eta^0 h - \lambda(r_q + \rho_q^-), -z_q + \eta^0 h - \lambda(r_q + \rho_q^-)\},$$

$$\widehat{\Phi}^{S_q \mathbf{B}^{0*}} = \min\{\varphi_{kq}, k = 1, ..., 6\},$$

$$\varphi_{1q} = -x_q + l^0 - \lambda(r_q + \rho_q^-),\ \varphi_{2q} = x_q - \lambda(r_q + \rho_q^-),$$

$$\varphi_{3q} = -y_q + w^0 - \lambda(r_q + \rho_q^-),$$

$$\varphi_{4q} = y_q - \lambda(r_q + \rho_q^-),\ \varphi_{5q} = -z_q + h^0 - \lambda(r_q + \rho_q^-),$$

$$\varphi_{4q} = z_q - \lambda(r_q + \rho_q^-)$$

$\widehat{\Phi}^{S_q\Omega^{0*}}$ is an adjusted phi-function for a sphere S_q of radius λr_q and the object Ω^{0*}.

We denote a point of global maximum of problem (9)-(10) by $\tilde{u}^* = (\tilde{x}_1^*, \tilde{y}_1^*, \tilde{z}_1^*, \tilde{x}_2^*, \tilde{y}_2^*, \tilde{z}_2^*, \tilde{\lambda}^* = 1)$.

4. Form a vector of feasible parameters

$$\varsigma^0 = (p^0, u_1^0, u_2^0),$$

assuming that

$u_q^0 = (x_q^0, y_q^0, z_q^0, \theta_q^0)$, $(x_q^0, y_q^0, z_q^0) = (x_q^{'*}, y_q^{'*}, z_q^{'*})$ and θ_q^0 is a vector of randomly generated rotation parameters of polyhedra $\mathbb{Q}_q, q = 1,2$.

Our FPPA algorithm returns the vector ς^0 to generate a starting point for a subsequent search for a local minimum of the problem (7)-(8).

6. Computational experiments

The results include a number of examples to demonstrate the effectiveness of the methodology. In all cases the input data of the example has been provided in [10]. For local optimisation, our programs use IPOPT (https://projects.coin-or.org/Ipopt) (see [19]) that only guarantees a local optimum for non-linear programming problems. We use computer AMD Athlon 64 X2 5200+.

Example 1 Clustering of objects A and B into a cuboid **B**, we believe this optimal but not proved**,** problem **P1,** see Figure 1, $F(u^*) = l^* \cdot w^* \cdot h^* = 1502.0771$, where $l^* = 16.4725$, $w^* = 4.000$, $h^* = 22.7966$ Running time is 3.21 sec.

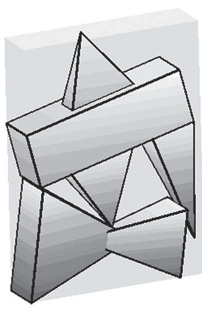

Fig. 1. Solution of problem P1 in Example 1

Example 2 Clustering of objects A and B into a cuboid **B**, we believe this optimal but not proved**,** problem **P1,** see Figure 2, $F(u^*) = l^* \cdot w^* \cdot h^* = 1399.9999$, where $l^* = 10.000$, $w^* = 10.000$, $h^* = 14.000$. Running time is 8.674 sec.

Fig. 2. Solution of problem P1 in Example 4

Example 3 Clustering of objects A and B into a cuboid **B**, we believe this optimal but not proved**,** problem **P1,** see Figure 3, $F(u^*) = l^* \cdot w^* \cdot h^* = 1152.000$, where $l^* = 4.000$, $w^* = 16.000$, $h^* = 18.000$ Running time is 4.93 sec.

Fig. 3. Solution of problem P1 in Example 5

Example 4 Clustering of objects A and B into a sphere **S**, we believe this optimal but not proved**,** problem **P2,** see Figure 4, $F(u^*) = r^* = 12.2274$, Running time is 2.351 sec.

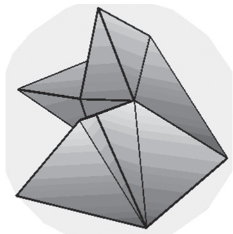

Fig. 4. Solution of problem P2 in Example 4

Example 5 Clustering of objects A and B into a sphere **S**, we believe this optimal but not proved**,** problem **P2,** see Figure 5, $F(u^*) = r^* = 11.2996$. Running time is 2.351 sec.

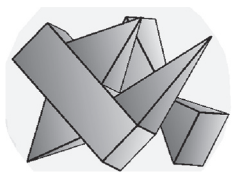

Fig. 5. Solution of problem P1 in Example 5

Example 6 Clustering of objects A and B into a cylinder **C**, problem **P3,** see Figure 6, $F(u^*) = \lambda^* = 0.682$. provided that r=20, h=40. Running time is 2.65 sec.

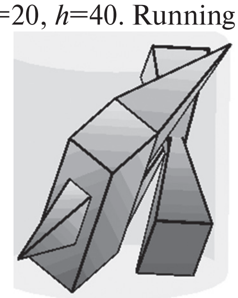

Fig. 6. Solution of problem P3 in Example 6

Example 3 and 5 are examples of global optimum proved by known global solutions.

7. Conclusions

In the paper a basic approach is presented to handle placement problems with irregular shapes (convex or non-convex polyhedra). We investigated the problem of enclosing two such objects by a cuboid, cylinder or sphere of minimal volume or homotetic coefficient by means of phi-function technique. The solution methodology can be applied to a wide range of problems in cutting and packing. The extension of the approach to the case of more than two objects, the problem of filling holes of arbitrary shapes and other forms of objectve functions is ongoing work for the near future publication.

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Resume

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OPTIMAL CLUSTERING OF POLYHEDRA

Background: Packing problems, also called placement or allocation problems, are interesting theoretically and have many important applications. Applications in industry include such problems as autonomously packing the hazardous waste into drums, which should then be melted in a plasma arc furnace, determining the placement of polycrystalline silicon nuggets during crucible packing as a key component of a robotic system to automated crucible packing process in semiconductor wafer production, creating the optimization frameworks for powder and FDM-based 3D printing that seeks to save printing time and the support material required to print 3D shapes, e.g., in space engeneering, automobile production, shipbuilding. It is well known that even the one-dimensional version of the problem of finding the optimal usage of a given resource, the classical knapsack problem, belongs to the class of NP-hard optimisation problems. For this reason, most of the work related to cutting and packing problems employ heuristic approaches. Nevertheless, the development of exact solution methods is an important task to broaden the range of optimal solvable cases.

Materials and methods: One of the successful concepts in the case of irregular objects, which lends itselft to exact approaches, is the phi-function technique. Using this approach leads, in general, to multi-extremal non-linear optimisation problems. Our tools permit the modelling of continuous object rotations, non-overlapping, containment and distance constraints. The concept allows the computation of high quality local optima, and in some cases, the global optimum. In this paper, we address the problem of determining the minimum size containing region to house two polyhedra.

Results: In the paper a basic approach is presented to handle placement problems with irregular shapes. We investigated the problem of enclosing two such objects by a cuboid, cylinder or sphere of minimal volume or homotetic coefficient by means of the phi-function technique.

Conclusion: The solution methodology can be applied to a wide range of problems in cutting and packing. The extension of the approach to the case of more than two objects, the problem of filling holes of arbitrary shapes and other forms of objectve functions is ongoing work for the near future publication.

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