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A hybrid algorithm for packing identical spheres into a container

Mhand Hifi*, Labib Yousef

EPROAD EA 4669, Université de Picardie Jules Verne, CURI, 7 rue du Moulin Neuf, Amiens 80000, France

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ABSTRACT

Packing identical spheres occur in several commercial and industrial contexts, like automated radio-surgical treatment planning and in materials science for studying the dynamic behavior of granular material systems. In this paper, a hybrid algorithm is proposed for approximately solving the identical sphere packing problem. Given a set of identical spheres and a large container (open or spherical container), the goal of the problem is to find a smallest container that contains all spheres without overlapping between spheres and between spheres and the container. The proposed algorithm combines both particle swarm optimization and an efficient continuous local optimization procedure. The swarm optimization generates a series of diversified populations of particles whereas the continuous optimization serves either to repair the infeasibility of solutions or improve their qualities. The performance of the proposed algorithm is evaluated on a set of standard benchmark instances and its obtained results are compared to those reached by the more recent methods available in the literature. The experimental part shows that the proposed approach remains competitive, where it is able to reach 47 new upper bounds out of the 93 tested instances.

1. Introduction

Packing identical spheres occur in several commercial and industrial contexts, like automated radio-surgical treatment planning where the problem is used as a tool for solving the radio surgical treatment planning (cf. Sutou & Dai, 2002) and, materials science where a random sphere packing problem is used as a model for studying the dynamic behavior of granular material systems (cf. Li & Ji, 2013). For these problems, it is often important to be able to get solutions with high-qualities. Fairly, simple deterministic and stochastic heuristics are often used for approximately solving these types of problems, but they generally well toward good solutions for some small instances whereas they provide mediocre solutions for more complex instances. In this paper, the Identical Sphere Packing (denoted ISP) is tackled with a hybrid algorithm that combines the particle swarm optimization and an efficient continuous local optimization. Two types of ISP are considered: the ISP with an *Open container* (denoted O-ISP), where the container has an unlimited length and, the ISP with a *spherical container* (denoted S-ISP), where its radius is unlimited.

An instance of each of both problems is characterized by a set N of n identical spheres, where each sphere $i \in N = \{1, \ldots, n\}$ is represented by its radius $r_i = 1$ and the container is either $\mathcal{P}$ with fixed width W and height H but unlimited length $L_0 = \infty$ or $\mathcal{S}$ of unlimited radius $S = \infty$. For both versions of the problem, the goal is to minimize the length L_0 (if the container $\mathcal{P}$ is open) or the radius R_0 (if the container $\mathcal{S}$ is spherical) such that all items of N are positioned in $\mathcal{P}$ or R_0, without overlapping between spheres and between spheres and the container.

On the one hand, O-ISP can be formulated as follows:

$$\text{Minimize} \quad L_0 \tag{1}$$

$$d(i,j) \geq (r_i + r_j), \ \ \forall (i,j) \in N^2, \ i < j \tag{2}$$

$$r_i \leq x_i \leq L - r_i, \forall i \in N \tag{3}$$

$$r_i \leq y_i \leq H - r_i, \forall i \in N \tag{4}$$

$$r_i \leq z_i \leq W - r_i, \forall i \in N \tag{5}$$

where $d(i,j) = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2}$, $(i,j) \in N \times N, i \neq j$. Eq. (1) denotes the objective function that minimizes the length L_0 of the target container $\mathcal{P}$. Eq. (2) represents the quadratic constraints that ensure the non-overlapping between any pair of distinct spheres. Eqs. from (3) to (4) represent the linear constraints

* Corresponding author.
E-mail addresses: hifi@u-picardie.fr, mhand.hifi@u-picardie.fr (M. Hifi), labib.yousef@u-picardie.fr (L. Yousef).

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Table 1
Function's overlapping for both problems: between the positioned spheres and between spheres and the container.

Between	O-ISP	S-ISP
sphere and container	$O_{i,x} = \max\left\{0, r_i + \lvert x_i\rvert - \frac{1}{2}L_0\right\}$ $O_{i,y} = \max\left\{0, r_i + \lvert y_i\rvert - \frac{1}{2}H\right\}$ $O_{i,z} = \max\left\{0, r_i + \lvert z_i\rvert - \frac{1}{2}W\right\}$	$O_{0,i} = \max\{0, d(i,0) + r_i - R_0\}$
sphere and sphere	$O_{i,j} = \max\{0, r_i + rj - d(i,j)\}$	$O_{i,j} = \max\{0, r_i + rj - d(i,j)\}$

that represent the sphere's feasibility when positioned into the container $\mathcal{P}$ of length L_0.

On the other hand, the problem S-ISP can be stated as follows:

$$\text{Minimize} \quad R_0 \tag{6}$$

$$d(i,j) \geq (r_i + r_j), \ \forall (i,j) \in N^2, \ i < j \tag{7}$$

$$d(0,i) \leq (R_0 - r_i), \forall i \in N \tag{8}$$

where $d(i,j) = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2}, (i,j) \in N, \times N, i \neq j$ and $d(0,i) = \sqrt{x_i^2 + y_i^2 + z_i^2}, i \in N$. Eq. (6) denotes objective function that minimizes the radius R_0 of the target container $\mathcal{S}$. Each Eq. (7) represents the quadratic constraints that ensure the non-overlapping between any pair of distinct spheres and each Eq. (8) denotes the quadratic constraints representing the sphere's feasibility when positioned into the container of radius R_0.

For both O-ISP and S-ISP, a packing can be represented by the following vector:

$$\overrightarrow{X} = (F, x_i, y_i, z_i, \ldots, x_n, y_n, z_n),$$

where F, $F = L_0$ for O-ISP (resp. $F = R_0$ for S-ISP), denotes the length (resp. radius) of the target container $\mathcal{P}$ (resp. $\mathcal{S}$) and $(x_i, y_i, z_i, \ldots, x_n, y_n, z_n)$ is the coordinates of positions of the n packed spheres.

In order to measure the infeasibility of a given packing $\overrightarrow{X}$, the amount of overlapping is measured following quantities represented in Table 1.

Hence, according to both terms of overlapping, following the couple of spheres or a sphere with the container, the first overlap $E(\overrightarrow{X})$ associated to the first version of the problem O-ISP is given as follows:

$$E(\overrightarrow{X}) = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} O_{i,j}^2 + \sum_{i=1}^{N} (O_{i,x} + O_{i,y} + O_{i,z})$$

and that associated to the second problem S-ISP is given as follows:

$$E(\overrightarrow{X}) = \sum_{i=0}^{N-1} \sum_{j=i+1}^{N} O_{i,j}^2.$$

The rest of the paper is organized as follows. Section 2 gives a literature review on the sphere packing problem. Section 3 describes the basic steps of the particle swarm optimization and its adaptation for solving both versions of the packing problem. Section 3.2 discusses the main principle of the proposed method and the cooperation used for either repairing infeasibility of the solutions or the improvement of the quality of the solutions at hand. Section 4 evaluates the performance of the proposed method on benchmark instances, where its achieved results are compared to those reached by recent algorithms available in the literature. Finally, Section 5 concludes by summarizing the contribution of the paper.

2. Related work

The ISP problem belongs to the Cutting and Packing family (Wascher, Haussner, & Schumann, 2007), which is considered as an old family of combinatorial optimization problems. The problem of packing identical spheres into the smallest container (parallelepiped or sphere) has received very little attention in the literature. Most published papers focus on packing (or cutting) items in two-dimensional supports whereas very few papers addressing the problem of packing spheres into specific supports, like container or open container, are available.

Among the available papers, Lochmann, Oger, and Stoyan (2006) addressed a statistical analysis for packing random spheres with variable radius distribution. Li and Ji (2013) studied a special problem of packing spheres into a cylinder container, where a dynamics-based collective method was proposed.

Farr (2013) discussed the problem of random close packing fractions of lognormal distributions of hard spheres, where a one-directional procedure-based method is tailored; that is an approach used in order to predict a close packing of spheres of lognormal distributions of sphere sizes.

Packing spheres into a container has also been addressed by Sutou and Dai. (2002) who proposed a global optimization approach. In Stoyan, Yaskow, and Scheithauer (2003) and Stoyan and Yaskow (2008), the authors described a mathematical model for packing spheres into an open container, where both height and width are fixed whereas the length is a variable to be determined. They proposed a neighbor search based upon extremum points for achieving a series of solutions.

M'Hallah, Alkandari, and Mladenović (2013) proposed a heuristic that is based on combining Variable Neighbor Search (VNS) with nonlinear programming solver. The method iterates moves of the current configuration and completes the partial configuration with a solver providing an approximate solution for a given nonlinear programming.

M'Hallah and Alkandari (2012) considered the principle used in M'Hallah et al. (2013) to solve the problem of packing identical spheres into the smallest containing sphere.

Soontrapa and Chen (2013) tackled the problem of packing identical spheres into a smallest containing sphere by using a random search following Monte Carlo's method.

Finally, Birgin and Sobral (2008) proposed twice-differentiable non-linear programming models for packing both circles and spheres into different containers where the containers may be circular, rectangular, etc. In order to reach a global solution for their proposed models, ALGENCAN solver was used for generating a multiple starts solutions (an extensive efficient models and methods for packing both circular and sphere problems were reviewed in Hifi & M'Hallah, 2009).

Particle Swarm Optimization (PSO) is considered as an evolutionary approach, where it has been proven to be very effective for many optimization (non)constraints problems (cf. Kennedy et al., 2001). However, using PSO for solving constraint optimization problems remains challenging because only few papers focused on solving these problems are available in the literature.