Universidad Autónoma de Nuevo León

Facultad de Ingeniería Mecánica y Eléctrica

Subdirección de Estudios de Posgrado

Bin packing applications in additive manufacturing

por

Aned Esquerra Arguelles

como requisito parcial para obtener el grado de

maestría en ciencias de la ingeniería

con orientación en Sistemas

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SUBDIRECCIÓN DE ESTUDIOS DE POSGRADO

Los miembros del Comité de Tesis recomendamos que la Tesis "Bin packing applications in additive manufacturing", realizada por el alumno Aned Esquerra Arguelles, con número de matrícula 1985276, sea aceptada para su defensa como requisito parcial para obtener el grado de Maestría en Ciencias de la Ingeniería con orientación en Sistemas.

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FIME
009

San Nicolás de los Garza, Nuevo León, junio 2020

"You were taught, with regard to your former way of life,
to put off your old self,
which is being corrupted by its deceitful desires;
to be made new in the attitude of your minds;
and to put on the new self,
created to be like God in true righteousness and holiness."

Ephesius. 4:22-24

Dedicatory

To my mother, of whom I am the result.

To my father, for inheriting his stubbornness.

To Adriano Alessandro, my beloved son to be the incentive of my everyday achievements.

To Carmen Luisa, my eternal love and wife for her constant and unconditional support and understand all the time that I have been away.

To my father Fidel Rodríguez Puertas, for his immeasurable patience all these years.

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First of all, to God for all the blessings received so far.

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Abstract

Aned Esquerra Arguelles.

Candidato para obtener el grado de Maestría en Ciencias de la Ingeniería con orientación en Sistemas.

Universidad Autónoma de Nuevo León.

Facultad de Ingeniería Mecánica y Eléctrica.

Título del estudio: Bin packing applications in additive manufacturing.

Número de páginas: 80.

Objetivos y método de estudio:
Objectives:

Develop avant-garde models for "Build Volume", "Void structures", and "Densest Layer Filling" problems focused on a novel vertexes-approach for their application in additive manufacturing.

Validate the models by experimenting on instances associated with three-dimensional printing problem typologies.

Propose a methodology to face problems in bin packing from several solution strategies.

.

Contribuciones y conclusiones:

Contributions:

Initiate a brand-new area of investigation with fresh vertexes-based model approaches to apply in 3D printing, to solve specific field problems.

Create an online public repository of far-out instances, models, results, and more resources to share with the BPP scientific community.

Conclusions:

Initials solutions obtained from global solvers mixed with inner-point solver strategies are a good starting point facing medium-sized densest filling layer problems and work extremely efficient in void structure situations.

Build volume problems can be treated by this model using an aggregation of objects with similar mechanical and physical properties inside the chamber with simple adaptations to objective functions.

The general problems described in the current research can be treated as multi-objective ones, but in general, is verified that a higher-order method of solution like decomposition and mixed strategies are required to obtain better quality parameters in a reasonable time.

Despite the developed exact models can not solve instances with a huge amount of items to pack, the case of densest filling layer applications so far, the developed model has proven its efficiency in void structures problems and build volume problems with some variations.

Firma del asesor: ______________________

Dr. Igor Semionovich Litvinchev

Chapter 1

INTRODUCTION

"If we knew what it was we were doing, it would not be called research, would it?"

ALBERT EINSTEIN.

Contents

1.1 Additive manufacturing

Additive manufacturing[1] is a set of tools and techniques for constructing three-dimensional objects from CAD/CAM data or digital models. This technology, also known as 3D printing frequently refers to a diversity of processes where raw materials melt, join and solidify under computerised controlled build-chambers to create three-dimensional articles by the primal matter deposition layered fusion, or another specific technique.

Late in the '90s, 3-D printing procedures were suitable barely for functional or aesthetic prototypes production, and their use was mainly in rapid prototyping, hence the association with the term 'rapid prototyping'.

As of 2019, additive technologies are viable as industrial-production-technology schema on account of the increased progress in precision, easy repeatability of processes, low waste primal ore, and a wide range of raw material to use, among other features. One of the essential benefits of 3D printing is the ability to compose complex shapes impossible to construct by hand, or traditional manufacturing approaches, including hollow parts or parts with internal truss structures to reduce weight. Also, fused deposition modelling becomes the most common 3D printing process in use.

The lastest years show notable advances in the rapid prototyping forefront: leading the production of titanium-alloy fully functional parts for the aero-spacial

[1]The term additive manufacturing can be used interchangeably with 3D printing.

and medical fields; powder bed fusion technology allows building hollow near-net shapes with accurate resolutions; directed energy-based high-tech offers the ability to add features on existing elements, remanufacture, and repair damaged ones; as well as producing parts directly from CAD data, see Figure 2.1 from page 17.

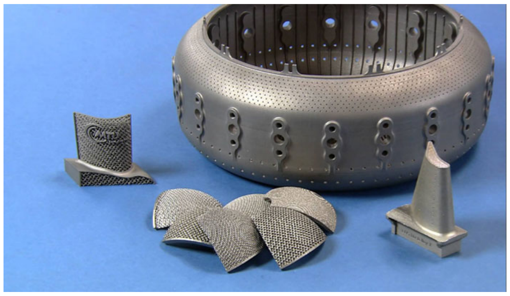
With industry 4.0 in full motion, the non-subtractive production arena is ultimately exciting and endless in opportunities, becoming a transformer agent in numerous domains and one of the most growing fields in the next decades, with applications in almost every aspect of modern life. Three-dimensional printing is revolutionising industries focused on industrial manufacturing, but with the advances in hi-tech, the possibilities are much broader.

1.1.1 General additive manufacturing benefits

1. Control prototyping and manufacturing costs.
2. Quick replacement of complex parts.
3. Ease of workability and waste reduction.
4. Reduced part counts and increased product complexity.

1.1.2 Applications of additive manufacturing

The backbone of additive manufacturing utilisation practically to date has been in the realm of engineering, especially to generate model prototypes. However, the potential of 3DP has increasingly been recognised in areas of commercial manufacture, in architecture, Materials Science, medicine, and so on due to its capacity to create supplies and devices matching, if not exceeding, the advantages of traditional consumer assets. This section presents various applications areas with an essential role in modern life.



(a) MTU Aero Engines parts, Source [1]

(b) Parts for Airbus. Source [1]

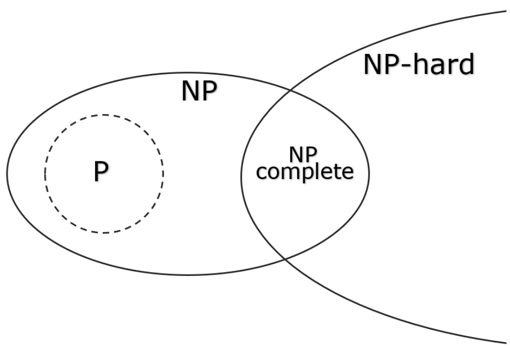
(c) Airbus injector part. Source [1]

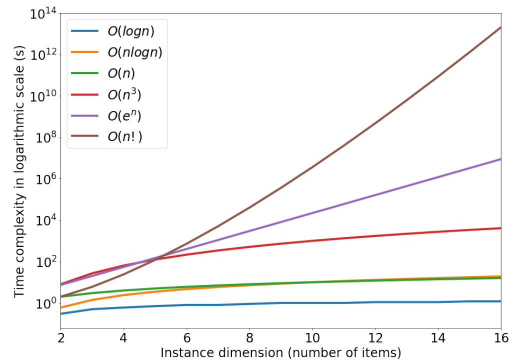
(d) Decorative items. Source [74]

FIGURE 1.1: 3D printing applications

In the pharmaceutical area, the discoverings and enhancing of 3-D printing systems can lead to the creation of a new dosage form designs, pre-clinical drugs development, on-demand production of medical devices, customised medications in clinical pharmacy practice, and the production of functional implants [3].

As the aerospace enterprise has a long history adopting and pioneering avant-garde technologies additive manufacturing fits right in with its historical trend, initially having a niche role in aerospace manufacturing like technology for rapid prototyping, however, as aerospace-oriented manufacture focuses on low-volume production of systems incorporating complex mechanical and electronic components [48].





(a) NP-hard problems diagram. Source [36] (b) Time complexity curves, based on [58]

FIGURE 1.2: NP-hard relationships [25][73] and time complexity in big-O notation

1.2 Bin packing problems

Bin packing problems are a class of mathematical optimisation problems where a set of objects, also known as items[2], e.g., projects budget items, geometrical objects, and metal granules, is restrained to a bigger one frequently called the container[3], this simplistic explanation gives the reader an erroneous idea about the complexity of the solution strategies of these problems.

Typically, the objective is either to bind one container as dense as possible or to restrict all items using a minimum number of vessels, maintaining a non-overlapping packing pattern between elements and receptacle boundaries.

Bin packing quandaries are notable cases of the C&P category, see Section 2.2 from page 18. There are numerous of variations of BPPs, e.g., 1BPP [52], 2DBPP, 3DBPP [10], linear, weighted packing, cost-based packing, sparse packing [67], irregular packing [39][11], among other classifications; all these problems are frequently combined with a variety of constraints [9] becoming strenuous ones. One of the most challenging aspects of this mathematical queries is the exponential

[2]This set may contain different-shaped, mono-sized regular, or irregular objects.

[3]Often a one-dimensional, three-dimensional or n-dimensional convex region, infrequently an infinite space or non-convex region.

growth of their solution search space with small increments in the number of items to bind, see Figure 1.2b from page 5, this is why they receive the name of combinatorial NP-hard problems [36][58][71] in computational complexity theory.

Packing problems have a wide range of real-life practical applications: logistics, i.e., containers loading [79][35]; materials science, i.e., [47]; in medicine; additive manufacturing; biology; nanotechnology; telecommunications, i.e., [51] [76] [62]; security services; architecture among other fields.

The objective function in a bin packing problem can vary from: maximising the area covered by a limited number of service centres; minimising the interference between service zones corresponding to different providers; maximising the volume of the container using dense packing; to place the objects sparse to keep distance between groups of similar ones.

1.3 Relationship between additive manufacturing and bin packing

As a parallel manufacturing process, AM enables manufacturing of different parts in a single build volume give rise to "Build Volume Packing" problems, see Figure 1.3 from page 7. A set of 3D items must be placed into containers or build volumes, see Figure 4.13 from page 65, optimising a particular objective subject to non-overlapping between items, and the edges of the container. The objectives vary from the densest packing (minimising space between the items) to the sparsest packing (maximising the minimal distance between the items).

In these problem typologies, modellers know the additive manufacturing items beforehand and design the best object layout inside the build volume. Generally, the build volume has the form of a prismoid, the following cases of "Building Volume

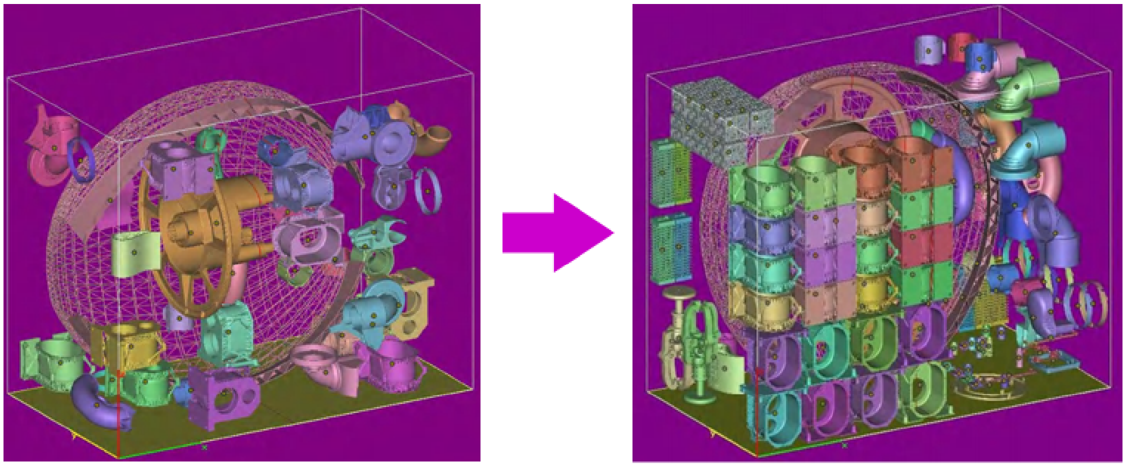


FIGURE 1.3: Build volume problem.

Problem[4]” various consider different object shapes:

1. **Densest packing**: the objects are placed in the container without overlapping and minimising the total space between the objects, with higher density ratios, the minimal distance between the objects is at least a given threshold.

2. **Sparsest packing**: the objects are placed in the container as distant as possible between them, and from the container border. This type of situation occurs when it is necessary to maintain parts separated to prevent possible deformations while cooling, or mechanical changes due to laser heat propagation.

3. **Cluster packing**: an object cluster is composed of items with similar features (mechanical properties, shapes, sizes or primal matter used for printing). The elements in the same batch are placed close enough to similar ones in a kind of densest packing. However, the distance between clusters must be sufficiently large to avoid low-quality end products or the detriment of parts characteristics. In this sense, this type of configuration considers packing clumps as the sparsest packing for macro-objects [66].

Additive manufacturing offers enormous geometrical freedom to create parts,

[4]These classes of problems belong to 3D optimised packing problems.

hollow structured systems are typical practices for printing primal matter, and time reduction in 3D printing of light-weighted parts. "Generating Void Structures[5]", is also a packing problem with holes standing for packing items, see Figure 1.4 from page 9. The number of holes, their shapes and sizes, positions and space orientations has to be defined minimising, e.g., the weight of the part without significant loss of its mechanical strength.

GVS is a design problem for manufacturing light-weighted hollowed structures or parts. Designing void structures is a particular variety of packing problem with the holes interpreted as objects placed into the piece. In contrast to the "Build Volume Packing", where the objects are given, in "Generating Void Structures" the number of holes, their shapes and sizes are defined subject to certain mechanical constraints. Generally, a mechanical strength engineer defines zones of the part suitable for hole introduction without losing significant mechanical characteristics; also the type of the holes allowed must be indicated, e.g., smooth or non-smooth, see Figure 1.4 from page 9. The difference resides in smooth holes, e.g. spheres or ellipsoids, are easier for finishing processes after printing and may provide more strength due to the absence of "corners". Alternatively, polyhedral holes may provide more weight savings under the same strength and fit tighter to technological constraints. Similarly, the holes have to be separated sufficiently one from another to avoid mechanical crash of the overall part under peak loads. The objective of the "Generating Void Structures" is minimising the weight of the part under mechanical constraints; this section presents several cases:

1. **Ellipsoidal holes**: ellipsoidal or/and spherical objects[6] have to be placed entirely in the convex 3D hollow zone without overlapping or distant enough one from another and the border of the container. The number of ellipsoids, their sizes, positions and space orientations are unknown and have to be defined maximising the total volume of the ellipsoids.

[5]Idem fon:bin-packing-classes

[6]This objects are hollow regions in the printed part.

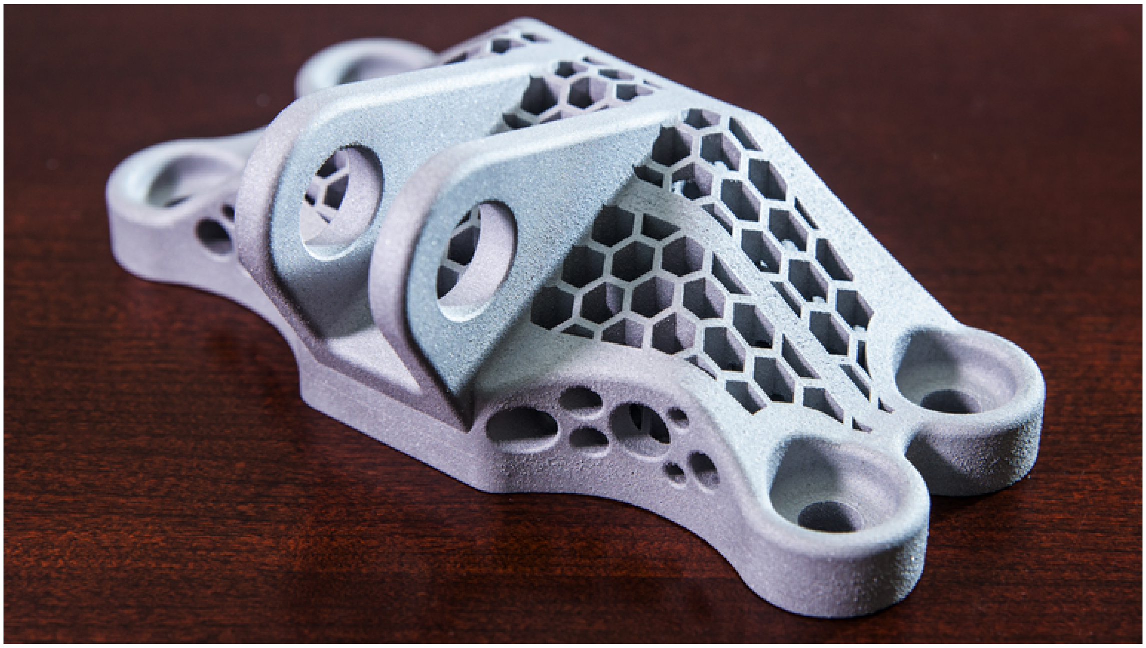


FIGURE 1.4: Generating void structures with smooth and non-smooth objects. Source [24]

2. **Polyhedral holes**: similar to the previous case, but using polyhedra[7] for the hollowing systems. *A priori* the modelling engineers fix the shapes of the polyhedra, increasing or decreasing polyhedra numbers in a homothetic manner. Alternatively, the operators fix only several vertices of the polyhedron, while the optimisation volume defines its shape.

Laser 3D printers operate with various raw materials, including metal particles, i.e., powders of titanium alloys are promising for the aerospace industry due to the attractive combination of high structural strength, low density, and tremendous corrosion resistance. There are two main approaches for manufacturing parts using 3D printing: a) fixation (alloying, sintering) of powder in the previously applied layer and b) direct layer-by-layer application of the already melted powder onto the substrate. In both cases, pores resulting from the sintering process are difficult to eliminate in the layer-by-layer technique. The quality of the powder is related to its packing density depending on the powder particles composition, their sizes and

[7]Idem to fon:hollow-section

shapes. This way a packing problem corresponding to the "Densest Layer Filling arises"[8], see Figure 1.5 from page 10.

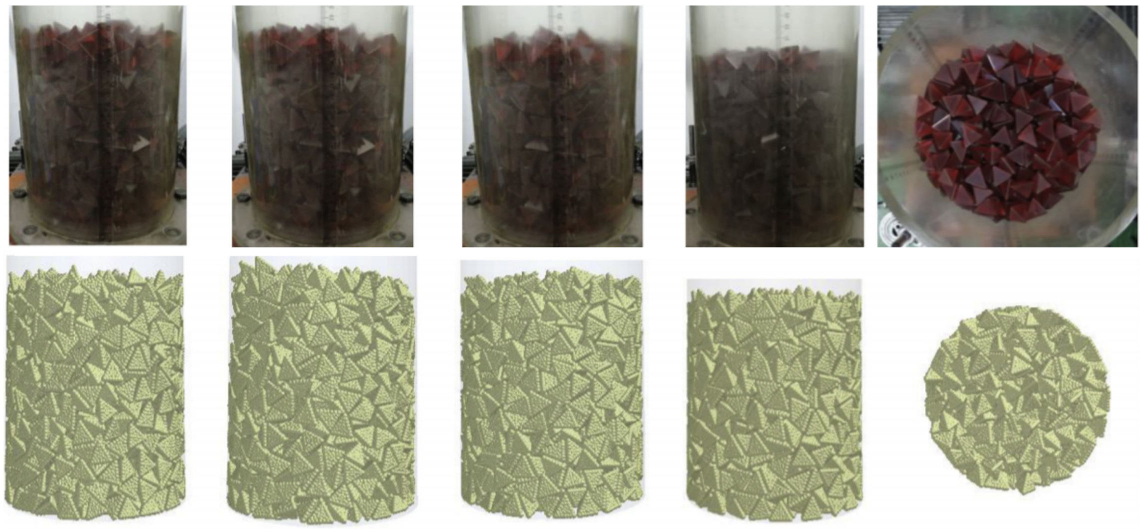


FIGURE 1.5: Snapshots of the densest filling layer packing morphologies of tetrahedral-shaped particles obtained via physical tryout and DEM simulations. Source [91]

This problem refers to the ore-alloys preparation used for additive manufacturing final processes. The quality of the powder is highly related to its packing density depending on the powder particles composition, their sizes and shapes. Usually, the powder engineers know a relative number of particles of a given size (relative frequency) and fulfilled the necessary conditions in the final packing. This section describes "Densest Layer Filling" for cuboidal layers cases:

1. **Spherical powder**: the spherical powder particles define the height of the layer resulting in the maximal density subject to a given relative frequency[40][49].
2. **Non-spherical powder**: similar to spherical, just involving non-spherical, i.e., polyhedral or cylindrical powder particles [41] [91] [63][90] [20].
3. **Mixed powder**: this is a mix of prior two approaches..

[8]Idem fon:bin-packing-classes

Modelling, validating and solving “Build Volume Packing”, “Generating Void Structures” and “Densest Layer Filling” problems; require different models, analytics, spatial and mathematical conditions, and involve several families of constraints adding complexity not only to the model but also to every instance type; in each type of problem, the dimensionality of the instances vary from one model to another.

1.4 Motivation

Several motivations are leading to start a research of bin packing applications in the additive manufacturing field: scientific ones related to the challenging and complex nature of problems associated with 3D printing “Densest Layer Filling” in large-scales production schemas; practicals ones related to the essential importance of these technologies in the future of manufacturing production; economic motivations due to forecast on the rise and inclusion on 3D printing in the global economy, and the destination of funds to investigate new trends, production workflows, and techniques.

1.5 Hypothesis

Through the generation of avant-garde model approaches, theories, and solution methods solve problems in additive manufacturing which nowadays remain unexplored with a significant improvement in modelling, elapsed times to find feasible or optimal solutions with excellent time responses.

1.6 Objectives

- Develop avant-garde models for "Build Volume", "Void structures", and "Densest Layer Filling" problems from a novel vertex-approach to apply in additive manufacturing.
- Demonstrate the validity of these models with experimentation on several kinds of instances, related to "Densest Layer Filling" of problem.
- Propose a cyclical methodology to face problems in bin packing from several solution strategies.

1.7 Expected contributions

- Open a brand-new area of investigation, with vertex-based model approaches to apply in 3D printing to solve specific field problems.
- Create an online public repository of recent 3D instances, vertex-based 3D models, tables of results, and experimentation imagery to share with the scientific community involved in bin packing research.
- Publish in a JCR journal a research article centred on a series of 3D vertex-based approach model for bin packing of mono-sized regular items.

1.8 Scope and limitations

The scope of the current study is bound to the activities listed next in this section. The investigation workflow follows a prior designed methodology, see Figure 3.1 from page 40, the process goes from the analysis of problem instances to the study of their mathematical formulations, and characteristics, it includes the development of a vertex-based baseline model, and the model validation through experimentation with different containers and objective functions, see Chapter 4 from page 45.

> The experimentation focus on packing regular tetrahedra[9] into different convex regular containers due to discrete computational resources and the lack of mathematical solver licensing limitations.
>
> The proposed instance complexity study lingers as an element of future work due to technical concerns with the massive growth of models search spaces.
>
> The investigation focuses its efforts on exact methods as the principal strategy used to find solutions; meta-heuristics, decompositions tactics, Q-neural networks, and other techniques remain as other elements of future work.

1.9 Thesis structure

This section concisely overviews the contents of this document chapter by chapter, describing the main course of actions taken in each one of them. Every topic gives the reader a description of the structured workflow developed by both: the author and the leading assessor.

1.9.1 Chapter 1: Introducing C&P problems and its applications to additive manufacturing

This chapter introduces additive manufacturing; it also overviews several essential characteristics of the C&P problem typologies. Furthermore, it exposes the relationship

[9] The models can manage a wide range of three-dimensional items, e.g., tetrahedra, cubes, octahedra, Plato's solids, and others.

Figure 1.6: Build chamber for large scale parallels additive manufacturing production. Source [2]

of these kinds of techniques with 3D printing in large production schemas and finally describes an approach using vertex to model structures and objects in CAD systems. It is about making a concise approach to the investigation subject, author motivations, research importance, analysis implications, scope and limitations, as well as how convenient is the vertex-base method to study of packing different three-dimensional elements in regular convex containers.

1.9.2 Chapter 2: Theory, assumptions and requirements

This chapter brings to the table the thesis theoretical framework, and is the fundamental pillar of the investigation. The analytical, experimental, and mathematical outcomes constitute the basis on which any further analysis, experiment or proposal for the development of the project will be supported; it also exposes the relevant related works to this research. The related areas follow from the research objectives, see Section 1.6 from page 12.

1.9.3 Chapter 3: Methodology and research workflow

This chapter outlines the scientific method present in the current research, in detail explains every stage step of the workflow process methodology design, it also gives some details about the instance design, and model mathematical formulation.

1.9.4 Chapter 4: Experimentation, materials, and methods

This chapter presents the experiment planning and serves as a blueprint for the experimentation execution and outcomes interpretation. It describes step by step the software involved in mathematical modelling; the solvers used and why their selection to execute the models; the tailored tools for 3D plotting, web-scrapping, instances generation, the data analysis; and the equipment related to run the models, shows and explains the mathematical formulation of the models. The design supports the research goals and hypotheses aiding the current investigation; it also provides the details of the experimental design including its parameters, variables, planning, expected participants, objects, instrumentation and procedures for data collection and analysis. A final evaluation based on an experimental design shows the validity of the insights.

1.9.5 Chapter 5: Conclusions, research limitations and future works

The last chapter summarises and exposes accomplished goals that support the initial hypothesis, it also reveals the outcomes resulting from the experimentation design and presents the drawbacks found during the research lifespan, and finally some areas of future work with ideas to overcome these obstacles.

Chapter 2

THEORY

"He who loves practice without theory is like the sailor who boards ship without a rudder and compass and never knows where he may cast."

LEONARDO DA VINCI.

Contents

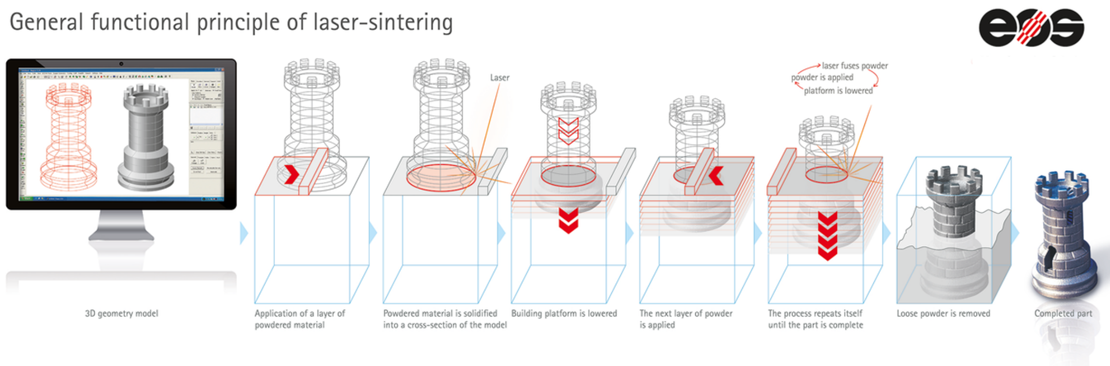


FIGURE 2.1: 3D printing workflow direct from CAD data. Source [24]

2.1 INTRODUCTION

Research on 3DBPP problems with different characteristics is plentiful. This section does not pretend to cover every single article in this branch of knowledge. Therefore, it is restricted to the review of some type of three-dimensional objects packing in several different containers with various methods and approaches, i.e., simulations using 3D vibrations and DEM techniques, exact methods, heuristics, see Table 2.1 from page 18. This section also refers to several excellent research works for reviews with possible applications to AM.

Despite the increasing computing power of today's vertical scaled-up workstations, there are still limitations as the processing speeds and fast computational storage involved is not enough to run the upcoming extended complex mathematical models optimally. However, there are considerable signs of progress with the inclusion of new horizontal computational integrated systems, even when those kinds of architectures mainly focused on Big Data applications. Hopefully soon, exact methods will overcome those drawbacks shortly, in a concordance of mathematicians efforts to discover and innovate new ways to improve models and these specific solution methods, as shown next in the compilation of the recent scientific articles on the subject.

This section also includes several papers on simulation, and physical packing experiments using DEM techniques for different mono-sized 3D particles. All the papers presented use techniques related to 3D vibrations and start from a random lose packing state to achieve a random close state in the final phases of the experimentation, the primary reason those investigations inclusion in this document resides in the outcoming ideas for further implementation of a GSA heuristic-based [64] in these experimentations, in future works.

Table 2.1: Problem typologies reviewed in the literature

Container type	3D Item class	Methods
Cylindrical	Ellipsoids	Exact, see Section 2.6.3.1
Prismoidal	Spheres	Simulations, see Section 2.6.3.2
Spherical	Tetrahedra	Heuristic and meta-heuristics, see Section 2.6.3.3
	Prisms	
	Other shapes	

2.2 C&P problems classification

Cutting and packing problems appear under various names in literature, e.g. cutting stock or trim loss problem, bin or strip packing problem, vehicle, pallet or container loading problems, nesting problem, knapsack problem etc. In 1990 appeared the first review paper exposing a consistent and systematic approach for a comprehensive typology integrating various kinds of problems [22], this typology is founded on the underlying logical structure of cutting, and packing problems. The primary purpose was to unify the different use of notions in the literature and to concentrate further research on particular types of problems, see Table 2.2 from page 19.

Table 2.2: A basic typology of C&P problems.

Objective	Items nature	Type of problem
Output maximisation	Identical	Identical item packing problem
	Weakly heterogeneous	Placement problem
	Strongly heterogeneous	Knapsack problem
Input maximisation	Arbitrary	Open dimension problem
	Weakly heterogeneous	Cutting stock problem
	Strongly heterogeneous	Bin packing problem

As the number of publications in the area of Cutting and Packing (C&P) increased considerably in the next two decades, the first typology of C&P problems introduced by Dyckhoff initially gave an excellent instrument for the classification of existing ones and incoming uncategorised problems appearing in new papers. However, over the years, some deficiencies of this typology became obvious, creating difficulties dealing with recent developments and preventing their acceptance. An improved typology was necessary partially based on Dyckhoff's original ideas introducing new categorisation criteria, defining problem categories different from those of Dyckhoff's [89].

2.3 Plato's solids

Plato's solids refer to five...., see Figure 2.2, from page 20,

2.4 Tetrahedra

The regular tetrahedron is the simplest Plato's solid [83]; Notwithstanding, in the study of its packing properties, several ancient Greek mathematicians, renowned

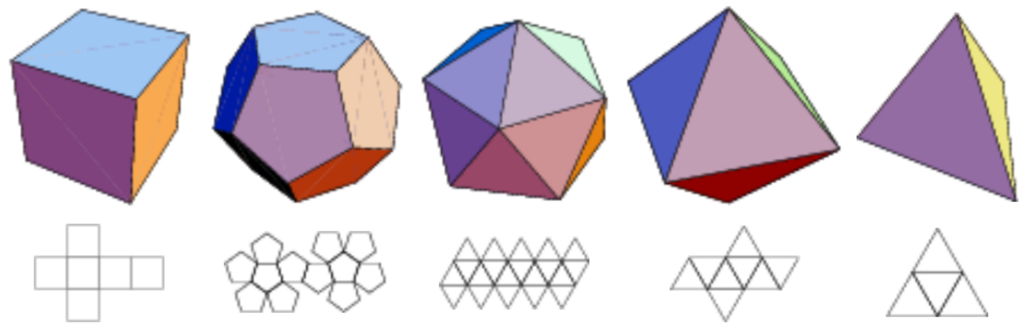


Figure 2.2: Plato's solid and their 2D representations. Source [83]

academics, and world-class scientists have made mistakes; many inquiries and interrogations about these structures persist unsolved. Currently, no one knows the density of its densest packings, the density of its densest translating packings, or the exact value of its congruent kissing number[1] [38] [21].

Nowadays, it is clear that regular tetrahedra cannot tile three-dimensional Euclidean spaces [32]. Our results suggest that the regular tetrahedron may not be able to pack as densely as the sphere, which would contradict a conjecture of Ulam. The regular tetrahedra might even be the convex body having the smallest possible packing density [14].

$$\theta = \cos^{-1}\left(\frac{AE + BF + CG}{\sqrt{A^2+B^2+C^2}\sqrt{E^2+F^2+G^2}}\right) \tag{2.1}$$

2.5 Non-overlapping and containment conditions

Let P, $G \subset \mathbb{R}^n$ be convex bounded polytopes defined by their vertices [45].

[1]The number of equivalent hyperspheres in n dimensions which can touch an equivalent hypersphere without any intersections, also sometimes called the "Newton number", contact number, coordination number, or ligancy.

$$P = \{x^s, s = 1, 2, 3...S\} \qquad G = \{y^l, l = 1, 2, 3...L\} \tag{2.2}$$

By convexity, a linear combination of their vertices can represent any point of P and G:

$$x \in P \Leftrightarrow x = \sum_s \lambda_s x^s, \quad \sum_s \lambda_s = 1, \quad \lambda_s \geq 0 \tag{2.3}$$

$$y \in G \Leftrightarrow y = \sum_l \mu_l y^l, \quad \sum_l \lambda_l = 1, \quad \lambda_l \geq 0 \tag{2.4}$$

By the definition $P \cap G \neq \varnothing$ if there exists a point belonging to both P and G. Thus, if $P \cap G \neq \varnothing$ there exists λ_s, μ_l such that:

$$\sum_s \lambda_s x^s = \sum_l \mu_l y^l, \quad \sum_s \lambda_s = 1, \ \lambda_s \geq 0, \quad \sum_l \mu_l = 1, \ \mu_l \geq 0. \tag{2.5}$$

Correspondingly, if system 2.5 has no feasible solutions, then $P \cap G = \varnothing$. To check out if 2.5 is feasible, consider the following optimisation problem:

$$\begin{aligned} z^* = \max \sum_s \lambda_s + \sum_l \mu_l \\ \sum_s \lambda_s x^s = \sum_l \mu_l y^l \\ \sum_s \lambda_s \leq 1, \quad \lambda_s \geq 0 \\ \sum_l \mu_l \leq 1, \quad \mu_l \geq 0 \end{aligned} \tag{2.6}$$

Note that 2.6 always has a feasible solution $\lambda_s = 0, \mu_l = 0$. Moreover, by constraints in 2.6, each term in the objective does not exceed 1. If $z^* = 2$ then the optimal solution to 2.6 fits 2.5 and hence $P \cap G \neq \varnothing$. Otherwise, for $z < 2$ we may conclude that 2.5 is infeasible and hence $P \cap G = \varnothing$.

The associated Lagrangian function to 2.6 has the following expression:

$$L(\lambda,\mu,v,\alpha,\beta)=\sum_s \lambda_s+\sum_l \mu_l+v\left(\sum_s \lambda_s x^s-\sum_l \mu_l y^l\right)-\alpha\left(\sum_s \lambda_s-1\right)-\beta\left(\sum_l \mu_l-1\right) \quad (2.7)$$

$$v\in\mathbb{R}_n, \qquad \alpha,\beta\geq 0$$

For fixed x^s, y^l the problem 2.6 is an LP problem. The corresponding dual has the form:

$$z^*=\min\{\alpha+\beta\} \quad (2.8)$$

$$\frac{\partial L}{\partial \lambda_s}=1+vx^s-\alpha\leq 0, \quad s=1,2...S \quad (2.9)$$

$$\frac{\partial L}{\partial \mu_l}=1+vy^l-\beta\leq 0, \quad l=1,2... \quad (2.10)$$

$$v\in\mathbb{R}^n,\alpha,\beta\geq 0. \quad (2.11)$$

By the strong duality theorem for LP we may state the non-overlapping condition $P\cap G=\varnothing$ in the form:

$$\alpha+\beta=\sum_s \lambda_s+\sum_l \mu_l<2 \quad (2.12)$$

$$1+v\cdot x^s-\alpha\leq 0 \quad (2.13)$$

$$1+v\cdot y^l-\beta\leq 0 \quad (2.14)$$

$$\sum_s \lambda_s x^s=\sum_l \mu_l y^l \quad (2.15)$$

$$\sum_s \lambda_s\leq 1, \quad \lambda_s\geq 0 \quad (2.16)$$

$$\sum_l \mu_l\leq 1, \quad \mu_l\geq 0 \quad (2.17)$$

$$v\in\mathbb{R}^n,\alpha,\beta,\mu_l,\lambda_s\geq 0 \quad (2.18)$$

System 2.12 has $S+T+n+4$ linear constraints and $S+L+n+4$ variables.

Note, that in the overall optimised packing problem coordinates x^s, y^l of the vertices are the variables to define. Then to fix the shape/size of the polytopes P and G, is mandatory to impose additional constraints.

For the convex container Ω, the containment conditions $P \subseteq \Omega$ are equivalent to:

$$x^s \in \Omega, \quad s = 1, 2, ...S \tag{2.19}$$

2.6 Articles and literature review

TABLE 2.3: List of latest reviewed bin packing articles related to the research topic.

Article			Instances						
Title	Ref.	Year	Cont. type	Dim.	Objects	R	MS	Size	Sol. method
Packing ellipsoids in an optimised cylinder	[65]	2020	Cylindrical	3D	Ellipsoids	Y	Y	Large	Exact
Lagrangian Approach to Modelling Placement Conditions in optimised Packing Problems	[45]	2020	*	*	*	*	Y	*	Exact
Experimental study on 3D vibrated packing densification of mono-sized dodecahedral particles	[41]	2020	Cylindrical	3D	Dodecahedra	Y	Y	Large	Simulation
Packing of different shaped tetrahedral particles: DEM simulation and experimental study	[91]	2020	Cylindrical	3D	Tetrahedra	N	N	Large	Simulation
A GRASP algorithm for multi-container loading problems with practical constraints	[4]	2020	Prismoidal	3D	Prismoidal	N	N	*	Meta-heuristics
An experimental study of packing of ellipsoids under vibrations	[40]	2020	Cylindrical	3D	Ellipsoids with several shapes	Y	Y	Large	Simulation
Multi-super-ellipsoid model for non-spherical particles in DEM simulation	[49]	2020	Cylindrical	3D	Ellipsoids	Y	Y	Large	Meta-heuristics
An optimised Covering Spheroids by Spheres	[57]	2020	Spherical	3D	Spheroids	Y	N	Large	Heuristics
Optimal layout of ellipses and its application for additive manufacturing	[68]	2019	Polygonal	2D	Ellipse	Y	Y	Large	Exact
A local search-based method for sphere packing problems	[31]	2019	Cuboidal	3D	Sphere	Y	Y	Large	Meta-heuristics
DEM simulation on the vibrated packing densification of mono-sized equilateral cylindrical particles	[63]	2018	Cylindrical	3D	Cylindrical	Y	Y	Large	Simulation
Evolutions of packing properties of perfect cylinders under densification and crystallisation	[47]	2018	Other shapes	3D	Cuboidal	Y	N	Large	Exact
BRKGA/VND Hybrid Algorithm for the Classic Three-dimensional Bin Packing Problem	[92]	2018	Prismoidal	3D	Prismoidal	N	N	Large	Meta-heuristics
Packing Irregular Objects in 3D Space via Hybrid optimisation	[50]	2018	Other shapes	3D	Other shapes	N	N	Large	Heuristics

TABLE 2.4: List of latest reviewed bin packing articles related to the research topic (cont.).

Article					Instances				
Title	Ref.	Year	Cont. type	Dim.	Objects	R	MS	Size	Sol. method
DEM dynamic simulation of tetrahedral particle packing under 3D mechanical vibration	[90]	2017	Cylindrical	3D	Tetrahedra	Y	Y	Large	Simulation
Maximally dense random packings of cubes and cuboids via a novel inverse packing method	[46]	2017	Other shapes	3D	Cylindrical	Y	N	Large	Exact
Voronoi analysis of the packings of non-spherical particles	[20]	2016	Other shapes	3D	Other shapes	Y	N	Large	Simulation
A dichotomous search-based heuristic for the three-dimensional sphere packing problem	[30]	2015		3D	Sphere	Y		Large	Meta-heuristics
A hybrid differential evolution algorithm for multiple container loading problem with heterogeneous containers	[42]	2015	Prismoidal	3D	Prismoidal	Y	N	Large	Meta-heuristics
A genetic algorithm for the three-dimensional bin packing problem with heterogeneous bins	[43]	2014	*	3D	*	N	N	Large	Meta-heuristics
An Estimation of Distribution Algorithm for the 3D Bin Packing Problem with Various Bin Sizes	[10]	2013	Cuboidal	3D	Cuboidal	N	N	Large	Exact
A biased random key genetic algorithm for 2D and 3D bin packing problems	[26]	2013	*	2D, 3D	*	N	N	Large	Meta-heuristics
Mathematical models of placement optimisation: two- and three-dimensional problems and applications	[75]	2012	Other shapes	2D, 3D	Several shapes	N	N	Medium	Exact
A Linear Programming Approach for the Three-Dimensional Bin-Packing Problem	[29]	2010	Prismoidal	3D	Cuboidal	N	N	Medium	Exact
DEM simulation on the vibrated packing densification of mono-sized equilateral cylindrical particles	[63]	2018	Cylindrical	3D	Cylindrical	Y	Y	Large	Simulation
Evolutions of packing properties of perfect cylinders under densification and crystallisation	[47]	2018	Other shapes	3D	Cuboidal	Y	N	Large	Exact
BRKGA/VND Hybrid Algorithm for the Classic Three-dimensional Bin Packing Problem	[92]	2018	Prismoidal	3D	Prismoidal	N	N	Large	Meta-heuristics

TABLE 2.5: List of 3D, 2D packing, and general topics related.

Title	Reference	Year	Type	Theme
Irregular packing problems: A review of mathematical models	[39]	2020	Review	Irregular packing models
A hybrid chaos firefly algorithm for three-dimensional irregular packing problem	[11]	2020	Scientific paper	Irregular packing algorithm
Sparsest packing of two-dimensional objects	[67]	2020	Scientific paper	Sparse packing in 2D
Analysis of irregular three-dimensional packing problems in additive manufacturing: a new taxonomy and dataset	[7]	2019	Review	Additive manufacturing
Nested packing of circular objects	[54]	2019	PhD. Thesis	Nested packing
Packing regular objects in a rectangular container	[53]	2016	MSc. Thesis	Regular packing
Constraints in container loading – A state-of-the-art review	[9]	2013	Review	Container loading constraints
Additive Manufacturing Technologies – Rapid Prototyping to Direct Digital Manufacturing	[8]	2012	Book review	Additive manufacturing
GSA: A Gravitational Search Algorithm	[64]	2010	Scientific paper	Heuristics
Disordered, quasicrystalline and crystalline phases of densely packed tetrahedra	[28]	2009	Scientific paper	Dense packing of tetrahedra
An improved typology of cutting and packing problems	[89]	2007	Review	CP classification
A typology of cutting and packing problems	[22]	1990	Review	CP classification
Reducibility Among Combinatorial Problems	[36]	1972	Scientific paper	Computational complexity

2.6.1 Additive manufacturing

In 2019, Luiz et al. present an article [7] reviewing existing general cutting and packing taxonomies and provides a new, more appropriate specification for classifying the problems encountered in AM. It comprises a clear-cut problem definition, a set of precise categorisation criteria for objectives and problem instances, and a simple notation. Furthermore, this review document establishes an improved terminology with terms that are familiar to, but not limited to, researchers and practitioners in the field of AM. Finally, this paper describes a new dataset used in the evaluation of existing and proposed computational solution methods for 3DIP problems encountered in additive manufacturing. It discusses the importance of this research for further underpinning work

Romanova et al. present a paper in 2019 with a study of a layout problem with a variable number of variable-sized ellipses placed into an arbitrary disconnected polygonal domain with a maximum packing factor [68]. The authors show and introduce some tools for mathematical modelling of placement constraints (distance constraints between ellipses and containment of ellipses into a polygonal domain) using the ϕ-function technique. These ϕ-functions allow formulating the layout problem in the form of a MIP model equivalent to a sequence of a non-linear programming sub-problems. The researchers propose and develop a new solution algorithm involving the feasible starting point algorithm and optimisation procedure to search for efficient local optimal solutions of the layout problem. The resulting algorithm can be used in the design of parts for *support-free* additive manufacturing, taking into account the conditions for its static-dynamic strength.

In 2019, Litvinchev et al. introduce a packing problem for irregular 3D objects approximated by polyhedra [44]. In this formulation, a cuboid of minimum height packs the objects under a finite number of continuous rotations, translations with minimum distance between articles. The problem has various applications and arises, e.g. in additive manufacturing. This study describes containment, distance and non-overlapping constraints using the ϕ-function technique. It also presents the related irregular packing problem in the form of a non-linear programming problem besides proposes a solution algorithm based on a fast starting point strategy and efficient local optimisation procedure.

2.6.2 Items packing

In a recent paper, Romanova et al. present an investigation on packing ellipsoids of revolution in a cylindrical container of minimum volume [65], the authors describe how to pack ellipsoids using continuous rotations and translations. They also introduce two non-linear mathematical programming models: one exact, and other approximated; this second model uses an optimised multi-spherical approximation of ellipsoids, both models used the ϕ-function technique to describe analytically non-overlapping and containment constraints. The authors introduce two solution approaches to solve the current packing problem, a set of computational results for up to 500 ellipsoids prove the efficiency of the proposed approaches.

In 2019, Hifi et al. present a study on sphere packing [31] where they study the three-dimensional sphere packing consisting in finding the highest density of a (sub)set of predefined spheres (small items) into a single three-dimensional container (large object) of given dimensions: cuboid of fixed dimensions or cuboid of variable length. The researchers tackle a problem with the prismoidal container of fixed dimensions by applying a local search-based method combining three principal features: (i) a best-local position procedure stage, (ii) an intensification stage and (iii) a diversification stage. The developed method also resolves the problem of packing a set of predefined spheres into a variable-length cuboidal/prismoidal container. Authors also present the method performance evaluation tested on a set of benchmark instances taken from the literature. The comparison of obtained results to those reached by their method shows the algorithms competitiveness for treated problems.

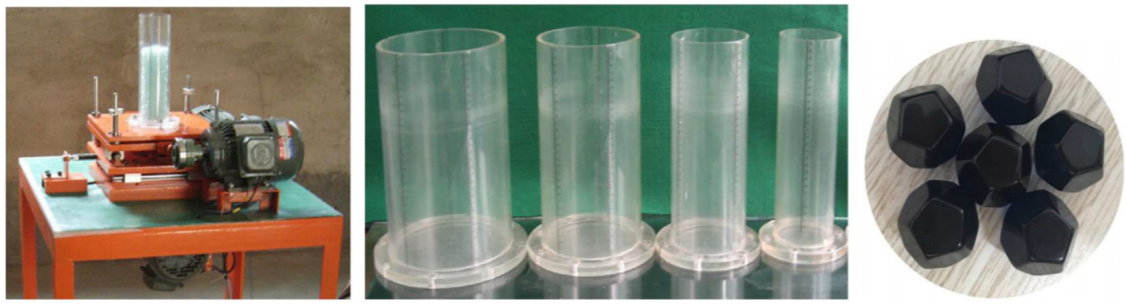
2.6.3 Solution methods

2.6.3.1 Exact methods

Litvinchev et al. propose in May 2020 novel procedures of packing 2D, and 3D elements in regular convex containers from vertex-based, and inequations-based models using a Lagrangian approach combined with KKT optimally conditions. The researchers prove the validity of the models and methods using several strategies and mathematical solvers for a range of randomly generated instances. They also provide a massive library of results fro extensive experimentation, next to the imagery, models, mathematical programming of the models, and instances in a public domain repository to investigation reproduction and consult [45].

In 2013, Yaxiong et al. present an investigation where the authors investigate a more general type of 3DBPP with bins of various sizes [10], unlike traditional bin packing problem where all bins are of the same size. The researchers propose a modified univariate marginal distribution algorithm (UMDA) for solving the problem with a strategy derived from the deepest bottom left packing method. The modified UMDA was experimentally compared with CPLEX and a genetic algorithm (GA) approach. The experimental study shows that the proposed algorithm performed better than GA and CPLEX for large-scale instances.

In 2010 Hifi et al. respectively solve a 3DBPP problem considering containers of identical dimensions to minimise the number of used containers [29], they use a mixed-integer linear mathematical formulation and introduce certain unique, valid constraints to improve the relaxed the lower bound of MILP1. After extensive experimentation, the researchers obtained satisfactory results showing a reliable and consistent execution of the proposed model before the tested instances.



(a) Vibration device (b) Cylindrical-shaped containers (c) Particles

Figure 2.3: Dodecahedral 3D vibration physical experiment using DEM technique. Source [41]

2.6.3.2 Simulations

In May 2020, Li et al. presented a new study on systematic physical experiments to densely packing of mono-sized regular dodecahedral particles exposed to 3D vibrations [41]. The research analyses the influences of various vibration conditions and container size on the packing density with optimised parameters, the way 3D CT non-destructive inspection characterise the microstructures obtained from different packings. The results show the possibility of experiment's reproduction of the transition from initial loose to final denser packing structure of mono-sized regular dodecahedral particles (a maximum packing density of 0.709) with proper control over the vibration conditions. Later microscopic analyses on the 3D computer reconstructed packing structures from experiments demonstrate the specific characteristics of the generated initial loose and final dense packings, see Figure 2.3 from page 30.

Also, in 2020, Zhao et al. present a DEM simulation and physical experiments study on packing different mono-sized tetrahedral particles under 3D vibrations [91]. In this study, researchers comprehensively investigate and optimise the effects of vibration conditions and particle shape on the packing densification during physical experiments. Similar characteristic microscopic properties such as coordination number (CN), particle contact type, radial distribution function (RDF), and particle orientations were numerically characterised and analysed. The results validate the resulting DEM model through physical experiments. Microscopic analysis indicates the minimum mean CN appears for tetrahedral particles with regular shape. The RDF exposes the effect of shape deviations from regular tetrahedral particles, the frequency of face-face, vertex-face and edge-edge contacts all drops out while that of edge-face contact increments. The cluster evolutions' validate the reduction or disappearance of two crucial local clusters (dimer and wagon wheel structures) as one of the principal reasons for density packing shrinkage of irregular tetrahedral particles.

In another recent paper, Li et al. experimentally study the packing of ellipsoidal particles with a range of aspect ratios under vibration conditions [40]. The authors investigate the effects of operational conditions such as dropping heights, feeding methods, and vibration modes on packing density systematically. The results indicate that packing density first increases with dropping height and then tends to be a particular value when dropping height is over 180dv. The relationship between packing density and aspect ratios gives an M-shaped curve, irrespective of operational conditions being consistent with literature observations. The packing density obtained by batch-wise feeding method is higher than the one obtained by the total feeding method, mainly when three-dimensional vibration is applied; the packing density increases proportionality to the vibration frequency and then decreases, i.e. there is an optimum frequency to achieve maximum packing density. The optimum frequency varies with vibration dimensions, and derives in a local particle orientation order under three-dimensional vibration with proper amplitude and frequency.

Quan Quian et al., in 2018 published a study of packing densification (a maximum packing density without wall effects can reach about 0.7166) of mono-sized equilateral cylindrical particles under mechanical vibration; this physical experiment is numerically reproduced using the discrete element method (DEM) [63]. The study analyses the influences of vibration frequency, amplitude and container size on the macro property (e.g. packing density) of each packing are studied. Meanwhile, various micro-properties including coordination number (CN), radial distribution function (RDF), local structures, contact types, particle position/orientation distributions, forces/stresses of the vibrated dense packing are characterised and compared with those of the loose initial poured packing. The outcoming results show that properly controlling vibration conditions can realise the transition of equilateral cylindrical particles from random loose packing (RLP) to random close packing (RCP).

In 2017, Bo Zhao et al. model the transition from random loose packing (RLP) to random close packing (RCP) of mono-sized regular tetrahedral particles under 3D mechanical vibration [90] by using the discrete element method, this paper presents, and systematically studies on the effects of vibration conditions and container size on the packing densification, the macro and micro properties such as packing density, coordination number (CN), particle contact type, RDF, particle orientation correlation, and forces between particles were characterised and analysed. The randomness of the obtained dense packings and corresponding densification mechanisms were also investigated.

Dong et al. present a structural analysis of the packings of identical non-spherical particles based on Voronoi cells [20]. The packings are generated by the discrete element method (DEM) simulations. The particles include axisymmetric ellipsoidal particles from oblates to prolates and cylindrical particles from disks to rods. The Voronoi cells are constructed under space discretisation and surface reconstruction, which is shown to be universal for different shapes. The effects of particle aspect ratio and sliding friction coefficient on the properties of Voronoi cells, including the reduced volume, reduced surface area and sphericity, are quantified. The reduced volume and surface area are found to observe log-normal distributions, while their mean values and standard deviations have different dependencies on particle shape and friction. By analyzing the correlations and using inherent relationships between different Voronoi cell properties, we establish a group of universal equations to predict these distributions according to particle sphericity and overall packing fraction. Such findings cannot only improve our understanding of the packings of non-spherical particles but also provide a basis for evaluating the transport properties and advancing the statistical mechanics theory for granular matter composed of non-spherical particles.

2.6.3.3 Heuristics and meta-heuristics

Alonso et al. in 2020, present a study of a real-life multi-container loading problem solved using a GRASP with improved methods for a company serving its customers: by first placing the products on pallets and then packing pallets on delivery trucks [4]; when the company ships numerous units of a product it requires homogeneous pallets, i.e., pallets containing only one product or weakly heterogeneous ones each layer corresponding to a single product, and finally strongly heterogeneous pallets with the remaining units of the products. The solutions to this problem have to satisfy five types of constraints: geometric constraints, the pallets are entirely inside the trucks and do not overlap each other; weight constraints, limiting the total weight a truck can bear and the maximum weight supported by each axle; constraints limiting the position of the cargo gravity centre; dynamic stability constraints, avoiding cargo displacements when the truck is moving; and constraints ensuring the delivery dates of products are respected.

Also, in 2020, Zhao et al. develop a novel heuristic solution method for solving three-dimensional irregular packing problems [11]. It introduces a three-grid approximation technique to approximate irregular objects. Then, authors design a hybrid heuristic method to place and compact each object where chaos search is embedded into the firefly algorithm to enhance the algorithm's diversity for optimising packing sequence and orientations. Results from several computational experiments demonstrate the effectiveness of the hybrid algorithm.

In 2018, Pankratov et al. present research motivated by packing non-spherical particles problem arising in natural sciences, e.g., in powder technologies. The concept of an ϵ-cover is introduced as an outer multi-spherical approximation of the spheroid with the proximity ϵ. The researchers proposed a fast heuristic algorithm to construct an optimise ϵ-cover giving a reasonable balance between the value of the proximity parameter ϵ and the number of spheres used, provided computational results demonstrate the efficiency of the approach [57].

In 2018, Zudio et al. present a variable neighbourhood descent (VND) inspired algorithm which improves the state-of-art biased random-key genetic algorithm (BRKGA), for the three-dimensional bin packing problem [92]. The constructive greedy-heuristic method to pack the boxes uses integer sequence to establish the order. The presented BRKGA/VND alternative supplies the initial and mutating the population on sorted box sequences. The devised composite method exhibits significantly superior average fitness through the generations, finding solutions with high quality faster. Authors test the novel approach with a standard set of 320 instances. The computational experiment proves that BRKGA/VND produces equal or better results compared to other state-of-art algorithms proposed in the literature. Data shows that BRKGA/VND hybrid variants systematically provide high-quality solutions at fewer iterations as opposed to the results attained by BRKGA.

Ma et al. in a 2018 paper consider the most general forms of irregular shape packing problems in 3D space, where both the containers and the objects can be of many shapes, where the free rotations of the objects are allowed [50]. The authors' propose a heuristic method for efficiently packing irregular objects by combining continuous optimisation and combinatorial optimisation. The initial strategy starts from the initial placement of an appropriate number of objects; then they optimise the positions and orientations of the objects using continuous optimisation. In combinatorial optimisation, and they further reduce the gaps between objects by swapping and replacing the deployed objects and inserting new objects. It demonstrates the efficacy of the authors' method with experiments and comparisons.

Hongteng et al. present, in 2018, a new practical problem treated as a decomposition into three three-dimensional packing problems: three-dimensional irregular packing with variable-size cartons problem, three-dimensional variable-size bin packing problem, and the single container loading problem [88]. Since the three sub-problems are NP-hard, searching for a suitable solution becomes more difficult. In this research, the authors developed mathematical models for each sub-problem and proposed three-stage heuristic algorithms to solve this new problem. They also conducted experiments with random instances generated by real-life cases. Computational results validate the algorithm efficiency and yield satisfactory results.

In this paper Hifi et al. solve the three-dimensional sphere packing problem by using a dichotomous search-based heuristic, the researchers define an instance of the problem by a set of n unequal spheres, and an object of fixed width and height and, unlimited length [30]. Its radius characterises each sphere, and the the problem aims to optimise the length of the object containing all spheres without overlapping. The proposed method employs a beam search combining three complementary phases:

Phase one: a greedy selection determining a series of single search subspace.

Phase two: a truncated tree search, using a width-beam search that explores some promising paths.

Phase three: a dichotomous search that diversifies the search.

Researchers evaluated the performance of the proposed method on benchmark instances found in reviewed literature and compared the obtained results to those reached by some novel methods. The proposed method is competitive, and it yields promising results.

In 2015, Xueping et al. consider multiple container loading problem, commonly known as the three-dimensional bin packing problem (3D-BPP), which deals with maximising container space utilisation while the containers available for packing are heterogeneous [42]. The problem has several applications in cargo transportation, warehouse management, medical packaging, container loading, and various fields of logistics. The authors develop a differential evolution (DE) algorithm hybridized with a novel packing heuristic strategy, best-match-first (BMF), which generates a compact packing solution based on a given box packing sequence and a container loading sequence. Authors evaluated the effectiveness of the developed algorithm on an assortment of industrial and randomly generated instances. The results determine the proposed algorithm outperforms existing solution approaches concerning quality.

In 2014, Li Xueping et al. present a genetic algorithm along with an innovative heuristic packing procedure [43] to solve industrial container loading strategies, the researchers use a novel packing heuristic procedure to converts box packing sequence and container loading sequence encoded in a chromosome to a compact packing solution, the genetic algorithm approach is used to evolve such sequences, this implementation of a hybrid strategy is first applied to 12 industrial instances and later on tested on randomly generated instances, the obtained results demonstrate that solutions with high quality can be found within a reasonable time.

In this paper, Gonçalves et al. present a novel biased random-key genetic algorithm (BRKGA) for 2D and 3D bin packing problems [26]. The approach uses a maximal-space representation to manage the free spaces in the bins. The proposed algorithm hybridises a novel placement procedure with a genetic algorithm based on random keys. The BRKGA is used to evolve the order in which the boxes are packed into the bins, and the parameters used by the placement procedure. Two new placement heuristics are used to determine the bin and the free maximal space where each box is placed. A novel fitness function that improves the solution quality significantly is also developed. The new approach is extensively tested on 858 problem instances and compared with other approaches published in the literature. The computational experiment results demonstrate that the new approach consistently equals or outperforms the other approaches, and the statistical analysis confirms that the approach is significantly better than all the other approaches.

Chapter 3

METHODOLOGY DESIGN

"The researcher suffers the disappointments, the long months spent in the wrong direction, the failures. But failures are also useful, because, well analyzed, they can lead to success. And for the researcher, there is no joy comparable to that of discovery, however small..."

SIR ALEXANDER FLEMING.

Contents

3.1 Introduction

The scientific method offers a set of techniques and procedures to obtain accurate theoretical understanding, experimental verification and validation by the use of reliable instruments eliminating any kind of subjectivity. This approach can provide useful and proven answers about many cases of study. The scientific community considers the scientific method as one of the most useful procedures since it allows the explanation of phenomena objectively, provide solutions to research problems and encourages the declaration of laws. Its construction is rigorous and logical in an orderly manner with clear, pure and complete principles seeking correction and enhancement to overcome, order and understand the gathered knowledge [87].

The scientific research is categorised according to the purpose, scope, design, source and focus of the activities involved; thus, the type of investigation influences the scientific method workflow.

3.2 Type of research

Following the related categories classification and the characteristics of the project carried out and described in this document, it can be grouped as applied quantitative-experimental-explicative research.

Applied:

Quantitative:

Experimental component:

Explicative research:

3.3 Research activities

To a better comprehension of the methodology used in this research, see Figure 3.1 of page 40.

1. Review related bibliography to find similarities and singularities with the proposed solution methods and models.
2. Develop new mathematical models and tailored algorithms focused on vertex approach to face additive manufacturing problems from a bin packing perspective.
3. Design and coding computational hybrid algorithms using a mixed-approach and starting point strategies to develop some optimisation algorithms to make solutions optimal or with minimal gaps.
4. Develop computational experimentation for various types (heterogeneity, size, quantity, and complexity) of simulated and real instances with different combinations of heuristics, meta-heuristics and exact methods and strategies.
5. Extend the previous model to large scale additive manufacturing problems like densest layer filling.

3.4 General procedure workflow

3.4.1 Modelling phase

In this methodology phase, incipient mathematical models representing the vertex-based approach and the conditions to obtain them are studied and tested, it also includes a thorough study of the mathematical structure of "optimal theoretical solutions" for several hand-made instances. This workflow milestone allows developing

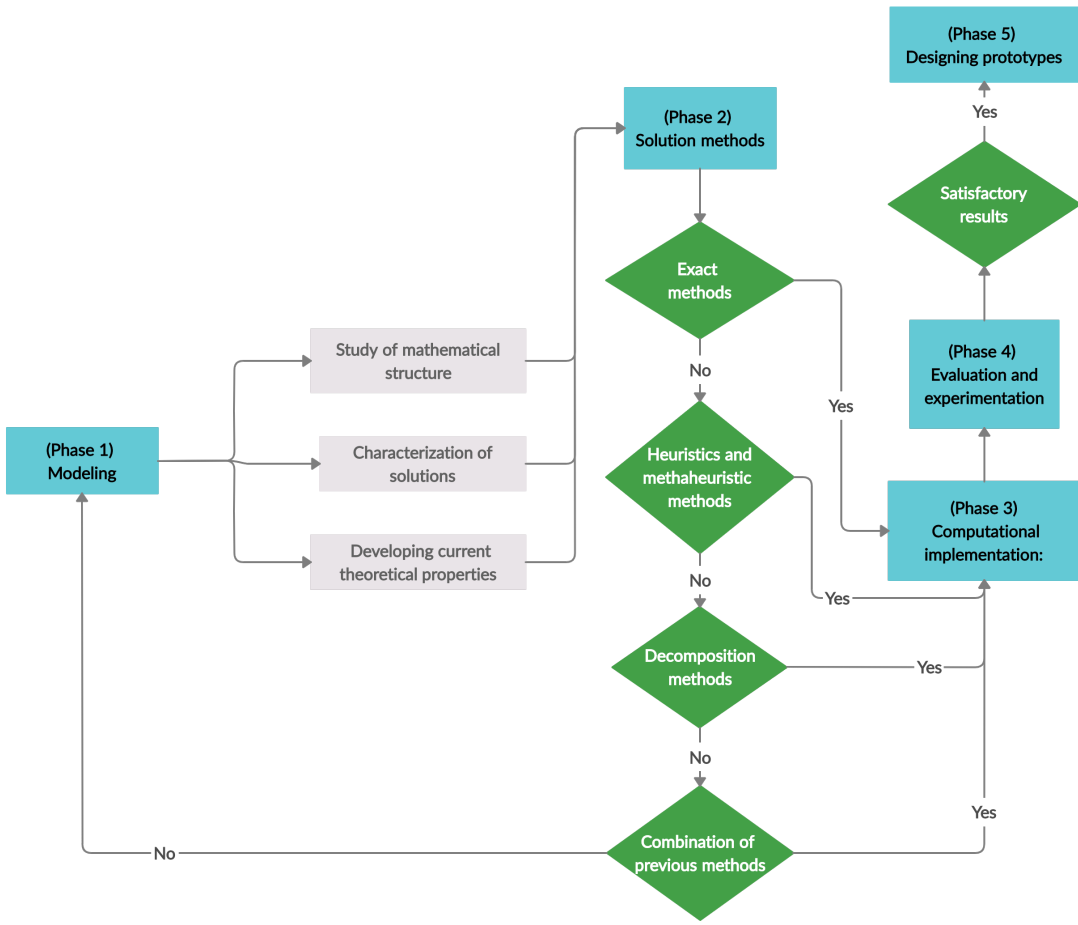


FIGURE 3.1: Flowchart of methodology cycle.

important theoretical properties, select an order in the testing of solution methods and other strategies to face this specific situation.

This stage has an a critical theoretical-algorithmic impact, focused on modelling packing non-overlapping, containment and other problem-specific conditions, and an iterative process of model improvement. The tools to use in this part are as simple as possible: adjacency matrix for three-dimensional object representation, distance metrics, and geometrical formulations.

3.4.2 Solution methods phase

From the results obtained in the modelling phase, and appropriate decision on selecting solution techniques is desirable. There are several ways presented in the reviewed literature to face non-linear optimisation problems, i.e., exact methods, heuristics and meta-heuristics, model decomposition, which today are state-of-the-art for solving hard optimisation problems.

The fact that packing problems are classified as NP-hard combined with a large number of instances makes developing solution methods a real challenge, Thus, is a must either developing exact methods to find the optimal global solution of the problem or building heuristics-based strategies guaranteeing right quality solutions in reasonable computation times.

3.4.3 Computational implementation phase

With the end of the solution methods, the computational implementation step is beginning, in this methodology stage expert criteria are required. Models implementation is a fundamental step with significant importance due to the inclusion of a variety of mathematical programming, general-purpose-high-level languages, available solvers and rendering and plotting tools, see Section 4.4 from page 50 as a part of the implementation.

3.4.4 Models

3.4.4.1 Model variables

X_{ijk} — Polytope vertex coordinates.

α_{ij} — Lagrangian multipliers.

β_{ij} — Lagrangian multipliers.

υ_{ijk} — Lagrangian multipliers

λ_{ijk} — Linear combinations vectors.

μ_{ijk} — Linear combinations vectors.

3.4.4.2 Model parameters

$i, i = \overline{1..p}$ — number of polytopes: this parameter defines the dimensionality of the instance, it refers to the number of small items to pack inside the container walls.

$j, j = \overline{1..s}$ — number of vertexes: defines the types of polytopes to pack.

$k, k = \overline{1..n}$ — number of dimensions: defines the format of the space, adjusting this parameter, the dimensions can be squeezed or extended.

d_{ikl} — Euclidean distance between points k and l of the polytope i: refers to the adjacency matrix of polyhedra structure.

3.4.4.3 Model objective function for packing in spherical-shaped containers

$$minimise \;\; r^1 \tag{3.1}$$

[1] r: for sphere or cylinder radius.

3.4.4.4 Model objective functions for packing in cylindrical-shaped containers

$$minimise \;\; r + h^2 \tag{3.2}$$

$$minimise \;\; r^2 * h \tag{3.3}$$

$$minimise \;\; (r-h)^2 + 9 * r^2 + 3 * h^2 \tag{3.4}$$

3.4.4.5 Model objective functions for packing in prismoidal-shaped containers

3.4.4.6 Model general constraints

$$\sum_{i=1}^{p}\sum_{j=1}^{s}\sum_{k=1}^{n}(X_{ijk} - X_{ij'k})^2 = dijj'^2 \tag{3.5}$$

$$\sum_{i=1}^{p}\sum_{j=1}^{s}\sum_{k=1}^{n}(X_{ijk} - X_{0k})^2 = r^2 \tag{3.6}$$

$$\sum_{i=1}^{p}\sum_{j=1}^{s}\sum_{k=1}^{n}\upsilon_{ijk} * X_{ijk} - \alpha_{ij} \leq -1 \tag{3.7}$$

$$\sum_{i=1}^{p}\sum_{j=1}^{s}\sum_{k=1}^{n}\upsilon_{ijk} * X_{i'jk} - \beta_{ij} \geq 1 \tag{3.8}$$

$$\sum_{i=1}^{p}\alpha_{ii'} + \beta_{ii'} < 2 \tag{3.9}$$

$$\sum_{i=1}^{p}\sum_{j=1}^{s}\sum_{k=1}^{n}\lambda_{ii'k} + \mu_{ii'k} = \sum_{i=1}^{p}\alpha_{ii'} + \beta_{ii'} \tag{3.10}$$

[2] h: cylinder height.

$$\sum_{i=1}^{p-1} \sum_{k=1}^{n} \lambda_{ii'k} \leq 1 \tag{3.11}$$

$$\sum_{i=1}^{p-1} \sum_{k=1}^{n} \mu ii'k \leq 1 \tag{3.12}$$

$$\forall i \neq i', j \neq j', k \neq k' \tag{3.13}$$

$$v_{ijk} \in \mathbb{R}^n, \alpha_{ij}, \beta_{ij}, \lambda_{ijk}, \mu_{ijk} \geq 0. \tag{3.14}$$

3.4.5 Experimentation and evaluation phase

In this methodology step, an experimental evaluation is carried out to assess the contribution of each of the features recorded that make up the solution method implemented. Adjusting algorithms parameters, analyzing real convergence, estimating limits for problem size, all are carried out using suitable experimental statistical design. Parametric or non-parametric analysis of variance allows establishing with statistical rigour the contribution to the solution quality of each of the components developed, as well as adequate comparison with existing methods if any.

Chapter 4

EXPERIMENTATION, MATERIALS AND METHODS

*"No amount of **experimentation** can ever prove me right; a single **experiment** can prove me wrong"*

ALBERT EINSTEIN.

Contents

4.1 Design

After the execution of 3456 experiments classified by container, e.g., 1296 for cylindrical containers, 1296 for prismoidal containers and 864 for spherical ones, to carry out the experimentation; several elements were taken into consideration: different containers types, the number of packing items, various strategies to improve the solutions, solvers and other factors that emerged as part of the solution analysis and previous model validations, see Table 4.1 from page 47.

Two main strategies[1] directed the second part of the experimentation: an initial point strategy using IPOPT solver solution as an entry point to BARON, and an initial point strategy using BARON solver with short execution times as an entry point to itself in a second execution.

4.2 Solvers selection

The solvers' selection involved a massive bibliographic revision of benchmark articles [37] on their performance on several sets of problems, other features reviewed for their inclusion in the research are: the availability on the mathematical modelling suites, type of access, licensing restrictions, API integration, usability and typology of problems to solve, among others.

4.2.1 Computational solvers

- BARON solver: is a computational system for solving non-convex optimisation problems to global optimality like purely continuous, purely integer, and mixed-integer non-linear problems. The Branch And Reduce Optimisation Navigator

[1] Strategies using LGO and other combinations arise in low-quality solution results.

Table 4.1: Experimentation summary

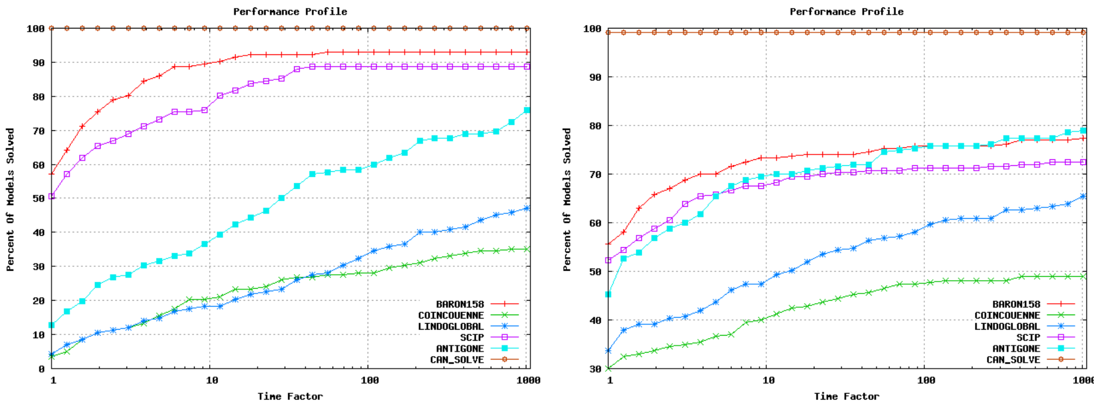
Container	**Solver**	**Items**	**Strategies**	**Tolerance**	**Objec. Function**	**Experiments**
Cylindrical	IPOPT, BARON, LGO	5, 7, 10, 14, 15, 20, 25, 30, 40, 50, 100, 200, 300	1) No initial solution.	from 10e-1 to 10e-7, step 10e-1	variable radius, variable height	1296
			2) Initial solution IPOPT		fixed radius, variable height	
			3) Initial solution BARON		variable radius, fixed height	
Spherical	IPOPT, BARON, LGO	5, 7, 10, 14, 15, 20, 25, 30, 40, 50, 100, 200, 300	1) No initial solution.	from 10e-1 to 10e-7, step 10e-1	fixed radius	864
			2) Initial solution IPOPT		variable radius	
			3) Initial solution BARON			
Prismoidal	IPOPT, BARON, LGO	5, 7, 10, 14, 15, 20, 25, 30, 40, 50, 100, 200, 300	1) No initial solution.	from 10e-1 to 10e-7, step 10e-1	variable length, variable width, fixed height	1296
			2) Initial solution IPOPT		variable length, fixed width, fixed height	
			3) Initial solution BARON		variable length, variable width, variable height	

receives its name from the combination of constraint propagation, interval analysis, and duality in its reduce armoury with enhanced branch and bound concepts as it weaves its way through the local minima and maxima of complex optimization problems in search of global solutions [70][77].

- IPOPT solver: is a software package for large-scale non-linear optimisation that implements an interior point search filter method search filter method that endeavours to find a local solution [12] [13], it is available from COIN-OR (http://www.coin-or.org) under the EPL (Eclipse Public License) open-source license. It includes the source code for IPOPT, wich means it is available free of charge, also for commercial purposes. However, if you give away software including IPOPT code (in source code or binary form) and you made changes to the IPOPT source code, you are required to make those changes public and to indicate which modifications you made. After all, the purpose of open source software developers is the constant evolution and refinement of the software. [6][15][61][81]

- LGO solver: is a solver suite system that has been developed and gradually extended for more than a decade. It now includes a suite of robust and efficient global and local non-linear solvers combining several search modes, providing a reliable, effective, and flexible set of solvers approach to a broad range of non-linear models. The solver suite approach enhances the reliability of the overall solution process. It integrates the following global scope algorithms: Branch-and-bound with adaptive partition and sampling-based global search (BB), Adaptive global random search (GARS), and Adaptive multi-start global random search (MS). The suit also includes the following local solver strategies: Heuristic global scope scatter search method (HSS), Bound-constrained local search, based on the effectiveness of an exact penalty function (EPM), constrained local search, based on the sequential model linearisation (SLP), constrained local search, based on a generalised reduced gradient approach (GRG) [72][23][60][59].

A systematic comparison of 1740 test problems shows that BARON has the



(a) 141 MINLPs from IBMLib (b) 250 MINLPs from MINLPLib

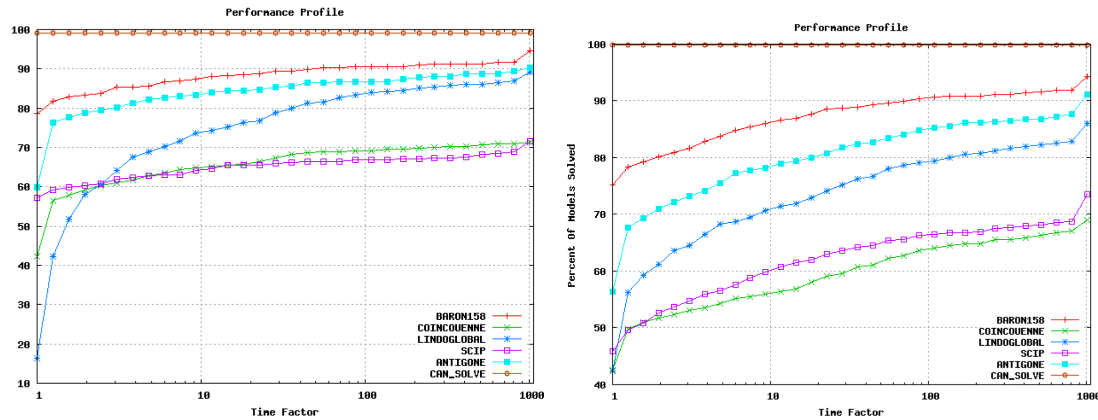
FIGURE 4.1: Solvers performance profile on mixed-integer non-linear problems. Source [69]

edge over other global codes for NLP/MINLP. The test problems used in this comparison were originated from GlobalLib, CMU/IBMLib, MINLPLib, and PrincetonLib, respectively. This test set includes all problems from these libraries that are accepted by all solvers. These and additional test problems are available in a variety of formats. Below we give performance profiles for individual test sets.

4.3 Instrumentation and equipment

All instances and solutions were pre-processed and processed, including solver execution in a Workstation HP Z230, with the current specifications:

- Intel(R) Xeon(R) 3.40 Ghz octa-core.
- 16 GB RAM DDR3
- 2TB HDD SATA 3 Gbits/s



(a) 369 NLPs from GlobalLib (b) 980 NLPs from PrincetonLib

Figure 4.2: Solvers performance profile on non-linear problems. Source [69]

4.4 Software and packages

The current research project involved several computer software ranging from general-purpose, see Section 4.4.1 from page 50, mathematical modelling programming languages, see Section 4.4.2 from page 51, computer cloud services, see Section 4.4.3 from page 54, to computational solvers, see Section 4.2 from page 46.

4.4.1 Programming languages and packages

The author used Python v3.7 programming language and packages extensively for secondary and supporting activities like developing an instances generator, web scraping NEOS-SERVER solver data files, three-dimensional instance plotting [34], initial two-dimensional instance plotting for prior model validations [33], instances data visualisation analysis [82], and analysis of results and other outcomes [78][80].

4.4.2 Mathematical modelling languages selection

Mathematical optimisation, also known as mathematical programming is a process that turns out a problem into an analytical model and then finds better solutions out of a myriad of possibilities. This non-trivial course of actions helps decision-makers to improve their proposals, optimise time-execution and saves a considerable number of resources. This section presents a deep-in review over benchmark articles, solvers and optimiser testing reports, analyses advantages and disadvantages on two groups of computational software.

Gurobi Optimizer: founded in 2008 by arguably the most experienced and respected team in optimisation circles claims to be the fastest and the most potent mathematical programming solver available for LP, QP and MIP (MILP, MIQP, and MIQCP) problems [56]. The development and maintenance team are continually looking to push the performance boundary for linear, quadratic, and mixed-integer programming forward, in presented test and evaluations the assured they have doubled the speed of their solver with each major release. The suite of products from Gurobi team represents new implementations, the latest mathematical and engineering improvements, computing hardware and programming environments to help meet the growing demands of business problems [55].

GAMS: is one of the preeminent tool providers for the optimisation industry, from multinational companies, universities, research institutions to governments in many different areas, e.g., including the energy and chemical industries, for economic modelling, agricultural planning, or manufacturing [18]. Started as a World Bank project by an economic modelling team in the 1970s, it was the first software system to join the language of mathematical algebra with traditional concepts of computer programming to describe and solve optimisation problems efficiently. By the foundation of the GAMS Development Corporation, in 1987, the mathematical modelling software became a commercial product. Nowadays, algebraic modelling is one of the most productive ways of implementing linear and non-linear models and decomposition methods for optimisation problems [17].

AMPL: designed to combine and extend the expressive capabilities and techniques of the existing mathematical modelling language while remaining easy to use for industrial and another type of applications. It is particularly notable for the naturalness of its syntax and the generality of its set and indexing expressions. It provides strong support for validation, verification and reporting of optimal solutions, through numerous alternatives for presenting data and results, Its extensive pre-processing routines can perform transformations serve to subdue problem size, turn piecewise-linearities to linear terms, and replace out selected variables. It is further characterised by its continuous improvement to help users' needs. New-fresh additions include looping and testing constructs for writing executable scripts in the command language, and facilities for establishing and working with several interrelated sub-problems [5].

After intensive review and experimentation on mathematical tools presented before, the mathematical modelling software AMPL was the final decision to use in this research, Next lines present the main reasons:

1. Easy to switch to other solvers with just a minimum of code adjustment.
2. Declarative AMPL models are regularly easier to read and are more high-level than the procedural code used to construct problems thought an API.
3. AMPL isolates the solver processes, which can be beneficial for significant issues, e.g, if any specific solver runs out of memory, this annoying issue will not affect AMPL.
4. AMPL provides a built-in functionality to import data from and export to databases and spreadsheets.
5. AMPL has an active ongoing community which is arguably more extensive than any other solver, including Gurobi. AMPL Google Group has more than 1700 members and rising.

TABLE 4.2: Comparison between GAMS, AMPL and Gurobi Optimizer

	GAMS	**AMPL**	**Gurobi**
Learning curve	Easy to learn	Easy to learn	Depends on the implementation and IDE used
Readability	Average	Easy	More complex: high-level than procedural code to solve problems via an API
Academic license	640.00 USD	Free and renewable	Free and renewable
Interface	Batch oriented	More flexible option of interactively exploring models and results	Python, R, Java
Environment-related	Higher use in industry modelling	Higher use in academic researches	Industry and academic in
Solvers included	Large set of solvers	Wide range	is sell independent and as is part of GAMS and AMPL
Problems solved	Depends on solvers installation	Depends on solvers installation	LP, QP and MIP (MILP, MIQP, and MIQCP)
Online community	Medium	Large	Small to medium
Syntaxis	Not intuitive	Intuitive and expressive	High-level language oriented
Documentation	Well documented	Well documented	Well documented
Design conception	Relies on more special conventions and reformulations	Designed with the idea of being much closer to mathematical notation	To work mainly from through API call using a high-level declarative language or included in modelling software.

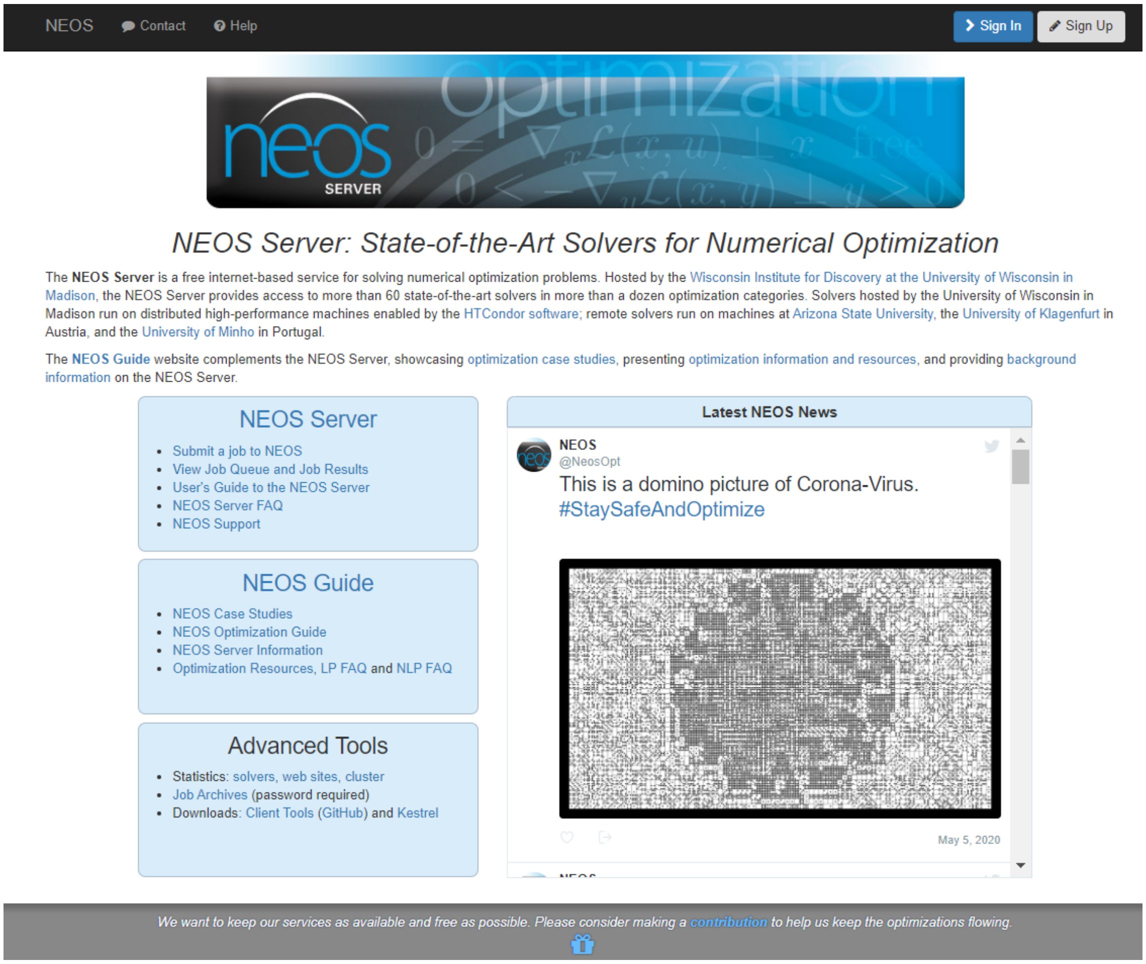


FIGURE 4.3: NEOS-server landing page, Source [84]

4.4.3 Cloud computing clusters

Besides the in-place computational power utilised to take out the experimentation concerning this research, See Section 4.3 from page 49, an extensive and intensive parallel experiment was executed using open services cloud solvers, like NEO-server [27][19][16] with different configurations and solvers, see Figures 4.5 and 4.4 from pages 56 and 55.

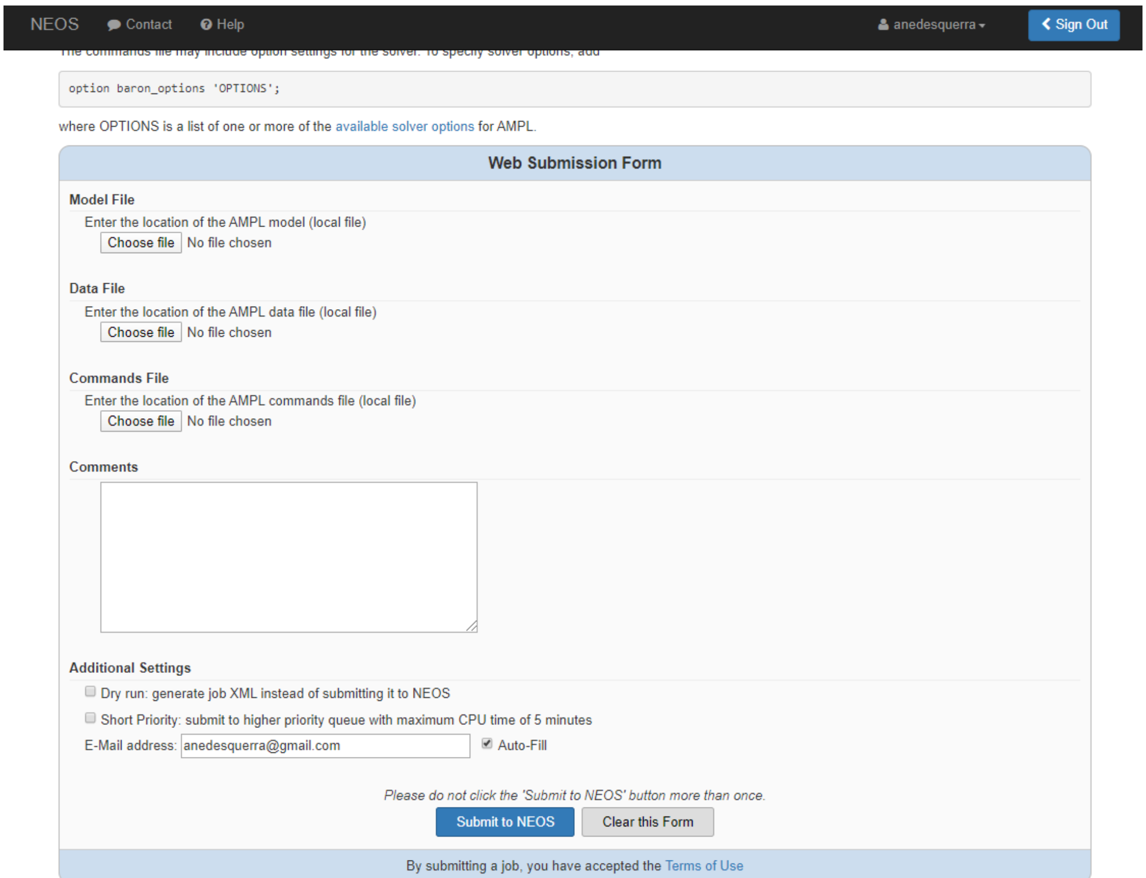


FIGURE 4.4: NEOS-server BARON interface, Source [85]

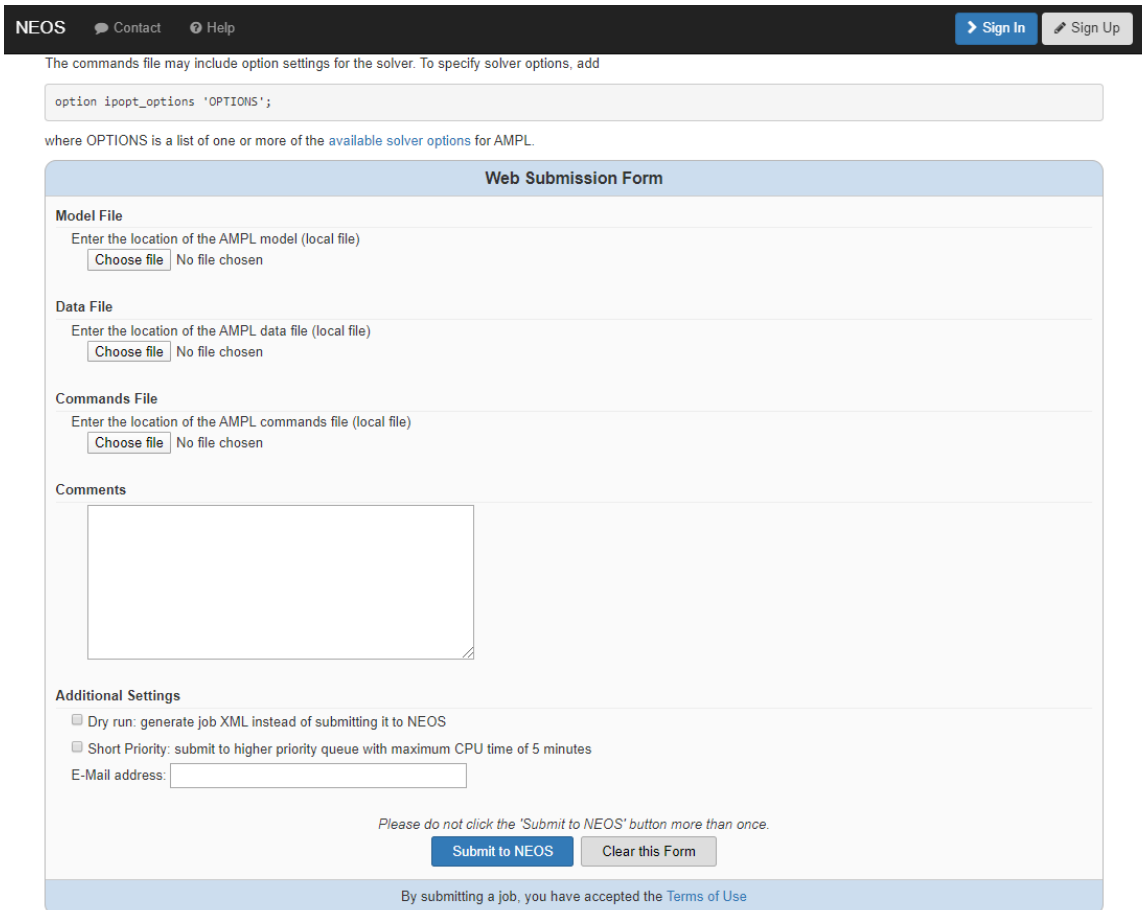


Figure 4.5: NEOS-server IPOPT interface, Source [86]

4.5 Results

4.5.1 Spherical-shaped container

TABLE 4.3: Model outcomes from homogeneous mono-sized tetrahedra packing instances in a spherical container.

# items	vars.	const.	cont. vol.	pack. vol.	time (s)	radius	density	iterations	tolerance	solution	feas. error
4	127	118	174.12	30.17	0.61	3.46	0.1733	82	1.0E-04	L.O.S.S[2]	3.4E-13
5	191	180	174.12	37.71	0.79	3.46	0.2166	254	1.0E-05	L.O.S.S	2.8E-08
6	268	255	211.33	45.25	1.35	3.70	0.2141	343	1.0E-04	L.O.S.S	3.8E-09
7	358	343	219.23	52.80	4.56	3.74	0.2408	649	1.0E-04	L.O.S.S	1.0E-06
8	461	444	239.40	60.34	4.22	3.85	0.2521	968	1.0E-04	L.O.S.S	2.5E-07
9	577	558	235.70	67.88	82.37	3.83	0.2880	1898	1.0E-04	L.O.S.S	1.2E-04
10	706	685	249.60	75.42	26.52	3.91	0.3022	2876	1.0E-04	L.O.S.S	6.8E-13
13	1171	1144	268.33	98.05	39.8	4.00	0.3654	1895	1.0E-04	L.O.S.S	1.0E-09
15	1546	1515	268.39	113.14	46.83	4.00	0.4215	1459	1.0E-02	L.O.S.S	1.2E-07
20	2711	2670	396.00	150.85	508.309	4.56	0.3809	2669	1.0E-04	L.O.S.S	1.5E-05
25	4201	4150	358.56	188.56	320.49	4.41	0.5259	1034	1.0E-04	L.O.S.S	5.0E-07
30	6016	5955	486.08	226.27	901.17	4.88	0.4655	3834	1.0E-05	O.S.F[3]	1.9E-07
35	8156	8085	549.04	263.99	1610.92	5.08	0.4808	6436	1.0E-04	L.O.S.S	1.5E-05
40	10621	10540	626.48	301.70	2148.04	5.31	0.4816	3239	1.0E-03	L.O.S.S	7.2E-08
50	16526	16425	816.88	377.12	2498.33	5.80	0.4617	1771	1.0E-04	L.O.S.S	1.0E-01
70	32236	32095	1090.39	527.97	12029.6	6.39	0.4842	6726	1.0E-03	L.O.S.S	1.2E-08
90	53146	52965	1382.12	678.82	15437	6.91	0.4911	6642	1.0E-03	L.O.S.S	1.2E-07
100	65551	65350	1513.96	754.25	25803.23	7.12	0.4982	8748	1.0E-04	L.O.S.S	1.4E-07

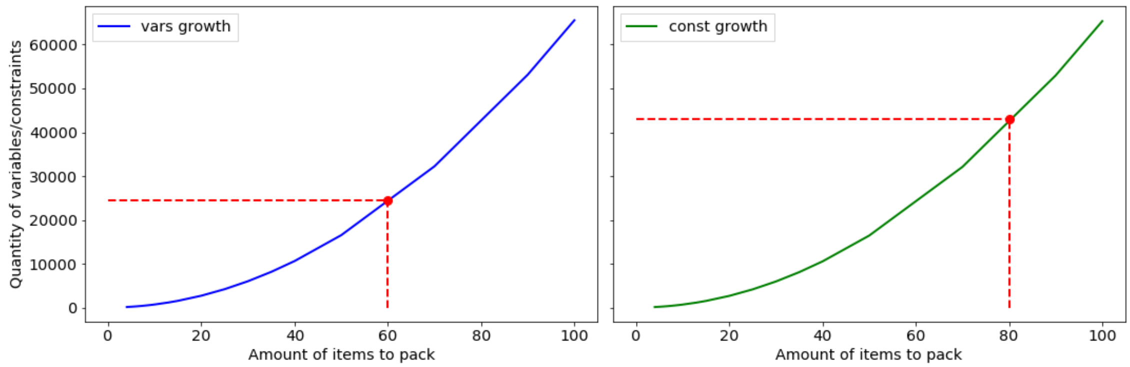


Figure 4.6: Model spatial complexity.

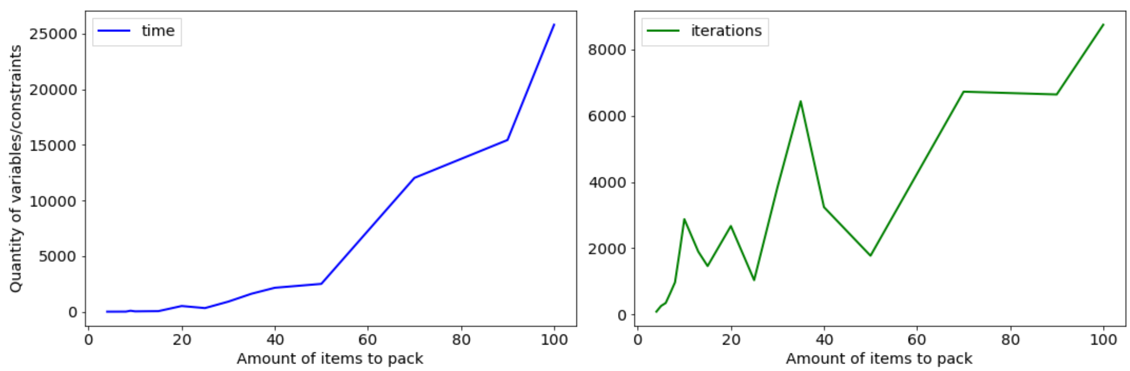


Figure 4.7: Model temporal behaviour.

4.5.2 Cylindrical-shaped container

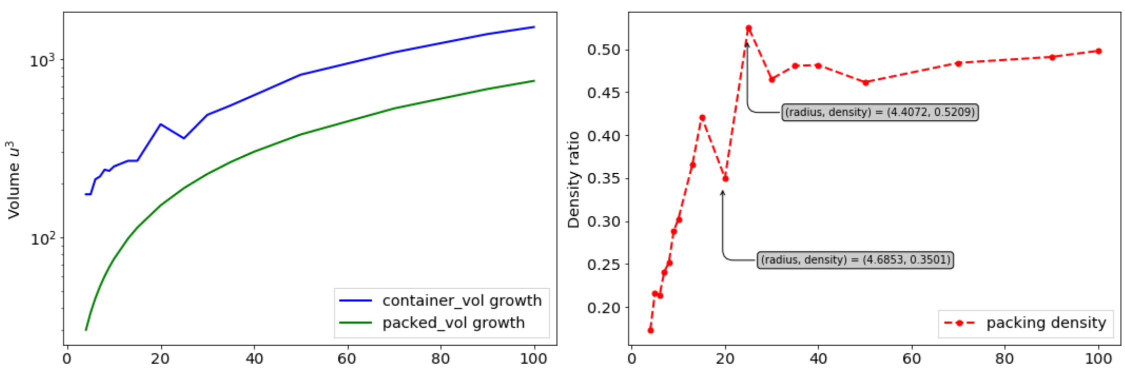
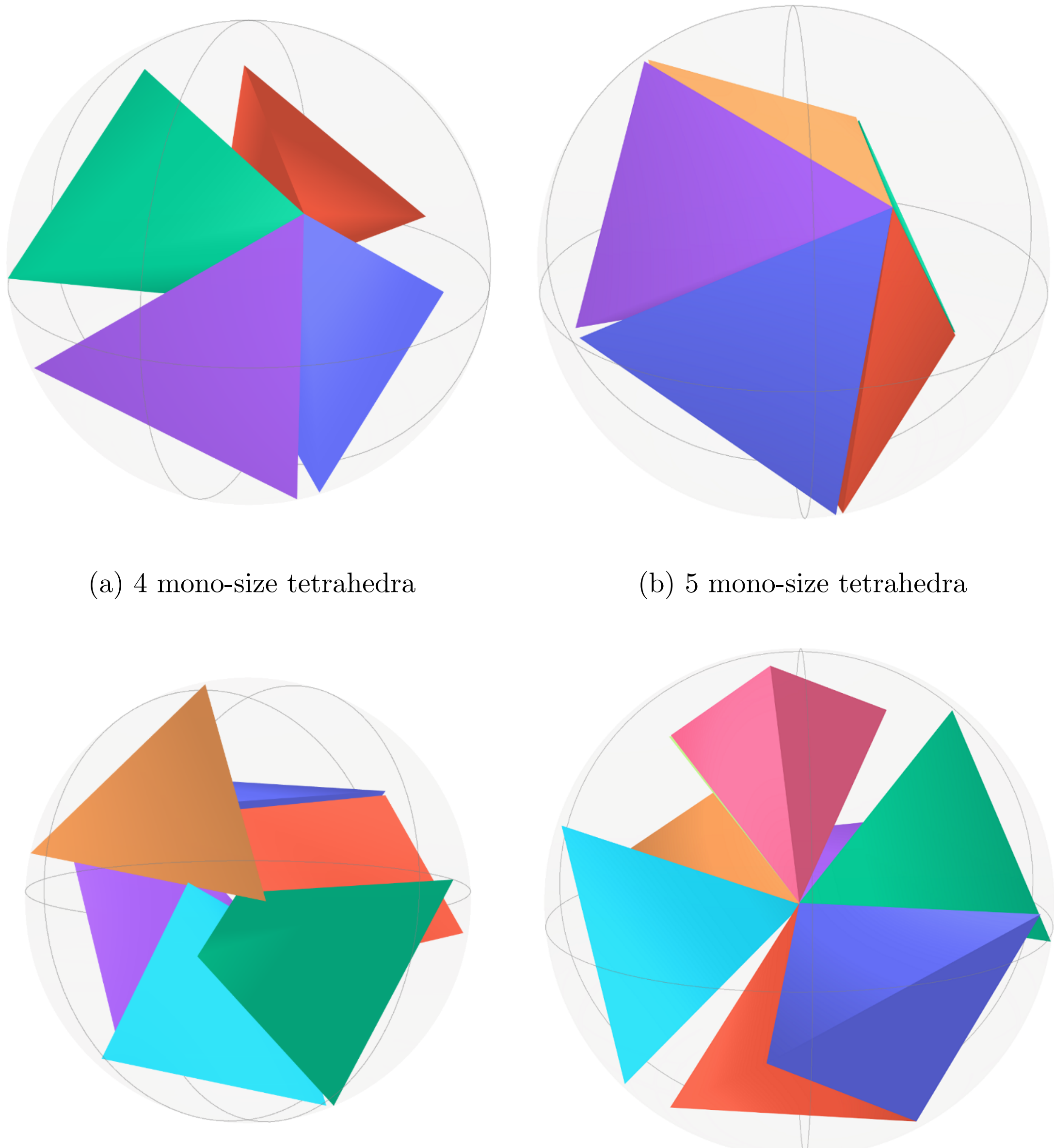


FIGURE 4.8: Density packing behaviour in spherical container.



(a) 4 mono-size tetrahedra

(b) 5 mono-size tetrahedra

(c) 6 mono-size tetrahedra

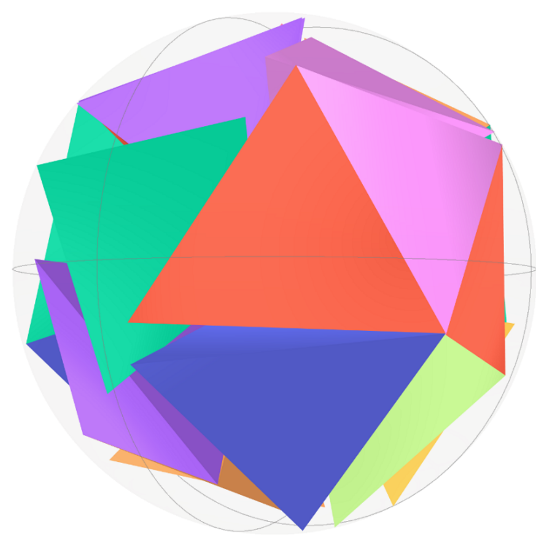
(d) 8 mono-sized tetrahedra

FIGURE 4.9: Small size instances of mono-sized tetrahedral packed in a spherical container

(a) 10 mono-size tetrahedra

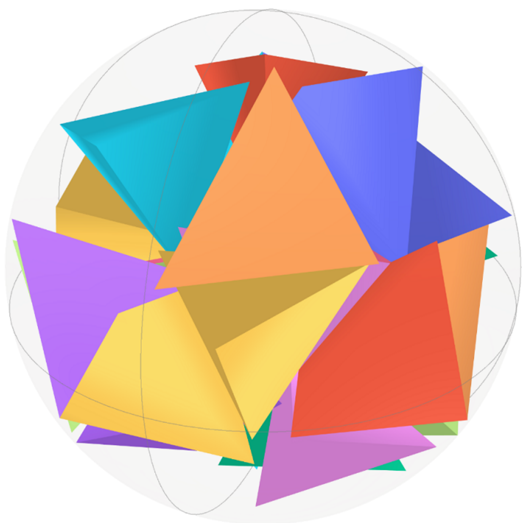
(b) 13 mono-size tetrahedra

(c) 20 mono-size tetrahedra



(d) 25 mono-sized tetrahedra

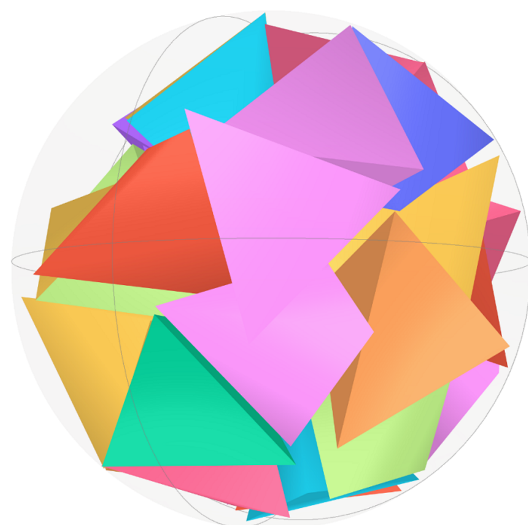
Figure 4.10: Small to medium size instances of mono-sized tetrahedral packed in a spherical container



(a) 30 mono-size tetrahedra

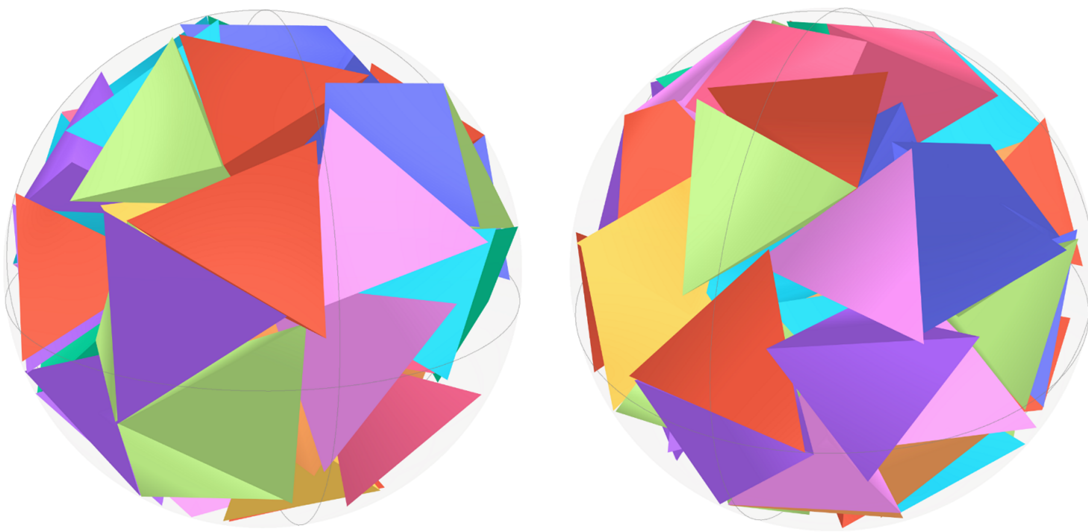
(b) 35 mono-size tetrahedra

(c) 40 mono-size tetrahedra



(d) 50 mono-sized tetrahedra

Figure 4.11: Medium size instances of mono-sized tetrahedral packed in a spherical container



(a) 70 mono-size tetrahedra (b) 90 mono-size tetrahedra

Figure 4.12: Medium to high sized instances of mono-sized tetrahedral packed in a spherical container.

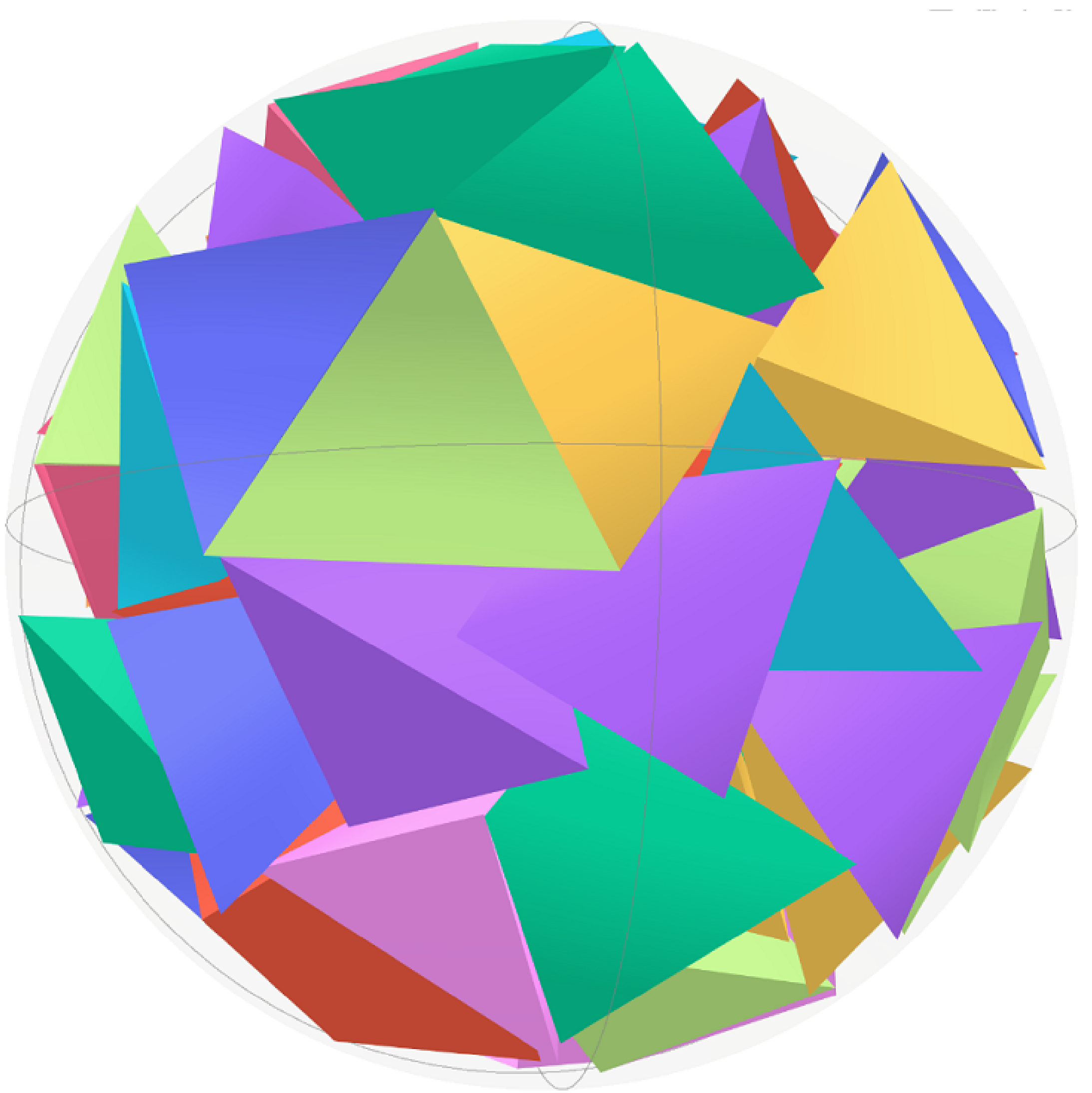
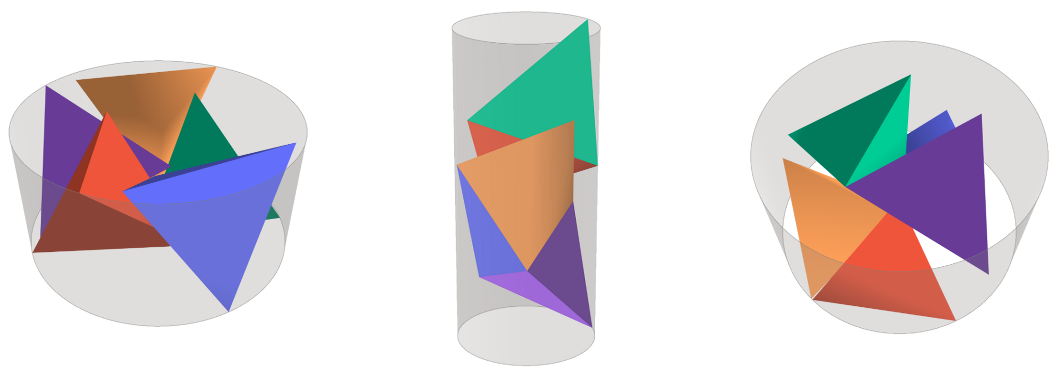


Figure 4.13: High sized instance of mono-sized tetrahedral packed in a spherical container - 100 mono-size tetrahedra.



(a) 5 mono-size tetrahedra (b) 5 mono-size tetrahedra (c) 5 mono-sized tetrahedra

FIGURE 4.14: Mono-sized tetrahedral packed in a cylindrical container with different objective functions.

Chapter 5

CONCLUSIONS

"So Einstein was wrong when he said, "God does not play dice." Consideration of black holes suggests, not only that God does play dice, but that he sometimes confuses us by throwing them where they can't be seen"

STEPHEN HAWKING.

Contents

5.1 Introduction

This chapter presents the current research conclusions, illustrates impressive outcomes about the problem analysis, exposes complex characteristics of the geometrical structures that define the packing elements, characterises solutions and modelling phases, and describes unexpected obstacles detected during the computational implementation. It also includes several further ideas arose to overcome those drawbacks as future work to continue delving and generating new knowledge in bin packing techniques applied to additive manufacturing.

5.2 Conclusions

- Initials solutions obtained from global solvers mixed with inner-point solver strategies are a good starting point facing medium-sized densest filling layer problems and work extremely efficient in void structure situations.
- Build volume problems can be treated by this model using an aggregation of objects with similar mechanical and physical properties inside the chamber with simple adaptations to objective functions.
- The multi-objective prospect could offer a different pathway to the solution of general problems described in the current research. In general, experimentation exposes a need for higher-order methods like decomposition, hybrid methods, meta-heuristics, novel approaches, as well as mixed strategies to obtain better quality parameters in a reasonable time.
- Despite the developed exact models can not solve instances with a massive amount of items to pack, the case of densest filling layer applications so far, the developed model has proven its efficiency in void structures problems and build volume problems with some variations.

5.3 Research limitations

- Alternative solution methods, such as heuristics, Meta-heuristics, neural networks and others, were nor implemented neither tested to deal with these typologies; therefore this limitation is included in future research in the bin packing applications in this field of knowledge.

- Since this approach is vertex-based, smooth surfaces like ellipsoid, cylindrical-shaped structures, must be created as mathematical approximations of themselves.
- This approach assumes the propagation of heat of sintering laser follows a linear or pseudo linear distribution, would be challenging the introduction of differential equations in the model to estimate this thermogenic process accurately.

5.4 Future works

- Test the vertex approach model against the inequation[1] approach model.
- Complete various instance complexity studies about the data generated.
- Extend the exact models to a broader range of structures combinations and non-convex containers.
- Extend the models to large-scaled bin packing problems.
- Design a GSA heuristic or meta-heuristic to test the previous models in time and solution quality parameters.
- Use reinforcement deep learnin with Q-learning to design neural network model to test the results of avant-garde models in time, solution quality parameters.

[1]A model developed in a separated parallel investigation to face others bin packing — additive manufacturing related-problems.

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Things to verify