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Tetrahedron packing using optimization

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Abstract

During this master thesis, we studied the tetrahedron packing problem using a purely optimization based approach. This problem consists in filling the space as densely as possible using regular unit edge tetrahedra that has fascinated humans for centuries. We start by introducing packing problems and the specific one about tetrahedron as well as their relevance in other domains. We continue by presenting an overview on the literature on the subject from the prism of the evolution of the packing density. Then, we present our approach, how it came about and how we managed to build models to put it into reality. Then taking our best model, we solve it using the IPOPT solver and apply a set of procedures in order to reach the best packing possible. The best we managed to get is 0.818978 not beating the best result to date but not being too far off. The different results are compared and analyzed. To finish this thesis and as a little sidetrack, we present how we performed a physical experiment using tetrahedral dices.

Contents

Chapter 1

Introduction

In this introduction, we will introduce the concept of packing, talk about its application to regular tetrahedra and present the plan for this master thesis.

1.1 The concept of packing

In this master thesis, we will talk about the packing of regular tetrahedra but packing is a much wider subject. It is an age-old art and science of arranging objects within a confined space to optimize its utilization and efficiency. From ancient civilizations packing goods for trade to modern-day engineers designing compact electronic devices, the concept of packing has played a pivotal role in human development and progress. The organization and arrangement of objects, whether tangible or intangible, have been fundamental to various aspects of our lives, influencing fields as diverse as materials science, logistics, architecture, and computer algorithms. Subsequently, we will present an overview of the concept of packing, by evoking its historical roots, theoretical underpinnings, and practical applications, as well as the challenges and innovations that have shaped this fascinating domain.

1.1.1 Historical perspectives on packing

The art of packing dates back to the early days of human civilization when nomadic tribes needed to pack their belongings efficiently for long journeys. Early examples of packing can be found in the well-organized storage systems of ancient Mesopotamian and Egyptian cultures. The emergence of trade and commerce further emphasized the importance of proper packing to maximize the volume of goods transported while minimizing damage and spoilage during transportation.

Packing techniques evolved with technological advancements and cultural exchanges. The Silk Road, for instance, witnessed the exchange of various packing methods among civilizations. Chinese merchants used intricate packing techniques to preserve goods like silk, porcelain, and tea during their long journeys across the Silk Road.

In the age of exploration, packing played a critical role in the voyages of discovery, as explorers had to pack provisions and equipment efficiently on their ships to sustain their journeys across vast oceans. The invention of cardboard boxes and other packing materials in the 19th century revolutionized the packaging industry and opened up new possibilities for transporting goods over long distances.

1.1.2 Theoretical foundations of packing

The theoretical study of packing gained momentum in the field of mathematics and computer science. Researchers explored the fundamental questions surrounding the optimal packing of geometric shapes, such as circles, squares, and spheres, within defined spaces. A packing of such geometric shapes is an arrangement of these shapes in space in a way such that they don't overlap. The quest to find efficient and dense packings led to the discovery of numerous packing problems, each with its unique set of constraints and objectives.

One of the earliest and most well-known packing problems is the packing of equally sized spheres. Notable contributions to this problem include the famous Kepler Conjecture, which hypothesized that the densest packing (with a density of 74%) can be achieved in a face-centered cubic or a hexagonal closed packed lattice (lattices are explained in section 2.2). The Kepler Conjecture was eventually proven by Thomas Hales in 1998, making it one of the most significant achievements in the field of discrete geometry.

The study of three-dimensional packings has gained substantial interest due to its relevance in materials science, crystallography, and soft matter physics. Tetrahedral packing, in particular, has attracted attention, given its prevalence in various molecular structures and composite materials.

1.1.3 Modern applications of packing

The significance of packing extends far beyond historical and theoretical contexts. In contemporary society, packing remains a pivotal aspect of various industries and technological advancements :

- Logistics and Supply Chain: Efficient packing in logistics is crucial for optimizing storage space, reducing shipping costs, and ensuring the safe transportation of goods. Innovations in packing materials, such as lightweight and durable packaging, have revolutionized the supply chain, enabling faster and more cost-effective delivery of products.

- Architecture and Urban Planning: Packing principles are employed in architectural design to optimize space utilization in buildings, urban spaces, and city planning. The concept of packing is evident in urban layouts, where the efficient arrangement of buildings, roads, and public spaces seeks to achieve harmonious and functional environments.

- Materials Science and Nanotechnology: In materials science, packing plays a significant role in determining the properties and behavior of materials. For instance, close-packed structures in crystals lead to higher mechanical strength, while porous packings enable unique properties in nanoporous materials with applications in filtration and catalysis.

- Electronics and Miniaturization: The drive for miniaturization in electronics has necessitated innovative packing techniques. Integrated circuits, for example, rely on precise and dense packing of transistors and other components on semiconductor wafers to achieve higher computational power and energy efficiency.

- Biological Systems: Packing is also vital in biological systems, where it influences the folding of proteins, the arrangement of DNA within chromosomes, and the organization of cellular structures. Understanding biological packing has implications for drug design, biotechnology, and medical research.

1.1.4 Challenges and innovations in packing

Despite centuries of exploration and research, packing remains a complex and multifaceted domain, with several challenges yet to be fully addressed. Some of the primary challenges in packing include:

- Packing Efficiency: Achieving the densest possible packing is a persistent challenge across different packing problems. Proving the optimality of certain packings and developing efficient algorithms to find near-optimal solutions remain active areas of research.
- Irregular Shapes and Constraints: Packing irregularly shaped objects within confined spaces introduces additional complexity. These challenges arise in fields like container loading, where irregularly shaped cargo must be arranged efficiently for transportation.
- Packing Stability: In certain applications, packing stability is a critical consideration. For instance, packing granular materials such as sand requires ensuring that the packing remains stable under various conditions, such as during transportation or structural loading.
- Real-World Constraints: Practical packing problems often involve real-world constraints, such as variations in shape and size of objects, weight limitations, and the need to accommodate fragile items.

Recent advances in computational power and optimization algorithms have paved the way for new approaches to packing. Innovations in materials and packaging technologies have also influenced packing solutions. Advanced materials with specific mechanical and thermal properties enable novel packing designs with enhanced functionality and performance. Additionally, advancements in 3D printing and additive manufacturing have led to new packing possibilities, enabling custom-designed packing solutions tailored to specific applications.

1.2 Tetrahedron packing

The previous section demonstrated the relevance of packing in general. The subject of this master thesis is the packing of regular tetrahedra[1] (the only non centrally symmetric regular platonic solid of the five). This problem is part of Hilbert's 18th problem. It has its own significant importance in various scientific and engineering disciplines. Understanding and optimizing tetrahedral packing arrangements can be useful in multiple domains, such as the following ones:

[1] It's important to note that throughout the remainder of this report, unless explicitly stated otherwise, the term "tetrahedron" will consistently refer to a regular unit edge tetrahedron

- Materials science: Tetrahedron packing can be used to study the packing of atoms in materials, such as metals and alloys. Understanding the packing of atoms is important for predicting the properties of materials, such as their strength, ductility, and conductivity. Tetrahedrons are present in various chemical contexts, such as crystal structures and molecular configurations like methane.

- Computer graphics: Tetrahedron packing can be used in computer graphics to create 3D models of objects and environments. It can also be used to simulate the behavior of fluids and other materials in computer-generated environments.

- Biology: DNA tetrahedrons are nanostructures formed by the pairing of four single-stranded DNA. They can be easily synthesized and have excellent biocompatibility and cellular permeability, making them a promising platform to construct biosensors and drug delivery systems for living cell studies. Lessons learned from packing could be useful to improve stability for drug delivery.

Overall, the relevance of tetrahedron packing stems from its pervasive presence in nature, its influence on material properties, and its applications in diverse scientific and engineering fields. By optimizing tetrahedral packing arrangements, researchers can unlock new possibilities for designing advanced materials, improving industrial processes, and gaining deeper insights into the intricate world of molecular and atomic structures. Furthermore, tetrahedron packing is an interesting mathematical problem in itself as all other packing problems.

All this explains the major wave of interest this subject received from researchers. However, despite considerable collective effort devoted to the study of this subject, the quest to identify the densest packing or establish the optimality of the current best remains fruitless.

1.3 Plan of this report

In this report, we will explain how this thesis went. We will start by taking a deep look into the literature on the subject of tetrahedron packing. Then based on that, we will present how we came up with the idea of this thesis. The different models built we be explained. Then, using the best model we will apply a set of optimization techniques and analyze the results. We will end this by a little physical experiment.

Chapter 2

Literature review

In this section, the scientific literature on the subject will be investigated with regards to the best results obtained (lattice and not) and the bounds on the density.

2.1 Aristotle's mistake

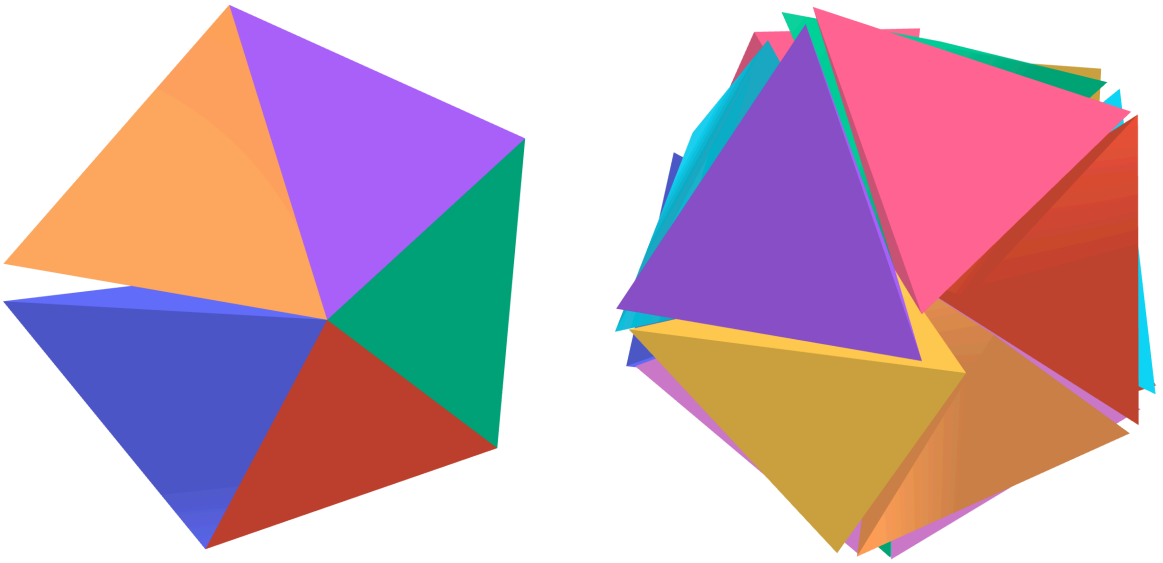
The tetrahedron packing problem has captured researchers' interest meaning the best density evolved over the past years as improved arrangement were found often using numerical search. In this section, we will present the most significant arrangements found and the methods that led to these.

The first mention of a result for this problem was given by Aristotle in his book *On the heavens* written in 350BC, he asserted that tetrahedron fill the space. The relevant passage is in the eighth chapter of the third book and its translation is "It is agreed that there are only three plane figures which can fill a space, the triangle, the square, and the hexagon, and only two solids, the pyramid and the cube." [1]. It is commonly believed that when he used the term pyramid, he was actually talking about tetrahedrons.

Regiomontanus (Johannes Müller von Königsberg) was the first to provide evidence suggesting the incorrectness of this assertion in the title present in a catalogue of his future publications. The translated title is "On the five equilateral bodies which are commonly designated regular, which of them clearly do fill a natural space and which do not, contra Averroes, the commentator on Aristotle" [13], unfortunately no copies were ever found, leaving the desire for a rigorous proof unfulfilled.

2.1.1 Not space filling proof

An intuitive reasoning can be used to prove that tetrahedra do not tile the space as presented by Lagarias and Zong [16] as well as Conway and Torquato [6]. The idea is to look at the dihedral angle in a tetrahedron (the angle between the two hyperlanes containing two faces of the tetrahedron), it is equal to $\arccos\left(\frac{1}{3}\right) \approx 70.53°$. This angle is clearly not a divider of 360° which poses a problem to get a perfect arrangement. If we try to pack 5 tetrahedra along the same edge, we leave a space equivalent to an angle of 7.35° empty (see Figure 2.1a). The same problem appears if we try to pack 20 tetrahedra around one vertex leaving an empty space of about 1.54 steradian (see Figure 2.1b). In the case of perfect perfect packing tiling the space, the tetrahedra would need to meet at the edges or at least vertices but as seen above this is not possible without leaving an empty space.



(a) 5 tetrahedra with one common edge (b) 20 tetrahedra with one common vertex

Figure 2.1: Space filling attempts

2.2 Best lattice packing

Embedded within the pursuit of the optimal packing lies a subtopic: the search for best lattice packing. In some cases, like for sphere packing, the best lattice packing ended up giving the best density for any packing as proved by Hales in 1998. In geometry, a lattice group in $\mathbb{R}^n$ is a subgroup of $\mathbb{R}^n$ with the addition as its operation. For example, a typical lattice in $\mathbb{R}^3$ is $\Lambda = \{\sum z_i \mathbf{a}_i | z_i \in \mathbb{Z}\}$ with $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ linearly independent. A lattice packing can be visualized as a packing where the tetrahedra are copied and placed on each point of the lattice.

The first person who tried to find the densest lattice packing is Minkowski in 1904 [17]. He started by proving the densest lattice packing of octahedra using a theorem on the densest lattice packings of centrally symmetrical convex bodies. He then proved that for a convex body K, $K+\Lambda$ is a lattice packing if no point of Λ except the origin is inside the difference body $D(K) = \{x - y : x, y \in K\}$. Using this and the densest lattice packing for the octahedra, he proposed $\frac{9}{38}$ as the densest lattice packing density for tetrahedra but he mistakenly thought that the difference body of a tetrahedron is an octahedron.

This mistake was corrected by Groemer in 1962 [10] who showed that the difference body of a tetrahedron is a cuboctahedron. A cuboctahedron is a convex body with 6 square faces and 8 triangular ones being quite different from an octahedron which is a polyhedron with 8 triangular faces. Using his findings, he presented a valid lattice packing with a density equal to $\frac{18}{49}$.

This density was proved to be optimal by Hoylman 1969 [12] using two lemmas also proved by Minkowski in [17]:

Lemma 1. *If $\{a_1, a_2, a_3\}$ is a basis for the lattice Λ, if a_1, a_2, a_3 are on the boundary of the difference body R, and if none of the lattice points $a_1 \pm a_2$, $a_1 \pm a_3$, $a_2 \pm a_3$, $a_1 \pm a_2 \pm a_3$, $2a_1 \pm a_2 \pm a_3$, $a_1 \pm 2a_2 \pm a_3$, $a_1 \pm a_2 \pm 2$ is interior to R, then Λ is admissible for R.*

Lemma 2. *If Λ is a critical lattice for the difference body R, then Λ has a basis $\{a_1, a_2, a_3\}$ such that a_1, a_2, a_3, and either*

- *$a_1 - a_2$, $a_2 - a_3$ and $a_3 - a_1$* ***or***
- *$a_1 + a_2$, $a_2 + a_3$ and $a_3 + a_1$*

all lie on lie on the boundary of R.

Using the fact that it is impossible for two points of the lattice to lie in the same triangular face of the cuboctahedron, there are 19 possible ways to put a_1, a_2 and a_3 on its faces which combined with either of the two possibilities of Lemma 2 gives 38 cases. By computing all these basis and the corresponding volume they yield, the smallest one is $\frac{196}{27}$ for the tetrahedron whose vertices are $(-1, 1, 1), (1, -1, 1), (1, 1, -1)$ and $(-1, -1, -1)$. Since the volume of this tetrahedron is equal to $\frac{8}{3}$, the best lattice for this tetrahedron has a density of $\frac{18}{49}$. This value is the same as the one found by Groemer. Furthermore, any tetrahedron can be transformed into the one studied above using affine transformations without changing the validity of the lattice nor the density of the packing. That means that best lattice packing for any regular tetrahedron has a density of $\frac{18}{49} \approx 0.367$.

2.3 Best packing evolution

We will here present how the subject of the best packing was studied and how the density evolved with the discovery of better packings. All the following packing results use the concept of fundamental cell. The idea behind it is to divide the space into small finite regions, often polyhedra that tile the space. The fundamental cell is the reference region that contains the tetrahedra and that will be copied to fully fill the space. Therefore, we can then consider that a polyhedron tiling the space and a corresponding arrangement of non overlapping tetrahedra, both inside polyhedron and with the copies, constitutes a valid packing. Then to compute the density of such packings, the following formula can be used:

$$\text{density} = \frac{NV_{\text{tetraheron}}}{V_{\text{fundamental cell}}}$$

with N being the number of tetrahedra in each cell.

The first modern tentative to find the best packing was by Conway and Torquato in 2006 [6]. They determined the fraction of the volume occupied by 20 tetrahedra fitted into a regular icosahedron (a polyhedron with 20 equilateral triangles as its faces), it amounts to 0.8567627. Then they used the best lattice packing of icosahedra as presented by Betke and Henk [2]. This packing has a density of 0.8363574, which combined with the volume fraction of the 20 tetrahedra per icosahedron gives a total packing density of 0.716559. The density identified by the authors stood as their optimal discovery, reigning as the highest at that time. This value falling below the optimal density for sphere packing (74%) prompted the authors to contemplate whether the packing of tetrahedra could potentially serve as a counterexample to Ulam's packing conjecture. This conjecture states that the optimal density for the packing of congruent spheres is smaller than

that for any other convex body. The discovery of better packings later eliminated that counterexample. Another conclusion, that this result allowed to make is that the best packing of tetrahedra cannot be a lattice packing as the non-Bravais lattice (a lattice in which the body orientations can change) studied here provided a nearly twice better density than the best lattice packing.

In 2008, Elizabeth Chen proposed a packing with a density of 0.7786157 [4] confirming that Ulam's conjecture is not contradicted by tetrahedrons. This result was obtained by building a combination of lattices of clusters of 9 tetrahedra. The clusters are composed of one central tetrahedron, 4 lower tetrahedra around one edge and 4 upper tetrahedra around the opposite edge (see Figure 2.2). The two groups of 4 tetrahedra can rotate around their attached edge and the rotation angles are called $-\frac{1}{9} \leq u, v \leq \frac{1}{9}$. The whole cluster can also be flipped, it is called positive when in initial orientation and negative when flipped. The packing is composed of layers, the central layer is composed of positive clusters and the layers alternate between positive and negative. Each layer has its own lattice depending on the orientation of its composing clusters. The packing obtained is periodic and crystallographic. All tetrahedra in the packing are ensured to have no intersection using separating hyperplanes (see section 3.1.3 for details on how this works). The optimal configuration was found using a method based on numerical optimization by following the next steps as described in the paper:

1. Write the equations of the virtual cluster vertices in terms of u and v
2. Write the equations of the virtual intersections between the cluster and its neighbors, in terms of the virtual cluster vertices, the lattice vectors a,b,c,d and extra intersection parameters (edge-to-edge or point-in-plane)
3. Solve for the abstract lattice vectors and extra intersection parameters, in terms of u and v
4. Write abstract expressions for the lattice volume and packing density in terms of u and v
5. Find the relative minimum of the lattice volume (They precise that they were only able to use numerical approximations because of the degree of the polynomial was too high)

This result was slightly improved by Torquato and Jiao to 0.782021 in 2009 [20]. To do this, they used another method based on optimization that they call adaptive shrinking cell (ASC). They start with 72 tetrahedra initially positioned as Chen proposed in her paper. The variables are the positions and orientations of the tetrahedra as well as the geometry of the fundamental cell (the cell is and stays a parallelepiped). They used the opposite of the packing density as objective function and a Monte Carlo based procedure with a Metropolis acceptance rule to optimize it. The optimization method is as follows : one tetrahedron or the cell is modified randomly, if that makes two tetrahedra overlap the modification is rejected, if the cell shrinks it is accepted and if it makes the cell bigger it is accepted with a defined probability. To check whether two tetrahedra overlap, they use the separating axis theorem (an other version of the theorem presented in section 3.1.3). The version they use states that two polyhedra are separated in space if the

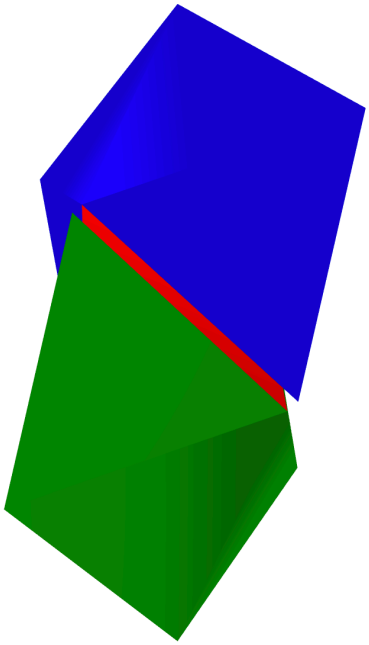


Figure 2.2: Chen's clusters, central tetrahedron in red, upper 4 in blue and lower 4 in green

projection of their vertices on an axis do not overlap. They also use the fact that this axis is either perpendicular to one face of the polyhedra or to a pair of edges (one from each polyhedron). This allows to only check 23 axis candidates (8 from faces and 15 form edge pairs) for each tetrahedron pair at each step. They were later able to further improve the density to 0.822637 by exploring a wider range of initial conditions (for example by using 314 instead of 72 tetrahedra) and optimization parameters [19].

The same year, Haji-Akbari, Engel et al. proposed two interesting results by using a more chemical approach to the problem [11]. They managed to obtain a density of 0.8324 by equilibrating an initially disordered fluid of 13,824 hard tetrahedra using a Monte Carlo simulation and then numerically compressing the result. The configuration obtained when equilibrating the fluid is a quasicrystal, that is why they decided to consider quasicrystal approximants as dense packing candidates. A quasicrystal approximant is a periodic crystal with local tiling structure identical to the one in a quasicrystal. This enabled the discovery of an even superior packing with a density of 0.8503. For the compression algorithm, they used a modified version of the isobaric Monte Carlo method where all volume changes are accepted even if they create an overlap (instead of rejecting them). The type of volume change (expansion or compression) is determined by comparing the acceptance probability p of translation moves to a target acceptance probability p_0. If $p < p_0$, a compression is applied and an expansion otherwise. The changes of volume are rescaling of the volume by a factor randomly chose between 1 and $1 \pm 0.002\Delta r$. The control parameter Δr corresponds to the maximum distance for the translations and is used to control the pressure in the system (lower equal higher pressure), it is exponentially lowered to 0 through the steps to obtain maximal compression.

In the beginning of 2010, a paper was published by Kallus, Elser and Gravel offering a packing with density of 0.8547 [15]. This result is particularly interesting because the

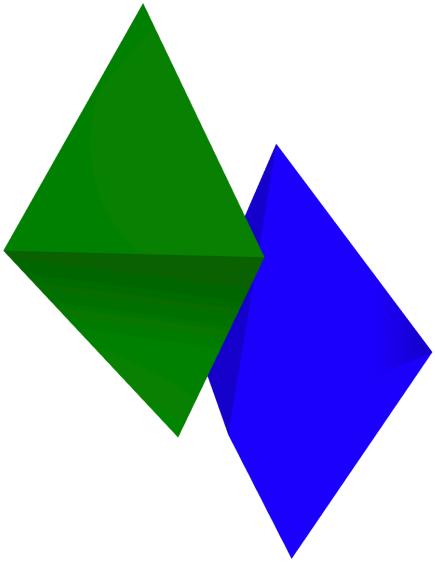


Figure 2.3: Bipyramidal dimers

trend up to that paper has been to increase the size of the fundamental cells and the number of tetrahedra in them, the packing presented here only consists of 4 tetrahedra per fundamental cell. They discovered this family of packings when looking at the results obtained using a numerical method. Their numerical method is an adapted version of the "divide and concur" approach to the constraint satisfaction from [8]. The difference with the results of the previous studies might be due to the fact that this method has dynamics that are highly non-physical allowing to find new configurations never seen up to that point. The packing they found can be described as double lattice of bipyramidal dimers (a single repeating unit is visible on Figure 2.3). A double lattice is the union of two lattices interconnected through an inversion operation centered around a specific point. The bipyramidal dimer is a polyhedron formed by two tetrahedra having one face in common. They built a one parameter family of double dimer packings based on a general monoclinic coordinates basis ($a \cdot b = b \cdot c = 0$). The reference tetrahedron is given by its vertices : $\frac{27}{28}a - \frac{7}{30}b + \frac{10}{39}c$, $\frac{1}{4}a - \frac{9}{10}b$, $\frac{1}{14}a + \frac{1}{10}b + \frac{5}{13}c$ and $\frac{3}{7}a + \frac{1}{10}b - \frac{5}{13}c$. The tetrahedron associated with this one to form a dimer is obtained by a 180° rotation around the axis $\left\{\frac{1}{4}a + tb | t \in \mathbb{R}\right\}$. The other dimer is obtained by inversion about the origin. The lattice is produced using translations following the vectors a, b and $\frac{1}{2}b + \frac{1}{2}c + xa$ where x is the single parameter of the lattice. When considering the coordinate system producing unit edge regular tetrahedra ($a = (2\sqrt{7}/5, 0, 0), b = (0, \sqrt{3}/2, 0)/textandc = (0, 0, 13\sqrt{3/14}/5)$), we see that the packing density is not influenced by the value of x. The packing is valid (the tetrahedra do not overlap) for $\frac{29}{56} \leq x \leq \frac{9}{14}$.

Shortly after, Torquato and Jiao inspired by the work of Kallus, Elser and Gravel discovered a packing with density 0.855506 [18]. They applied the adaptive shrinking cell method to packings with smaller number of particles per fundamental cell (ranging from 2 to 32). The configuration that gave the best result is composed of 4 tetrahedra forming two contacting dimers. To obtain, the best packing density they increased the one-parameter approach to the lattice description (from Kallus et al.) to two parameters. The fact that the obtained packing has less symmetry than the one from Kallus et al. and has a better density can be explained by the fact that tetrahedra are not centrally

symmetrical polyhedra. They also proposed a candidate upper bound for the packing density of 0.880755 but it has not yet been proved.

2.3.1 Best packing to date

The best result to date with a density of 0.856347 was presented in 2010 by Chen, Engel and Glotzer [5]. They managed to find this result using two different methods:

- An analytical method based on a three parameter family of double dimer packings, taking generalization a step further than the two previous attempts. They start by defining the lattices : L^+ for the positively orientated dimer is spanned by $a+b, b+c, c+a$ and L^- for the negatively orientated dimer which is offset by $d+a$. The positive dimer has vertices $(2,2,2),(2,-1,-1),(-1,2,-1),(-1,-1,2)$ and $(-2,-2,-2)$ and the negative dimer is the same but inverted about the origin. The lattices are essentially:

$$\begin{aligned} L^+ &= \{n_a a + n_b b + n_c c | n_a + n_b + n_c = 0 \mod 2\} \\ L^- &= \{n_a a + n_b b + n_c c | n_a + n_b + n_c = 1 \mod 2\} + d \end{aligned}$$

  with the vectors a, b, c, d parameterizing the lattices. These four 3-dimensional vectors mean that the set of all configurations is a 12-dimensional linear space. Some of the configurations in this space are not valid packings because some tetrahedra overlap. To ensure that no overlap occur, 9 constraints preventing the neighbors of the dimer at the origin to have any intersection with it are written. These constraints limit the linear space a 3-dimensional one called $\mathcal{P}'$ where the lattice vectors can be written as:

$$\begin{aligned} a &= \left\langle \frac{27}{10} + u,\ \frac{21}{20} - v,\ -\frac{3}{20} + 2u + v \right\rangle \\ b &= \left\langle -\frac{3}{10} - u,\ \frac{51}{20} + v,\ \frac{27}{20} - 2u - v \right\rangle \\ c &= \left\langle -\frac{129}{160} - u + 2v + 2w,\ -\frac{237}{320} + \frac{1}{2}u - v + 3w,\ \frac{753}{320} + \frac{1}{2}u - v + w \right\rangle \\ d &= \left\langle \frac{1}{10} + u,\ -\frac{1}{20} + u - v,\ -\frac{1}{20} + u - v \right\rangle \end{aligned}$$

  The space $\mathcal{P}'$ is even more restrict to a linear space only containing the double dimer packings:

$$\mathcal{P}'' = \left\{ \langle u, v, w \rangle \in \mathcal{P}' : \left| \frac{1}{2}u + 2v \right| \leq \frac{33}{320} \wedge |v| \leq \frac{3}{64} - w \right\}$$

  The volume of the unit cell is given by $V = |\det[a+b, b+c, c+a]| = \frac{9}{25}(117 + 60u^2 - 80uv + 80v^2)$. In $\mathcal{P}''$, there are two points that provide the best density of $\frac{4000}{4671}$: $\langle u, v, w \rangle = \pm\frac{3}{320}\langle 2, 5, 0 \rangle$.

- A numerical compression method employing the same classic isobaric Monte Carlo scheme as before. They applied this method to initially random configurations containing between 1 and 16 tetrahedra. A very interesting phenomenon arose from these : the optimal packings for 4,8,12,16 tetrahedra all contain dimers.

The packing of regular tetrahedra proposed in this paper have a density remaining the best to this day. Although an entire decade has passed, no superior outcome has emerged. Furthermore, there exists no substantiated evidence that this serves as an upper bound for the tetrahedron packing density. Therefore, the search for a better result remains an relevant field of study.

2.4 Bounds

The current best lower bound is determined by the most favorable packing density achieved thus far, specifically amounting to 85.63% as of the present moment. The underpinnings of this result are presented in the above section of this report.

As seen before in the section 2.1, Aristotle thought that tetrahedron tiled the space, an affirmation that was proved to be wrong in the 15th century. The first non trivial upper bound was presented by Gravel, Elser and Kallus in 2010 [9]. The upper bound they give is equal to $1 - 2.5\,10^{-25}$. This result is obtained by finding a lower bound to the volume fraction not occupied by tetrahedrons in a sphere centered on the edge of one tetrahedron of the packing and not containing any tetrahedron vertex. Then this bound is used in conjunction with a lower bound found on the size of the set of disjoint spheres (still centered on edges and containing no vertex) in a packing of N tetrahedra to build a lower bound on the minimal fraction of space "lost". This bound is then converted to an upper bound on the tetrahedron packing density. As stated by the authors, this bound is not tight and there is room for improvement; however, no attempts to investigate it further appear to have been undertaken.

2.5 Physical experiment

Above we have seen many theoretical approach to the search of the densest tetrahedron packing. Here, we will take a look at a physical experiment conducted by Jaoshvili, Esakia, Porrati and Chaikin [14]. They used tetrahedral dice to estimate the packing density. The dice are not perfect tetrahedra: they only fill 96% of the circumscribed tetrahedron or 116% of the inscribed one. They used 1000 tetrahedra that they put in containers of different sizes which were shaken and then tetrahedra were added until it was not possible anymore. They mainly used cylinders of different radii. To measure the density achieved they weighed a fluid of known density when filling the empty container and with the dice in it. Using the densities measured for the different radii, they extrapolate the maximal value (for a cylinder of infinite radius) to be 0.76 ± 0.02. This result is relatively close to the ones of the packings with a number of tetrahedra of the same order.

Chapter 3

Optimization models

As we have seen in the literature review, the best packing density result dates back to more than 10 years ago. Since then, no new approach has managed to improve this result. The methods which proved to provide the best densities are the analytical construction of an admissible space of packings for a specific configuration (ex: the packing of two dimers) and the use of Monte Carlo based numerical methods for more general problems with a defined number of tetrahedra. It is easy to notice that any problem of packing is an optimization problem where there is an objective to maximize (the density) and a set of constraints to satisfy (mainly preventing overlaps). Here, we would like to study how the tetrahedron packing problem can be formulated as an optimization problem. In essence, the goal is to build a model allowing to find the fundamental cell giving the best density for a given number of tetrahedra in it. We will present here 4 iterations of the model.

3.1 Model 1: naive approach

This first version of the model was built to assess the feasibility of the objectives we set ourselves. The aim was then to make the simplest model possible using a naive approach to solve all problems that presented themselves. The model can be divided into 3 main parts : the formulation of the tetrahedra, the objective function and the constraints ensuring no overlap between tetrahedra occur. Each will be explained in details in the next subsections.

3.1.1 Tetrahedron formulation

The most important part of the model is how the tetrahedra are actually formulated. A unit edge regular tetrahedron in $\mathbb{R}^3$ is subject to 6 degrees of freedom. Its position and orientation can be uniquely defined using a point in space (3 degrees: (x, y, z)) and three rotation angles. However, the most basic way to describe a tetrahedron is using the coordinates of its vertices. That is what we chose to use, all the vertex coordinates are set to be variables and with the use of constraints on the distances between each vertex we only get valid tetrahedra. The validity of this approach in terms of degrees of freedoms can be verified as follows: the variable vertex coordinates produce $4 * 3 = 12$ degrees of freedom and we have 6 constraints on the distances thanks to the same number of different pairs of vertices. Combining the two, the expected 6 degrees of freedom are recovered.

3.1.2 Objective function

The value we want to maximize for this problem is the density, given by $\frac{NV_{\text{tetrahedron}}}{V_{\text{fundamental cell}}}$. As the number of tetrahedra and their volume are defined beforehand, we choose the objective to be the minimization of the volume of the fundamental cell. For this first model, we restrict the fundamental cell space to only rectangular parallelepipeds. It is clear that all parallelepipeds are valid fundamental cells because they tile the space using copies of themselves along their edges. To ensure that all tetrahedra are well fully inside the cell we just have to bound the components of their vertex coordinates by 0 and the corresponding edge length of the parallelepiped. The objective function is then simply given by the volume of the parallelepiped i.e. the products of its constituting edge lengths.

3.1.3 No intersection constraints

The conceptualization of the set of constraints to ensure that the tetrahedra don't overlap is the most tricky part of the model conception. It can be done by individually constraining each pair of tetrahedra to have no overlap. As a tetrahedron is fundamentally the convex hull of its vertices, it is a convex set. That allows the use of the separating hyperplane theorem which states that [3]:

Theorem 1. *Let A and B be two disjoints convex sets, i.e. $A \cap B = \emptyset$, then there exists $a \neq 0$ and b such that $a^T x \leq b$ for all $x \in A$ and $a^T x \geq b$ for all $x \in B$.*

Using this, the constraints boil down to always making sure it is possible to find a separating hyperplane between the pair of tetrahedra. It can be done by creating hyperplane variables a and b for each tetrahedron pair and ensuring that the tetrahedra are on either side by writing the inequalities. b can even always be set to 1 because only 3 degrees of freedom are needed for an hyperplane in $\mathbb{R}^3$. The only situation in which that could cause a problem is if the hyperplane needs to contain $(0, 0, 0)$ fortunately that will never happen thanks to the definition of the fundamental cell. The inequalities can only be checked on the vertices as each tetrahedron is their convex hull. This constraint has been tested and works fine but there is an even smarter way to formulate it, we can check that the other tetrahedron is on the other side of the hyperplane found by taking the convex combination of the 4 hyperplanes containing the faces of the other tetrahedron. The vertices of the second tetrahedron are necessarily on the other side because of the construction of the hyperplane, the corresponding inequalities don't need to be checked. This allows to exchange 4 inequality constraints for one equality (the convex combination). For example, the constraints separating the tetrahedra I and J write as follows (with a_1, a_2, a_3, a_4 being the convex combination coefficients associated with that pair, $v_{I,p}$ the vector containing the coordinates of the pth vertex of the tetrahedron p and $r \in \{1, 2, 3, 4\} \setminus \{p\}$):

$$
\begin{aligned}
&a_1 + a_2 + a_3 + a_4 = 1 \\
&\sum_{p=1}^{4} a_p \left(v_{I,p} - \frac{\sum_{q \in \{1,2,3,4\} \setminus \{p\}} v_{I,q}}{3} \right)^T (v_{J,1} - v_{I,r}) \leq 0 \\
&\sum_{p=1}^{4} a_p \left(v_{I,p} - \frac{\sum_{q \in \{1,2,3,4\} \setminus \{p\}} v_{I,q}}{3} \right)^T (v_{J,2} - v_{I,r}) \leq 0 \\
&\sum_{p=1}^{4} a_p \left(v_{I,p} - \frac{\sum_{q \in \{1,2,3,4\} \setminus \{p\}} v_{I,q}}{3} \right)^T (v_{J,3} - v_{I,r}) \leq 0 \\
&\sum_{p=1}^{4} a_p \left(v_{I,p} - \frac{\sum_{q \in \{1,2,3,4\} \setminus \{p\}} v_{I,q}}{3} \right)^T (v_{J,4} - v_{I,r}) \leq 0
\end{aligned}
$$

3.1.4 Full formulation

Here, we present the full model written under the classic form for an optimization problem. The presented problem is for the packing of N tetrahedra.

$$
\begin{aligned}
\underset{x}{\text{minimize}} \quad & h_1 * h_2 * h_3 \\
\text{subject to} \quad & h_i \geq v_{J,k}\left[i\right], \\
& 1 = \sum_{p=1}^{3} \left(v_{J,k}[p] - v_{L,k}[p] \right)^2, \\
& 1 = \sum_{p=1}^{4} a_{J,L,p}, \\
& \sum_{p=1}^{4} a_{J,L,p} \left(v_{J,p} - \frac{\sum_{q \in \{1,2,3,4\} \setminus \{p\}} v_{J,q}}{3} \right)^T (v_{L,k} - v_{J,r}) \leq 0, \\
& i \in \{1,2,3\} \quad J \in \{1,\ldots,N\} \quad L \in \{J+1,\ldots,N\} \quad k \in \{1,2,3,4\} \\
& r \in \{1,2,3,4\} \setminus \{p\}
\end{aligned}
\tag{3.1}
$$

The different variables are as follows:

Variable	Bounds	Description
h_i		Length of the ith vector of the fundamental cell, its constituting vectors are $(h_1, 0, 0), (0, h_2, 0)$ and $(0, 0, h_3)$
$v_{J,k}[i]$	≥ 0	ith coordinate component of the kth vertex of the tetrahedron J
$a_{J,L,p}$	≥ 0	pth coefficient for the convex combination of the hyperplanes for the tetrahedron pair (J, L)

3.2 Model 2: tetrahedra protruding

The previous model was a working model but it was too restrictive in the sense that it was preventing tetrahedron to protrude from the faces of the fundamental cell. In

this section, we will explain how the model was adapted to allow this behavior. No full formulation will be given as no new idea in terms of implementation are used, only the addition and modification constraints.

3.2.1 No intersection constraints

These changes have the biggest impact of the enforcement of the absence of overlap. We now have to consider the fact that the tetrahedra may overlap with copies of other tetrahedra or even themselves. This behavior can be observed on Figure 3.1 where the packing is correct with respect to the constraints of the previous model as the 6 "base" tetrahedra don't overlap and the centers are inside the cell. However, it is obviously not a valid packing when we try to tile the space by copying the fundamental cell.

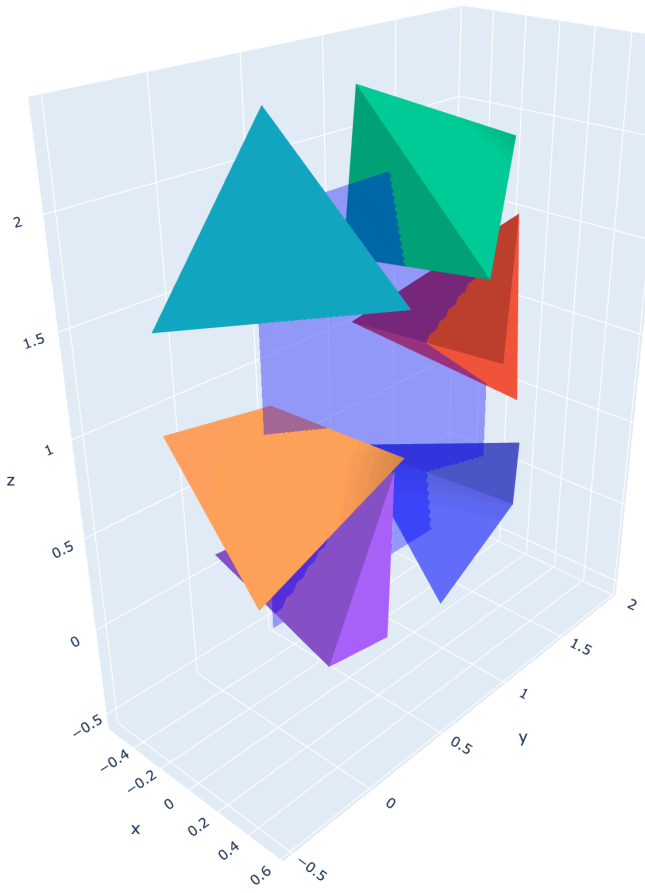


Figure 3.1: (Model 2) Centers in the fundamental cell and no copies constraints. The fundamental cell is transparent blue.

This means that we have to add new constraints taking into account the copies the tetrahedra for the tiling. For that, each tetrahedron in the original fundamental cell must have no intersection with all the others copies around it. The fundamental cell is in contact with 26 of its copies: 6 with faces in common, 12 with edges and 8 with vertices. Fortunately, all these don't need to be included as we can take advantage of the

symmetries. When checking for overlaps between the base and copied cell, we are both preventing overlap through one face, edge or vertex and its opposite because the part on the copy in contact with the base cell corresponds to its opposite part of the base cell. That means we have 13 copies to consider, amounting to $26N^2$ hyperplanes to be found. The copies of the tetrahedra can easily be found by translating them using a combination of the cell vertices : $k_1(h_1, 0, 0) + k_2(0, h_2, 0) + k_3(0, 0, h_3)$. The constraints to avoid the overlaps are the same as in 3.1.3. The values of the coefficients (k_1, k_2, k_3) are :

- Face copies : $(1, 0, 0), (0, 1, 0), (0, 0, 1)$
- Edge copies : $(1, 1, 0), (1, -1, 0), (1, 0, 1), (1, 0, -1), (0, 1, 1), (0, 1, -1)$
- Vertex copies : $(1, 1, 1), (1, -1, -1), (1, 1, -1), (1, -1, -1)$

3.2.2 Objective function

The fundamental behavior of the objective function remains largely consistent. Two versions were developed. The first one forces only one vertex per tetrahedron to be inside the fundamental cell. To put this into constraints, we choose one and require it to be inside. The choice of an arbitrary vertex should not pose any problem as they are interchangeable, it only adds a bit of complexity for the solver as valid configurations are eliminated. However, problems are still observed, we get results like the one visible on Figure 3.2 where the tetrahedra are mainly outside the fundamental cell. This configuration does not present any intersection between tetrahedra when considering the first layer of copies around the cell but not anymore with further copies. Indeed, we observe an intersection when considering the copy given by $(k_1, k_2, k_3) = (-2, -2, 0)$. That could be solved by adding new layers of copies to the constraints but that does have a high cost as the number of copies grows according to $\frac{(2*n_{\text{layers}}+1)^3-1}{2}$ (while still using symmetry). That is why a second idea based on forcing the centers to be inside the cell is used. It solves the problem by making sure most of the tetrahedron volume is contained in the fundamental cell but has the big disadvantage of potentially being too restrictive.

The constraints on h_i's now become:

$$h_i \geq \frac{\sum_{k=1}^{4} v_{J,k}[i]}{4} \tag{3.2}$$

3.3 Model 3: translations and rotations of reference tetrahedron

In this model, we try to change the description of the tetrahedra from the coordinates of all their vertices to 3 rotations and a translation only giving them the 6 degrees of freedom of movement they deserve. This change influences the objective function.

The idea behind this model is to use a reference regular tetrahedron centered on the origin, it is first rotated around the origin and then translated. In order to still be able to use the same constraints on intersections, the vertex coordinates are computed and put into constraints. The conversion works as follows:

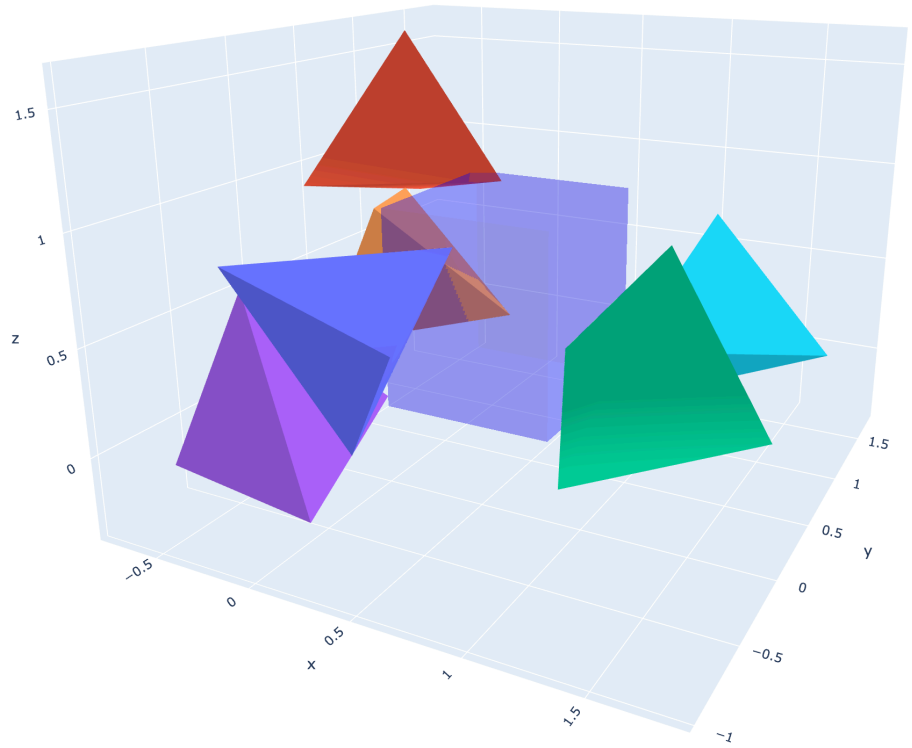


Figure 3.2: (Model 2) One vertex in the fundamental cell. The fundamental cell is transparent blue.

$$v_{J,k} = x_{\text{trans},J} + \tag{3.3}$$

$$\begin{pmatrix} \cos(\alpha_J)\cos(\beta_J) & \cos(\alpha_J)\sin(\beta_J)\sin(\gamma_J) - \sin(\alpha_J)\cos(\gamma_J) & \cos(\alpha_J)\sin(\beta_J)\cos(\gamma_J) + \sin(\alpha_J)\sin(\gamma_J) \\ \sin(\alpha_J)\cos(\beta_J) & \sin(\alpha)\sin(\beta_J)\sin(\gamma_J) + \cos(\alpha_J)\cos(\gamma_J) & \sin(\alpha_J)\sin(\beta_J)\cos(\gamma_J) - \cos(\alpha_J)\sin(\gamma_J) \\ -\sin(\beta_J) & \cos(\beta_J)\sin(\gamma_J) & \cos(\beta_J)\cos(\gamma_J) \end{pmatrix} v_{\text{ref},k} \tag{3.4}$$

where α_J, β_J and γ_J are respectively the yaw, pitch and roll angles for the tetrahedron J, $x_{\text{trans},J}$ the translation vector for the tetrahedron J and $v_{\text{ref},k}$ the coordinates of the k vertex of the reference tetrahedron. This change has the side benefit of giving a direct access to the centers of the tetrahedra through $x_{\text{trans},J}$. It is easier to use in the constraints on the size of the fundamental cell introduced in 3.2.

3.4 Model 4: parallelepipedic fundamental cell

For this model, the fundamental cell was modified in order to accept more general parallelepipeds not required to be rectangular. Such parallelepipeds are described by 3 vectors of the form : $(c_{1,x}, 0, 0), (c_{2,x}, c_{2,y}, 0), (c_{3,x}, c_{3,y}, c_{3,z})$. The objective function is still the volume of the cell which is :

$$V_{\text{cell}} = \left| \det \begin{bmatrix} c_{1,x} & c_{2,x} & c_{3,x} \\ 0 & c_{2,y} & c_{3,y} \\ 0 & 0 & c_{3,y} \end{bmatrix} \right| = c_{1,x} * c_{2,y} * c_{3,z}$$

Unfortunately, one problem arises from this formulation: the model considers very flat fundamental cells valid because when the third vector describing parallelepiped is long

and at a very low angle with the hyperplane $z = 0$ the copies "on top" are also translated to the side allowing the tetrahedra to protrude very much above and below without being in contact with one tetrahedron from the first layer of copies. These fundamental cells are often even too flat and wide to be able to see the tetrahedra when looking at the whole cell. This phenomenon is due to the fact that we only check for intersections with the first layer of copies. This problem is similar to what happened with model 2 but here it cannot be solved by only adding layers of copies because as long $c_{3,z}$ is very small, the parallelepiped can be enlarged to avoid intersections while the number of constraints from the addition of layers is prohibitive. One solution is to bound the angles between the vectors of the parallelepiped using the fact that $\cos(\angle(c_i, c_j)) = \frac{(c_i \cdot c_j)}{\|c_i\|\|c_j\|}$. This was tested with $\frac{\pi}{4}$ and $\frac{3\pi}{4}$ as bounds but the model was still producing solutions with overlaps with further layers. We gave up on that idea and thought about what was the core cause of the problem. It is caused by the fact that the copy layers that are checked do not "isolate" the base cell from the layers not checked in the sense that protruding tetrahedra from both can be in contact through the checked layers. A solution would be to force the first layer to isolate, i.e. to have a minimal distance between any two points on parallel faces of the fundamental cell further apart than two tetrahedra can stick out of the cell. A tetrahedron whose center is inside the cell can at most protrude of $\sqrt{\frac{3}{8}}$ from a face (this is the distance between any vertex and the center of the tetrahedron). The minimal distance between two parallel faces is given by $c_{3,z}$, $\frac{c_{1,x}c_{2,y}c_{3,z}}{\sqrt{(c_{1,x}c_{3,z})^2+(c_{1,x}c_{3,y})^2}}$ or $\frac{c_{1,x}c_{2,y}c_{3,z}}{\sqrt{(c_{2,y}c_{3,z})^2+(c_{2,x}c_{3,z})^2+(c_{2,x}c_{3,y}-c_{2,y}c_{3,x})^2}}$, therefore bounding them from below by $2\sqrt{\frac{3}{8}}$ would solve the problem. Sadly, that bound is too restrictive and leads to the convergence towards local infeasibility points especially with small numbers of tetrahedra. That is why we decide to add one layer of copies to the constraints to be able to lower the bound to $\sqrt{\frac{3}{8}}$, solving the convergence problems. It is important to note that that takes the number of copies to check from 13 to 62. That significantly increases the number of constraints per tetrahedron but we can still use one layer of copies and the higher lower bound for the distance inside the cell for problems with a higher number of tetrahedra, where it has the most impact on the number of constraints and the least on density.

To enforce the tetrahedron centers to be inside the tetrahedron, we cannot use bounds on the coordinates of the centers as before. The region inside of the fundamental cell cannot be defined that way anymore. We have to use the fact that all the points inside the parallelepiped are given by a linear combination of its constituting 3 vectors presented above. Essentially for any point x in the parallelepiped we have $x = \sum_{i=1}^{3} k_i c_i$ with $0 \leq k_i \leq 1$. We just have to add the constraints from this to ensure the centers are inside.

3.4.1 Full formulation

The full model is given by :

$$
\begin{aligned}
\underset{x}{\text{minimize}} \quad & c_{1,x} * c_{2,y} * c_{3,z} \\
\text{subject to} \quad & \sum_{i=1}^{3} k_{i,J} c_i = x_{\text{trans},J}, \\
& c_{3,z} \geq \sqrt{\frac{3}{8}}, \\
& \frac{c_{1,x} c_{2,y} c_{3,z}}{\sqrt{(c_{1,x} c_{3,z})^2 + (c_{1,x} c_{3,y})^2}} \geq \sqrt{\frac{3}{8}}, \\
& \frac{c_{1,x} c_{2,y} c_{3,z}}{\sqrt{(c_{2,y} c_{3,z})^2 + (c_{2,x} c_{3,z})^2 + (c_{2,x} c_{3,y} - c_{2,y} c_{3,x})^2}} \geq \sqrt{\frac{3}{8}}, \\
& v_{J,k} = x_{\text{trans},J} + M_{\text{rot}}(\alpha_J, \beta_J, \gamma_J) v_{\text{ref},k} \\
& 1 = \sum_{p=1}^{4} a_{J,L,p}, \\
& \sum_{p=1}^{4} a_{J,L,p} \left(v_{J,p} - \frac{\sum_{q \in \{1,2,3,4\} \setminus \{p\}} v_{J,q}}{3} \right)^T (v_{L,k} - v_{J,r}) \leq 0, \\
& 1 = \sum_{p=1}^{4} b_{M,O,p,s}, \\
& \sum_{p=1}^{4} b_{M,O,p,s} \left(v_{M,p} - \frac{\sum_{q \in \{1,2,3,4\} \setminus \{p\}} v_{M,q}}{3} \right)^T \left(v_{L,k} - v_{J,r} - \sum_{q=1}^{3} d_{s,q} c_q \right) \leq 0, \\
& i \in \{1,2,3\} \quad j \in \{1,2,3\} \setminus \{i\} \quad k \in \{1,2,3,4\} \quad r \in \{1,2,3,4\} \setminus \{p\} \\
& s \in \{1, \ldots, 62\} \quad J \in \{1, \ldots, N\} \quad L \in \{J+1, \ldots, N\} \quad M\{1, \ldots, N\} \\
& O \in \{1, \ldots, N\}
\end{aligned}
\tag{3.5}
$$

All the variables are described below:

Variable	Bounds	Description
c_i	≥ 0	Vectors describing the parallelepiped (when a variable is added alongside the index it designates the corresponding coordinate)
$k_{i,J}$	$\geq 0, \leq 1$	ith coefficient of the linear combination of the parallelepiped vectors giving the center of the tetrahedron J
$v_{J,k}$	≥ 0	Coordinates of the kth vertex of the tetrahedron J
$x_{\text{trans},J}$		Vector describing the translation applied to the reference tetrahedron to get the tetrahedron J
$M_{\text{rot}}(\alpha_J, \beta_J, \gamma_J)$		Matrix describing the rotation applied to the reference tetrahedron to get the tetrahedron J (depends on $(\alpha_J, \beta_J, \gamma_J)$ the yaw, pitch and roll angles). See 3.4 for details.
$a_{J,L,p}$	≥ 0	pth coefficient for the convex combination of the hyperplanes for the tetrahedron pair (J, L)
$b_{M,O,p,s}$	≥ 0	pth coefficient for the convex combination of the hyperplanes for the tetrahedron M and the sth copy of O
$d_{s,q}$	≥ 0	qth coefficient for the combination of cell vectors giving the translation for sth copy of any tetrahedron

Chapter 4

Solving and analysis

In this section, we will solve the packing problem using the models presented above and one off the shelves solver. We will start by introducing the software used, the parameters and the results. Optimization strategies will be presented. The results will then be analyzed and comparisons between the models and to the literature results will drawn.

4.1 Experimental setup

The software used to formulate models and solve the problem is the community edition of AMPL. AMPL (A Mathematical Programming Language)[1] is a versatile and robust programming language designed for formulating and solving complex optimization problems. It offers the possibility to write models in an user-friendly syntax. One very big advantage of AMPL is its Python api which allows to more easily control the solving process. The solver that was used is IPOPT (interior point optimizer)[2], an open source solver for large-scale nonlinear optimization problem. That fits really well with our problem as we have both a nonlinear objective function and nonlinear constraints. Solving took place on a standard personal computer.

To assess the validity of all the solutions, a validation code was written in Python. It works with a variable number of copy layers and uses two different strategies to check for intersections. The first one is the same as the first one presented in 3.1.3. It uses a SAT solver (z3) to find valid hyperplanes separating each tetrahedron pair. The second one takes advantage of the fact that we have the definitive arrangement of tetrahedra. That allows us to use a collision detection based approach, like what is usually done in video games [7]. It consists in trying multiple hyperplane candidates for each pair (23, similarly to what was done in the literature). The candidates are either containing one face or their normal vector is perpendicular to an edge pair (one from each tetrahedron). This second verification technique is much cheaper in computing cost allowing to check for larger numbers of copy layers.

4.2 Model comparison

In this section, we will compare the results and performances of the 4 models presented in Chapter 3. For each of them, we will measure the time taken to solve and the density for a

[1] https://ampl.com
[2] https://coin-or.github.io/Ipopt/

solving with uninitialized variables, all constraints active at all time and for $4, 6, 8, 11, 16$ tetrahedra. The only exceptions are the results contained in between parenthesis, they were obtained through multiple solves with a progressive addition of constraints to keep the solving time under a reasonable limit. All packings are valid and were checked using the validation code against 10 layers of copies. The results are visible in the following table:

N	Model 1		Model 2		Model 3		Model 4	
	Run time	Density	Run Time	Density	Run time	Density	Run time	Density
4	1.8s	30.68%	52.6s	55.89%	9.6s	61.57%	63.2s	57.35%
6	5.5s	37.9%	76.5s	50.34%	31.2s	56.63%	309.1s	54.1%
8	15.4s	42%	10390.7s	60.54%	50.6s	52.19%	701.2s	58.42%
11	37.2s	40.5%	(118.5s)	(62.46%)	215.3s	56.53%	4858.58s	48.75%
16	149.46s	40.83%	(434.2s)	(59.51%)	1724.6s	55.22%	(3283.2s)	(49.33%)

Table 4.1: Model performance comparison

We start by taking a look at the run time, this value was measured by the solver. It is important to note that it is subject to variations as the conditions like the heat have a significant impact on processing power. They will only be used to get a rough idea of the order of magnitude of time necessary for solving. We observe that going from model 1 to model 2 implies a significant increase in run time as expected because of the additions of the copy constraints to allow the tetrahedra to protrude. The 3rd model which switches the tetrahedron description to 3 angles and 3 coordinates (the only 6 degrees of freedom necessary) was successful in making the model more efficient, which is translated into better run times. And finally, as anticipated, the model 4 is less efficient than model 3 as it has many more constraints to satisfy.

Now considering the densities, we can clearly see on the Figure 4.1 that model 1 is by far the worse. That is totally understandable as it requires the tetrahedra to be entirely inside the fundamental cell. We clearly see that the impact of this is less when we have more tetrahedra. That is explained by the fact that the boundary effect gets less and less significant as the fundamental cell grows relative to the tetrahedron size. For the other models, we cannot really observe any pattern in the relation between the number of tetrahedra and the density at the exception that models 3 and 4 seem to work better with smaller numbers. We also observe that the results seem to stay quite similar between the configurations with 11 and 16 tetrahedra for all models, that is unexpected given that in the literature even numbers of tetrahedra (and especially multiples of 4) always pack better. That can be explained by the fact that our model fails to produce dimers that according to the results of the literature allow for denser packings. One other quite surprising result is the better performances generally demonstrated by the model 3 compared to the model 4 despite the fact that the model 4 was built to introduce more freedom in the fundamental cell shape choice. It was supposed to allow for better densities. That is probably explained by the level of complexity of the model introduced by the new set of constraints to avoid overlap niche scenarios.

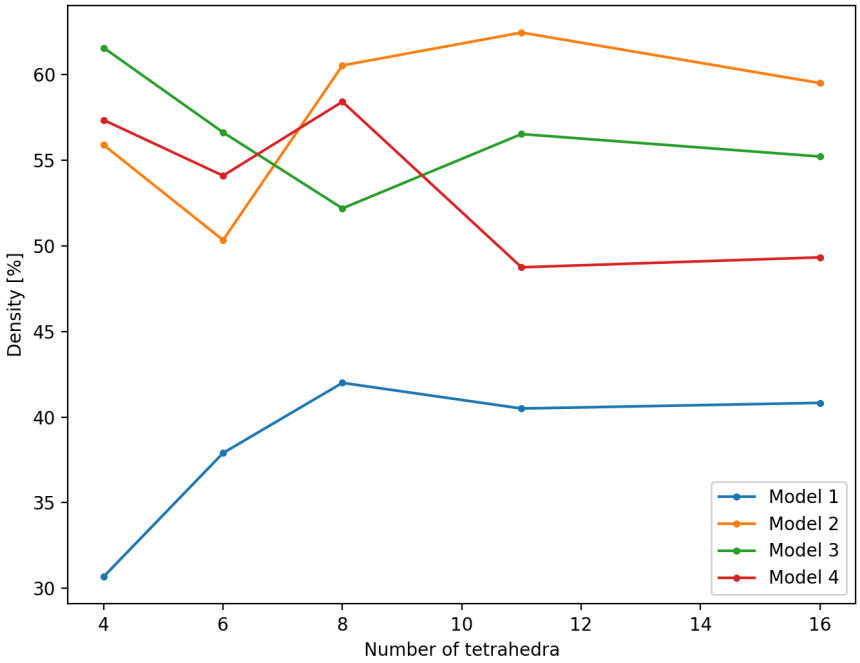


Figure 4.1: Evolution of the densities in function of the number of tetrahedra for the 4 models

4.3 Solving procedures

In this section, we will present all the procedures we used to try and get the best result possible. They will all be applied to the model supposed to be the best, the 4th as it is the more general one in terms of admissible fundamental cells and placement of the tetrahedra in them. Furthermore, it is quite constraint intensive which makes it the perfect candidate for some of the following techniques.

4.3.1 Initial conditions

The first improvement we would like to try is the use of intelligent initial conditions. We will try one bad initial condition, one average and a good initial condition all with 4 tetrahedra. They are all visible on Figure 4.2. The good initial condition is the best result of the paper from Kallus et al. [15] but with the tetrahedra translated outside the fundamental cell. The bad initial condition gave a density of 49.7%, the average one 61% and the good 59.4%. We clearly see that it is not the initial condition expected to be the best that produces the best result although it is quite close to the average one. The arrangement of the tetrahedra looks similar, but the fundamental cell is smaller for the average one, giving it the best density. That might be due to the fact that the initial fundamental cell is better suited to the tetrahedra in the average whereas it is perturbed in the good case. In the good case, the initial condition violates the "center in" constraint. That was actually experimentally proven: when using a more appropriate placement of the cluster, we observed that the good initial condition beat the average one. We see that both are better than the bad initial condition stressing the importance

of good initial conditions. However, the densities are only marginally better than the one with the standard initialization of the solver (visible in Table 4.1). Using the standard initialization seems to not hurt the result too much which is a good thing because building good initial conditions can be tricky.

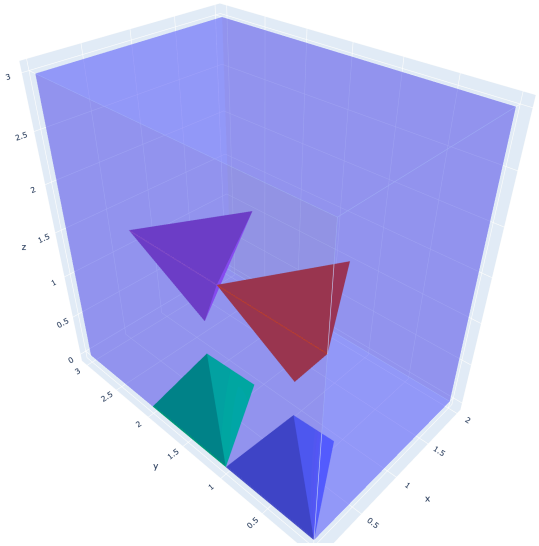
4.3.2 Adaptive constraint enforcement

The second enhancement we would like to explore involves the modification of the set of active constraints (in the sense that they need to be satisfied). We have already seen in 4.2 that solving multiple times with an increasing number of constraints up to the full set of constraints can greatly help reduce the run time. A smaller run time has the advantage to allow to test more complex configurations with more tetrahedra per fundamental cell or more layers of copies. It helps by allowing the solving of complex problems to start with an initial solution that already satisfies some of the constraints. For the model 2, we worked with the constraints for the intersections with the copies. We solved a first time with no constraints using copies then we added back the copies with a face in common, and the ones with an edge or a vertex in common. We tried to apply this the configurations with $4, 6$ and 8 tetrahedra and the impact on the densities turned out to be small (at most 4% better and 1% worse).

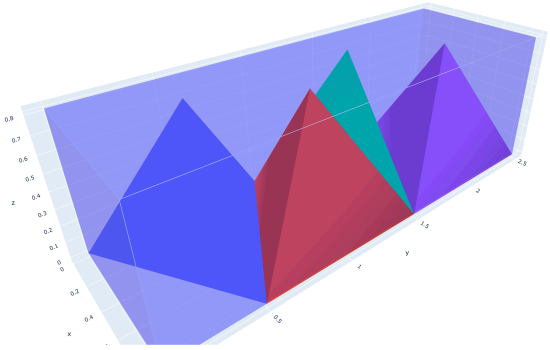
Another way to adapt the constraints can be to change them. That is possible with the model 4 where we can select the number of copy layers considered and adapt the lower bound on the distances between faces of the cell in consequence. We tried to successively solve for 1 to 4 layers of copies and found that the following densities for 4 tetrahedra packings: $25.7\%, 62.7\%, 56.8\%$ and 39.1%. We see that adding layers beyond 2 does not help the result get better, probably because of the added complexity and because the bound was already not limiting the cell size. We see that solving before for 1 layer then for 2 improves the result compared to solving directly with 2 (Table 4.1).

4.3.3 Dimer particles

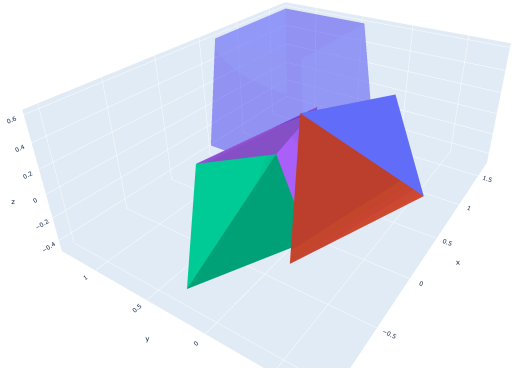
The results from the literature seem to indicate (particularly [5]) that dimers are the optimal way to arrange a pair of tetrahedra for numbers of tetrahedra which are multiples of 4. A modified version of the model 4 was created, in this version all the tetrahedra have a copy of themselves along one of their faces. The rest stays the same, the intersection are still considered tetrahedron to tetrahedra even though it is probably more efficient to consider them dimer to dimer, but this was done for ease of use. It is also more relevant that way for a comparison with the classic version. It was tested with 2, 3 and 4 dimers. The 2 dimers gave a density of 65.25%, the 3 gave 53.9% and the 4 gave 60.7%. As expected, it did not improve the density for the configuration with 6 tetrahedra. It was only marginally better for 8 tetrahedra but had a very positive impact when working with 4 tetrahedra. That is normal because the double dimer is the configuration that produced the best density ever but our density stays far off the best one. One big disadvantage of this strategy is that solving it is much slower than the equivalent free tetrahedra model (5 to 6 times slower for 4 tetrahedra per cell). The solver does not seem to be able to continuously shrink the fundamental cell, it has to re-enlarge it multiple times probably to make the dimers change position.



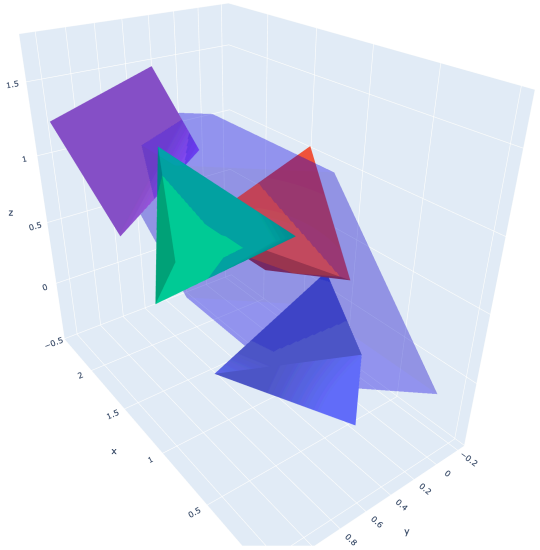
(a) Bad initial condition



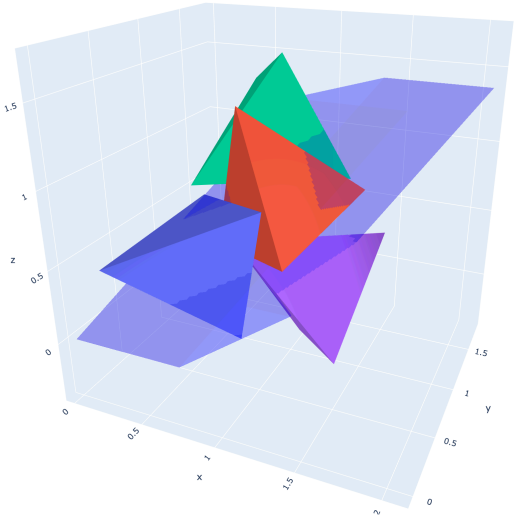
(b) Average initial condition



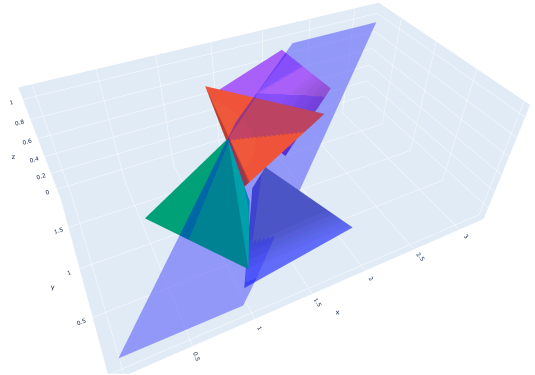
(c) Good initial condition



(d) Solution bad initial condition



(e) Solution average initial condition



(f) Solution good initial condition

Figure 4.2: Space filling attempts

4.3.4 Multiple successive runs

Another test we have performed is checking if making the tetrahedra from a previous solution "explode" and solve again improves the density. We would like to see if solving from a modified solution can help find better packings. The idea behind the "explosion" is to take the tetrahedra apart from each other to facilitate the access to other configurations. To do that, we computed the center of the cluster of tetrahedra by taking the average of the center coordinates of all the tetrahedra. Then the tetrahedra are translated according to the vector $\epsilon(\text{center}_{\text{tetrahedron}} - \text{center}_{\text{cluster}})$ where ϵ is the explosion factor. The underlying concept is to take further away the tetrahedra that are already further away from the cluster center because they are the ones that are less well packed and that are probably in contact with the boundaries of the fundamental cell. This technique was tested with 4 tetrahedra and for multiple values of ϵ, the result are on Figure 4.3. We see that using multiple runs yields improvements in densities. The value of ϵ does not appear to make a big difference, as we observe a similar comportment for $\epsilon = 0$. Furthermore, the behavior through the runs appears quite random and more problem related than influenced by ϵ. We can deduce that is more the fact that we run multiple successive solves that is beneficial. It is in fact some sort of a multi start scheme where we solve the problem for multiple different initial conditions in terms of tetrahedron placement. Despite all this, the best density our model has ever produced (81.9%) comes from the 11th run with $\epsilon = 0.2$. That is why, we try a bigger number of solves, 300 to be precise, with $\epsilon = 0.2$. We are limited in the number of solves because they are quite slow (around 60s per solve). That did not a improve the best density. The same was observed with other values of ϵ. On the other hand, this method allows to reliably find packings with densities of around 75% beating by a big margin our previous ones. That also means that the best packing was found by luck and that it would be beneficial to solve from a larger number of different initial valid configurations.

4.3.5 Combining everything

Here, we will try and get the best packing possible by combining all the above procedures that proved to improve the result. We will use the model 4 with 4 tetrahedra using an initial condition, force particles to be dimers and run multiple successive solves. Unfortunately, that did not produce any better packing. We were even more limited in the number of successive runs as the time needed to solve a problem with dimers is longer. Therefore, the combination of the multiple runs and the dimer particles is not really a good idea as they work against one another. Furthermore, the idea of an intelligent initial condition is not very relevant in the case of multiple successive runs as most run won't use it.

4.4 Comparison with the literature

Our best packing density is 0.818978 which is not significantly distant from the best density ever found of 0.856347. Both packings are visible on Figure 4.4. We see that they are quite close but our packing is two tetrahedra along the faces of a dimer rather than two dimers against one another. It looks like, ours is like this because of the "center in" constraints, the two single ones cannot get together into a dimer without violating these constraints.

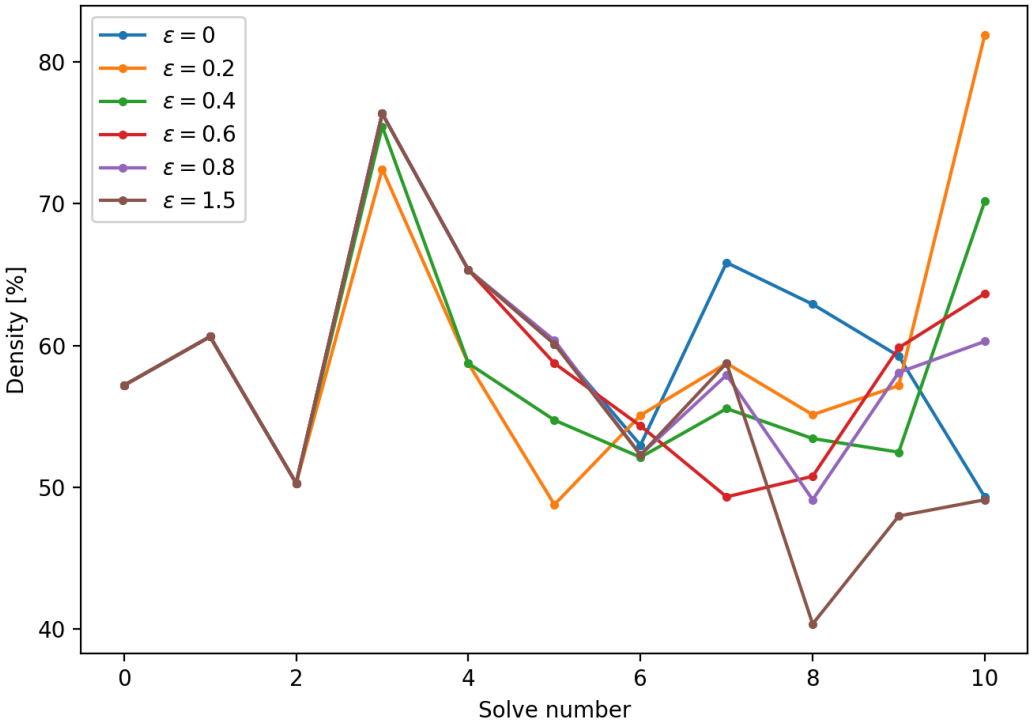
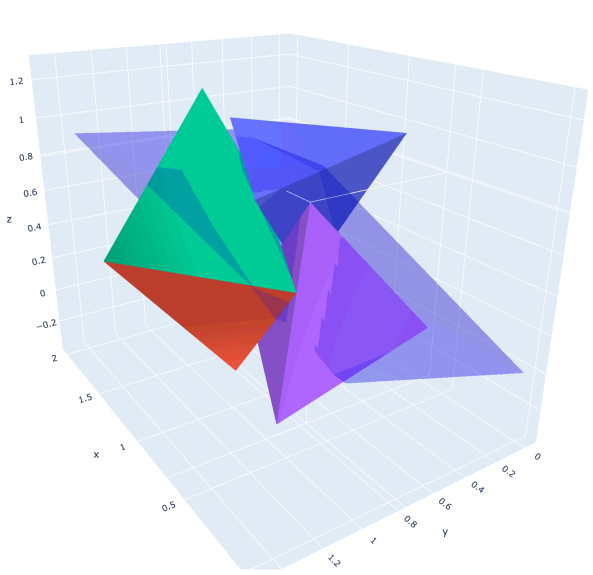
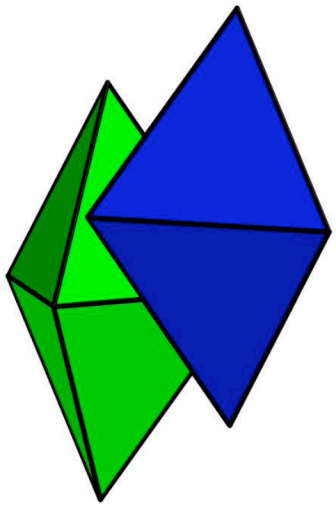


Figure 4.3: Evolution of the densities after successive solving for multiple values of the explosion factor ϵ

When using the results from the literature as initial conditions, the model does always produce a much worse solution. That is due to the comportment of the solver which always increases the size of the fundamental cell even if the constraint on the centers inside the cell are satisfied. You can see the same effects on Figure 4.3 where $\epsilon = 0$ when resolving from the same state (a valid one) the solver can produce a worse solution.



(a) Best packing from our models



(b) Best packing ever from [5]

Figure 4.4: Best packing comparision with state of the art

Chapter 5

Physical experiment

While during this thesis we focused on optimizing tetrahedron arrangements, there's an intriguing detour we have made to quickly experiment with the physicality of the packing problem. This experiment lets us investigate something interesting, even though it is not exactly related to the main topic. Without going too deep, we would like to see what packing density can easily be achieved in a real environment and compare it with the ones we managed to obtain using our optimization scheme. For that, we have used 300 tetrahedral dices that we put into a homemade rectangular box (see Figure 5.1). Once filled, we measured the minimal height at which a closing top in contact with the top tetrahedra and parallel to the bottom face of the box could be. That height combined with the other dimensions of the box gave us the volume of a valid fundamental cell of $726.18\,\mathrm{cm}^3$. Evaluating the volume of each tetrahedra turned out to be a bit more difficult as they have rounded vertices, measuring at 2 cm but if we look at the intersections of the prolongation of the edges we get 2.25 cm. That means that we have a density that goes from 38.9% to 55.5% depending on the edge length we use. This interval is too large to draw any conclusion from it. That is why, inspired by the paper [14], we decided to use water to measure the empty volume between the tetrahedra. We put a plastic bag into our box, filled it up to the height we measured earlier and weighed the volume of water. Then, we put the tetrahedra back in the box and added water up to the top of the tetrahedra. The density is given by $1 - \frac{\text{weight}_{\text{full of tetrahedra}}}{\text{weight}_{\text{empty}}}$. We obtained a value of around 56% which is even higher than the upper bound we found above. That might be due to the fact that despite the shaking the water may not have well penetrated through all the interstices between the tetrahedra underestimating $\text{weight}_{\text{full of tetrahedra}}$. This second measurement whilst probably not perfect indicates that the real value is probably more towards the upper density value. These densities are not far off the ones obtained using optimization models. They are subject to stricter constraints in the sense that the tetrahedra can't protrude through the box's faces but they are larger scale experiments with a larger number of tetrahedra than what we were able to use on our models. That helps mitigate the stricter constraints' influence because the more tetrahedra are used and the larger the box becomes the closer we get to the real space filling problem with infinite bounds.

Figure 5.1: Homemade box for the physical experiment

Chapter 6

Conclusion

In conclusion, this thesis explored the intricate world of tetrahedron packing. We started by taking a look at all the reasons that make this problem relevant. Its significance across numerous real world domains and the human curiosity made more clear why it has been on many scientist's interest list for centuries. We've delved into the most important research results that led to the best known packing to date. That showed that the methods used were often the same and are more than one decade old. That sprinkled our interest for an entirely optimization based approach to solve this problem.

We set ourselves to build a model that would be able to be solved by an off the shelves solver and that would yield state of the art level packings. We gradually built on a originally naive model to get to the desired level of generality. That required a deep understanding of the geometry of the problem and its various limit cases.

Once our model was ready, we used it in conjunction with many different optimization procedures to try and get the best result possible. We managed to get a density of 81.9% for the packing of 4 tetrahedra per fundamental cell. That did not allow us to beat the state of the art but it is close enough to consider that it was worth trying and that it may be interesting to keep optimizing our approach. To evaluate the quality of our packings and to do something a bit more fun we also quickly explored the world of physical experiments.

Whilst our best packing is quite good, it could probably be improved. New optimization procedures, like the freezing of variable or a proper multi start approach, could be used on the same model and with the same solver. It would also be a good idea to use commercial solvers to see if they can get better results. Another big area for improvement is the model itself, it would be ideal to keep the same level of generality in the admissible solutions but find formulation that allow to get rid of constraints (mainly the ones involving copies of the cell).

In closing, this thesis presents a purely optimization based approach to the problem of tetrahedron packing that will hopefully inspire people to build on this to reach new heights in packing density. The best impact this thesis could ever have is to bring back the interest to this problem, allowing the discovery of new ways to tackle this problem that will lead to improvements in densities and to a better understanding of the world around us.

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Appendix A

Best packing coordinates

This is the coordinates of the tetrahedron vertices and the vectors of the fundamental cell for the best packing we obtained using our models.

The tetrahedra:

$$
\begin{aligned}
v_{1,1} &= (1.7408534447, 0.5542742068, 0.9453351426) \\
v_{1,2} &= (0.8364281236, 0.9515823329, 0.7898967581) \\
v_{1,3} &= (0.9305721559, -0.0317669462, 0.9453351587) \\
v_{1,4} &= (1.2551681462, 0.3726175031, 0.0902850664)
\end{aligned}
$$

$$
\begin{aligned}
v_{2,1} &= (1.3833475361, 1.4865692471, 0.4189286389) \\
v_{2,2} &= (0.5730662440, 0.9005280986, 0.4189286302) \\
v_{2,3} &= (1.4774915677, 0.5032199544, 0.5743669541) \\
v_{2,4} &= (1.2305186626, 0.8446934721, -0.3324958915)
\end{aligned}
$$

$$
\begin{aligned}
v_{3,1} &= (0.5730663072, 0.9005282228, 0.4189286191) \\
v_{3,2} &= (1.4774916071, 0.5032200508, 0.5743670102) \\
v_{3,3} &= (1.0587515423, 1.0821847760, 1.2739787633) \\
v_{3,4} &= (1.3833476093, 1.4865693574, 0.4189287626)
\end{aligned}
$$

$$
\begin{aligned}
v_{4,1} &= (0.5216018900, 0.1185020088, 0.0397059625) \\
v_{4,2} &= (1.3318831969, 0.7045431367, 0.0397059402) \\
v_{4,3} &= (0.6744308139, 0.7603777724, 0.7911304924) \\
v_{4,4} &= (0.4274578763, 1.1018513054, -0.1157323386)
\end{aligned}
$$

The fundamental cell:

$$
\begin{aligned}
c_1 &= (0.8431139290, 0, 0) \\
c_2 &= (0.3832635288, 0.7538493728, 0) \\
c_3 &= (0.7922338647, 0.6035803905, 0.9056292724)
\end{aligned}
$$

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