

Approximation of partitions of least perimeter by Γ -convergence : around Kelvin's conjecture

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Abstract

In this paper we propose a numerical process to approximate optimal partitions in any dimension. The key idea of our method is to relax the problem into a functional framework based on the famous result of Γ -convergence obtained by Modica and Mortolla.

Keywords: Kelvin's conjecture, foams, γ -convergence, optimal tiling

1 Introduction

We study in this article the problem of dividing a region $C \subset \mathbb{R}^N$ into pieces of equal volume such as to minimise the surface of the boundary of the partition. Physically this problem can be reformulated in: what is the most efficient soap bubble foam of C (see [14]) ?

If $C = \mathbb{R}^2$, Hales proved in 1999 that any partition of the plane made of regions of equal area has a perimeter at least equal that of the regular hexagonal honeycomb tiling (see [8] or [13]).

The problem when $C = \mathbb{R}^3$ has been first raised by Lord Kelvin in 1894. He conjectured that a tiling made of shapes which are closed from truncated octahedra may be optimal. This conjecture was motivated by the fact that this tiling satisfies Plateau's first order optimality conditions (see for instance the book of Plateau [9] translated by K. Brakke). Ten years ago, the two physicists D. Weaire and P. Phelan found a better tiling than the one of Kelvin (see [15]). This tiling is made of two kinds of cells: one with 14 sides and the other with 12. This last structure is up to now the best candidate for solving Kelvin's problem.

In this paper we propose a numerical process to approximate optimal partitions in any dimension. The key idea of our method is to relax the problem into a functional framework based on the famous result of Γ -convergence obtained by Modica and Mortolla (see [12], [11] or [1] for a different approach).

In the first section we give a rigorous mathematical framework to the question of dividing a bounded set C into peaces of equal volume with the smallest boundary measure. In a second section we extend this framework to the case $C = \mathbb{R}^3$. In both situations, we prove by a direct approach the well-posedness of our problems. In a third part, we describe how the result of Modica and Mortolla on phase transitions leads to a numerical algorithm to approximate optimal partitions. To conclude we illustrate the efficiency of our numerical process on different geometrical situations. In our experiments, we were able to recover

both Kelvin's and Weaire and Phelan's tilings starting with uniform random distribution of densities.

2 Dividing a bounded subset of \mathbb{R}^N

Let $n \in \mathbb{N}$ and C a compact regular subset of \mathbb{R}^N . We are first going to give a rigorous mathematical framework to the question of dividing C into n peaces of equal volume such that the boundary of the partition has the smallest measure. For this purpose, let us consider the following natural partitioning problem:

$$\inf_{(\Omega_i)_{i=1}^n \in \mathcal{O}_n} \mathcal{J}_n(\Omega_1, \dots, \Omega_n) \quad (1) \quad \boxed{\text{P1}}$$

with

$$\mathcal{J}_n(\Omega_1, \dots, \Omega_n) = \sum_{i=1}^n \mathcal{H}^{N-1}(\partial\Omega_i) \quad (2)$$

where \mathcal{H}^{N-1} stands for the $(N-1)$ -dimensional Hausdorff measure and \mathcal{O}_n defined by

$$\mathcal{O}_n = \{(\Omega_i) \text{ measurables} \mid \cup_{i=1}^n \Omega_i = C, \Omega_i \cap \Omega_j = \emptyset \text{ if } i \neq j \text{ and } |\Omega_i| = \frac{|C|}{n} \text{ for } i = 1 \dots n\} \quad (3) \quad \boxed{\text{constr}}$$

where $|\Omega_i|$ is the Lebesgue measure of the set Ω_i . Notice that the two first equalities in (3) have to be understood up to a set of measure zero. We claim that the problem (1) is well posed:

thm1 **Theorem 2.1** *It exists at least one family $(\Omega_i^*)_{i=1}^n \in \mathcal{O}_n$ such that:*

$$\mathcal{J}_n(\Omega_1^*, \dots, \Omega_n^*) = \inf_{(\Omega_i)_{i=1}^n \in \mathcal{O}_n} \mathcal{J}_n(\Omega_1, \dots, \Omega_n)$$

.

Proof We notice first that it is equivalent to show that the problem of minimising

$$\hat{\mathcal{J}}_n(\Omega_1, \dots, \Omega_n) = \sum_{i=1}^n \mathcal{H}^{N-1}(\partial\Omega_i \setminus \partial C) \quad (4)$$

among sets of \mathcal{O}_n has a solution since $\hat{\mathcal{J}}_n - \mathcal{J}_n$ is equal to the constant $\mathcal{H}^{N-1}(\partial C)$. Now, we apply the standard direct method of the calculus of variations: Consider a minimising sequence $((\Omega_i^k)_{i=1}^n)_k$ of partitions. That is

$$\lim_{k \rightarrow +\infty} \hat{\mathcal{J}}_n(\Omega_1^k, \dots, \Omega_n^k) = \inf_{(\Omega_i)_{i=1}^n \in \mathcal{O}_n} \hat{\mathcal{J}}_n(\Omega_1, \dots, \Omega_n).$$

It is clear from the previous limit that for k large enough, every set Ω_i^k has a finite perimeter with respect to the $N-1$ Hausdorff measure. This implies classically that every such set Ω_i^k is a set of Cacciopoli's type. More precisely, the characteristic function $\chi_{\Omega_i^k}$ is in the space

$BV(C)$, the normed space of functions of bounded variations in C (for a precise definition of $BV(C)$ and its main properties, see [6] and [2]). Additionally, we have

$$\|\chi_{\Omega_i^k}\|_{BV(C)} = \mathcal{H}^{N-1}(\partial\Omega_i^k \setminus \partial C).$$

By a standard compactness argument (see for instance [6] page 176), there exists a subsequence of $(\Omega_i^k)_{i=1}^n$ (still denoted using the same index) that converges in $L^1(C)^n$ to a n -tuple $(\Omega_i^*)_{i=1}^n$. By the $L^1(C)^n$ convergence, every limit set Ω_i^* is still of volume $|C|/n$. Let us prove that $(\Omega_i^*)_{i=1}^n$ is optimal for our problem. The convergence in $L^1(C)$ implies the convergence almost everywhere in C of each $\chi_{\Omega_i^k}$. As a consequence the following constraints are still satisfied at the limit:

$$\cup_{i=1}^n \Omega_i^* = C, \quad \Omega_i^* \cap \Omega_j^* = \emptyset \text{ if } i \neq j. \quad (5) \quad \boxed{\text{E1}}$$

Moreover, the norm of $BV(C)$ is lower semi-continuous, that is

$$\forall i = 1 \dots n, \quad \mathcal{H}^{N-1}(\partial\Omega_i^* \setminus \partial C) \leq \liminf_k \mathcal{H}^{N-1}(\partial\Omega_i^k \setminus \partial C). \quad (6) \quad \boxed{\text{E2}}$$

Equations (5) and (6) prove the theorem. \square

From the previous proof, we deduce that problem (1) is equivalent to the functional optimisation problem:

$$\inf_{(u_i)_{i=1}^n \in \mathcal{X}_n} J_n(u_1, \dots, u_n) \quad (7) \quad \boxed{\text{P1f}}$$

where

$$J_n(u_1, \dots, u_n) = \sum_{i=1}^n \int_C |Du_i| \quad (8)$$

is the sum of all the BV norms of each function u_i and

$$\mathcal{X}_n = \{(u_i) \mid \forall i = 1 \dots n, u_i \in BV(C, \{0, 1\}), \int_C u_i = \frac{|C|}{n}, \sum_{i=1}^n u_i(x) = 1 \text{ a.e. in } C\}. \quad (9)$$

We will establish in section 4 a relaxed functional formulation also based on BV spaces which will be the key point of our numerical approach.

3 Dividing a torus: a sub-problem of Kelvin's conjecture

In this section we would like to extend the previous optimisation problem restricted to bounded domains to partitions of all \mathbb{R}^N . We first recall an existence result obtained by F. Morgan in [7] which gives a rigorous mathematical formulation of Kelvin's problem in \mathbb{R}^N :

Theorem 3.1 *Consider the partitions of \mathbb{R}^N into countable measurable sets (Ω_i) of unit volume. For all such partitions, we define:*

$$F((\Omega_i)) = \limsup_{r \rightarrow +\infty} \frac{\mathcal{H}^{N-1}(B(0, r) \cap (\cup_i \partial\Omega_i))}{|B(0, r)|} \quad (10) \quad \boxed{\text{morgancos}}$$

where $|B(0, r)|$ is the volume of the ball of radius r centered at the origin. Then, there exists a partition which minimises F among all admissible partitions.

As noticed by F. Morgan, such a partition is not unique: a compact perturbation around the origin does not change the previous superior limit. We describe below how we are going to parametrise partitions of \mathbb{R}^N . In order to approximate numerically a solution of Kelvin's problem we will focus on a sub-problem involving only a finite number of sets having some property of periodicity. Consider the unit cube $C = [0, 1]^N$ and $(\Omega_i)_{i=1}^n$ a finite partition of C in n measurable sets which satisfy:

$$\forall i = 1 \dots n, \quad \forall x \in \partial C, \quad \chi_{\Omega_i}(x) = \chi_{\Omega_i}(\hat{x}) \quad (11) \quad \boxed{\text{perconstr}}$$

where \hat{x} is roughly speaking x modulus 1. More formally, \hat{x} is by definition the unique element of $[0, 1]^N$ which is in the class of x in $(\mathbb{R}/\mathbb{Z})^N$. To every family $(\Omega_i)_{i=1}^n$ having the property (11) we associate the set:

$$E = \mathbb{R}^N \setminus \left(\bigcup_{l \in \mathbb{Z}^N} \tau_l \left(\bigcup_{i=1}^n \partial \Omega_i \right) \right) \quad (12) \quad \boxed{\text{E3}}$$

where τ_l is the translation of vector l . If we assume that every connected components of E is of volume $\frac{|C|}{n}$, we obtain up to an homothecy an admissible partition for Kelvin's problem. Moreover the cost F introduced by Morgan of this homothetic partition (O_i) can be easily computed and we have:

$$F((O_i)) = \frac{\mathcal{J}_n^{\text{per}}(\Omega_1, \dots, \Omega_n)}{n^{1/3}}$$

where

$$\mathcal{J}_n^{\text{per}}(\Omega_1, \dots, \Omega_n) = \mathcal{H}^{N-1}(\partial E \cap C). \quad (13) \quad \boxed{\text{P1per}}$$

Let us point out some important facts. First, every partition of \mathbb{R}^N can not be described in the previous way. Nevertheless, it is clear that letting n tend to infinity, it is possible to approximate (in the sense of Morgan's cost functional) every partition by the previous construction. Second, it is not true that every family $(\Omega_i)_{i=1}^n$ of sets of volume $\frac{|C|}{n}$ which satisfies (11) produces always by (12) a set which connected components are all of volume $\frac{|C|}{n}$. A family of parallel strips may satisfy (11) and produces a set E with unbounded connected components. It is intuitively clear that this kind of partition would not be optimal for $\mathcal{J}_n^{\text{per}}$, at least for n large. We will not consider this difficulty in the following and we will observe in section 6 that those cases do not appear numerically. Finally, notice that in the definition (13), the pieces of ∂E which are included in ∂C are counted. This detail makes an important difference with the one presented in the previous section where the standard norm of the space BV was enough to compute the perimeter associated to each set $(\Omega_i)_{i=1}^n$. This technical aspect will have a major importance regarding the relaxed formulations that we will introduce in the next section.

As in the previous section, we give a rigorous mathematical formulation in a functional context of the previous construction. Let $\tilde{C} = [-1, 2]^N$, and consider the space

$$\mathcal{X}_n^{per} = \{(u_i) \mid \forall i = 1 \dots n, u_i \in BV^{per}(\hat{C}, \{0, 1\}) \int_C u_i = \frac{|C|}{n}, \sum_{i=1}^n u_i(x) = 1 \text{ a.e. in } C\} \quad (14)$$

where

$$BV^{per}(\hat{C}) = \{u \in BV(\hat{C}) \mid u(x) = u(\hat{x}), \text{ a.e. } x \text{ in } \hat{C}\} \quad (15)$$

and \hat{x} is defined as before. In order to optimise an energy similar to (13) we define

$$J_n^{per}(u_1, \dots, u_n) = \sum_{i=1}^n \int_C |Du_i|. \quad (16) \quad \boxed{\text{P1perf}}$$

Since C is a closed set, notice that the jumps of u_i which are on the boundary of C are counted in the cost (16). Based on the same arguments as the proof of theorem 2.1 we have the existence result:

thm2 **Theorem 3.2** *There exists at least one family $(u_i^*)_{i=1}^n \in \mathcal{X}_n^{per}$ such as:*

$$\mathcal{J}_n^{per}(u_1^*, \dots, u_n^*) = \inf_{(u_i)_{i=1}^n \in \mathcal{X}_n^{per}} \mathcal{J}_n(u_1, \dots, u_n).$$

4 Relaxation of the perimeter and Γ -convergence

The main difficulty in solving numerically problems (7) or (16) is related to the approximation of irregular functions which are characteristic functions. In order to tackle this point we introduce a relaxation of those problems based on the famous Γ -convergence result of Modica and Mortola. The main feature of this relaxation is to make it possible to approximate optimal “true partitions” in n pieces by an n -tuple of regular functions optimal for some relaxed functionals. We first recall Modica and Mortola’s theorem which will be used to establish our relaxed formulations.

MM **Theorem 4.1** *(L. Modica and S. Mortola see [11] and [12]) Let $0 < V < |C|$ and W a continuous positive function which vanishes only at 0 and 1 and set $\sigma = 2 \int_0^1 \sqrt{W(u)} du$. For all $\varepsilon > 0$, consider*

$$F^\varepsilon(u) := \begin{cases} \varepsilon \int_C |\nabla u|^2 + \frac{1}{\varepsilon} \int_C W(u) & \text{if } u \in W^{1,2}(C) \cap X, \\ +\infty & \text{otherwise} \end{cases} \quad (17)$$

and

$$F(u) := \begin{cases} \sigma \mathcal{H}^{N-1}(Su) & \text{if } u \in BV(C, \{0, 1\}) \cap X, \\ +\infty & \text{otherwise} \end{cases} \quad (18)$$

where X is the set of functions $u \in L^1(C)$ which satisfy $\int_C u = V$ and Su is the set of essential singularities of u (see [6] or [2]). Then the functionals F^ε Γ -converge to F in X and every sequence of minimisers (u_ε) is precompact in X (endowed with the L^1 norm).

We establish a simple relaxation of problem (7) which is easily obtained from previous theorem and [3]. Let us point out that Baldo in [3] already proposed a vectorial formulation of Modica and Mortola's result very close from our setting. The main difference between his approach and our formulation is that we only consider scalar potentials w under the additional linear constraint $\sum_{i=1}^n u_i(x) = 1$ almost everywhere. In that way we avoid to deal with polynomials of high degree which could create important difficulties from the numerical point of view.

Theorem 4.2 (*Relaxation of problem (7)*) *Consider C a bounded open set of \mathbb{R}^n and W a continuous positive function which vanishes only at 0 and 1 and set $\sigma = 2 \int_0^1 \sqrt{W(u)} du$. For $n \in \mathbb{N}^*$, let X be the space of functions $u = (u_i) \in L^1(C)^n$ which satisfy $\int_C u_i = \frac{1}{|C|}$, $\forall i = 1 \dots n$ and $\sum_{i=1}^n u_i(x) = 1$ almost everywhere x in C . For all $\varepsilon > 0$, consider*

$$F^\varepsilon(u) := \begin{cases} \varepsilon \sum_{i=1}^n \int_C |\nabla u_i|^2 + \frac{1}{\varepsilon} \sum_{i=1}^n \int_C W(u_i) & \text{if } u \in (W^{1,2}(C))^n \cap X, \\ +\infty & \text{otherwise} \end{cases} \quad (19) \quad \boxed{\text{P1frel}}$$

and

$$F(u) := \begin{cases} \sigma \sum_{i=1}^n \mathcal{H}^{N-1}(Su_i) & \text{if } u \in BV(C, \{0, 1\})^n \cap X, \\ +\infty & \text{otherwise} \end{cases} \quad (20)$$

where Su_i is the set of essential singularities of u_i . Then the functionals F^ε Γ -converge to F in X and every sequence of minimisers u^ε is precompact in X (endowed with the L^1 norm).

Proof We follow the classical proof of Modica and Mortola. First we establish the compactness part of the theorem: suppose that (u^ε) is a sequence of minimisers of the functionals F^ε . For each $i = 1 \dots n$, we apply the compactness result of theorem 4.1 to the sequence u_i^ε . Classically, the precompactness of each components of the sequence u^ε gives the precompactness of the sequence (u^ε) by a diagonal argument.

As in the standard proof we decompose the Γ -convergence results into two steps: let (u^ε) converging in X to u . We have to show first that

$$\liminf F^\varepsilon(u^\varepsilon) \geq F(u).$$

Again we apply theorem 4.1 to each sequence u_i^ε for $i = 1 \dots n$. Since the \liminf of a finite sum is greater than the sum of the \liminf of each sequence, we have

$$\begin{aligned} \liminf F^\varepsilon(u^\varepsilon) &= \liminf \sum_{i=1}^n \left(\varepsilon \int_C |\nabla u_i|^2 + \frac{1}{\varepsilon} \sum_{i=1}^n \int_C W(u_i) \right) \\ &\geq \sum_{i=1}^n \liminf \varepsilon \int_C |\nabla u_i|^2 + \frac{1}{\varepsilon} \sum_{i=1}^n \int_C W(u_i) \\ &\geq F(u). \end{aligned} \quad (21) \quad \boxed{\liminf 1}$$

Finally, let us prove that every value obtained by the Γ -limit can be approximated by a sequence of values obtained by F^ε . Let $u \in BV(C, \{0, 1\})^n \cap X$, we look for a sequence $(u^\varepsilon) \subset (W^{1,2}(C))^n \cap X$ such as

$$\limsup F^\varepsilon(u^\varepsilon) \leq F(u).$$

This none trivial regularisation of a partition can be constructed with the same ideas as Baldo's in [3]. The main point is to restrict the study to polygonal partitions of finite perimeter which satisfy the same volume constraints. More precisely, for all $u \in BV(C, \{0, 1\})^n$ and for all $i = 1 \dots n$ we define $S_i = u_i^{-1}(1/2)$. The family S_i is sometimes called a Caccioppoli partition that is a partition of C into sets (S_i) of finite perimeters. From [3] lemma 3.1, we deduce that there exists a sequence of polygonal partitions (S_i^ε) such as $\forall i = 1 \dots n$,

- $|S_i^\varepsilon| = \frac{|C|}{n}$,
- $\mathcal{H}^{N-1}(\partial S_i^\varepsilon \cap \partial C) = 0$,
- $\mathcal{H}^{N-1}(\partial S_i^\varepsilon \cap \partial C) \rightarrow \mathcal{H}^{N-1}(\partial S_i \cap \partial C)$ when $\varepsilon \rightarrow 0$.

Now, for a given polygonal partitions we can use a standard regularisation process (see [12] or [3]) to construct a sequence (u^ε) which satisfies the volume constraints, the equality $\sum_{i=1}^n u_i^\varepsilon(x) = 1$ almost everywhere x in C and also the inequality

$$\limsup F^\varepsilon(u^\varepsilon) \leq F(u). \quad (22) \quad \boxed{\text{limsup1}}$$

The inequalities (21) and (22) prove the Γ -convergence. \square

We now give a relaxation result for the periodic case:

$\boxed{\text{thper}}$

Theorem 4.3 (*Relaxation of problem (16)*) Consider $C = [0, 1]^n$, $\hat{C} = [-1, 2]^n$ and W a continuous positive function which vanishes only at 0 and 1 and set $\sigma = 2 \int_0^1 \sqrt{W(u)} du$. For $n \in \mathbb{N}^*$, let X be the space of functions $u = (u_i) \in L^1(C)^n$ which satisfy $\int_C u_i = \frac{1}{|C|}$, $\forall i = 1 \dots n$ and $\sum_{i=1}^n u_i(x) = 1$ for almost everywhere x in C . For all $\varepsilon > 0$, consider

$$F^\varepsilon(u) := \begin{cases} \varepsilon \sum_{i=1}^n \int_C |\nabla u_i|^2 + \frac{1}{\varepsilon} \sum_{i=1}^n \int_C W(u_i) & \text{if } u \in (W^{1,2}(C))^n \cap X, \hat{u} \in (W^{1,2}(\hat{C}))^n \\ +\infty & \text{otherwise} \end{cases} \quad (23) \quad \boxed{\text{P1fperfre}}$$

and

$$F(u) := \begin{cases} \sigma \sum_{i=1}^n \int_C |Du_i| & \text{if } u \in BV(C, \{0, 1\})^n \cap X, \hat{u} \in BV(\hat{C}, \{0, 1\})^n \\ +\infty & \text{otherwise} \end{cases} \quad (24)$$

where Su_i is the set of essential singularities of u_i and \hat{u} is the 1-periodic extension of u to \hat{C} . Then the functionals F^ε Γ -converge to F in X and every sequence of minimisers (u^ε) is precompact in X (endowed with the L^1 norm).

Proof Let (u^ε) be a sequence of minimisers for functionals F^ε . As in the previous theorem, we use the compactness part of theorem 4.1 applied to the sequence of 1-periodic extensions (\hat{u}^ε) to obtain the precompactity in X . Now we consider (u^ε) converging in X to u . We want to prove that:

$$\liminf F^\varepsilon(u^\varepsilon) \geq F(u).$$

Notice that this fact is not an immediate consequence of theorem 4.1. The main difference comes from the fact that the jumps of u on ∂C are counted in the cost functional F . The idea is to move a little bit the set C in order to avoid this “bad” situation and then apply the standard Modica-Mortola’s theorem. We first establish that up to a small translation of vector a , the measure $D\hat{u}$ has a support intersected with $a + \partial C$ which is negligible with respect to the \mathcal{H}^{N-1} measure. Since u is a characteristic function of a set of finite perimeter, the structure theorem on the reduced boundary (which is exactly the jump set of u) claims that the measure $D\hat{u}$ has a support which is contained (up to a set of 0 \mathcal{H}^{N-1} measure) in a union of countable C^1 compact hypersurfaces. Let $\delta > 0$, F_a be a face of the cube C of normal vector a and E one of those smooth hypersurfaces. Since F_a and E are both manifolds of dimension $N - 1$ we can apply a classical consequence of Thom’s transversality theorem which asserts that for almost all δ the two manifolds $F_a + \delta n_a$ and E are transverse (see [5] for instance). As a consequence $(F_a + \delta n_a) \cap E$ is an empty set or a smooth manifold of dimension exactly $N - 2$. Then $(F_a + \delta n_a) \cap E$ is negligible with respect to the measure \mathcal{H}^{N-1} for almost all $\delta > 0$. We can apply the previous arguments to each hypersurface which covers the support of $D\hat{u}$ and to all the faces of C . In that way we prove that there exists a vector a such as

$$\begin{cases} (C + a) \subset \hat{C} \\ \int_{\partial(C+a)} |Du| = 0. \end{cases} \quad (25) \quad \boxed{\text{nocharge}}$$

Now setting $C_a = C + a$, we have

$$\begin{aligned} \liminf F^\varepsilon(u^\varepsilon) &= \liminf \varepsilon \sum_{i=1}^n \int_C |\nabla u_i^\varepsilon|^2 + \frac{1}{\varepsilon} \sum_{i=1}^n \int_C W(u_i^\varepsilon) \\ &= \liminf \varepsilon \sum_{i=1}^n \int_{C_a} |\nabla u_i^\varepsilon|^2 + \frac{1}{\varepsilon} \sum_{i=1}^n \int_{C_a} W(u_i^\varepsilon) \\ &\geq \sum_{i=1}^n \int_{C_a} |Du_i| \\ &= \sum_{i=1}^n \int_{\bar{C}_a} |Du_i| \\ &= \sum_{i=1}^n \int_{\bar{C}} |Du_i| \end{aligned}$$

where the second and the last equalities are a consequence of the periodicity of the functions (u_ε) and u . The inequality is obtained using the limsup part of the theorem 4.1 applied to the open set C_a and the third equality comes from (25).

The limsup part of the proof can be established exactly with the same ideas as in the non periodic case. The only difference is that the elements of the sequence must be in $W^{1,2}(\hat{C})^n$, which can be achieved with very small modifications of the energy F_ε associated to the element. \square

5 The minimisation algorithm

The two previous theorems have two major advantages to approximate optimal partitions. First it makes it possible to work with regular functions under linear constraints. Additionally, it gives us the opportunity to replace a strongly not convex problem by a smooth sequence of optimisation problems depending of ε which are close from being convex for $\varepsilon \gg 1$. We base our optimisation strategy on this observation. We start to solve the relaxed problems (19) or (23) with ε large. Since in this case those problems are almost convex, we can expect to find by standard descent method a good approximation u_ε of the solution. Then we increase the value of ε step by step and solve the new optimisation problems starting the optimisation process with the previous numerical solution. Observe that our strategy does not give any warranty to identify in the end of the process a global optima of the original problem since branching in a wrong direction may occur when ε tends to 0. Nevertheless, we observe in our experiments that this approach is surprisingly efficient for our problems.

Based on the above ideas we can now describe our optimisation algorithm. In order to simplify the notations we restrict our description to the dimension $N = 2$ and $C = [0, 1]^2$. It is straightforward to adapt our method to the case $N = 3$. We decompose the domain C into a M^2 grid with spacing $h = 1/(M - 1)$. Consider a renumbering operator $K : (0, M - 1) \times (0, M - 1) \mapsto (0, M^2 - 1)$ such $K(k, l) = lM + k$. Our unknowns are the components of the discrete fields $(U_i^\varepsilon)_{k,l}$ as $(U_i^\varepsilon)_{K(k,l)}$ (which we abbreviate as $(U_i^\varepsilon)_K$ when there is no risk of confusion) depending on whether we want to insist on the spatial relation between the components. We approximate the gradient of functions u_i^ε by standard first order finite difference operators δ_x and δ_y , defined for any discrete vector field U by:

$$[\delta_x U]_{k,l} = \frac{U_{k+1,l} - U_{k,l}}{h}, \quad (26)$$

$$[\delta_y U]_{k,l} = \frac{U_{k,l+1} - U_{k,l}}{h}. \quad (27)$$

If the index (k, l) corresponds to a boundary point, the previous gradient is computed considering the boundary conditions of the problem. In the case of a bounded domain we simply use Dirichlet conditions whereas in the torus case we use the periodicity of the grid. The discretisation of cost functionals (19) and (23) are directly deduced from the expression (26). Let us call F_d^ε that discrete cost functional.

To complete the description of our discretisation we describe now the linear constraints imposed on the discrete values $(U_i^\varepsilon)_{k,l}$. On one hand we have the volume constraints imposed on the functions u_i^ε

$$\sum_{k,l} (U_i^\varepsilon)_{K(k,l)} = \frac{M^2}{n}, \quad \forall i = 1 \dots n, \quad (28) \quad \boxed{\text{contrvol}}$$

and the pointwise non overlapping constraints

$$\sum_i (U_i^\varepsilon)_{K(k,l)} = 1, \quad \forall k, l = 0 \dots M-1. \quad (29) \quad \boxed{\text{controver}}$$

Let us denote by Π the linear projection operator on the constraints (28) and (29). More precisely, regarding the unknown as an array of size $M^2 \times n$, the constraints on that array $(a_{i,j})$ may be written:

$$\begin{cases} \sum_j a_{i,j} = c_i \quad \forall i = 1 \dots n \\ \sum_i a_{i,j} = d_j \quad \forall j = 0 \dots M^2 - 1 \end{cases} \quad (30) \quad \boxed{\text{constrarr}}$$

where $c_i = 1$ for all $i = 1 \dots n$ and $d_j = \frac{M^2}{n}$ for all $j = 1 \dots M^2$. Let us note that the previous constraints must satisfy the compatibility condition

$$\sum_i c_i = \sum_j d_j \quad (31) \quad \boxed{\text{compcond}}$$

which is true in our case since $\sum_i c_i = M^2$ and $\sum_j d_j = n \frac{M^2}{n} = M^2$. One consequence of the previous compatibility condition is that the set of all $n + M^2$ constraints of (30) is not of maximal rank. It is not difficult to see that keeping the $n + (M^2 - 1)$ first constraints gives a free system of constraints.

We describe in the first Algorithm a few step to compute in an efficient way the projected array $(b_{i,j}) := \Pi((a_{i,j}))$ when $n \ll M^2$ for any fixed vectors (c_i) , (d_j) which satisfy (31). Notice that the more time consuming step in the previous algorithm is the resolution of the linear system $C|_{(n-1) \times (n-1)} (\lambda_j)|_{n-1} = (d_j)|_{n-1}$ which is only of size $(n-1)^2$. In all the experiments that we carried out, n was always less than $1e2$ which leads to a fast projection algorithm.

To finish our description, we give the successive steps of our optimisation in the second Algorithm (we refer to [10] for technical details on the conjugated gradient algorithm and the choice of the line search methods).

Finally, if the domain C is not a square or a cube, we simply consider a squared or cubic domain which contains C and impose the additional Dirichlet constraints:

$$(U_i)_K = 0, \quad \forall i = 1 \dots n$$

if K corresponds to a grid point which is outside of C . The previous algorithms are easily adapted to this more general situation.

6 Numerical results

We were able to run a series of large computations on 2D and 3D problems. We first address problem (1) when C is a disk (see figure 2) and a triangle (figure 3). All the 2D computations

Algorithm 1 Projection on the linear constraints

1. $(e_i) := (2 \sum_j a_{i,j} - 2c_i)$
2. $(f_j) := (2 \sum_i a_{i,j} - 2d_j)$
3. Define the matrix $C = (c_{k,l})$ of size $n \times n$ by

$$\begin{cases} c_{k,l} = -\frac{M^2}{n} \text{ if } k \neq l \\ c_{k,k} = M^2 - \frac{M^2}{n} \end{cases}$$
4. $(d_j) := (f_j) - \frac{2}{n} \sum_i e_i$
5. Compute the unique vector (λ_j) of size $n \times 1$ with $\lambda_n = 0$ such as $C|_{(n-1) \times (n-1)} (\lambda_j)|_{n-1} = (d_j)|_{n-1}$ where the notation $C|_{(n-1) \times (n-1)}$ stands for the matrix of size $(n-1) \times (n-1)$ obtained from C by extracting the $n-1$ first rows and $n-1$ first columns. The definitions of $(\lambda_j)|_{n-1}$ and $(d_j)|_{n-1}$ are similar.
6. $S := \sum_j \lambda_j$
7. $(\eta_i) := \frac{(e_i) - S}{n}$
8. $A_{\text{orth}} := (\eta_i) * 1_{1 \times n} + 1_{M^2 \times 1} * \text{Transpose}((\lambda_j))$ where $1_{k \times l}$ is the matrix of size $k \times l$ which coefficients are all equal to 1 and $*$ is the standard matrix multiplication.
9. $B := A - A_{\text{orth}}$

Algorithm 2 Numerical optimisation by Γ -convergence**Require:** $\varepsilon_{\text{initial}}, \varepsilon_{\text{final}}, (U_i^{\varepsilon_{\text{initial}}}), \omega, \delta > 1$ (tolerance)

- 1: $\varepsilon := \varepsilon_{\text{initial}}, (U_i^\varepsilon) := (U_i^{\varepsilon_{\text{initial}}})$
- 2: **repeat**
- 3: Compute (V_i^ε) the solution of $\min F_d^\varepsilon((V_i))$ among arrays (V_i) which satisfy constraints (28) and (29) (up to a tolerance δ). This step is carried out by a standard projected conjugated gradient algorithm (based on the previous projection algorithm) starting from (U_i^ε) .
- 4: $(U_i^{\varepsilon/\omega}) := (V_i^\varepsilon), \varepsilon := \varepsilon/\omega$
- 5: **until** $\varepsilon > \varepsilon_{\text{final}}$

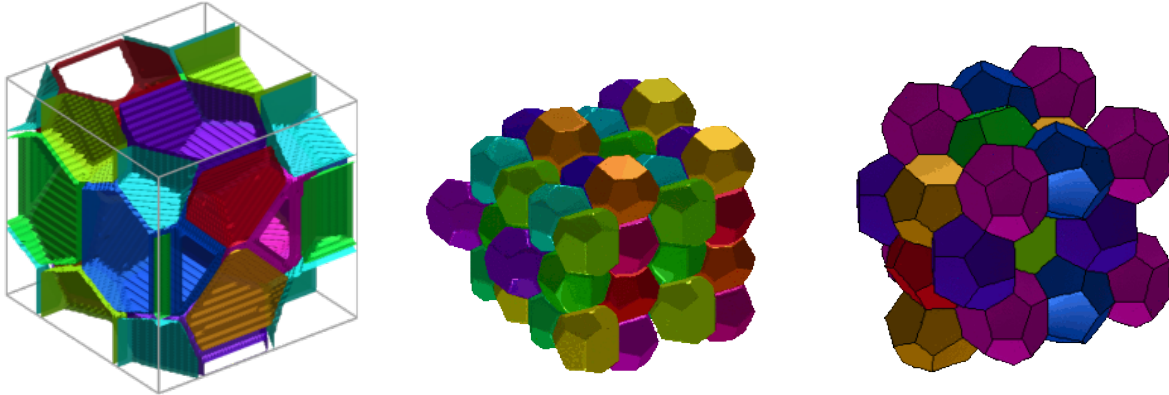


Figure 1: Switching from a density representation to a boundary description

fig:f0

have been done on a grid of dimension (253×253) . We set $\varepsilon_{\text{initial}} = 1$, $\varepsilon_{\text{final}} = 1e - 3$, the tolerance parameter $\delta = 1e - 6$ and $\omega = 1.1$. We always start our optimisation process with an array $(U_i^{\varepsilon_{\text{initial}}})$ made of uniform random values in $[0, 1]$. As expected, our numerical solutions are made of local patches satisfying the 120 degrees angular conditions. Moreover some symmetries of the set C are preserved for small values of n .

We performed 3D computation for problem (13) with n from 8 to 21 (see figure 4) on grids of dimension $(128 \times 128 \times 128)$. As a post treatment, we used the very efficient local optimisation software “Evolver” (see [4]) developed by Ken Brake to obtain a finer description of optimal tilings. Let us point out that most of the geometrical structure was already contained in the parametrisation of the tiling given by the density functions (U_i) at the end of our algorithm. In figure 1 we represent in the first picture the level sets $\{U_i = \frac{1}{2}\}$ for $i = 1 \dots n$. In the second picture we draw the periodic reconstruction of the densities without any surface optimisation. Notice that a small gap remains between the level sets. In the last picture, we display the result of the optimisation performed by “Evolver”.

With $n = 16$ we observe that we obtain Kelvin’s tiling only made of truncated octahedra. With $n = 8$, starting again from a complete random array, we recover the famous tiling obtained by D. Weaire and P. Phelan which is made of exactly two kinds of cells. We give below the values corresponding to the cost functional ...for $n = 8$ to 21. Unfortunately we were not able to find a better tiling than the one discovered by D. Weaire and P. Phelan.

Finally, we tried to beat Weaire and Phelan’s tiling by considering optimal cutting of sets C which already tile the space. Namely, we approximated optimal cuttings of a truncated octahedron, a triangular prism, a rhombic dodecahedron and one hexagonal prism (see figure 5). We then computed the cost (13) associated to the tilling deduced from the previous optimal cutting. The array below sum up the optimal values in the periodic and none periodic cases of the functional.

We sum up our results in table 6. The first column gives different values of Morgan’s cost functional obtained by the periodic tilings and the second one gives the values obtained by the optimal cutting of sets which already tile the space. We observe that none of such tiling gave a better cost than the ones obtained by periodic boundary conditions.

able-newton

n	Morgan's cost, see (10)	n	Bounded convex polyhedra C	Morgan's cost
8	2.644175	6	Truncated octahedron	2.852505
16	2.653171	10	Truncated octahedron	2.924930
20	2.655404	6	Rhombic dodecahedron	2.934629
21	2.657727	8	Truncated octahedron	2.942078
22	2.666318	8	Rhombic dodecahedron	2.945360
12	2.671376	10	Rhombic dodecahedron	2.956432
17	2.675445	4	Rhombic dodecahedron	2.984274
19	2.680236	2	Rhombic dodecahedron	2.987346
18	2.681586	2	Truncated octahedron	3.004914
13	2.683315	3	Truncated octahedron	3.009927
15	2.689541	4	Truncated octahedron	3.014228
10	2.692954	4	Hexagonal prism	3.021674
9	2.693281	6	Hexagonal prism	3.051920
14	2.694757	8	Triangular prism	3.061425
11	2.695891	2	Hexagonal prism	3.078461

Table 1: Optimal values for the periodic case (2 first columns) and different polyhedral cuttings (three last columns).

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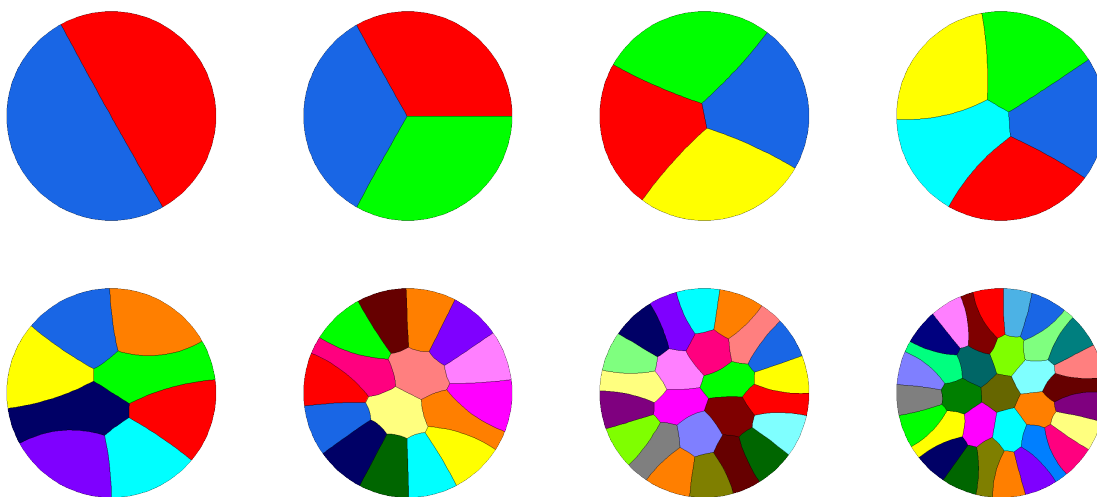


Figure 2: Tiling of the disk with 2, 3, 4, 5, 8, 16, 24, 32 cells

fig:f1

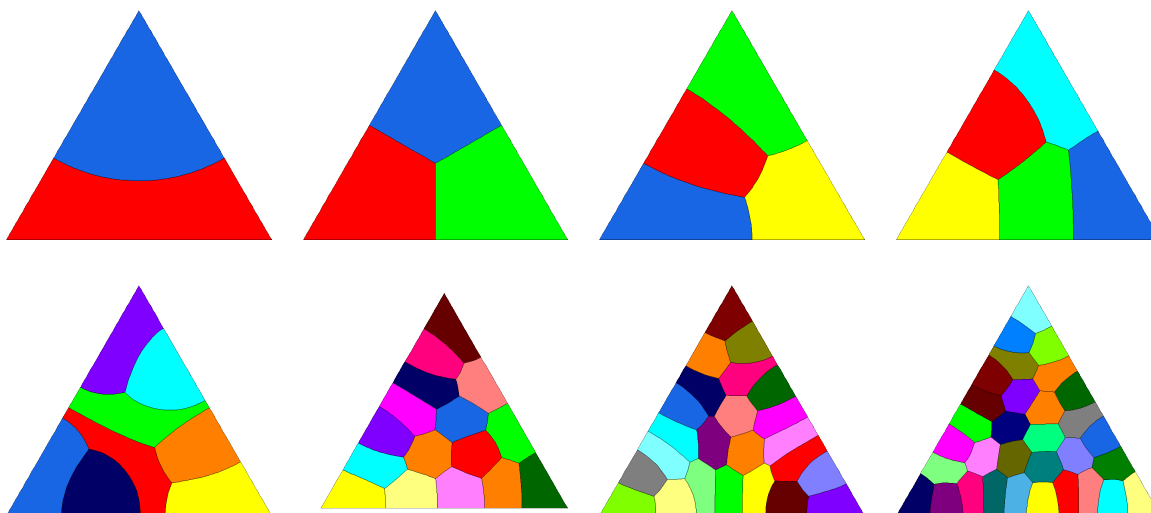


Figure 3: Tiling of the triangle with 2, 3, 4, 5, 8, 16, 24, 32 cells

fig:f2

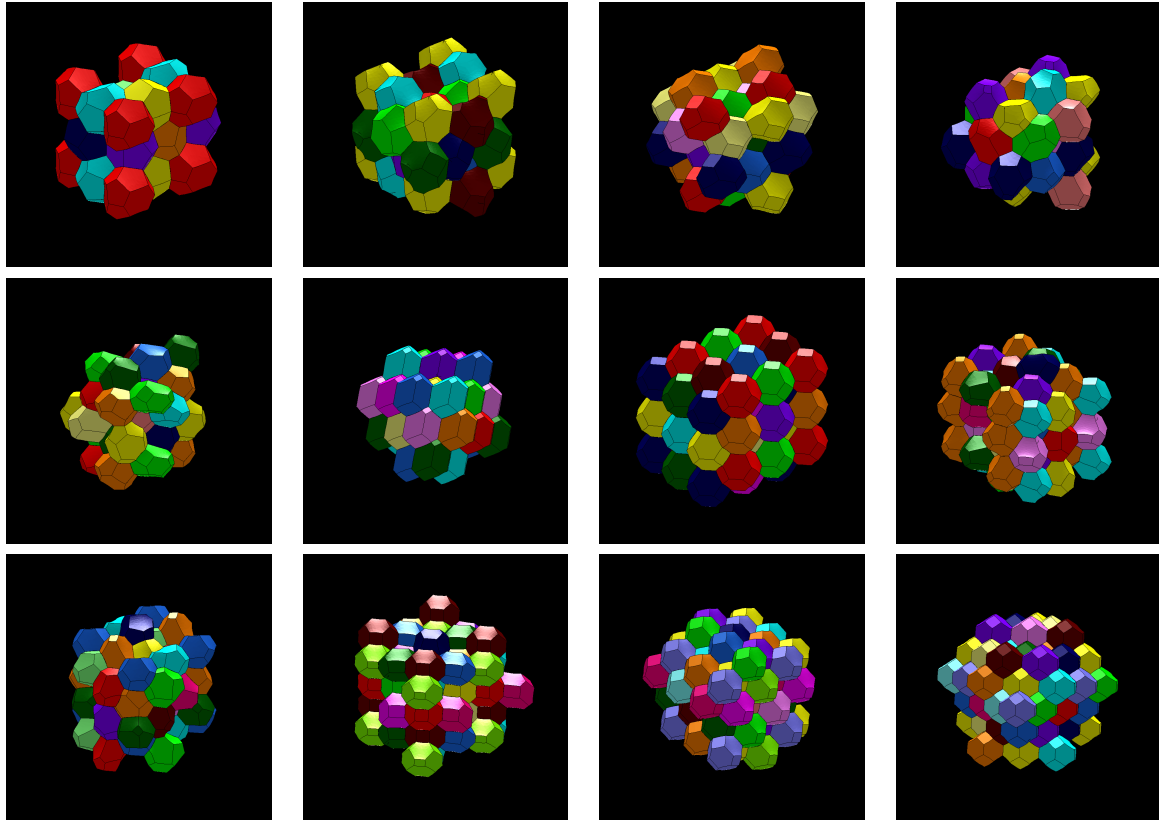


Figure 4: Periodic tilings of the space by 8, 10, 12, 13, 14, 15, 16, 17, 18, 19 20, 21 cells

fig:f3

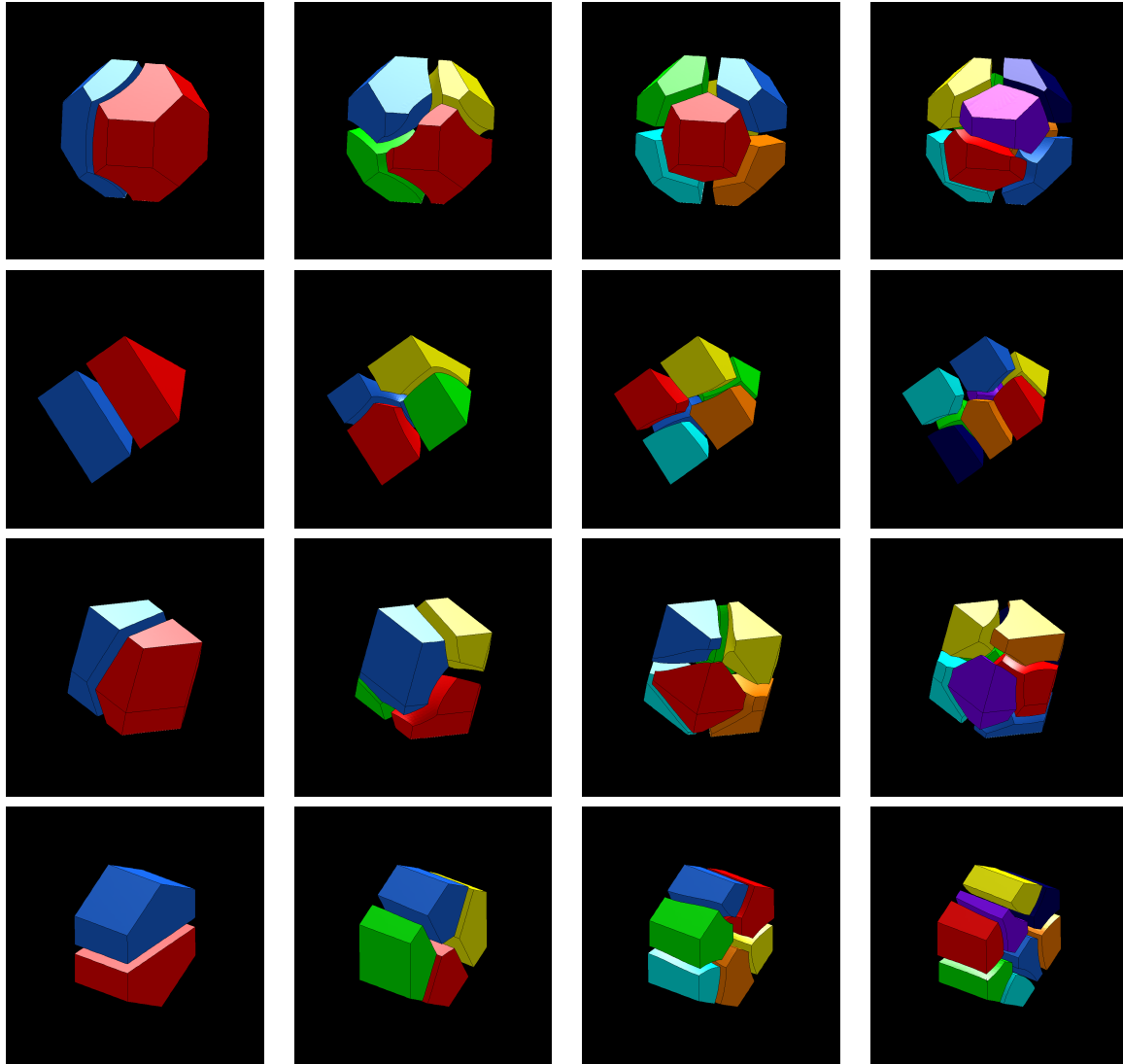


Figure 5: None periodic tilings

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