

Approximation of Partitions of Least Perimeter by Γ -Convergence: Around Kelvin's Conjecture

Édouard Oudet

CONTENTS

- 1. Introduction
- 2. Dividing a Bounded Subset of \mathbb{R}^N
- 3. Dividing a Torus: A Subproblem of Kelvin's Conjecture
- 4. Relaxation of the Perimeter and Γ -Convergence
- 5. The Minimization Algorithm
- 6. Numerical Results
- Acknowledgments
- References

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

1. INTRODUCTION

The aim of our work is to investigate the problem of dividing a region $C \subset \mathbb{R}^N$ into pieces of equal volume so as to minimize the surface of the boundary of the partition. Physically, this problem can be reformulated thus: what is the most efficient soap-bubble foam of C (see [Thomson 87])?

If $C = \mathbb{R}^2$, Hales proved in 1999 that any partition of the plane consisting of regions of equal area has a perimeter at least equal to that of the regular hexagonal honeycomb tiling (see [Hales 01] or [Morgan 09]).

The problem when $C = \mathbb{R}^3$ was first raised by Lord Kelvin in 1894. He conjectured that a tiling mode truncated octahedra is optimal. This conjecture was motivated by the fact that such a tiling satisfies Plateau's first-order optimality conditions (see, for instance, [Plateau 73]). Ten years ago, the two physicists D. Weaire and P. Phelan found a better tiling than Kelvin's (see [Weaire and Phelan 94]). This tiling includes two kinds of cells: 14-sided cells and 12-sided cells. 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 [Modica and Mortola 77, Modica 87], or see [Alberti 00] for a different approach).

In the next section, we provide a rigorous mathematical framework for the problem of dividing a bounded set C into pieces of equal volume with the smallest boundary

measure. In the next 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. Then 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 a uniform random distribution of densities.

2. DIVIDING A BOUNDED SUBSET OF \mathbb{R}^N

Let $n \in \mathbb{N}$ and let C be a compact regular subset of \mathbb{R}^N . First, we provide a rigorous mathematical framework for the question of dividing C into n pieces of equal volume such that the boundary of the partition has the smallest measure. Let us consider the following natural partitioning problem:

$$\inf_{(\Omega_i)_{i=1}^n \in \mathcal{O}_n} \mathcal{J}_n(\Omega_1, \dots, \Omega_n) \tag{2-1}$$

with

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

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

$$\mathcal{O}_n = \{(\Omega_i) \text{ measurable} \mid \cup_{i=1}^n \Omega_i = C, \Omega_i \cap \Omega_j = \emptyset \text{ if } i \neq j \text{ and } |\Omega_i| = \frac{|C|}{n} \text{ for } i = 1, \dots, n\}, \tag{2-3}$$

where $|\Omega_i|$ is the Lebesgue measure of the set Ω_i . Notice that the first two equalities in (2-3) have to be understood up to a set of measure zero. We claim that the problem (2-1) is well posed:

Theorem 2.1. *There 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 observe first that it suffices to show that the problem of minimizing

$$\hat{\mathcal{J}}_n(\Omega_1, \dots, \Omega_n) = \sum_{i=1}^n \mathcal{H}^{N-1}(\partial\Omega_i \setminus \partial C) \tag{2-4}$$

among sets of \mathcal{O}_n has a solution, since $\hat{\mathcal{J}}_n - \mathcal{J}_n$ is equal to the constant $\mathcal{H}^{N-1}(\partial C)$. We apply the standard direct

method of the calculus of variations: Consider a minimizing 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 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 [Evans and Gariepy 92] and [Ambrosio et al. 00]). Additionally, we have

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

According to a standard compactness argument (see, for instance, [Evans and Gariepy 92, p. 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 an 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:

$$\cup_{i=1}^n \Omega_i^* = C, \quad \Omega_i^* \cap \Omega_j^* = \emptyset \text{ if } i \neq j. \tag{2-5}$$

Moreover, the norm of $BV(C)$ is lower semicontinuous. That is, for all $i = 1, \dots, n$,

$$\mathcal{H}^{N-1}(\partial\Omega_i^* \setminus \partial C) \leq \liminf_k \mathcal{H}^{N-1}(\partial\Omega_i^k \setminus \partial C). \tag{2-6}$$

Equations (2-5) and (2-6) prove the theorem. □

From the previous proof, we deduce that problem (2-1) is equivalent to the functional optimization problem

$$\inf_{(u_i)_{i=1}^n \in \mathcal{X}_n} J_n(u_1, \dots, u_n), \tag{2-7}$$

where

$$J_n(u_1, \dots, u_n) = \sum_{i=1}^n \int_C |Du_i| \tag{2-8}$$

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

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

In Section 4 we establish a relaxed functional formulation also based on BV spaces that will be the key point of our numerical approach.

3. DIVIDING A TORUS: A SUBPROBLEM OF KELVIN'S CONJECTURE

In this section, we extend the previous optimization problem restricted to bounded domains to partitions of all \mathbb{R}^N . We first recall an existence result obtained in [Morgan 08] that 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*

$$F((\Omega_i)) = \limsup_{r \rightarrow +\infty} \frac{\mathcal{H}^{N-1}(B(0, r) \cap (\cup_i \partial\Omega_i))}{|B(0, r)|}, \quad (3-1)$$

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

As observed by Morgan, such a partition is not unique: a compact perturbation around the origin does not change the previous limit superior. We describe below how to parameterize partitions of \mathbb{R}^N . In order to approximate numerically a solution of Kelvin's problem, we will focus on a subproblem 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 into n measurable sets that satisfy

$$\forall i = 1, \dots, n, \forall x \in \partial C, \chi_{\Omega_i}(x) = \chi_{\Omega_i}(\hat{x}) \quad (3-2)$$

where \hat{x} is, roughly speaking, x modulo 1. More formally, \hat{x} is by definition the unique element of $[0, 1]^N$ that is in the class of x in $(\mathbb{R}/\mathbb{Z})^N$. To every family $(\Omega_i)_{i=1}^n$ having the property (3-2) we associate the set

$$E = \mathbb{R}^N \setminus \left(\bigcup_{l \in \mathbb{Z}^N} \tau_l \left(\bigcup_{i=1}^n \partial\Omega_i \right) \right), \quad (3-3)$$

where τ_l is the translation of the vector l . If we assume that every connected component of E is of volume $|C|/n$, we obtain up to an homothety 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

$$\mathcal{J}_n^{\text{per}}(\Omega_1, \dots, \Omega_n) = \mathcal{H}^{N-1}(\partial E \cap C). \quad (3-4)$$

Let us point out some crucial features. First, not every partition of \mathbb{R}^N can be described in the previous way. Nevertheless, it is clear that if we let 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 $|C|/n$ that satisfies (3-2) always produces by (3-3) a set all of whose connected components are of volume $|C|/n$. A family of parallel strips may satisfy (3-2) and produce 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.

Noteworthy in the definition (3-4) is that the pieces of ∂E that are included in ∂C are counted. This detail makes an important distinction from that presented in the previous section, where the standard norm of the space BV was sufficient to compute the perimeter associated with each set $(\Omega_i)_{i=1}^n$. This technical aspect will have major importance regarding the relaxed formulations that will be introduced in the next section.

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

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

where

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

and \hat{x} is defined as before. In order to optimize an energy similar to (3-4), we define

$$J_n^{\text{per}}(u_1, \dots, u_n) = \sum_{i=1}^n \int_C |Du_i|. \quad (3-5)$$

Since C is a closed set, observe that the jumps of u_i that are on the boundary of C are counted in the cost (3-5). Based on the same arguments as in the proof of Theorem 2.1, we have the following existence result.

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

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

4. RELAXATION OF THE PERIMETER AND Γ -CONVERGENCE

The main difficulty in solving numerically problems (2–7) and (3–5) is related to the approximation of irregular functions that 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 report here Modica and Mortola’s theorem, which will be used to establish our relaxed formulations.

Theorem 4.1. [Modica 87, Modica and Mortola 77] *Let $0 < V < |C|$, let W be a continuous positive function that vanishes only at 0 and 1, and set $\sigma = 2 \int_0^1 \sqrt{W(u)} du$. For all $\varepsilon > 0$, consider*

$$F^\varepsilon(u) := \begin{cases} \varepsilon \int_C |\nabla u|^2 + \frac{1}{\varepsilon} \int_C W(u) & \text{if } u \in W^{1,2}(C) \cap X, \\ +\infty & \text{otherwise,} \end{cases} \quad (4-1)$$

and

$$F(u) := \begin{cases} \sigma \mathcal{H}^{N-1}(Su) & \text{if } u \in \text{BV}(C, \{0, 1\}) \cap X, \\ +\infty & \text{otherwise,} \end{cases} \quad (4-2)$$

where X is the set of functions $u \in L^1(C)$ that satisfy $\int_C u = V$, and Su is the set of essential singularities of u (see [Evans and Gariepy 92] or [Ambrosio et al. 00]). Then the functionals F^ε Γ -converge to F in X , and every sequence of minimizers (u_ε) is precompact in X (endowed with the L^1 norm).

We establish below a simple relaxation of problem (2–7) that is easily obtained from the previous theorem and [Baldo 90]. Let us point out that in [Baldo 90] there was already proposed a vectorial formulation of Modica and Mortola’s result very close to our setting. The main difference between his approach and our formulation is that we consider only scalar potentials w under the additional linear constraint $\sum_{i=1}^n u_i(x) = 1$ almost everywhere. So we avoid dealing with polynomials of high degree, which could create important difficulties from the numerical point of view.

Theorem 4.2. (Relaxation of problem (2–7)) *Consider a bounded open set C of \mathbb{R}^n and W a continuous positive function that 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 $u = (u_i) \in L^1(C)^n$ that satisfy $\int_C u_i = \frac{|C|}{n}$, $\forall i = 1, \dots, n$, and $\sum_{i=1}^n u_i(x) = 1$ for almost all x in C . For all $\varepsilon > 0$, consider*

$$F^\varepsilon(u) := \begin{cases} \varepsilon \sum_{i=1}^n \int_C |\nabla u_i|^2 + \frac{1}{\varepsilon} \sum_{i=1}^n \int_C W(u_i) & \text{if } u \in (W^{1,2}(C))^n \cap X, \\ +\infty & \text{otherwise,} \end{cases} \quad (4-3)$$

and

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

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 minimizers u^ε is precompact in X (endowed with the L^1 norm).

Proof: Following the classical proof of Modica and Mortola, we first establish the compactness part of the theorem: Let us hypothesize that (u^ε) is a sequence of minimizers 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 component of the sequence u^ε implies 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) converge in X to u . First, it has to be shown 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

$$\begin{aligned} \liminf F^\varepsilon(u^\varepsilon) &= \liminf \sum_{i=1}^n \left(\varepsilon \int_C |\nabla u_i|^2 + \frac{1}{\varepsilon} \sum_{i=1}^n \int_C W(u_i) \right) \quad (4-4) \\ &\geq \sum_{i=1}^n \liminf \varepsilon \int_C |\nabla u_i|^2 + \frac{1}{\varepsilon} \sum_{i=1}^n \int_C W(u_i) \geq F(u). \end{aligned} \quad (4-5)$$

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 $u \in \text{BV}(C, \{0, 1\})^n \cap X$. We look for a

sequence $(u^\varepsilon) \subset (W^{1,2}(C))^n \cap X$ such that

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

This nontrivial regularization of a partition can be constructed with the same ideas as those in [Baldo 90]. The main point is to restrict the study to polygonal partitions of finite perimeter that satisfy the same volume constraints. More precisely, for all $u \in \text{BV}(C, \{0, 1\})^n$ 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, which is a partition of C into sets (S_i) of finite perimeters. From [Baldo 90, Lemma 3.1], we deduce that there exists a sequence of polygonal partitions (S_i^ε) such that $\forall i = 1, \dots, n$, the following hold:

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

Now, for a given polygonal partition we can use a standard regularization process (see [Modica and Mortola 77] or [Baldo 90]) to construct a sequence (u^ε) that satisfies the volume constraints, the equality $\sum_{i=1}^n u_i^\varepsilon(x) = 1$ for almost all x in C , and also the inequality

$$\limsup F^\varepsilon(u^\varepsilon) \leq F(u). \tag{4-6}$$

The inequalities (4-5) and (4-6) prove the Γ -convergence. □

Now let us give a relaxation result for the periodic case:

Theorem 4.3. (Relaxation of problem (3-5).) *Consider $C = [0, 1]^n$, $\hat{C} = [-1, 2]^n$, and W a continuous positive function that 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 $u = (u_i) \in L^1(C)^n$ that satisfy $\int_C u_i = \frac{|C|}{n}$, $\forall i = 1, \dots, n$, and $\sum_{i=1}^n u_i(x) = 1$ for almost all x in C . For all $\varepsilon > 0$, consider*

$$F^\varepsilon(u) := \begin{cases} \varepsilon \sum_{i=1}^n \int_C |\nabla u_i|^2 + \frac{1}{\varepsilon} \sum_{i=1}^n \int_C W(u_i) & \text{if } u \in (W^{1,2}(C))^n \cap X, \hat{u} \in (W^{1,2}(\hat{C}))^n, \\ +\infty & \text{otherwise,} \end{cases} \tag{4-7}$$

and

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

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 minimizers (u^ε) is precompact in X (endowed with the L^1 norm).

Proof: Let (u^ε) be a sequence of minimizers 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 precompactness 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 originates from the fact that the jumps of u on ∂C are counted in the cost functional F .

The idea is to move slightly the set C in order to avoid this “bad” situation and then apply the standard Modica–Mortola theorem. We first establish that up to a small translation of vector a , the measure $D\hat{u}$ has a support intersecting with $a + \partial C$ that 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 that is contained (up to a set of \mathcal{H}^{N-1} measure zero) in a union of countable C^1 compact hypersurfaces.

Let $\delta > 0$, F_a a face of the cube C with normal vector a , and E one of the 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 that asserts that for almost all δ , the two manifolds $F_a + \delta n_a$ and E are transverse (see [Demazure 89], for instance). As a consequence, $(F_a + \delta n_a) \cap E$ is the 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 $\delta > 0$.

Previous arguments can be applied to each hypersurface that covers the support of $D\hat{u}$ and to all the faces of C . So we have proved that there exists a vector a such that

$$(C + a) \subset \hat{C}, \quad \int_{\partial(C+a)} |Du| = 0. \tag{4-8}$$

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

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

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 lim sup part of Theorem 4.1 applied to the open set C_a , and the third equality comes from (4-8).

The lim sup part of the proof can be established with exactly the same ideas as in the aperiodic 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 with the element. \square

5. THE MINIMIZATION ALGORITHM

The two previous theorems exhibit two major advantages to approximate optimal partitions. First, they make it possible to work with regular functions under linear constraints. Additionally, they give us the opportunity to replace a strongly nonconvex problem by a smooth sequence of optimization problems depending on ε that are close to being convex for $\varepsilon \gg 1$. Our optimization strategy is based on the latter observation. First solve the relaxed problems (4-3) and (4-7) with ε large. Since in this case those problems are almost convex, we can expect to find by a standard descent method a good approximation u_ε of the solution.

Then the value of ε is increased step by step and the new optimization problem is solved by starting the optimization process with the previous numerical solution. Note that our strategy does not give any guarantee that at the end of the process we can identify a global optimum of the original problem, since branching in a wrong direction may occur as ε tends to 0. Nevertheless, we observe in our experiments that this approach is surprisingly efficient for our problems.

Relying on the above strategy, we can now describe our optimization algorithm. In order to simplify the notation, 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

an $M \times M$ 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 that $K(k, l) = lM + k$. Our unknowns are the components of the discrete fields $(U_i^\varepsilon)_{k,l}$ or $(U_i^\varepsilon)_{K(k,l)}$ (which we abbreviate as $(U_i^\varepsilon)_K$ when there is no risk of confusion) depending on whether we 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

$$[\delta_x U]_{k,l} = \frac{U_{k+1,l} - U_{k,l}}{h}, \quad [\delta_y U]_{k,l} = \frac{U_{k,l+1} - U_{k,l}}{h}. \quad (5-1)$$

If the index (k, l) corresponds to a boundary point, the previous gradient is computed by 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 discretization of the cost functionals (4-3) and (4-7) are directly deduced from the expression (5-1). Let us call that discrete cost functional F_d^ε .

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

$$\sum_{k,l} (U_i^\varepsilon)_{K(k,l)} = \frac{M^2}{n}, \quad \forall i = 1, \dots, n, \quad (5-2)$$

and the pointwise nonoverlapping constraints

$$\sum_i (U_i^\varepsilon)_{K(k,l)} = 1, \quad \forall k, l = 0, \dots, M - 1. \quad (5-3)$$

Let us denote by Π the linear projection operator on the constraints (5-2) and (5-3). 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

$$\begin{aligned} \sum_j a_{i,j} &= c_i \quad \forall i = 1, \dots, n, \\ \sum_i a_{i,j} &= d_j \quad \forall j = 0, \dots, M^2 - 1, \end{aligned} \quad (5-4)$$

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

$$\sum_i c_i = \sum_j d_j, \quad (5-5)$$

which is true in our case, since

$$\sum_i c_i = M^2 \quad \text{and} \quad \sum_j d_j = n \frac{M^2}{n} = M^2.$$

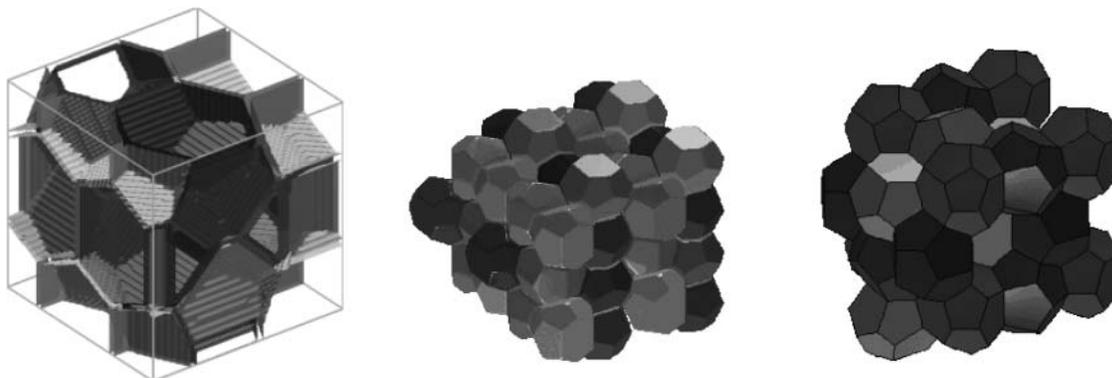


FIGURE 1. Switching from a density representation to a boundary description.

One consequence of the previous compatibility condition is that the set of all $n + M^2$ constraints of (5-4) is not of maximal rank. It is not difficult to see that keeping the first $n + (M^2 - 1)$ constraints gives a free system of constraints.

Notice that it is straightforward to compute the projected array $(b_{i,j}) := \Pi((a_{i,j}))$ in an efficient way when $n \ll M^2$ for any fixed vectors (c_i) , (d_j) that satisfy (5-5). In all the experiments that we carried out, n was always less than 100, which leads to a fast projection step.

Finally, we describe the successive steps of our optimization in Algorithm 5 (we refer to [Kelley 99] for technical details on the conjugated gradient algorithm and the choice of the line search methods).

Algorithm 1 Numerical optimization by Γ -convergence.

Require: $\varepsilon_{\text{initial}}$, $\varepsilon_{\text{final}}$, $(U_i^{\varepsilon_{\text{initial}}})$, ω , $\delta > 1$ (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) that satisfy constraints (5-2) and (5-3) (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** $\varepsilon > \varepsilon_{\text{final}}$

Finally, if the domain C is not a square or a cube, we simply consider a square or cubic domain that 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 that 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 (2-1) when C is a disk (see Figure 2) and a triangle (Figure 3). All the 2D computations were done on a grid of dimension (253×253) . We set $\varepsilon_{\text{initial}} = 1$, $\varepsilon_{\text{final}} = 10^{-3}$, the tolerance parameter $\delta = 10^{-6}$ and $\omega = 1.1$. We always start our optimization process with an array $(U_i^{\varepsilon_{\text{initial}}})$ consisting of uniform random values in $[0, 1]$. As expected, our numerical solutions consist of local patches satisfying the 120-degree angular conditions. Moreover, some symmetries of the set C are preserved for small values of n .

We performed 3D computations for problem (3-4) with n from 8 to 21 (see Figure 4) on grids of dimension $(128 \times 128 \times 128)$. As a posttreatment, we used the very efficient local optimization software Evolver (see [Brakke 92]) developed by Ken Brakke to obtain a finer description of optimal tilings. Let us point out that most of the geometric structure was already contained in the parameterization 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 optimization. Notice that a small gap remains between the level sets. In the last picture, we display the result of the optimization performed by Evolver.

With $n = 16$ we observe that we obtain Kelvin's tiling, only made of truncated octahedra. With $n = 8$, starting

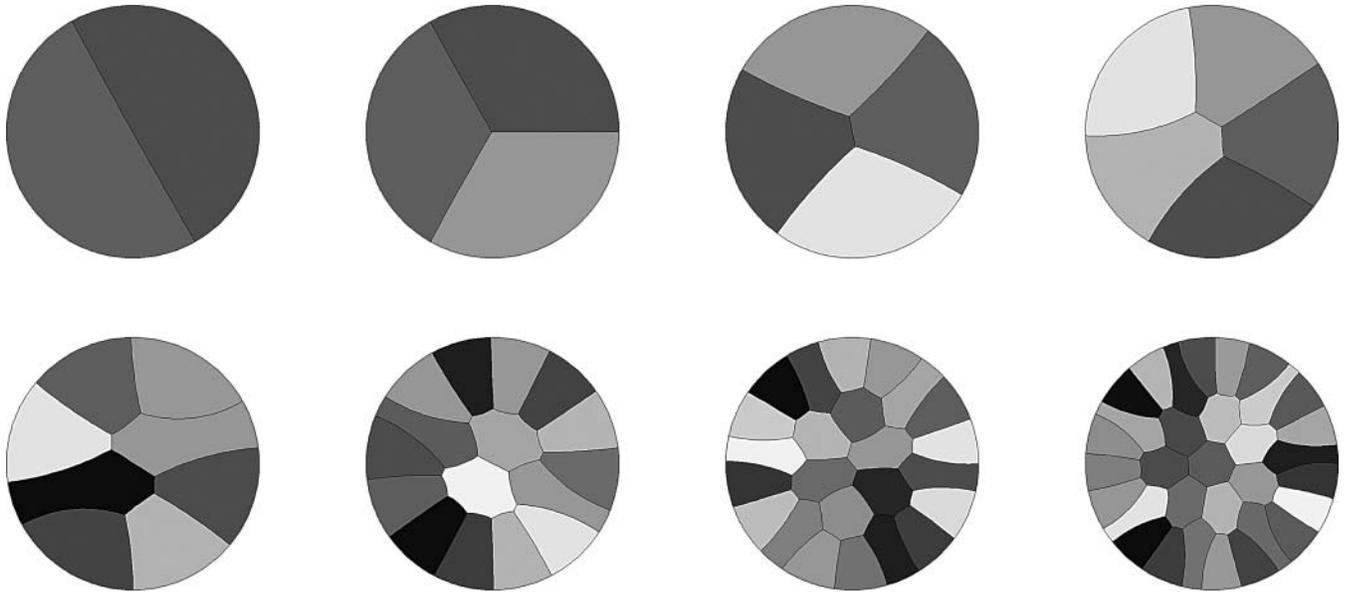


FIGURE 2. Tiling of the disk with 2, 3, 4, 5, 8, 16, 24, 32 cells.

again from a complete random array, we recover the famous tiling obtained by D. Weaire and P. Phelan consisting of exactly two kinds of cells. We give below the values corresponding to the cost functional for $n = 8$ to

21. No better tiling than the one reported by D. Weaire and P. Phelan was suggested.

Finally, we tried to outperform Weaire and Phelan's tiling by considering an optimal cutting of sets C that

n	Morgan's Cost; see (3-1)	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 (first two columns) and different polyhedral cuttings (last three columns).

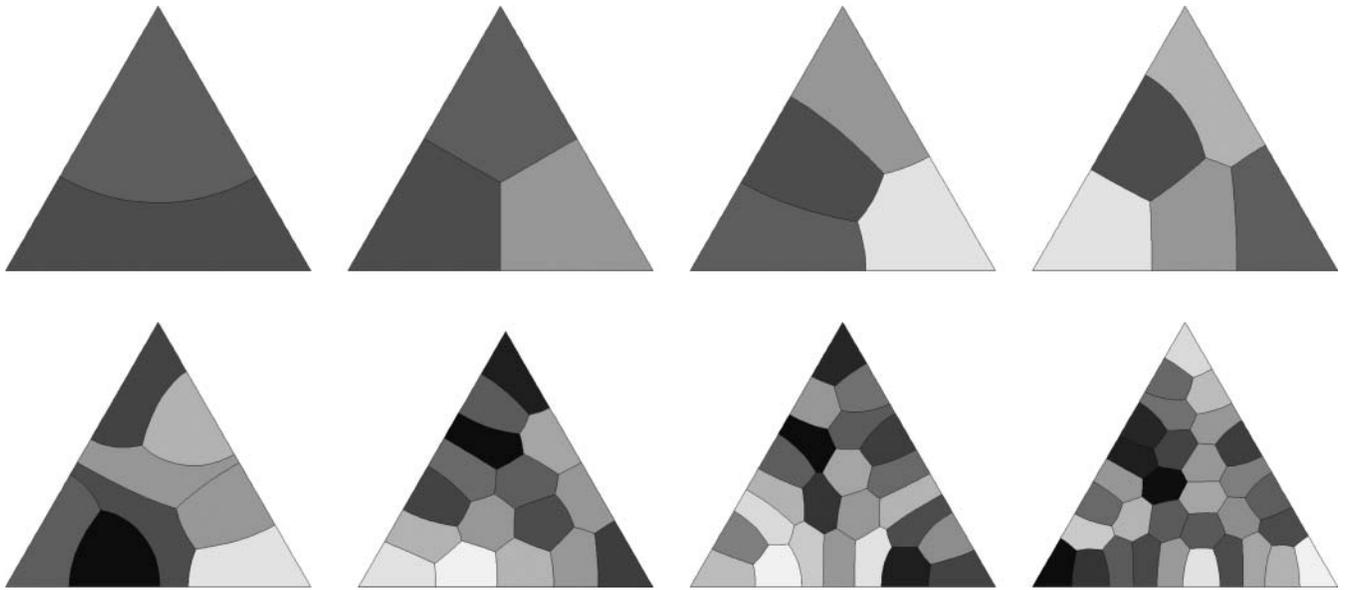


FIGURE 3. Tiling of the triangle with 2, 3, 4, 5, 8, 16, 24, 32 cells.

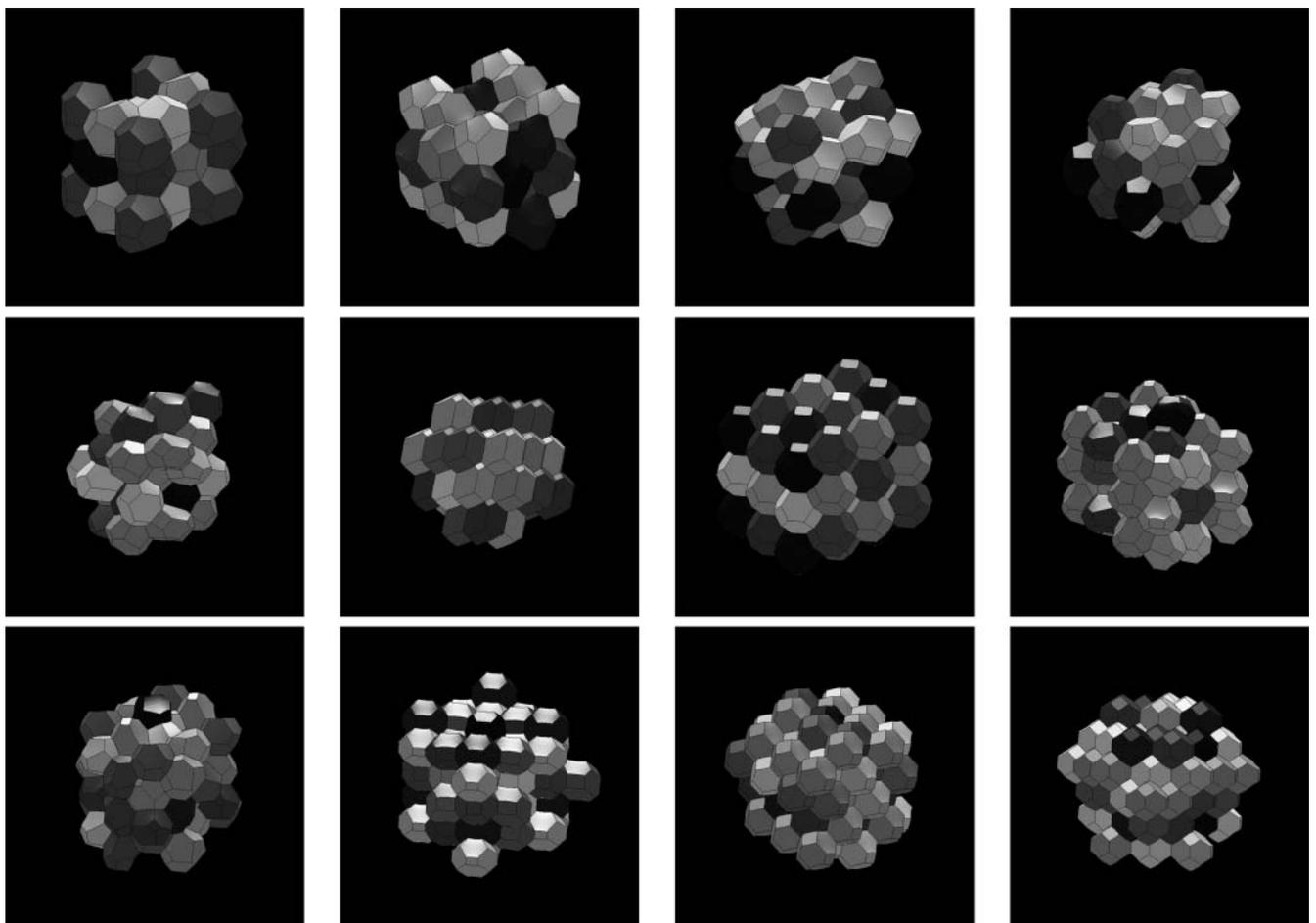


FIGURE 4. Periodic tilings of the space by 8, 10, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21 cells.

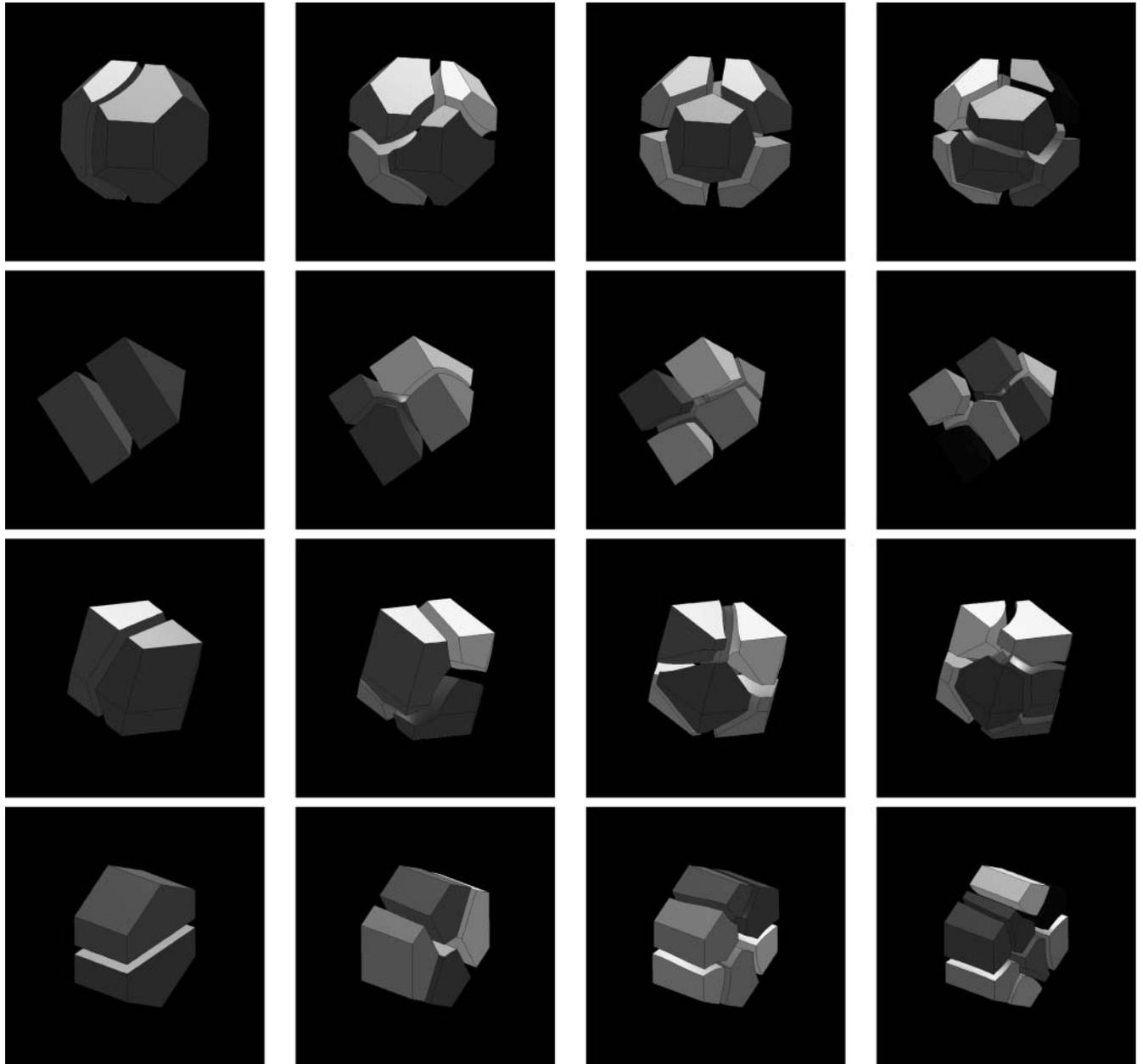


FIGURE 5. Aperiodic tilings.

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 (3–4) associated with the tiling deduced from the previous optimal cutting. The array below sums up the optimal values in the periodic and aperiodic cases of the functional.

Our results are summarized in Table 1. The first column provides different values of Morgan's cost functional

obtained by the periodic tilings, and the second column gives the values obtained by the optimal cutting of sets that already tile the space. We observe that no tiling gave a better cost than those obtained by periodic boundary conditions.

ACKNOWLEDGMENTS

Alessandro Giacomini is warmly thanked for his help in the proof of the relaxation result of Theorem 4.3.

Professor K. Brakke contributed to the current version of the paper through many fruitful comments on the use of his software Evolver.

REFERENCES

- [Alberti 00] G. Alberti. “Variational Models for Phase Transitions, an Approach via Γ -Convergence.” In *Calculus of Variations and Partial Differential Equations (Pisa, 1996)*, pp. 95–114. Berlin: Springer, 2000.
- [Ambrosio et al. 00] Luigi Ambrosio, Nicola Fusco, and Diego Pallara. *Functions of Bounded Variation and Free Discontinuity Problems*, Oxford Mathematical Monographs. New York: Oxford University Press, 2000.
- [Baldo 90] Sisto Baldo. “Minimal Interface Criterion for Phase Transitions in Mixtures of Cahn–Hilliard Fluids.” *Ann. Inst. H. Poincaré Anal. Non Linéaire* 7:2 (1990), 67–90.
- [Brakke 92] Kenneth A. Brakke. “The Surface Evolver.” *Experiment. Math.* 1:2 (1992), 141–165.
- [Demazure 89] Michel Demazure. *Bifurcations and Catastrophes*, Universitext, Geometry of Solutions to Nonlinear Problems. Berlin: Springer-Verlag, 2000.
- [Evans and Gariepy 92] Lawrence C. Evans and Ronald F. Gariepy. *Measure Theory and Fine Properties of Functions*, Studies in Advanced Mathematics. Boca Raton: CRC Press, 1992.
- [Hales 01] T. C. Hales. “The Honeycomb Conjecture.” *Discrete Comput. Geom.* 25:1 (2001), 1–22.
- [Kelley 99] C. T. Kelley. *Iterative Methods for Optimization*, Frontiers in Applied Mathematics 18. Philadelphia: SIAM, 1999.
- [Modica 87] Luciano Modica. “The Gradient Theory of Phase Transitions and the Minimal Interface Criterion.” *Arch. Rational Mech. Anal.* 98:2 (1987), 123–142.
- [Modica and Mortola 77] Luciano Modica and Stefano Mortola. “Un esempio di Γ^- -convergenza.” *Boll. Un. Mat. Ital. B (5)* 14:1 (1977), 285–299.
- [Morgan 08] F. Morgan. “Existence of Least-Perimeter Partitions.” *Philos. Mag. Lett.* 88:9–10 (2008), 647–650.
- [Morgan 09] Frank Morgan. *Geometric Measure Theory*, 4th edition. Amsterdam: Elsevier/Academic Press, 2009.
- [Plateau 73] Joseph Plateau. *Statique Expérimentale et Théorique des Liquides soumis aux Seules Forces Moléculaires*, 1873. (Translation by K. Brakke available online at <http://www.susqu.edu/brakke/aux/downloads/Plateau-Fr.pdf>.)
- [Thomson 87] William Thomson, Lord Kelvin. “On the Division of Space with Minimum Partitional Area.” *Philos. Mag. Lett.* 24:151 (1887), 503.
- [Weaire and Phelan 94] D. Weaire and R. Phelan. “A Counter-example to Kelvin’s Conjecture on Minimal Surfaces.” *Forma* 11:3 (1996), 209–213. (Reprint of *Philos. Mag. Lett.* 69:2 (1994), 107–110.)

Édouard Oudet, Laboratoire de mathématiques, Université de Savoie, Campus scientifique, 73376 Le Bourget-du-lac, France (Edouard.Oudet@univ-savoie.fr)

Received September 15, 2009; accepted July 19, 2010.