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Novel structures for optimal space partitions

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Abstract

Partitioning space into polyhedra with a minimum total surface area is a fundamental question in science and mathematics. In 1887, Lord Kelvin conjectured that the optimal partition of space is obtained with a 14-faced space-filling polyhedron, called tetrakaidecahedron. Kelvin's conjecture resisted a century until Weaire and Phelan proposed in 1994 a new structure, made of eight polyhedra, obtained from numerical simulations. Herein, we propose a stochastic method for finding efficient polyhedral structures, maximizing the mean isoperimeter Q, instead of minimizing total area. We show that novel optimal structures emerge with non-equal cell volumes and uncurved facets. A partition made of 24 polyhedra, is found to surpass the previous known structures. Our work suggests that other structures with high isoperimeter values are still to be discovered in the pursuit of optimal space partitions.

1. Introduction

The Kelvin problem [1–4] is a search for the space-filling arrangement of equal volume cells having a minimal surface area. Kelvin conjectured [1] that such a structure (noted K) has a unique cell type with 14 facets. Two truncated octahedra, forming the Kelvin unit cell of a cubic lattice, are illustrated in figure 1(a).
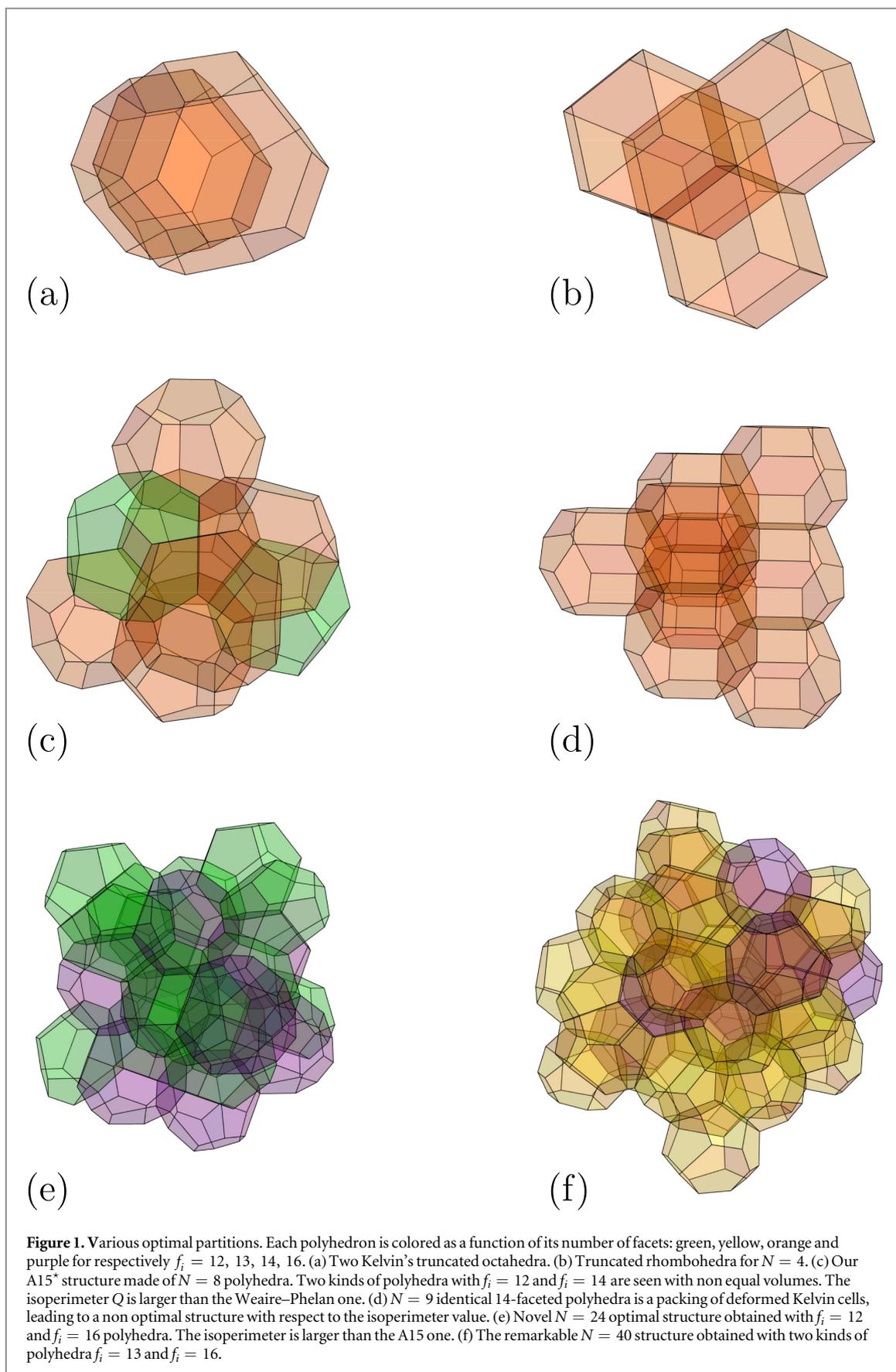
Since the free energy of soap films is related to surface energy, foams are thought to be paradigms of optimal partition problems. However, they also obey Plateau's rules stating that facets meet on edges at 120° implying curved facets and edges. In 1994, Weaire and Phelan [2] studied numerically surface minimization of foam cell structures, and discovered a new structure (noted WP) which is composed of two kinds of polyhedron though they both have equal volumes: irregular dodecahedron and tetrakaidecahedron resulting in a lower average face number 13.5. $N = 8$ polyhedra are needed to form a cubic unit cell. The WP structure presents slightly curved facets.

After its discovery, the WP structure has been recognized to be close to the family of Frank and Kasper structures [5]. The latter crystallographic architectures are composed of polyhedra of various facet numbers but exhibiting only pentagonal and hexagonal uncurved facets. In particular, the A15 crystallographic structure, being close to WP, looks similar to the one illustrated in figure 1(c).

In order to characterize arbitrary space partitions, let us consider N polyhedra constituting a unit cubic cell that can be replicated in three dimensions. <u>In this work, we consider only uncurved facets</u>. Each polyhedron labeled i is described by a volume V_i, an area A_i and a facet number f_i. These geometrical characteristics can be averaged over the structure leading respectively to V, A and f. In addition, the isoperimeter Q_i of each element i is defined by

$$Q_i = 36\pi \frac{V_i^2}{A_i^3} \tag{1}$$

for which values are situated in between 0 (lamellar polyhedron) and 1 (hypothetic spherical polyhedron). The average isoperimeter is mathematically given by

Figure 1. Various optimal partitions. Each polyhedron is colored as a function of its number of facets: green, yellow, orange and purple for respectively $f_i = 12, 13, 14, 16$. (a) Two Kelvin's truncated octahedra. (b) Truncated rhombohedra for $N = 4$. (c) Our A15* structure made of $N = 8$ polyhedra. Two kinds of polyhedra with $f_i = 12$ and $f_i = 14$ are seen with non equal volumes. The isoperimeter Q is larger than the Weaire–Phelan one. (d) $N = 9$ identical 14-faceted polyhedra is a packing of deformed Kelvin cells, leading to a non optimal structure with respect to the isoperimeter value. (e) Novel $N = 24$ optimal structure obtained with $f_i = 12$ and $f_i = 16$ polyhedra. The isoperimeter is larger than the A15 one. (f) The remarkable $N = 40$ structure obtained with two kinds of polyhedra $f_i = 13$ and $f_i = 16$.

$$Q = \frac{1}{N} \sum_{i=1}^{N} Q_i \qquad (2)$$

Table 1. Noticeable novel structures found with an isoperimeter Q larger than the value of the Kelvin structure. The first three rows correspond to Kelvin, Frank and Kasper A15, and Weaire–Phelan classical structures. For each structure, the table gives the number N of polyhedra constituting the unit cell, the isoperimeter Q, the isoperimeter Q', the mean facet number f, the cell types in terms of facets, and the mean volume fluctuations v.

Name	N	Q	Q'	f	f_i's	v
K	2	0.75337	0.75337	14.00	{14}	0
A15	8	0.76102	0.76098	13.50	{12, 14}	0
WP	8	—	0.764	13.50	{12, 14}	0
A15*	8	0.76175	0.76181	13.50	{12, 14}	0.01353
	24	0.76130	0.76504	13.33	{12, 16}	0.10063
	36	0.75544	0.75884	13.56	{12, 13, 14, 15, 16}	0.10972
	37	0.75490	0.75909	13.57	{12, 13, 14, 15, 16}	0.11723
	38	0.75459	0.75785	13.58	{12, 13, 14, 15, 16}	0.10596
	40	0.75592	0.75758	13.60	{13, 16}	0.07155
	56	0.75502	0.76319	13.50	{11, 12, 13, 14, 15, 16}	0.16537

and measures in some way the average sphericity of polyhedra in the structure. However, an alternative definition of the isoperimeter is often considered in physics, i.e.

$$Q' = 36\pi \frac{V^2}{A^3} \qquad (3)$$

for which area and volumes are averaged independently allowing for searching area minimization with a fixed volume distribution. Indeed, by considering the constraint $V_i = 1/N$, the Kelvin problem is equivalent to the maximization of Q'. Moreover, for identical polyhedra, like in the Kelvin structure, $Q = Q'$. However, these observables are slightly different when polyhedron shapes and/or volumes are different, e.g. in the A15 structure. As a reference in our work, both values of Q and Q' are given in table 1 with five digits for respectively the K, Frank and Kasper A15 and WP structures.

The WP structure presents still the highest known Q' (and Q) value for equal volume polyhedra. It is slightly surpassing A15 but has curved facets. It should be also noted that the Frank and Kasper structure σ considering 30 non-equal volume polyhedra is surpassing the A15 isoperimeter [10, 11]: $Q'_\sigma = 0.7624$. However, when relaxing this sigma structure with Plateau rules [4], the curved structure is found to have higher area than WP.
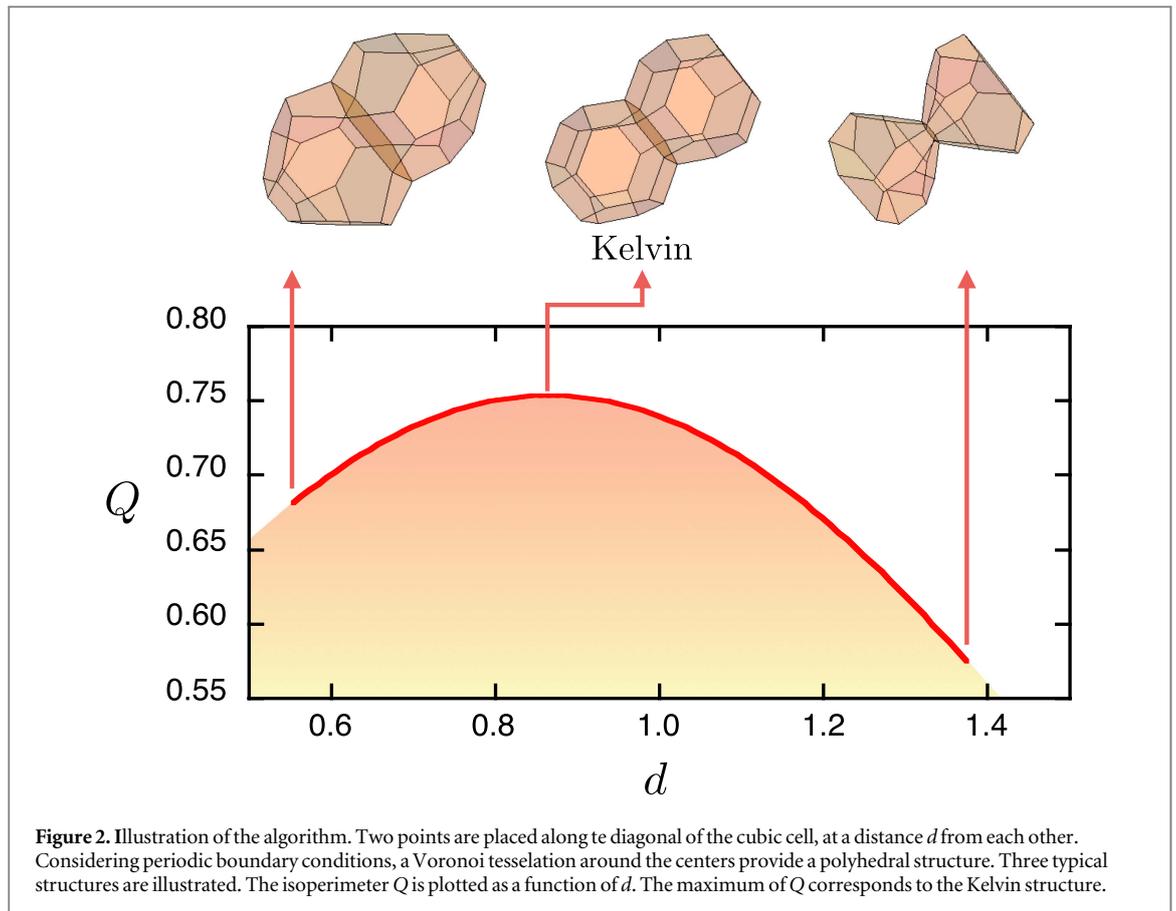
The space partition challenge remains since some other structure with a higher isoperimeter value might be found [6]. For example, theoretical works [6–8] have conjectured that the ideal mean facet number is $f = 13.3973$, which is much lower than the values for K and A15 structures. A numerical method has also been proposed to explore efficient structures but only K partition has been surpassed [9].

In the present paper, we propose a way to explore novel optimal uncurved structures in a cubic lattice cell by suppressing the equal volumes constraint, such that Q becomes the relevant observable. By optimizing the isoperimeter Q, high Q' values may also be reached, as we will discover below.

2. Numerical method

We consider N points in a cube instead of managing the many (and variable) degrees of freedom when one places vertices, edges and faces of a cellular structure. For a set of N points, a Voronoi tesselation [12] is calculated, giving rise to polyhedral structures. Our algorithm calculates the area A_i and the volume V_i of each Voronoi cell i providing Q using equation (1). Any displacement of the points will change the structure. The degrees of freedom in the system is therefore given by a constant $3(N - 1)$ variables corresponding to relative positions of points around a central one. In the high dimensional space of the $3(N - 1)$ coordinates, Q could be represented by a landscape.

A stochastic algorithm has been developed for optimizing Q by changing the coordinates of the points, i.e. finding the highest point of the landscape. It is mainly based on simulated annealing [13]. In this algorithm, the N points are initially placed randomly in a centered unit cube. This initial configuration leads to an isoperimeter $Q = Q_0$ of the corresponding Voronoi tesselation. A fixed point is then chosen and will keep its coordinates during the entire simulation. At each iteration t the other $N - 1$ points are moved via a gaussian noise term $N(0, \sigma)$, where the standard deviation $\sigma(Q, T)$ is a function of the regarded isoperimeter Q and the dimensionless simulated temperature $T = T_0/(1 + t)$ which decreases along the simulation. At each iteration t, the new positions of the points allow to calculate the corresponding Voronoi tesselation and a new hypothetic isoperimeter q. If $q > Q$, the new, favorable, configuration is adopted. However, if $q < Q$ the new confuguration is not systematically rejected allowing the system to flee a local maximum. In that case, the system

Figure 2. Illustration of the algorithm. Two points are placed along te diagonal of the cubic cell, at a distance *d* from each other. Considering periodic boundary conditions, a Voronoi tesselation around the centers provide a polyhedral structure. Three typical structures are illustrated. The isoperimeter *Q* is plotted as a function of *d*. The maximum of *Q* corresponds to the Kelvin structure.

adopts its new, defavorable configuration with a probability $P(q, Q) = \exp((q - Q)/T)$ and keeps its old configuration with a propability $1 - P(q, Q)$. After long and multiple runs, the best structures are determined.

Our method is illustrated by the plot in figure 2 for the $N = 2$ case. Two points are placed along the diagonal of the cubic cell at a distance *d* between each other. The Voronoi tesselation considering the periodic boundary conditions is built providing two identical polyhedra. Three different cases are illustrated. The maximum value of $Q(d)$ corresponds to the Kelvin structure which emerges naturally at $d = \sqrt{3}/2$.

The numerical method has been performed for several values of *N* between 2 and 64. For large *N* values, the high dimensional phase space seems to be rugged and the system may be trapped in one of the numerous local maxima of *Q*, the structure is recorded and then strongly modified by popping a randomly chosen polyhedron and by nucleating another one elsewhere, in order to visit another part of the phase space. Very long simulations are therefore needed to explore a large number of possible structures in a high dimensional space. Although millions of iterations are needed to obtain small structures, billions of iterations were performed for large *N* values.

Please note that the proposed algorithm is not relevant for total area minimization. Since the volumes V_i are free variables, maximizing Q' by moving Voronoi centers will inevitably lead the system to heterogeneous structures where some polyhedra tend to vanish, providing large volume differences.

3. Results

Figures 1(b)–(f) presents selected structures maximizing the isoperimeter *Q*. The case $N = 4$ leads to a partition of identical rhombohedra, illustrated in figure 1(b), having a low isoperimeter $Q_4 = 0.74048$. The first interesting case is found for the $N = 8$ case leading to a partition similar to A15, but slightly different ! It possesses in fact the same symmetry elements than A15, but the cells are characterized by non equal volumes. It corresponds to the A15 family of Frank and Kasper structures. We note this structure A15*, that is illustrated in figure 1(c). We define the mean volume difference by

$$v = \frac{1}{\langle V \rangle} \sqrt{\frac{1}{N} \sum_{i=1}^{N} (V_i - \langle V \rangle)^2}. \tag{4}$$
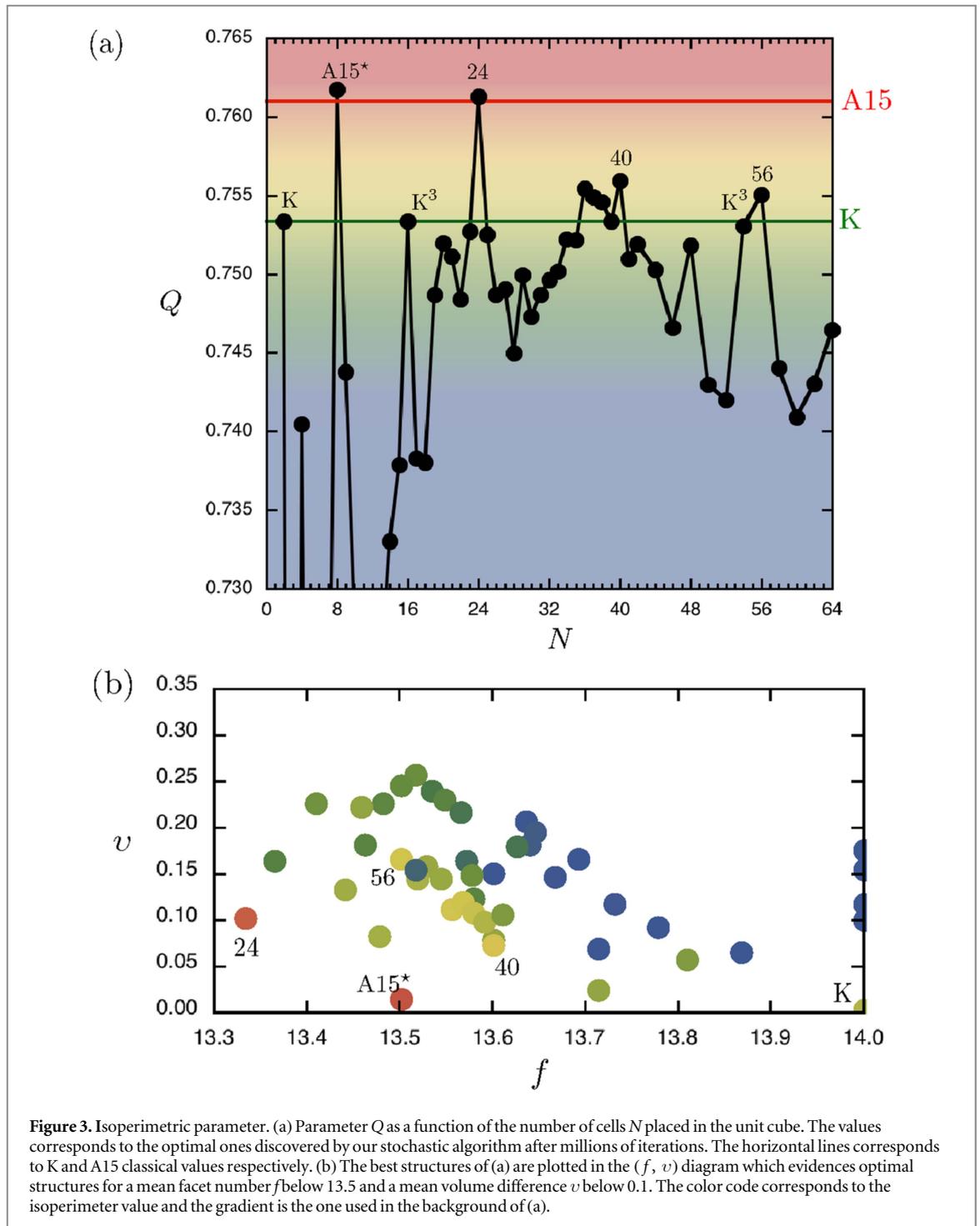
Figure 3. Isoperimetric parameter. (a) Parameter Q as a function of the number of cells N placed in the unit cube. The values corresponds to the optimal ones discovered by our stochastic algorithm after millions of iterations. The horizontal lines corresponds to K and A15 classical values respectively. (b) The best structures of (a) are plotted in the (f, υ) diagram which evidences optimal structures for a mean facet number f below 13.5 and a mean volume difference υ below 0.1. The color code corresponds to the isoperimeter value and the gradient is the one used in the background of (a).

This observable measures the deviation from the equal volume constraint. The structure A15⋆ is characterized by $\upsilon = 0.01353$. In fact, the dodecahedra volumes are slightly reduced by a factor 0.976 and tetrakaidecahedra are sightly enlarged by a factor 1.008. The isoperimeter $Q_{A15^\star} = 0.76175$ is higher than Q_{A15}. This result proves that our algorithm is efficient in order to search for optimal structures.

Figure 1(d) illustrates the $N = 9$ case which has an isoperimeter lower than Q_K, but is formed by equal cell volumes. The cells are 14 facets polyhedra, being deformed tetrakaidodecahedra. For values of $N = \{2, 4, 7, 9, 12\}$, our algorithm converges towards equal volume 14 faceted cells.

By increasing again the number N of cells, one reaches the case $N = 16 = 2 \times 2^3$ reducing trivially to the Kelvin structure that is replicated in the three main directions. We note this replicated structure K³. This replication is also expected for $N = 54 = 2 \times 3^3$ while the replication of A15⋆ should be found for $N = 64 = 8 \times 2^3$. The simulations for $N = 54$ are close to the expected structure K³, the $N = 64$ case is far

from reaching the optimal structure due to the high dimensionality and the complexity of the phase space. Much longer computation runs are needed to produce replicated structures A15$^{\star 3}$ and K^3 for high N values.

Above $N = 16$, we have found other structures with high isoperimeters. A remarkable structure with $N = 24$ is illustrated in figure 1(e). It is composed of 12 and 16 faceted polyhedra leading to $Q_{24} = 0.76130$, i.e. slightly below $Q_{A15^{\star}}$, but larger than Q_{A15}. The volume difference between 12- and 16-faceted polyhedra is significant ($\upsilon = 0.10063$) and the average face number is the lowest obtained in our simulations: $f = 13.33$, i.e. close to the ideal number conjectured earlier. The $N = 24$ structure is remarkable for both extreme isoperimeter and f values.

The case $N = 40$ is another noticable structure, having 13 and 16 faceted polyhedra, as illustrated in figure 1(f). It has a large isopermieter, much larger than the Kelvin's one. It should be noted that this structure does not belong to Frank–Kasper structures since the 13 faceted polyhedra possess each a square facet. Frank–Kasper structures are therefore not the only way to explore optimal structures.

Figure 3(a) presents the best isoperimeter Q values obtained as a function of selected values of N between 2 and 64. Horizontal lines denote respectively Kelvin and A15 classical values, known before our work. The novel structures, noted A15* and 24, are seen to beat the known values. A series of other structures are in between K and A15 like the surprising case $N = 40$. Although the data are scattered, the positions of successive maxima of $Q(N)$ can be emphasized. They seem to form a suite 8, 24, 40 and 56, i.e. $(2k + 1)8$ with k being an integer. The neighbors of those selected structures seem also to reach high isoperimeter values (close to and even larger than Q_K). This conjecture should be confirmed with additional simulations for larger N values.

Figure 3(b) shows the average volume difference υ as a function of the mean facet number f for the best structures found in our simulations with N going from 2 to 64. The color code corresponds to the one of the isoperimeter in figure 3(a). The data points are seen grouped in a triangular region close to the $\upsilon = 0$ axis. The color gradient corresponding to the isoperimeter value reveals that best structures are found for υ values between 0 and 0.1 and a mean facet number from 13.3 to 13.5. We conjecture that other structures can be found in this region by providing extensive simulations using our algorithm.

Let us consider the isoperimetric values Q' of our remarkable structures, as listed in table 1. First, it should be noticed that $Q' > Q$ in most cases, and thus, by optimizing Q, we generally obtain high Q' values. The second and most important result is that the $N = 24$ structure surpasses all reported optimal structures !

4. Summary

In summary, we studied space partitions with non-equal volume polyhedra, optimizing the isoperimeter Q. We discovered novel structures. One of them exhibits a Q' value larger than the Weaire–Phelan and σ case, known to possess the largest isoperimeters before this work. It is composed of 24 polyhedra and has the lowest known average facet number. In addition, remarkable structures have been found, like the one composed of 13 and 16 faceted polyhedra for $N = 40$.

The exploration of space partitions is still under progress and future extensive simulations may provide key elements for finding new remarkable structures. Non cubic lattice cells can be explored also to obtain even higher Q and/or Q' values. Considering non planar interfaces may also improve a little bit the values of both isoperimeters, but this requires additional numerical simulations, left for future studies.

Acknowledgments

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