A new counter-example to Kelvin's conjecture on minimal surfaces

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Abstract

A new counter-example to Kelvin's conjecture on minimal surfaces [1] has been found. The conjecture stated that the minimal surface area partition of space into cells of equal volume was a tiling by truncated octahedra with slightly curved faces [K]. Phelan and Weaire found a counter-example [2] whose periodic unit includes two different tiles, a dodecahedron and a polyhedron with 14 faces [A15]. Successively, Sullivan showed the existence of a whole domain of partitions [3] by polyhedra having only pentagonal and hexagonal faces that included A15.

Here is presented a new partition with lower surface area than K containing quadrilateral, pentagonal and hexagonal faces. These and other new partitions have been generated via the Voronoi diagram of spatially periodic sets of points obtained as local maxima of the stationary solution of the 3D Swift-Hohenberg [4] partial differential equation in a triply periodic boundary, with pseudorandom initial conditions.

The geometrical problem that seems to have its solution in real foams of partitioning space into cells of equal volume with the least interfacial area has not yet been solved. The solution to the bi-dimensional problem, also known as the honeycomb conjecture, has only recently been given a formal proof by Thomas Hales [5]. A possible solution to the three-dimensional problem was given more than a century ago by William Thomson, better known as Lord Kelvin, who was also the first to formally state it [1].

Kelvin conjectured that the partition made by a packing of identical truncated octahedra with slightly curved faces [K], had the minimum surface area among all the possible equal volume partitions of space. The truncated octahedron is a polyhedron with 14 faces, 8 of which are hexagons and the remaining 6 are quadrilaterals as shown in Figure 1. In the partition considered by Kelvin all the edges were curved. The quadrilateral faces were flat, and the hexagonal ones were slightly curved, this way further reducing the total interfacial area of the partition when compared to the flat-faced version of the truncated octahedron.

In 1993, Robert Phelan and Denis Weaire, using Ken Brakke's program Surface Evolver [6], showed the existence of a partition [A15] having less area than that found by Kelvin [2]. The partition, also known as the Weaire-Phelan structure, has two different cell shapes, namely a cubicly deformed pentagonal

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Figure 1: A truncated octahedron. This polyhedron is space-filling.

dodecahedron and an axially squashed 14-hedron with 12 pentagonal and 2 hexagonal faces as in Figure 2.

Shortly after the discovery, John Sullivan described a class of mathematical foams known as tetrahedrally close-packed structures, which included A15. Many of these structures have been known for a long time as Frank-Kasper phases [7, 8]. All the structures belonging to this domain are made of polyhedral cells having only pentagonal and hexagonal faces. He constructed infinite families of periodic structures as convex combinations of a finite set of basic structures [3].

This showed that not only A15 had less area than K, but infinitely many other structures (the terms structure, partition, foam and tiling are used as synonyms here) could be constructed with such a property. The polyhedral cells used in these structures are of four distinct kinds having 12, 14, 15 and 16 faces. All contain 12 pentagons plus respectively 0, 2, 3 and 4 hexagons. These are the only combinatorially possible simple polyhedra with 12 to 16 faces containing only pentagons and/or hexagons where the hexagons are not adjacent, as shown by the program plantri [9]. A simple polyhedron is a polyhedron in which each vertex belongs to exactly three edges.

Since the only faces that occur in the partitions found have from 4 to 6 sides, a polyhedra nomenclature based on this fact consisting of three numbers has been considered. Each polyhedron is assigned three numbers X-Y-Z that represent the number of quadrilaterals (X), pentagons (Y) and hexagons (Z). This naming system, called simplified signature, although not always univocal in defining the topology as with the Schlegel diagram [10], presents the advantage of a much more concise form of identification of the polyhedron, very similar to the signature used in the software application 3dt [11], and for this reason it

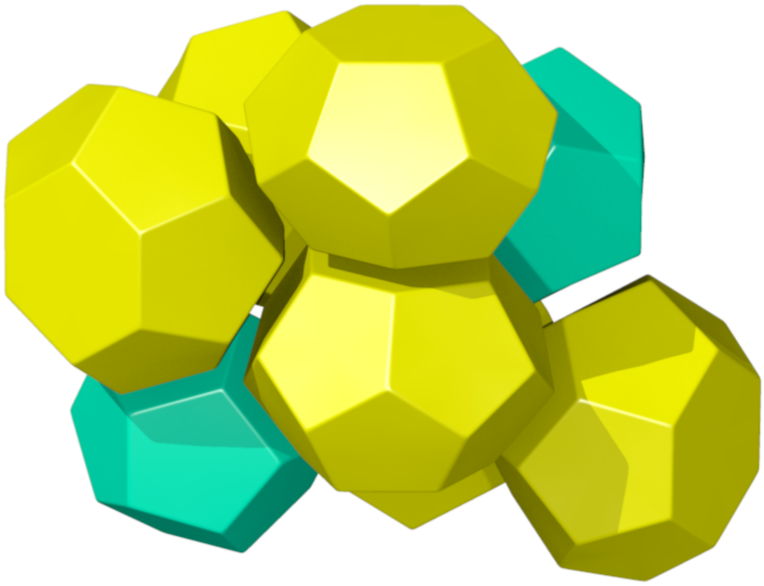

Figure 2: The periodic unit of the Weaire-Phelan structure contains 8 polyhedra, two 0-12-0 (cyan) and six 0-12-2 (yellow).

will be used to describe the polyhedral composition of the structures found in this work.

One method of generating foams is by Voronoi partitions in three dimensions. All that is needed is a set of points in a three-torus, which is a three-dimensional region (a parallelepiped) whose boundaries are connected to themselves. The three-torus is the unit cell of the structure, which is periodically repeated in the three directions in space. Generation methods that start from random sets of points have already been used with interesting results [12].

Here is proposed a method based on a partial differential equation that shows a pattern forming behaviour, the Swift-Hohenberg equation [4, 13]. A script has been written using the software Matlab that solves the following equation:

$$\frac{\partial u}{\partial t} = au - (\nabla^2 u + 1)^2 u + bu^2 - u^3 \tag{1}$$

on a periodic cube of prescribed size L using the Fast Fourier Transform. The coefficients a and b in Equation 1 affect the final pattern. The values needed for homogeneously distributed maxima to appear in the stationary state are respectively close to 0.1 and 1. The unit cell was chosen to be cubical for simplicity. A version of the code that computes Equation 1 in a cuboid as also been written and a more general implementation working in a parallelepiped might help. Solutions with non-cubic symmetry arise in a cubic region only if a multiple of their unit cell has cubic symmetry. This is always the case, the only problem being the fact that the structure might be very large.

The solution for the function $u = u(x, y, z, t)$ has been found to converge from pseudorandom initial conditions to a stationary state. The three-dimensional

	simplified signature	sp. gr.	c	z
K	[6-0-8]	$Im\bar{3}m$	5.306	14
P42a	2[2-8-4]+2[1-10-2]+2[1-10-3]+[0-12-2]	$C12/c1$	5.303	13.71
A15	[0-12-0]+3[0-12-2]	$Pm\bar{3}n$	5.288	13.5

Table 1: Simplified signature, space group of the most symmetrical configuration, minimum cost c of the equal-volume partition and average number of faces per cell z, for all the known basic periodic partitions whose cost is less or equal to that of K.

coordinates of the local maxima of the function $u = u(x, y, z, t)$ in this final state have been extracted. The method has been run a finite number of times, and the results have been compared for congruence. Successively L has been incremented and the coordinates at the stationary state have been recorded again. It has been found that for large values of L the patterns formed appear locally but not globally ordered. For certain values of the parameter L the system converges to a state where the maxima are arranged on parallel lines in space, all having the same orientation, in a hexagonal packing fashion. The partition obtained from such an arrangement is a cylindrical hexagonal honeycomb.

Another issue is that many of the simpler patterns appear for different values of L. These values are the multiples of the fundamental lattice distance for a given pattern. Thus more complex patterns might be hidden by the simpler ones when looking for a solution for a given size L.

In general, since the average distances between the local maxima are roughly constant, increasing the size of the cubic region in which the equation is calculated increases the number of the local maxima within the same region. This allows structures with different level of complexity to be found simply acting on the size of the periodic boundary L.

The patterns obtained from such a setup were BCC, HCP, A15, P20, C15 [14, 3], P36, K11 [15], P42. Those starting with the letter P have not been found in the literature.

Using Sullivan's vcs software [16] the Voronoi partition for each set was created. This software uses the gift-wrapping algorithm for the determination of the Voronoi vertices and for this reason is not stable when more than four Voronoi planes meet at a point. Since some of the new partitions found were non-simple, a small random quantity has been added to the coordinates of the points to avoid algorithm instabilities.

A tiling (or partition) is non-simple if it is not simple. A tiling is simple if every face contained in it is shared by two adjacent tiles, every edge by three incident faces, and every vertex by four incident edges.

The partitions have been imported into Surface Evolver, where the added errors have been eliminated by deletion of the edges shorter than a given value. A number of additional simple foams has been created directly in Surface Evolver by *popping* vertices of non-simple ones. The outcome of this operation is not a unique structure since there are $3^m + 4^n$ different combinations, if m is the number of 8-connected vertices and n that of 6-connected vertices in the original non-simple foam. However, this number can be drastically reduced due to symmetry considerations.

The periodic graph of the nets constituted by the edges of the partitions have

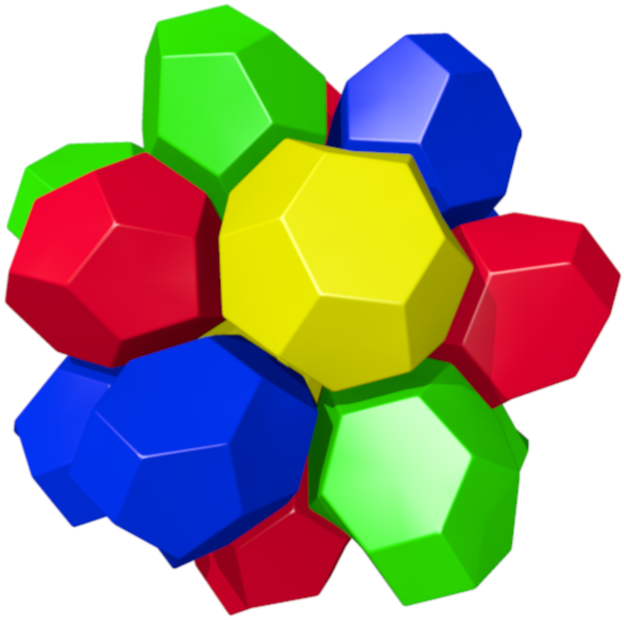

Figure 3: The unit cell of the new partition P42a contains 14 polyhedra of 4 different kinds. Four 1-10-2 (red), two 0-12-2 (yellow), four 1-10-3 (green) and four 2-8-4 (blue).

been analysed by Systre [17] so that the primitive net could be identified and the number of tiles in the partition therefore reduced to its minimum possible. This helped in the case of P42, where the 42 tiles have been reduced to 14.

Four out of the 81 simple partitions derived from the P42 non-simple case showed less surface area than K. Figure 3 shows a picture of the tiling of the unit cell of the structure with the lowest cost, which has been named P42a. The fundamental unit is made of ten 14-hedra and four 13-hedra. The average number of faces, 13.71 is very close to the value of 13.70 found by Matzke's experimental work on the three-dimensional shape of bubbles in foams [18] and not too far from the optimal value [19].

The space groups for each of the foams produced were determined by 3dt. The application is part of the Gavrog Project [11]. Table 1 reports the data for K, A15 and P42a for comparison. The space group refers to the maximum symmetrical structure, while the cost is obtained by constraining the structure to have tiles of the same volume. The cost of a foam is given by:

$$c = A/V^{2/3} \tag{2}$$

where A is the average interfacial area per tile and V is the volume of each tile. The Surface Evolver code used for the calculation of foams properties and parameters (including their cost) has been provided by Sullivan. The code for the relaxation of the periods has been written by the author.

The method described, opportunely tuned, could lead to numerical proofs of the Kelvin problem and to the honeycomb problem considered by Tóth [20].

All the pictures have been generated with 3dt. Tiles are represented slightly detached one from the other for a better visualization.

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