COVERING POLYHEDRAL TORI

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Abstract. Covering a toroidal surface by quadrilaterals and their transformation by leapfrog and other operations are illustrated.

INTRODUCTION

Carbon nanotubes and their closed, circular forms with toroidal shape have been identified among the laser irradiated graphite products. [1-3] A torus can be viewed as a tube with joint ends and, conversely, a tube can be understood as a cut torus. Since a torus is covered by a continuous surface, any edge-vertex lattice embedded on that surface will generate a polyhedral torus. As they can get rise from a graphite sheet, by a zone-folding process, [4-6] it is conceivable to take the single-wall products as the objects of the covering problems herein discussed. For general aspects in covering a graph, the reader can consult refs. [7,8] We limit here to square-like tori and their transforms, obtainable by applying some simple operations.

TESSELLATING A TORUS

The most simple covering of a toroidal surface is by a rectangular (i.e. square-like) net (Figure 1). When gluing, the tube ends can be forced offset, the resulting lattice being twisted (see below). In our procedure it is called a v-twisting (i.e., vertex columns are vertically shifted).
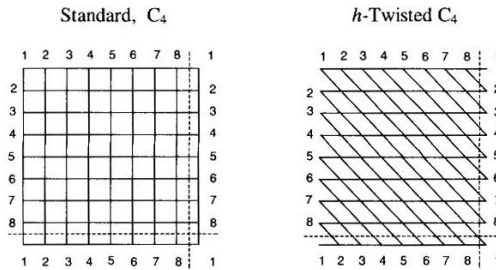
Standard, C_4 h-Twisted C_4

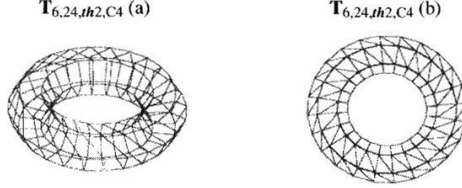FIGURE 1. Standard C_4 faces and a h-twisted pattern.

When the twisting shifts vertex rows horizontally it results in a **h**-twisted pattern (see Figure 1). Twisting can be achieved either to the right or to the left hand side. It is easier understood if addressed to cyclic permutations. Examples are given below.

$\mathbf{T}_{6,12,C4}$ (nontwisted) $\mathbf{T}_{6,12,tv6,C4}$

$\mathbf{T}_{6,24,th2,C4}$ (a) $\mathbf{T}_{6,24,th2,C4}$ (b)
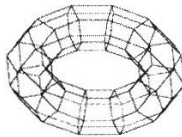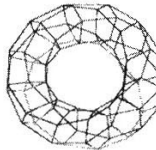
The name of a torus $\mathbf{T}_{c,n,C4}$, generated by moving a c-membered cycle around another n-membered cycle [9] must be completed by adding the twisting specifications: th and tv, a third letter for the sense (e.g., thr – twist, horizontal, rectus), followed by the number of *twisted row faces* (integers, between 1-c, and 1-n, respectively).

For generating a rhomboidal pattern, pi/4 rotated with respect to the original square faces of the torus, a transformation like that shown in Figure 2 is proposed. The term "horizontal" reminds that horizontal edges are moved.
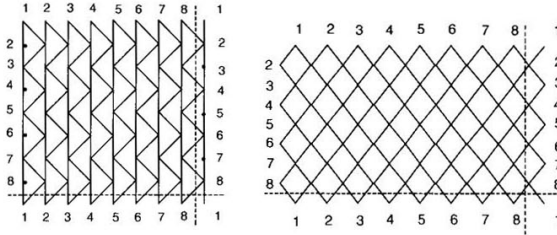

FIGURE 2. Rhomboidal patterns rh

Nice tori can be thus obtained (see below): $\mathbf{T}_{6,12,rh,C4}$ is further transformed by adding *vertical* edges in each of its faces to give $\mathbf{T}_{6,12,rh,v,C3}$, a sequence of square bipyramids, joined by a common triangle. If *horizontal* edges are added to $\mathbf{T}_{6,12,rh,C4}$ one obtains the transform $\mathbf{T}_{6,12,rh,h,C3}$. Both derived structures are regular graphs of degree 6, covered by triangles

(i.e., deltahedranes [10] – denoted by C_3 in the name of structure).

$\mathbf{T}_{6,12,rh},C4$

$\mathbf{T}_{6,12,rh,v},C3$

$\mathbf{T}_{6,12,rh,\,h},C3$
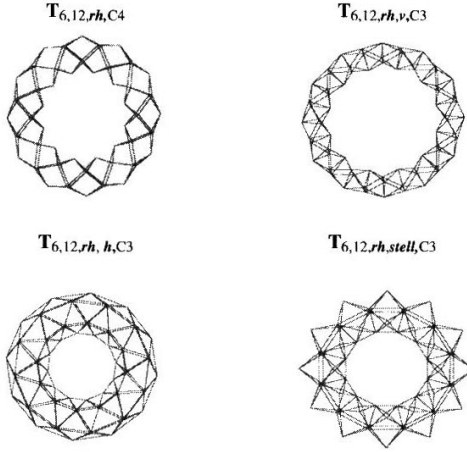
$\mathbf{T}_{6,12,rh,stell},C3$

In continuing, let's add to structure $\mathbf{T}_{6,12,rh}$, alternatively, horizontal and vertical edges, so that no two original rhomboidal faces, sharing a common edge, have the same h or v added edge. It results in a deltahedrane $\mathbf{T}_{6,12,rh,stell},C3$, meaning the omnicapped transform (see the next section) of the $\mathbf{T}_{3,12,C4}$ rectangular lattice. Each of its faces is capped (stellated) by pyramid-like relief. Such a structure can be made, of course, by adding a vertex over the center of each square-like face, followed by joining it by each of the four corners.

LEAPFROG

Leapfrog transformation of a single-wall torus involves the stellation of its faces followed by dualization. [10]

Note that a torus is a closed surface. A combinatorial representation of a closed surface is called a map M. [11] Stellation and dualization are operations on maps.

Let denote in a map: v - number of vertices; e - number of edges; f - number of faces and d - vertex degree. An asterisk * will mark the corresponding parameters in the transformed map.

Stellation St of a map consists of adding a new vertex in the center of its faces followed by connecting it with each boundary vertex. It is also called a *capping* operation or *triangulation*. [10,11]

The resulting omnicapped map shows the relations:

$$St(M): \qquad v^* = v + f$$
$$e^* = 3e$$
$$f^* = 2e$$

so that the Euler's relation: $v - e + f = 2 - 2g$ (v, e, f, g being respectively the number of vertices, number of edges, number of faces, and genus) is obeyed. Note that a torus is of genus one while a sphere or a cylinder are of genus zero.

Dualization Du of a map can be achieved by locating a point in each of its faces. Two such points are joined if their corresponding faces share a common edge. The new edge is called the *edge dual Du(e)* and the transformed map, the (Poincaré) *dual Du(M)*. The vertices of *Du(M)* represent the faces of M and *vice-versa*. Thus the following relations exist:

$$Du(M): \qquad v^* = f$$
$$e^* = e$$
$$f^* = v$$

Dual of the dual recovers the map itself: $Du(Du(M)) = M$.

Leapfrog Le is a composite operation. It can be written as:

$$Le = Du(St(M)) \qquad\qquad (1)$$

Within the leapfrog process, the dualization is made on the stellated map (Figure 3). A sequence of stellation-dualization rotates parent n-gonal faces by *pi/n*. [12-14]
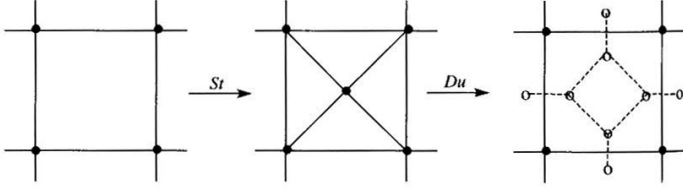
FIGURE 3. Fate of a square-like face by Leapfrog;
circles denote the vertices in *Le* transform.

Consider the basic relations in a map:

$$\sum nf_n = 2e \qquad (2)$$

$$\sum d\,v_d = 2e \qquad (3)$$

A map embedded in a torus can be a regular d graph (i.e. a graph having all its vertices of the same degree d). From (2) and (3) it follows that:

$$v = (1/d)\sum nf_n \qquad (4)$$

where the subscript n means the n-gonal face.

Theorem 1.

The number of vertices in the leapfrog transform Le(M) is d times larger than in the original map M, irrespective of the type of tessellation.

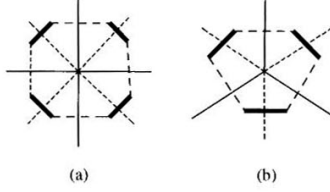For demonstration, let's go back to the dualization process (Figure 4):

<center>(a)   (b)</center>

FIGURE 4. Dualization of the omnicapped faces around a four-degree (a)
and three-degree (b) vertex

Note that a bounding polygon is formed around each original vertex. Also note that, as a consequence of the involved triangulation, the vertex degree in $Le(M)$ is *always* 3. In other words, the dual of a triangulation is a *cubic net*. [11]

Two cases usually appear:

Case (a): $d = 4$; the bounding polygon is an octagon ($n = 8$).

$$v^* = (1/d^*)[nf_n + 8f_8] = (1/d^*)[nf_n + 8v] \qquad (5)$$

By virtue of (4), $v = nf_n/d = nf_n/4$, so that eq 5 becomes:

$$v^* = (1/3)[nf_n + 8(nf_n/4)] = nf_n \qquad (6)$$

The ratio v^*/v (i.e. the multiplication factor in the leapfrog process) is:

$$v^*/v = nf_n/(nf_n/4) = 4 \qquad (7)$$

Case (b): $d = 3$; the bounding polygon is a hexagon ($n = 6$).

$$v^* = (1/d^*)[nf_n + 6f_6] = (1/3)[nf_n + 6v] \qquad (8)$$

In this case $v = nf_n/3$, so that (8) becomes:

$$v^* = (1/3)[nf_n + 6(nf_n/3)] = nf_n \tag{9}$$

and the multiplication ratio:

$$v^*/v = nf_n/(nf_n/3) = 3 \tag{10}$$

At this stage, we can generalize:

$$v^* = (1/d^*)[\sum nf_n + 2dv] = (1/3)[\sum nf_n + 2d(\sum nf_n/d)]$$
$$= 3\sum nf_n/d^* \tag{11}$$

$$v^*/v = (3\sum nf_n/d^*)/(\sum nf_n/d) = 3(d/d^*) \tag{12}$$

Since d^* is always 3 in $Le(M)$, *the multiplication ratio depends only of the vertex degree in the original map*, irrespective of the face boundary polygons.

A *simpler demonstration* takes into account eq 3, the fact that the map is a d regular graph and the observation that each edge in M shares two vertices in $Le(M)$. Thus,

$$v^* = 2e = dv \tag{13}$$

$$v^*/v = dv/v = d \tag{14}$$

By completion,

$$Le(M): \quad v^* = dv = 2e$$
$$e^* = 3e$$
$$f^* = f + v$$

Leapfrog transformation can be achieved by a different sequence of simple operations: $Le = Tr(Du(M))$. It is the well-known way of dualization of dodecahedron to icosahedron followed by its truncation in obtaining the C_{60} fullerene. The goal of such a transformation is to *isolate* the *pentagons* appearing on the mapped sphere, in fullerenes.

In square tori, the *pi/4* rotation, appearing by *Le*, would produce *rhomboidal* lattices (Figure 5) that are quite difficult to implement in transforming a square-like net.
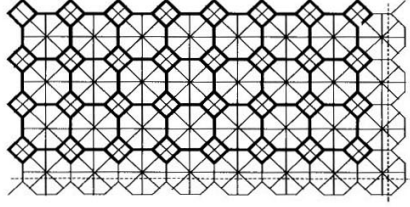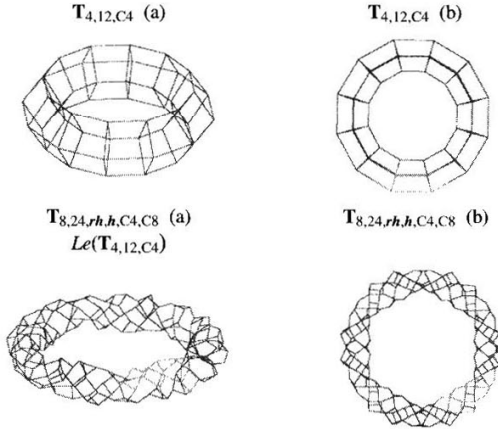
FIGURE 5. Dualization within *Le* transformation of a square-like net.

A square torus and its leapfrog transform are illustrated in the following:

$\mathbf{T}_{4,12,C4}$ (a) $\mathbf{T}_{4,12,C4}$ (b)

$\mathbf{T}_{8,24,rh,h,C4,C8}$ (a) $\mathbf{T}_{8,24,rh,h,C4,C8}$ (b)
$Le(\mathbf{T}_{4,12,C4})$

DUAL OF MEDIAL

Medial *Me* is an important operation of a map. [11] It is achieved as follows: put the new vertices as the midpoints of the original edges. Join two vertices if and only if the original edges span an angle. More exactly, the two edges must be incident and consecutive within a rotation path around their common vertex in the original map.

The medial graph is a subgraph of the line-graph. [15] In the line-graph each original vertex gives rise to a complete graph while in the medial graph only a cycle C_d (1.e., a d-membered cycle, d being the vertex degree) is formed. All medials are 4-valent graphs and $Me(M) = Me(Du(M))$. The transformed parameters are:

$$Me(M): \quad \begin{aligned} v^* &= e \\ e^* &= 2e \\ f^* &= f + v \end{aligned}$$

The medial operation rotates parent n-gonal faces by pi/n.

Dual of medial is a composite operation (Figure 6):
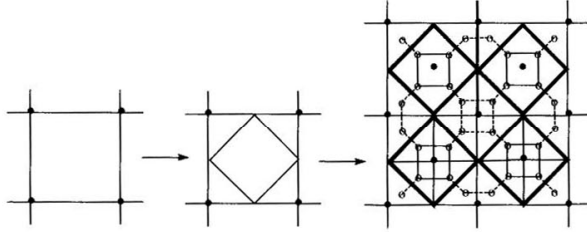
$$Dm = Du(St(Me(M))) \tag{15}$$

FIGURE 6. Stages in a *Dual of medial Dm* transformation of a square net..

Theorem 2.

The vertex multiplication ratio in a Dm transformation is 2d, irrespective of the face boundary polygons. It preserves the initial mutual orientation of all parent faces.

With the observation that each vertex v of M gives rise to twice d new vertices in $Dm(M)$ it is easily to demonstrate that:

$$v^* / v = 2dv / v = 2d \tag{16}$$

and it does not depends on the kind of polygonal faces. The multiplication is twice that induced by Le. Since its consisting simple operations rotate the parent n-gonal faces by an

even number of *pi/n*, the global result of *Dm* is the conservation of their original mutual orientation. The transformed parameters are:
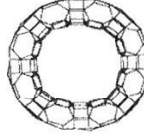
$$Dm(M): \quad v^* = 2dv = 4e$$
$$e^* = 6e$$
$$f^* = f + v + e$$

This operation is particularly applicable to square tori, with a multiplication ratio 8. The expansion is eventually anisotropic, over the two dimensions ($c \times n = 4 \times 2$, and *vice-versa*, for a *h*- and *v*-net, respectively) as illustrated below for the *Dm* transforms of $T_{4,8,C4}$:
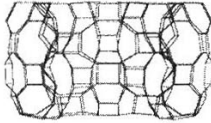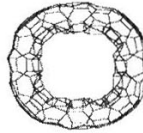
$T_{16,16,h,C4,C8}$ (a)
$Dm(T_{4,8,C4})$; 1
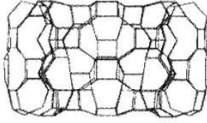
$T_{16,16,h,C4,C8}$ (b)

$T_{8,32,v,C4,C8}$ (a)
$Dm(T_{4,8,C4})$; 2

$T_{8,32,v,C4,C8}$ (b)

Of course, the two tori: $T_{16,16,h,C4,C8}$ (1) and $T_{8,32,v,C4,C8}$ (2) represent one and the same structure. Note that the bounding polygon is an octagon, as expected for a 4-valent regular graph (see above, the medial graph).

Q-Transformation

There exists another transformation that preserves the initial orientations of all parent faces in the map. It is called the *quadrupling* transformation *Q*. [13,14] The *Q* operation can be viewed as a particular case of *Dm*:

$$Q = Du(St(Mer(M)))$$ (17)

with *Mer* being a *reduced medial*, where the face around each original vertex collapses into this vertex, that preserves its original valency (Figure 7).
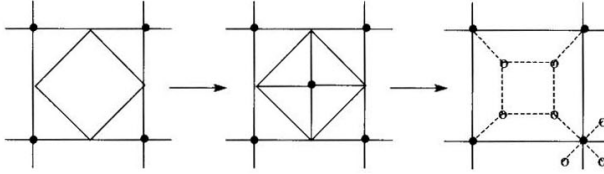

FIGURE 7. *Q* operation in a square face.

Theorem 3.

The vertex multiplication ratio in a Q transformation is $d + 1$ irrespective of the type of tiling the original map.

Keeping in mind that for each vertex v in M results d new vertices in $Q(M)$ and the old vertices are preserved, the demonstration is immediate:

$$v^* = vd + v$$ (18)

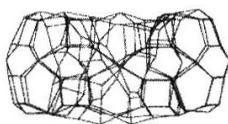and the multiplication ratio:

$$v^*/v = v(d+1)/v = d+1$$ (19)

Q operation involves two *pi/n* rotations, so that the initial orientation of the polygonal faces is conserved.

The transformed parameters are:

$$Q(M): \qquad v^* = v + 2e = v + dv$$
$$e^* = 4e$$
$$f^* = f + e$$

In square nets, this operation leads to nonregular graphs (degree 3 and 4) - as illustrated below:

$Q(\mathbf{T}_{4,8,C4,C6})$ (a)

$Q(\mathbf{T}_{4,8,C4,C6})$ (b)

This operation works well in trivalent maps (e.g. the polyhex tori), with $3 + 1 = 4$, multiplication ratio, and conserving the regular degree 3.

CONCLUSIONS

A square-like toroidal net can be transformed in a variety of derivatives by applying suitable operations. Amond the above discussed operations, some occur with preserving the original valency (i. e., 4 - see the rhomboidal transformation). Some others (e.g., *Le* and *Q* operations) change, partially or totally the initial valency to cubic valency (i.e., 3). Only the novel *Dm* operation is able to transform a square-like torus (a regular graph of degree 4) into a regular, cubic torus, with preserving the original mutual orientation of all parent faces.

In opposition to polyhex tori, more agreed by organic chemists, the square-like tori and their transforms are expected to appear in some supramolecular inorganic compounds (see polyoxometalates [16])

REFERENCES

[1] Iijima, S, *Nature* (London), **1991**, *354*, 56.

[2] Liu, J.; Dai, H.; Hafner, J. H.; Colbert, D. T.; Smalley, R. E.; Tans, S. J.; Dekker, C. Fullerene "crop circles". *Nature* (London), **1997**, *385*, 780-781

[3] Martel, R.; Shea, H. R.; Avouris, P. *Nature* (London), **1999**, *398*, 299.

[4] Kirby, E. C.; Mallion, R. B.; Pollak, P. Toroidal polyhexes. *J. Chem. Soc. Faraday Trans.* **1993**, *89*, 1945-1953.

[5] John, P. E. Kekulé count in toroidal hexagonal carbon cages. *Croat. Chem. Acta,* **1998**, *71*, 435-447.

[6] Ceulemans, A.; Chibotaru, L. F.; Bovin, S. A.; Fowler, P. W. The electronic structure of polyhex carbon tori. *J. Chem. Phys.* **2000**, *112*, 4271-4278.

[7] Gross, J. T.; Tucker, T. W. *Topological Graph Theory*; Wiley Interscience, 1987.

[8] Pisanski, T.; Žitnik, A.; Graovac, A.; Baumgartner, A. Rotagraphs and their generalizations, *J. Chem. Inf. Comput. Sci.* **1994**, *34*, 1090-1093.

[9] Diudea, M. V.; Graovac, A.; A. Generation and graph-theoretical properties of C$_4$-tori. *Commun. Math. Comput. Chem. (MATCH)*, this volume.

[10] King, R. B. Applications of Graph Theory and Topology in Inorganic Cluster and Coordination Chemistry, CRC Press, 1993.

[11] Pisanski, T.; Randić, M. Bridges between Geometry and Graph Theory. In: C. A. Gorini, Ed., *Geometry at Work. A Collection of Papers Showing Applications of Geometry. Math. Assoc. Amer. Notes* , **2000**, *53*, 174-194.

[12] Fowler, P. V.; Steer, J. I. The leapfrog principle: a rule for electron counts of carbon clusters. *J. Chem. Soc. Chem. Commun.* **1987**, 1403-5.

[13] Fowler, P. V.; Cremona, J. E.; Steer, J. I. Systematics of bonding in non-icosahedral carbon clusters. *Theor. Chim. Acta* **1988**, *73*, 1-26.

[14] Brinkmann, G.; Fowler, P. W.; Yoshida, M. New non-spiral fullerenes from old: generalized truncation of isolated-pentagon-triple carbon cages. *Commun. Math. Comput. Chem. (MATCH)*, **1998**, **38**, 7-17.

[15] Harary, F. *Graph Theory*, Addison - Wesley, Reading, M.A., 1969.

[16] Muller, A.; Kogerler, P.; Kuhlman, Ch. A variety of combinatorially linkable units as disposition: from a giant icosahedral Keplerate to multi-functional metal-oxide based network structures. *Chem. Commun.* **1999**, 1347-1358.