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COMPOSITE OPERATIONS ON MAPS

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ABSTRACT. A map *M* is a combinatorial representation of a closed surface. Convex polyhedra, starting from the Platonic solids and going to spherical fullerenes, can be generated by applying some operations on maps. Three composite map operations: leapfrog, chamfering and capra, play a central role in the fullerenes construction and their electronic properties. Generalization of the above operations leads to series of transformations, characterized by distinct, successive pairs in the Goldberg multiplication formula *m*(*a*,*b*). Parents and products of most representative operations are illustrated.

INTRODUCTION

A map *M* is a combinatorial representation of a (closed) surface.[1,2] Let: *v, e, f* – be the number of vertices, edges, faces, *d* – the vertex degree and *s* – the face size, in the map. A subscript "0" will mark the corresponding parameters in the parent map.

Some basic relations in a map, have been discovered by Euler:[3,4]

$$\sum d\, v_d = 2e \tag{1}$$

$$\sum s\, f_s = 2e \tag{2}$$

where v_d and f_s are the number of vertices of degree *d* and number of *s*-gonal faces, respectively and (d, $s \geq 3$). The two relations are joined in the famous formula:

$$v - e + f = 2(1-g) \tag{3}$$

with *g* the genus[5] of a graph (*i.e.*, the number of holes performed on a plastic sphere to make it homeomorphic to the surface on which the given graph is embedded; $g = 0$ for a planar graph and 1 for a toroidal graph).

The nuclearity of fullerene polyhedra can be counted by the Goldberg's[6] relation:

$$m = (a^2 + ab + b^2);\ a \geq b;\ a + b > 0 \tag{4}$$

which predicts the multiplication factor $m = v/v_0$ in a 3-valent map transformed by a given operation (see below). The *m* factor is related to the formula giving the volume of truncated pyramid, of height *h*: $V = mh/3$, coming from the ancient Egypt.

This paper is organized as follows: the second section presents some classical composite operations, with definitions given in terms of simple map operations; the third section deals with generalized operations, inspired from the Goldberg's representation of polyhedra in the (*a*,*b*) "inclined coordinates"; the forth section presents some molecular realization of these composite operations. The last two sections give a summary of the paper and references, respectively.

CLASSICAL COMPOSITE OPERATIONS

We limit here to the most important composite operations, meaning the basic, simple operations, such as: Dual, Medial, Stellation, Truncation, Snub, etc., are known. The reader can consult some already published papers.[1,2,7]

Leapfrog *Le* (*tripling*) operation[8-12] can be written as:

$$Le(M) = Du(P_3(M)) = Tr(Du(M)) \tag{5}$$

where P_3 is a particular case of the *Polygonal* P_s *capping* (s = 3, 4, 5), realizable[13,14] by (i) adding a new vertex in the center of the face, (ii) putting s-3 points on the boundary edges and (iii) connecting the central point with one vertex (the end points included) on each edge. In this way the parent face is covered by trigons (s = 3), tetragons (s = 4) and pentagons (s = 5). The P_3 operation is also called *stellation* or (centered) *triangulation*.

A sequence of stellation-dualization rotates the parent s-gonal faces by π/s. Leapfrog operation is illustrated, for a pentagonal face, in Figure 1.

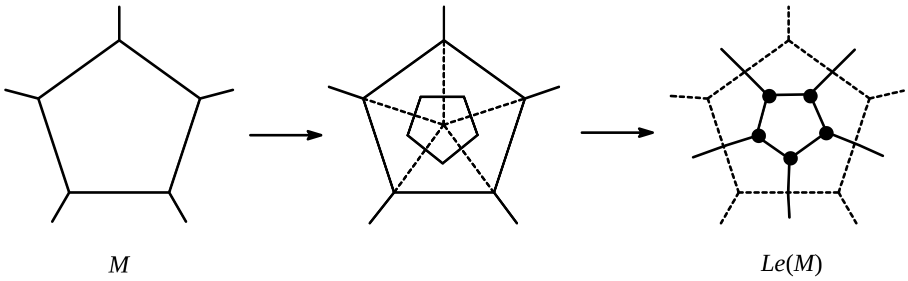

Figure 1. Leapfrogging a pentagonal face of a trivalent map

A bounding polygon, of size $2d_0$, is formed around each original vertex. In the most frequent cases of 4- and 3-valent maps, the bounding polygon is an octagon and a hexagon, respectively.

The complete transformed parameters are:

$$Le(M): \quad v = s_0 f_0 = d_0 v_0\ ;\ e = 3e_0\ ;\ f = v_0 + f_0\ ;\ m(1,1) = 3 \tag{6}$$

In trivalent maps d_0 = 3, so that $Le(M)$ is also called the *tripling* operation. Note that the vertex degree in $Le(M)$ is *always* 3, as a consequence of the dualization of a triangulation.

A nice example of using *Le* operation is: *Le*(Dodecahedron) = Fullerene C_{60}. The leapfrog operation can be used to insulate the parent faces by surrounding bounding polygons.

Chamfering (*quadrupling*) *Q* is another composite operation, achieved by the sequence:[6,13,14]

$$Q(M) = E_{-}(Tr_{P_3}(P_3(M))) \tag{7}$$

where E_{-} means the (old) edge deletion in the truncation Tr_{P3} of the new, face centered, vertices introduced by the P_3 capping (Figure 2). The old vertices are preserved.

The complete transformed parameters are:

$$Q(M): \quad v = (d_0 + 1)v_0;\ e = 4e_0;\ f = f_0 + e_0;\ m(2,0) = 4 \tag{8}$$

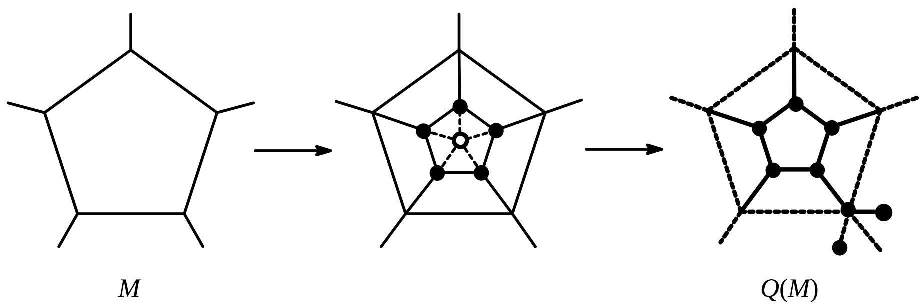

Figure 2. Quadrupling a pentagonal face of a 3-valent map.

Q operation leaves unchanged the initial orientation of the polygonal faces. Note that, the chamfering of a 4-valent map is not a regular graph anymore (because of mixing the new trivalent vertices with the parent 4-valent ones). Only a 3-valent map is chamfered to a 3-regular graph.

Q insulates the parent faces always by hexagons. An example of this operation is: *Q* (Dodecahedron) = Fullerene C_{80}.

The "chamfering" (edge chamfering being equivalent to vertex truncation)[6] is most often called "quadrupling", by the vertex multiplication $m = 4$, in trivalent maps.

Capra *Ca* (*septupling*) - the goat, is the Romanian corresponding of the *leapfrog* English children game. It is a composite operation,[15] necessarily coming third, by the Goldberg's multiplying factor $m(2,1) = 7$.

The transformation can be written as:[14]

$$Ca(M) = Tr_{P_5}(P_5(M)) \tag{9}$$

with Tr_{P5} meaning the truncation of new, face centered, vertices introduced by the P_5 capping (Figure 3). Note that, P_5 involves an E_2 (*i.e.*, edge trisection) operation. *Ca* insulates any face of *M* by its own hexagons, which are not shared with any old face (in contrast to *Le* or *Q*).

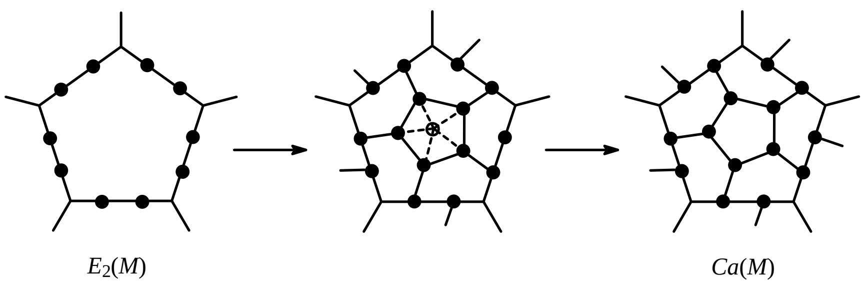

Figure 3. Capring a pentagonal face of a 3-valent map.

Table 1 lists the net parameters in Capra transforms,[15] either in simple or iterative application on finite objects.

According to the *m*-value in trivalent maps, Capra is the *septupling* S_1 operation. A second septupling operation S_2 was defined in ref. 13.

Only a 3-valent regular map leads to a regular 3-valent graph by Capra; clearly, maps/graphs of degree greater than 3 will not be regular anymore.

Table 1.

The transformed parameters by the iterative *Ca* operation

Operation	Parameter
$Ca(M)$	$v_1 = v_0 + 2e_0 + s_0 f_0 = (2d_0 + 1)v_0$
	$e_1 = 7e_0$
	$f_1 = s_0 f_0 + f_0$
$Ca_2(M)$	$v_2 = v_1 + 2e_1 + \sum s f_{1,s} = (16 d_0 + 1)v_0$
	$e_2 = 7^2 e_0$
	$f_2 = \sum s f_{1,s} + f_0 = 8 s_0 f_0 + f_0$
$Ca_n(M)$	case $d_0 > 3$
	$v_n = 8 v_{n-1} - 7 v_{n-2}$; $n \geq 2$

GENERALIZED OPERATIONS

One of us (P. E. J.) has proposed a generalization of operations on maps, inspired from the work of Goldberg,[6] and its representation of polyhedra in the (*a*,*b*) “inclined coordinates” (60^o between axes). The nuclearity multiplicity factor *m* for trivalent maps is given by eq. (4).

Figures 4 and 5 illustrate the method on the hexagonal face. The points of the “master” hexagon must lie either in the center of a lattice hexagon or on a lattice vertex, so that in the center of the parent hexagon must be a new hexagon. The edge length of the parent hexagon is counted by the primitive lattice vectors (*x*,*y*).

A similar procedure was used by Coxeter,[16] who built up icosahedral polyhedra/fullerenes as dual master triangular patches, represented by pairs of integers.

For the (3,2) Cut operation - Figure 5 b, the central face and first connected atoms were cut off.

Some of the generalized composite operations, corresponding to non-prime *m*, can be expressed as operation sequences, as shown in Table 2. It is obvious that (*a*,*a*) and (*a*,0) operations provide achiral products (*e.g.*, fullerenes of the full I_h point group symmetry) while (*a*,*b*), $a \neq b$, result in chiral transformed maps (*e.g.*, fullerenes of therotational *I* point group symmetry) . The (*a*,0) operations produce non-rotated maps. The above generalized operations, as implemented in the software package CageVersatile,[17] work on any face and vertex-degree type maps.

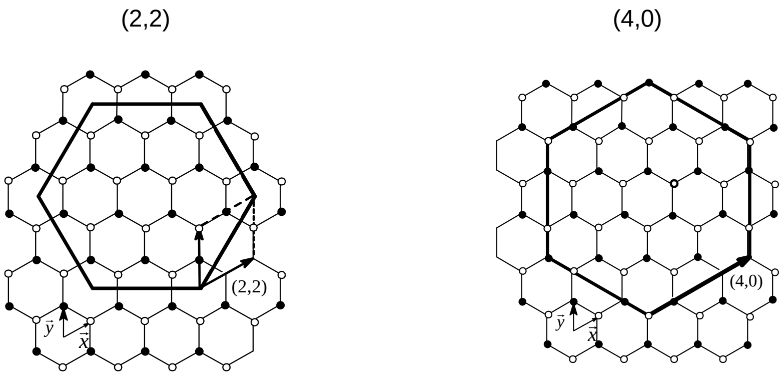

Figure 4. Generalized (*a*, *a*) and (*a*, 0) operations

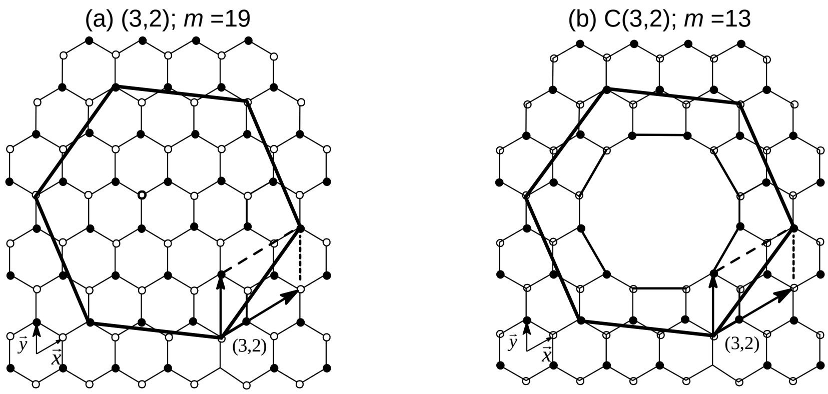

Figure 5. Generalized (*a*, *b*) operation: *a* = *b* + 1 (5a) and (central face and first connected atoms) “cut” C(*a*,*b*) (5b),the last one corresponding to *m*(3,1) =13 factor.

In case of trivalent regular maps, relations (1) and (2) can be rewritten as:

$$3 \cdot v_0 = 2 \cdot e_0 = s_0 \cdot f_0 \tag{10}$$

Keeping in mind the multiplication factor *m* (see (4)), the number of vertices in the transformed map is:

$$v_1 = m \cdot v_0 \tag{11}$$

Eq 10 leads to:

$$3 \cdot v_1 = 3 \cdot m \cdot v_0 = 2 \cdot e_1 \tag{12}$$

$$e_1 = \frac{3}{2} \cdot m \cdot v_0 = \frac{3}{2} \cdot m \cdot \frac{2}{3} e_0 = m \cdot e_0 \tag{13}$$

Table 2.

Inclined coordinates (a, b), multiplication factor $m = (a^2 + ab + b^2)$, number of atoms N and operation symbols (running on the dodecahedral C_{20} fullerene)

	(a, b)	m	N	Operation	Obs.
1	(1, 0)	1	20	I	Identity
2	(1, 1)	3	60	$Le_{1,1}$	Rotated by π / s; achiral
3	(2, 0)	4	80	$Q_{2,0}$	Non-rotated; achiral
4	(2, 1)	7	140	$Ca_{2,1}$	Rotated by $\pi / 2s$; chiral
5	(2, 2)	12	240	$Le_{1,1}$, $Q_{2,0}$	Rotated by π / s; achiral
6	(3, 0)	9	180	$Le_{1,1}$, $Le_{1,1}$	Non-rotated; achiral
7	(3, 1)	13	260	-	Rotated; chiral
8	(3, 2)	19	380	-	Rotated; chiral
8'	C(3, 2)	13	260	-	Rotated; chiral
9	(3, 3)	27	540	$Le_{1,1}$, $Le_{1,1}$, $Le_{1,1}$	Rotated by π / s; achiral
10	(4, 0)	16	320	$Q_{2,0}$, $Q_{2,0}$	Non-rotated; achiral
11	(4, 1)	21	420	$Le_{1,1}$, $Ca_{2,1}$	Rotated; chiral*
12	(4, 2)	28	560	$Q_{2,0}$, $Ca_{2,1}$	Rotated by $\pi / 2s$; chiral
13	(4, 3)	37	740	-	Rotated; chiral
14	(4, 4)	48	960	$Le_{1,1}$, $Q_{2,0}$, $Q_{2,0}$	Rotated by π / s; achiral
15	(5, 0)	25	500	-	Non-rotated; achiral
16	(5, 1)	31	620	-	Rotated; chiral
17	(5, 2)	39	780	-	Rotated; chiral
18	(5, 3)	49	980	$Ca_{2,1}$, $Ca_{2,1}$	Chiral/ achiral*
19	(5, 4)	61	1220	-	Rotated; chiral
20	(5, 5)	75	1500	-	Rotated; achiral

***** achiral, when the sequence $CaR(CaS(M))$ is used.

The above operations introduce new hexagons, keeping the original faces. Thus, the number of faces of any size s in M_1 is:

$$f_{1,s} = f_{1,6} + f_0 \tag{14}$$

Relation (10) becomes:

$$2 \cdot e_1 = \sum s \cdot f_{1,s} = 6 \cdot f_{1,6} + s_0 \cdot f_0 \tag{15}$$

Substitution of e_1 in (15) leads to:

$$f_{1,6} = \frac{m-1}{6} \cdot s_0 \cdot f_0 \tag{16}$$

$$f_{1,s} = \frac{m-1}{6} \cdot s_0 \cdot f_0 + f_0 \tag{17}$$

For the n^{th} iterative operation, one deduces:

$$v_n = m^n \cdot v_0 \tag{18}$$

$$e_n = m^n \cdot e_0 \tag{19}$$

$$f_{n,s} = \frac{m^n - 1}{6} \cdot s_0 \cdot f_0 + f_0 \tag{20}$$

Relations (18) to (20) hold for all the presented operations running on a trivalent regular M_0. In other words, the above relations are true for the 3-valent Platonic solids: tetrahedron *T*, cube *C* and dodecahedron *D*.

For other degree maps, in case of *Le*, *Q* and *Ca* operations, some relations are above presented.

We stress here that, in contrast to the Coxeter[16] procedure our method operates on the original graph (not its dual) which enables the embedding on any kind of close or open surface. Moreover, extensions by "cutting" the master faces have not been explored in the cited literature. Thus, a large palette of polyhedral structures, useful in modeling nanostructures, is available.

MOLECULAR REALIZATION

This section illustrates the “molecular” realization or, in other words, the transformation of molecules (such as graphitoids) by the mathematical operations.

It is well-established that *Le* operating on fullerenes provides Clar fullerenes.[2] The *Q* and *Ca* operations are more related to each other.

Recall that, according to the Clar theory, any polyhedral map may be looked for a perfect Clar structure[2,18] PCS (Figure 6), which is a disjoint set of faces (built up on all vertices in *M*) whose boundaries form a 2-factor. A *k*-factor is a regular *k*-valent spanning subgraph. A PCS is complementary to a Fries structure,[19] which is a Kekulé structure having the maximum possible number of benzenoid (alternating single-double edge) faces. A Kekulé structure is a set of pairwise disjoint edges/bonds of the molecule (over all its atoms) that coincides with a perfect matching and a 1-factor in Graph Theory. A trivalent polyhedral graph, like that of fullerenes, has a PCS if and only if it has a Fries structure.[2] Such structures represent *total resonant sextet* TRS benzenoid molecules and it is expected to be extremely stable, in the valence bond theory.[2,20] Leapfrog *Le* is the only operation that provides PCS transforms.

By extension, Diudea[13] proposed a corannulenic system (Figure 7). A perfect corannulenic structure PCorS is a *disjoint set* of (supra) faces covering all vertices in the molecular graph. The associated Fries-like structure is defined as above but its construction will avoid the corannulenic core vertices.

Among the above three classical composite operations: *Le*, *Q* and *Ca*, none is able to provide a PCorS. It is, however, possible by the operation sequence *Le*(*Q*(*M*)) or *Q*(*Le*(*M*)), as shown in Figure 7. This sequence is equivalent to the generalized (2,2) operation.

The PCorS superimposes over PCS. Thus, any PCorS is necessarily a PCS. The supra-organized corannulenic units are expected to contribute to the stability of the whole molecule.

As above mentioned, operations (*a*,*b*), $a \neq b$, provide chiral transformed maps. It is, however, possible that the horizontal edge of the parent hexagon be inclined either to the right or to the left, thus resulting pair operations and enantiomeric products (see Figure 5).

Figure 6. The transform of dodecahedron - C_{20}, by generalized operation (3,0), leading to perfect Clar PCS structure.

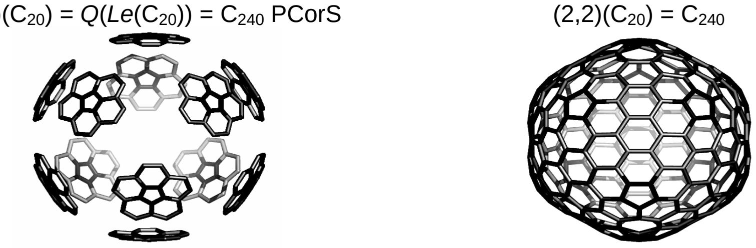

Figure 7. The transform of dodecahedron - C_{20}, by generalized operation (2,2), leading to and perfect corannulenic PCorS structure.

Since pentangulation (2,1) of a face can be done either clockwise or counter-clockwise, it results in an enantiomeric pair of objects: *CaS*(*M*) and *CaR*(*M*), in terms of the sinister/rectus stereochemical isomers.[15] Figure 8 illustrates of such a pair derived from the Dodecahedron.

Figure 8. Enantiomeric pair of the (2,1) Capra transforms of C_{20}

If a composite operation includes an even repetition of a pro-chiral operation, the sequence of one kind pro-chiral operation will lead to either a chiral transform or an achiral object, the last one in case of 1:1 ratio of pro-enantiomeric operations (see Figure 9).

(5,3)(*C*) = *CaS*(*CaS*(*C*)); *m* = 49; *N* = 392
(Rotated; chiral)

(7,0)(*C*) = *CaR*(*CaS*(*C*)); *m* = 49; *N* = 392
(Non-rotated; achiral)

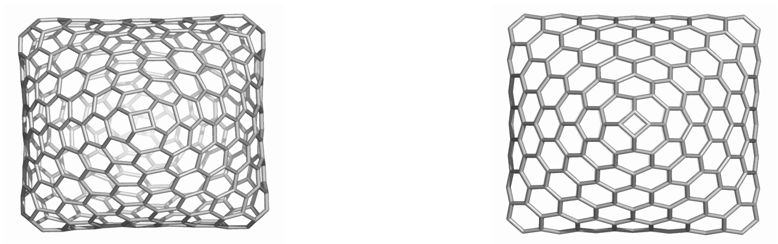

Figure 9. Pair of Capra transforms of the Cube

Other pro-chiral operations are further illustrated: the (3,2) and C(3,2) cut operations working on the dodecahedron (Figure 10). For the procedure working on a hexagonal face see Figure 5.

(3,2)(*D*); *m* =19; *N* =380

C(3,2)(*D*); *m* =13; *N* =260

(a)

(b)

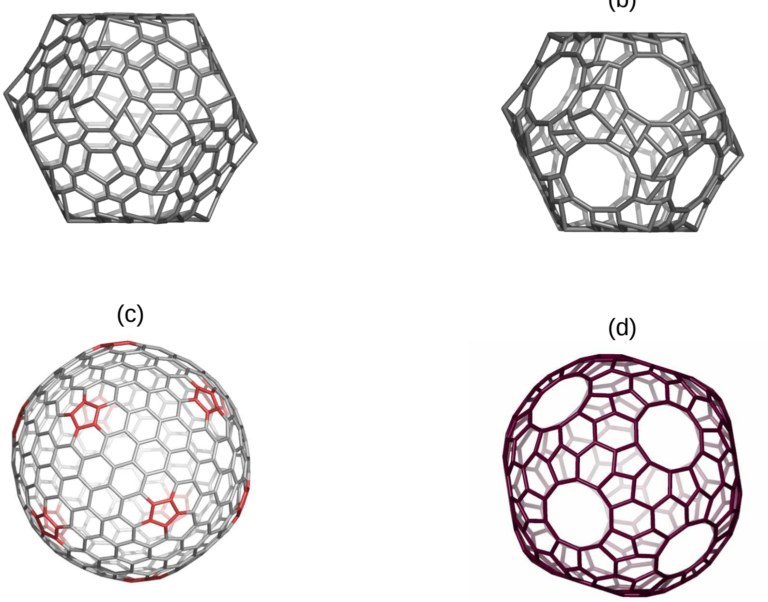

Figure 10. (3,2) and C(3,2) operations performed on the Dodecahedron, non-optimized (a, b) and optimized (c, d).

CONCLUSIONS

Convex polyhedra, starting from the Platonic solids and going to spherical fullerenes, can be generated by map operations.

Three composite map operations: leapfrog, chamfering and capra have been analyzed with respect to their lattice elements.

Generalization of the above operations provided a series of transformations, characterized by distinct, successive pairs in the Goldberg multiplication formula $m(a,b)$.

Parents and products of most representative operations have been illustrated, for finite cages.

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