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Extension of Euler Formula in Multi-Shell Polyhedra

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Abstract. Operations on maps are geometric-topological transformations enabling modification of a given covering of a polyhedral covering. They can be extended to work on all rings of a 3D network, thus generating finite multi-shell polyhedra or infinite periodic units. The obtained structures are evaluated by an extension of Euler formula which accounts for all the distinct elements of a finite CW-complex.

1. Introduction

A map is a combinatorial representation of a (closed) surface S.[1,2] Let us denote in a map: v – the number of vertices, e – the number of edges, f – the number of faces and d – the vertex degree.

Recall some basic relations in a map:

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

$$\sum n\, f_n = 2e \tag{2}$$

where v_d and f_n are the number of vertices of degree d and number of n-gonal faces, respectively. The two relations are joined in the famous Euler (1758) formula:[3]

$$\chi(S) = v - e + f \tag{3}$$

with χ being the Euler *characteristic* of a graph.[4] This formula is useful for checking the consistency of an assumed structure. For a convex polyhedron, which is homeomorphic to a sphere, $\chi = 2$. Positive/negative χ values indicate positive/negative curvature of a surface.

The first rigorous proof of Euler's formula is due to Cauchy. For other proofs, the reader can consult ref. 5.

The Euler characteristic of a closed, orientable, surface is related to its genus g (*i.e.*, the number of tori, in a connected sum decomposition of the surface, or the number of cuts that turn a cyclic structure into a tree - for a sphere, $g = 0$):

$$\chi(S) = 2(1-g) \tag{4}$$

A surface is *orientable*, when it has two sides, or it is *non-orientable*, when it has only one side, like the Möbius strip. In case of a non-orientable surface, the Euler characteristic reads:

$$\chi(S) = 2-n \tag{5}$$

where n is the number of *cross-caps* attached to the sphere to make it homeomorphic to that non-orientable surface.[6]

The Euler characteristic can also be found by integrating the Gaussian curvature K of a surface (the Gauss-Bonnet theorem).[7,8]

$$\int_S KdS = 2\pi\chi(S) \tag{6}$$

A discrete analog of the Gauss-Bonnet theorem is Descartes' theorem[22,23] that states the "total defect" of a polyhedron, measured in full circles, is proportional to the Euler characteristic of the polyhedron:

$$\sum_p^S \phi_p = 2\pi\chi(S) \tag{7}$$

For any finite CW-complex, the Euler characteristic χ can be defined as the alternating sum:[9]

$$\chi = k_0 - k_1 + k_2 - k_3 + \dots, \tag{8}$$

where k_n denotes the number of cells of dimension n in the complex. It can also be defined by using the Betti numbers, in terms of homology groups.[10]

Several transformations (*i.e.*, operations) on maps are known and used for various purposes. Among the basic map operations, the most important are dualization, truncation, medial, and the composite operations: leapfrog, chamfering and capra. The reader can find more about map operations in some recent monographs.[11,12] In the hereafter discussion, these transformations are operated basically on the Platonic objects (Figure 1).

Figure 1. The five Platonic polyhedra.

2. Operations in Multi-Shell Polyhedra

Motivation of this study originates in the theory of hyper-cube,[13] expressed by the "cube-into-cube" ^{2}C geometrical representation (Figure 2a) and the experimental existence of "onion"-fullerenes, as well.

Among the basic map operations we focused here on the medial *Med* operation. This is because "bisection" (the other name used for *Med*) is the most natural operation in nature and Cubeoctahedron (shown as double-shell polyhedron in Figure 2b) could intercalate within the cubic crystalline network. In the top of figures, lattice data and ring *r* counting polynomials are given.

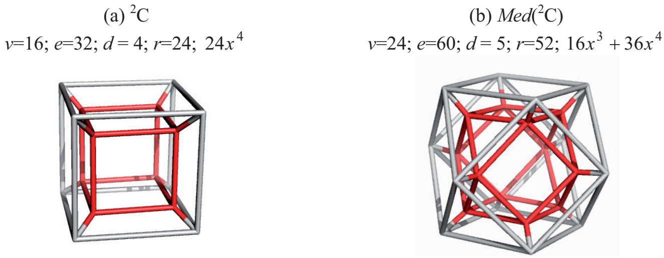


Figure 2. Double-shell polyhedra

Other map operations can also be used for modifying the faces of a "polyhedron-into-polyhedron", either as closed or open structures, as shown in Figures 3 and 4.

A particular result is obtained when the *Med* operation is performed on the "point-into-polyhedron" and acts on *all rings* (see the subscript *_all* at the end of operation name): it leads to a structure type in which *the parent and its transform coexist* (Figure 5).

(a) $Ca(^2\mathrm{C}))$
v=112; e=224; r=144; $96x^4 + 48x^6$

(b) $Op(Ca(^2\mathrm{C})))$
v=160; e=296; r=156; $108x^4 + 48x^7$

Figure 3. Capra transform (a) and the corresponding open structure (b)

(a) $Q(^2\mathrm{C}))$
v=64; e=128; r=84; $60x^4 + 24x^6$

(b) $Op(Q(^2\mathrm{C})))$
v=112; e=200; r=96; $72x^4 + 24x^8$

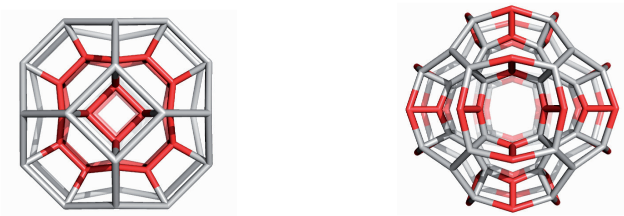


Figure 4. Chamfering transform (a) and its open structure (b)

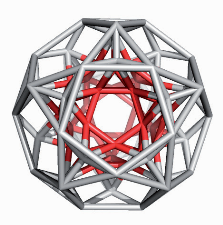
(a) *Med*(CP))_*all*
v=20; e=60; r=56; $44x^3 + 12x^4$

(b) *Med*(OP))_*all*
v=18; e=60; r=58; $52x^3 + 6x^4$

Figure 5. *Med*(MP)_*all* transforms of cube (a) and octahedron (b)

Two *all-Med* transforms, obtained from identical "polyhedron-into-polyhedron" ^{n}P are shown in Figure 6. The procedure was also applied on toroidal ^{2}P structures (Figure 7). A series of interesting structures could be obtained by applying the *all*-operations on the array of 12 dodecahedra (Figure 8).

(a) $Med(^2D))\_all$
v=80; e=240; r=214; $160x^3+30x^4+24x^5$



(b) $Med(^2I))\_all$
v=72; e=240; r=214; $160x^3+30x^4+24x^5$

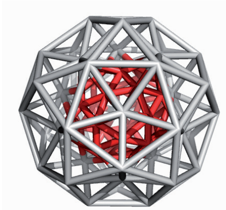
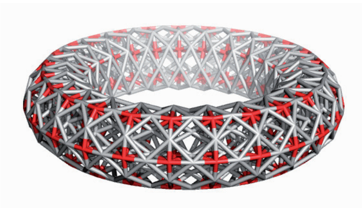


Figure 6. All-*Med*(M) transforms of multi-shell dodecahedron (a) and icosahedron (b)

(a) *Med*(^{2}TOR(4,4)[5,25])_all
v=625; e=2000; r=1750; $1000x^3+750x^4$



(b) *Med*(^{2}TOR(4,4)[5,25])_all (slide)
v=40; e=100; f_3=40; f_4=20; g = 1

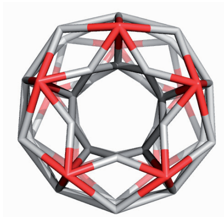
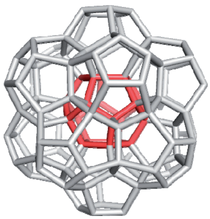
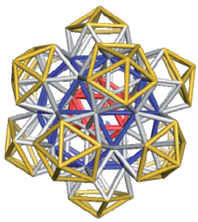


Figure 7. Medial of a double shell toroidal structure

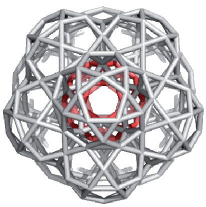
(a) 12×D
v=130; e=230; r=114; $114x^5$



(b) *Du*(12×D)
v=114; e=390; r=310; $310x^3$



(c) *Med*(12×D)
v=230; e=570; r=424; $280x^3+114x^5$



(d) *Le*(12×D)
v=570; e=960; r=424; $50x^3+114x^5+260x^6$

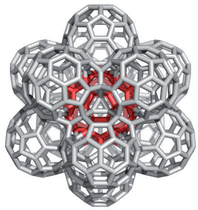


Figure 8. Double-shell polyhedra derived from the 12-array of dodecahedra

Cubeoctahedron could play the role of tetrapodal repeat unit used in the design of spongy carbon architectures.[11,12] Thus, spongy-structures derived from the dodecahedron and cube can be designed by the aid of *Med* operation (Figure 9).

(a) *Med*(*Med*(OP))_*all* v=60; e=156; r=112; $52x^3 + 60x^4$

(b) *Med*(*Med*(IP))_*all* v=150; e=390; r=274; $130x^3 + 120x^4 + 24x^5$

(c) 12×*Med*(*Med*(IP))_*all* v=870; e=2430; r=1818; $810x^3 + 780x^4 + 228x^5$

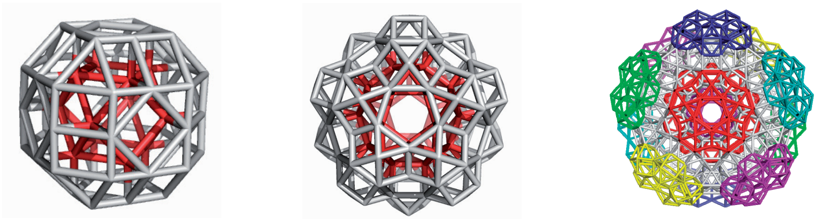


Figure 9. Spongy-structures

The discussed structures have been performed by our original software: CVNET,[14] TORUS[15] and JSCHEM[16].

3. Euler Extended Formula for Multi-Shell Polyhedra.

The Euler formula relates the basic map parameters to the *χ-characteristic* of the surface *S* and the genus *g* of a graph embedded into *S*. In multi-shell polyhedra, the map (a 2D lattice) is changed by a 3D lattice and faces are correspondingly changed by *hard rings* (i.e., those elementary rings that are not the sum of other, smaller rings). In a 3D lattice, an edge can share more than two rings, this fact generating serious problems in counting SSSR (smallest set of smallest rings). Within this paper, the rings are also counted in terms of the ring polynomial.

Let consider the evaluation of Euler χ-characteristic as an alternating sum (eq 8) of the number of cells k_n of dimension n in a finite CW-complex. In a multi-shell polyhedral structure, the cells of dimension n=3 must be accounted, and the Euler formula can read as:

$$v - e + r - p(s-1) = \chi(G) \qquad (9)$$

where p is the number of k_3-cells (i.e., elementary polyhedra) while s is the number of shells; in case of s=1, the classical Euler formula is recovered (after identifying r with f). The results of application of eq 9 are presented in Tables 1 to 7.

Table 1. Euler-Extended Formula in Multi-Shell Platonic ^{n}P Polyhedra

	Object (^{n}P): Ring Polynomial	d	$v-e+r-p(s-1)=\chi$	p
1	^{2}C: $24x^4$	4	16-32+24-6=2	f(C)
2	^{3}C: $42x^4$	5 (8), 4 (16)	24-52+42-6×2=2	f(C)
3	^{2}D: $30x^4+24x^5$	4	40-80+54-12=2	f(D)
4	^{3}D: $60x^4+36x5$	5 (20), 4 (40)	60-130+96-12×2=2	f(D)
5	^{2}I: $40x^3+30x^4$	6	24-72+70-20=2	f(I)
6	^{3}I: $60x^3+60x^4$	7 (12), 6 (24)	36-114+120-20×2=2	f(I)
7	^{2}O: $16x^3+12x^4$	5	12-30+28-8=2	f(O)
8	^{3}O: $24x^3+24x^4$	6 (6), 5 (12)	18-48+48-8×2=2	f(O)
9	^{2}T: $8x^3+6x^4$	4	8-16+14-4=2	f(T)
10	^{3}T: $12x^3+12x^4$	5 (4), 4 (8)	12-26+24-4×2=2	f(T)

Table 2. Euler-Extended Formula in Double-Shell Closed/Open Polyhedra

	Object (^{n}P): Ring Polynomial	d	$v-e+r-p=\chi$	p
1	*Ca*(^{2}C): $96x^4+48x^6$	4	112-224+144-30=2	f(*Ca*(C))
2	*Q*(^{2}C): $60x^4+24x^6$	4	64-128+84-18=2	f(*Q*(C))
3	*Op*(*Ca*(^{2}C)): $108x^4+48x^7$	4(112), 3(48)	160-296+156-24=-4	f(*Op*(*Ca*(C)))
4	*Op*(*Q*(^{2}C)): $72x^4+24x^8$	4(64), 3(48)	112-200+96-12=-4	f(*Op*(*Q*(C)))

Table 3. Euler-Extended Formula in Double-Shell Polyhedra (*Med*(MP)_*all* of Platonics)

	Object (MP): Ring Polynomial	d	$v-e+r-p=\chi$	p
1	CP: $44x^3+12x^4$	6	20-60+56-14=2	f(*Med*(C))
2	DP: $110x^3+24x^5$	6	50-150+134-32=2	f(*Med*(D))
3	IP: $110x^3+20x^4+12x^5$	10(12), 6(30)	42-150+142-32=2	f(*Med*(I))
4	OP: $52x^3+6x^4$	8(6), 6(12)	18-60+58-14=2	f(*Med*(O))
5	TP: $24x^3+6x^4$	6	10-30+30-8=2	f(*Med*(T))

In case of identically transformed shells, p equals the number of faces of the parent map (Tables 1 and 2). When all rings are "operated", the vertex number of the parent map is added (Table 4).

Table 4. Euler-Extended Formula in Multi-Shell *Med*(^{n}P)_*all* Polyhedra

	Object (^{n}P): Ring Polynomial	d	$v-e+r-p(s-1)=\chi$	p
1	^{2}C: $64x^3+24x^4$	6	32-96+88-22=2	f(*Med*(C)) + v(C)
2	^{3}C: $120x^3+42x^4$	8 (12), 6 (40)	52-168+162-22×2=2	f(*Med*(C)) + v(C)
3	^{2}D: $160x^3+30x^4+24x^5$	6	80-240+214-52=2	f(*Med*(D)) + v(D)
4	^{3}D: $300x^3+60x^4+36x^5$	8 (30), 6 (100)	130-420+396-52×2=2	f(*Med*(D)) + v(D)
5	^{2}I: $160x^3+30x^4+24x^5$	10 (12), 6 (60)	72-240+214-44=2	f(*Med*(I)) + v(I)
6	^{2}O: $64x^3+24x^4$	8 (6), 6 (24)	30-96+88-20=2	f(*Med*(O)) + v(O)
7	^{3}O: $120x^3+42x^4$	8 (24), 6 (24)	48-168+162-20×2=2	f(*Med*(O)) + v(O)
8	^{2}T: $40x^3+6x^4$	6	16-48+46-12=2	f(*Med*(T)) + v(T)
9	^{3}T: $60x^3+24x^4$	8 (6), 6 (20)	26-84+84-12×2=2	f(*Med*(T)) + v(T)

Table 5. Euler-Extended Formula in Double-Shell Toroidal Polyhedra

	Object: Ring Polynomial	d	$v-e+r-p=\chi$	p
1	^{2}TOR(4,4)[7,7]: $49x^4$	5	98-245+196-49=0	f(TOR(4,4)[7,7])
2	*Med*(^{2}TOR(4,4)[7,7])_*all*: $392x^3+294x^4$	8 (49), 6 (196)	245-784+686-147=0	f(*Med*(TOR(4,4)[7,7]))+ f(TOR(4,4)[7,7]) =98+49
3	*Med*(^{2}TOR (4,4)[5,25])_*all*: $1000x^3+750x^4$	8 (125), 6 (500)	625-2000+1750-375=0	f(*Med*(TOR(4,4)[5,25]))+ f(TOR(4,4)[5,25]) =250+125

Table 6. Euler-Extended Formula in Multi-Shell Convex Polyhedra

	Object: Ring Polynomial	d	$v-e+r-p=\chi$	p
1	(12×D): $114x^5$	3 (60), 4(70)	130-230+114-12=2	f(D)
2	*Du*(12×D)_*all*: $310x^3$	10 (42), 5 (72)	114-390+310-32=2	f(I) + v(I)
3	*Med*(12×D)_*all*: $280x^3+114x^5$	4 (120), 6 (110)	230-570+424-52=2	f(D) + 2f(I)
4	*Le*(12×D)_*all*: $50x^3+114x^5+260x^6$	3 (360), 4 (210)	570-960+424-32=2	$f(C_{60})$

Table 7. Euler-Extended Formula in Spongy Polyhedra

	Object: Polynomials	d	$v-e+r-p=\chi$	p
1	*Med*(*Med*(IP))_*all*: $R(G)=130x^3+120x^4+24x^5$	6 (90), 4 (60)	150-390+274-32=2	f(*Med*(I))
	$F(G)=100x^3+120x^4+0x^5$	faces	150-390+220-0=-20	g=11
2	12×*Med*(*Med*(IP))_*all*: $R(G)=810x^3+780x^4+228x^5$	4 (180), 6 (690)	870-2430+1818-256=2	256=130+114+12
	$F(G)=580x^3+780x^4+0x^5$	faces	870-2430+1360-0=-200	g=101
3	*Med*(*Med*(OP))_*all*: $R(G)=52x^3+60x^4$	6 (36), 4 (24)	60-156+112-14=2	f(*Med*(O))
	$F(G)=40x^3+48x^4$	faces	60-156+88-0=-8	g=5

The objects derived from the array of 12 dodecahedra (Figure 8 and Table 6) open the way to the quasi-crystals[17] of fullerenes. Our energetic calculations have shown good stability for such 3D conglomerates.

Spongy structures, (Figure 9) are of particular interest because of their hollows/channels. When consider the rings and all the cells filling the space, g=0, as for any spherical polyhedron. When only the faces are considered, the multi-tori character is revealed, and corresponding high genera (Table 7). The deleted triangles in 12×*Med*(*Med*(IP))_*all* (Table 7, second row) equal the number of edges (230) in the 12×D array (Table 6, first row) while the pentagons are now channels. In case they will be synthesized, *e.g.*, by using appropriate MOFs, a catalytic activity can be predicted,[18] like that of the natural zeolites. Energetic and crystallographic calculations are in progress.

4. Conclusions

The map operations enable modification of a given polyhedral tessellation. More over, they can be applied on 3D lattices to give multi-shell polyhedra. Among these operations, the Medial was particularly useful in generating finite objects or infinite periodic units. The designed multi-shell polyhedra obey the novel extension of the well-known Euler formula which accounts for the distinct elementary polyhedra glued together (by identification of common features) in more complex architectures.

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