Volume 31 Number 2 February 2010 ISSN 0195-6698

ELSEVIER

European Journal of Combinatorics

Editors-in-Chief: P. Ossona de Mendez and P. Rosenstiehl

European Journal of Combinatorics 31 (2010) 649–675

Contents lists available at ScienceDirect

European Journal of Combinatorics

journal homepage: www.elsevier.com/locate/ejc

Some problems, I care most

Michel Deza

Ecole Normale Superieure, Paris, France
JAIST, Ishikawa, Japan

ARTICLE INFO

Article history:
Available online 19 April 2009

Ten problems

I. Perfect matroid designs
II. (a) Infinite hypermetrics
    (b) l_1-embedding of complexes
III. (a) Fullerenes: IQ, Skyrmions, viruses
    (b) Space fullerenes
IV. (a) Zigzags and railroads in fullerenes
    (b) Zigzags and Lins triality of maps
V. (a) Three classes of exotic plane graphs
    (b) Ambiguous boundaries of polycycles
VI. Extreme physical distances

I. Perfect Matroid Designs

P.J. Cameron and M. Deza, *Designs and Matroids*, in Handbook of Combinatorial Designs, 2nd ed. by C. J. Colbourn and J. Dinitz, Discrete Math. and Appl. **42**, Chapman and Hall/CRC, 2006, Ch. VII.10 (847–851).

Perfect Matroid Designs

- A perfect matroid design, or PMD, is a matroid M, of rank r such that all flats of rank i, $0 \leq i \leq r$, have the same cardinality f_i.
  The tuple $(f_0, f_1, \dots, f_r)$ is the type of M.

E-mail address: Michel.Deza@ens.fr.

doi:10.1016/j.ejc.2009.03.019

- The geometrisation of a PMD of type $(f_0, f_i, \dots, f_r)$ is a PMD of type $(f_0', f_1', \dots, f_r')$, where $f_i' = (f_i - f_0)/(f_1 - f_0)$. In particular, $f_0' = 0, f_1 = 1$.
- PMDs are (Deza, 1978) the extremal case for family A of k-subsets of a given v-set intersecting pairwise in $l_0, l_1 \dots, l_t$ elements. Namely, for $v > v_0(k)$, it holds:
  $|A| \leq \prod_{0 \leq i \leq t} \frac{v - l_i}{k - l_i}$ with equality if and only if A is the hyperplane family of a PMD with type $(l_0, l_1, \dots, l_t, k, v)$.

Known necessary conditions for PMD

If there exists a PMD of type $(0, 1, f_2, \dots, f_r)$, then:

1. $\prod_{i \leq k \leq j-1} \frac{f_l - f_k}{f_j - f_k}$ is a non-negative integer for $0 \leq i < j \leq l \leq r$;
2. $f_i - f_{i-1}$ divides $f_{i+1} - f_i$ for $2 \leq i \leq r - 1$;
3. $(f_i - f_{i-1})^2 \leq (f_{i+1} - f_i)(f_{i-1} - f_{i-2})$ for $1 \leq i \leq r - 1$.

The above necessary conditions are not sufficient; for example, (R. M. Wilson), no PMD of type (0, 1, 3, 7, 43) or (0, 1, 3, 19, 307) exists.

All known geometric PMDs

They are truncations of the following 5 examples:

- Free matroids, with $f_i = i$ for all i.
- Finite projective spaces over a field GF_q, with $f_i = \frac{q^i - 1}{q - 1}$.
- Finite affine spaces: the points are the vectors in a vector space of rank r over GF_q and $f_i = q^i$.
- Steiner systems $S(t, k, v)$: the hyperplanes are the blocks. These PMDs have rank $t + 1$ and $f_i = i$ for $i < t, f_t = k, f_{t+1} = v$.
- Triffids (Hall triple systems) of type $(0, 1, 3, 9, 3^n)$.

Triffids and their algebraic siblings

So, a triffid is any PMD of rank 4 with type $(0, 1, 3, 9, 3^n)$.
Those PMDs are equivalent to each of following structures:

- Hall triple system: a Steiner triple system $S(2, 3, 3^n)$ on E, $|E| = 3^n$, such that, for any point $a \in E$, there exists an involution for which a is a unique fixed point.
- Finite exponent 3 commutative Moufang loop: a finite commutative loop $(L, \cdot)$, such that, for any $x, y, z \in L$, it holds $(x \cdot x) \cdot x = 1$ and $(x \cdot x) \cdot (x \cdot z) = (x \cdot y) \cdot (x \cdot z)$.
- Distributive Manin quasigroup: a groupoid $(Q, \circ)$, such that all translations are automorphisms and the relation $x \circ y = z$ is preserved under permutation of the variables.
- Restricted Fischer pair (G, F): a group G having commutative center $\{1\}$ and generated by a subset F with $x^2 = 1 = (xy)^3$ and $xyx \in F$ (for any $x, y \in F$).

The problem of PMD existence

- To decide the wide gap between known examples of PMD and necessary conditions. For example, it is not known whether there is a PMD of type (0, 1, 3, 13, 183), (0, 1, 3, 13, 313), or (0, 1, 3, 15, 183).
- U. S. R. Murty, H. P. Young and J. Edmonds, *Equicardinal matroids and matroid-designs*, in Proc. 2nd Chapel Hill Conference on Combinatorial Structures and Applications, 498–547, Gordon and Breach, New York, 1970.

- M. Deza and G. Sabidussi, *Combinatorial structures arising from commutative Moufang loops*, Chapter VI in Quasigroups and Loops: Theory and Applications, ed. by O.Chein et al., Sigma Series in Pure Mathematics **8**, 151–160, Heldermann, Berlin, 1990.

IIa. Hypermetrics

Hypermetric inequalities

- If $b \in \mathbb{Z}^n$, $\sum_{i=1}^n b_i = 1$, then hypermetric inequality is:

$$H(b)d = \sum_{1 \le i < j \le n} b_i b_j d(i,j) \le 0.$$

- If $b = (1, 1, -1, 0, \dots, 0)$, then $H(b)$ is triangle inequality.
- If $b = (1, 1, 1, -1, -1, 0, \dots, 0)$, then $H(b)$ is pentagonal inequality.
- The hypermetric cone HYP_n is the set of all d such that $H(b)d \le 0$ for all b.
- The cone HYP_n has full dimension $\binom{n}{2}$.
- HYP_n is defined by an infinite set of inequalities, but it is polyhedral (Deza–Grishukhin–Laurent, 1993).

Three cones

A cut semi-metric on $\{1, \dots, n\}$, for $S \subset \{0, \dots, n\}$, is:

$$\delta_S(i,j) = \begin{cases} 1 & \text{if } |S \cap \{i,j\}| = 1, \\ 0 & \text{otherwise.} \end{cases}$$

Cut cone CUT_n is generated by all δ_S; metric cone MET_n is generated by all n-vertex semi-metrics. Deza, 1960:

- $CUT_n \subset HYP_n \subset MET_n$ for all $n \ge 3$;
- $HYP_n = MET_n$ if and only if $n = 3, 4$;
- $CUT_n = HYP_n$ if and only if $3 \le n \le 6$.
- The facets ($3\binom{n}{3}$, 1 orbit) of MET_n and extreme rays ($2^{n-1} - 1$, $\lfloor \frac{n}{2} \rfloor$ orbits) of CUT_n are simple.

  But direct computation of HYP_n, $n \ge 7$, is too hard.

The cone HYP_7

Deza and Dutour, 2004: HYP_7 has 3773 facets in 14 orbits below and 31170 extreme rays in 29 orbits (incl. 3 of CUT_7).

$(1, 1, -1, 0, 0, 0, 0)$	$(1, 1, 1, -1, -1, 0, 0)$
$(1, 1, 1, 1, -1, -2, 0)$	$(2, 1, 1, -1, -1, -1, 0)$
$(1, 1, 1, 1, -1, -1, -1)$	$(2, 2, 1, -1, -1, -1, -1)$
$(1, 1, 1, 1, 1, -2, -2)$	$(2, 1, 1, 1, -1, -1, -2)$
$(3, 1, 1, -1, -1, -1, -1)$	$(1, 1, 1, 1, 1, -1, -3)$
$(2, 2, 1, 1, -1, -1, -3)$	$(3, 1, 1, 1, -1, -2, -2)$
$(3, 2, 1, -1, -1, -1, -2)$	$(2, 1, 1, 1, 1, -2, -3)$

First 10 orbits above are also of facets of CUT_7 (among its 38780 facets in 36 orbits).

MET_7 has 105 facets (1 orbit) and 55226 extreme rays (46).

HYP_8 has $\ge$7126560 extreme rays in $\ge$381 orbits.

Finite hypermetrics

- Assouad and Deza, 1979: a rationally-valued $d \in MET_n$ belongs to CUT_n iff λd, for a scale λ, is an isometric subspace of the path-metric of a hypercube graph H_m.
- Assouad, 1982: $d \in HYP_n$ iff d^2 is an isometric subspace of Euclidean space $(\mathbb{R}^{n-1}, l_2)$, generating a lattice.
  If $d = d_{path}(G)$ of n-vertex graph G, then $d \in HYP_n$ if and only if the above lattice is a root lattice.
- If $d = d_{path}(G)$ of n-vertex graph G, then $d \in MET_n$.
  Deza and Terwilliger, 1987: $d_{path}(G) \in HYP_n$ iff $2d$ is an isometric subspace of a direct product of copies of $\frac{1}{2}H_m$ $(m \geq 7)$, $K_{m\times 2}$ $(m \geq 7)$ and the Gosset graph G_{56}.
  Shpectorov; Deza–Grishukhin, 1993: $d_{path}(G) \in CUT_n$ if and only if $2d_{path}(G)$ is an isometric subspace of a direct product of copies of $\frac{1}{2}H_m$ and $K_{m\times 2}$ only.

Problem: Infinite hypermetrics

- Wanted: infinitary version of the above theory.
  Elements of HYP_∞ correspond to "towers of lattices" since any finite sub-hypermetric correspond to a lattice.
  Example of difficulties: garland of hyperoctahedra $K_{m\times 2}$, $m \to \infty$, is not scale-isometric subspace of H_∞ (even of Z_∞), while any of its n-point metric subspaces belongs to CUT_n (equivalently, l_1-embeddable).
- Some infinite hypermetrics are not Lipschitz-embeddable into l_1, while any of their finite subspaces is l_1-embeddable.
  Arora, Lovasz et al, 2005, using Deza–Maehara, 1990: for every $n \geq 2$, some n-point hypermetrics require distortion at least of order $(\log_n)^{0.6}$ for embedding into l_1.
- If (X, d) is a finite hypermetric space, then (X, d^2) is an isometric subspace of an Euclidean sphere $(\mathbb{S}^m, l_2)$.
  For which infinite hypermetrics it holds?
- A Banach space is isometric to a subspace of a Hilbert space if and only if it satisfies the parallelogram law. But, Neyman, 1984: any l_p with $p \neq 2$ cannot be characterized by a finite number of equalities or inequalities.
  But all $\leq n$-point l_1-metrics are: $<\infty$ linear inequalities.
- Mendel and Naor, 2006: metric cotype 2, first non-trivial non-linear (on squared distances) inequality in l_1.
- More information on hypermetrics, l_1-embedding and scale hypercube embedding are in books:
  M. Deza and M. Laurent, *Geometry of Cuts and Metrics*, Springer-Verlag, 1997, and its follow-up
  M. Deza, V.P. Grishukhin and M. Shtogrin, *Scale isometric polytopal graphs in hypercubes and cubic lattices*, Imperial College Press, World Scientific, 2004.

IIb. l_1-embedding of complexes

M. Deza, M. Dutour and S. Shpectorov, *Isometric embedding of Wythoff polytopes into cubes and half-cubes*, Ars Mathematica Contemporanea **1** (2008) 99–111.

l_1-embedding of graphs

- A metric d is l_1-embeddable if it embeds isometrically into the metric space l_1^k for some dimension k.
- An n-point metric d is l_1-embeddable iff $d \in CUT_n$
  (The path-metric d_G of) a finite graph G is l_1-embeddable iff there exists its scale λ embedding into a hypercube H_m, i.e., a vertex mapping $\phi : G \to \{0, 1\}^m$, such that $d(\phi(x), \phi(y)) = \lambda d_G(x, y)$.
- Scale 1 embedding is isometric hypercube embedding,
  scale 2 embedding is isometric half-cube embedding.

- H_m embeds in $J(2m, m)$ and $J(m, s)$ embeds in $\frac{1}{2}H_m$.
  The Johnson graph $J(m, s)$ is formed by all s-subsets of $\{1, \dots, m\}$ with subsets S, T being adjacent if $|S \Delta T| = 2$.
- A complex X embeds into H_m or $\frac{1}{2}H_m$ if its skeleton embeds into hypercube H_m with scale 1 or 2.

Regular (convex) polytopes

A regular polytope is a polytope, whose symmetry group acts transitively on its set of flags. The list consists of:

Regular polytope	Group
Regular polygon P_n	$I_2(n)$
Icosahedron and Dodecahedron	H_3
600-cell and 120-cell	H_4
24-cell	F_4
γ_d (hypercube) and β_d (cross-polytope)	B_d
α_d (simplex)	$A_d = Sym(d+1)$

There are 3 regular tilings of Euclidean plane ((3^6), (6^3), $(4^4) = \delta_2 = \mathbb{Z}^2$) and infinity of (p^q) on hyperbolic plane $\mathbb{H}^2$.

All non-polytopal regular tilings of dimension $d \geq 3$, are: Euclidean $\delta_d = \mathbb{Z}^d$, two sporadic tilings of $\mathbb{R}^4$ and 15, 7, 5 tilings of $\mathbb{H}^d$ with $d = 3, 4, 5$, respectively.

l_1-embedding of regular tilings

- Deza–Shtogrin, 2000: all l_1-embeddable (skeletons of) d-dimensional ($d \geq 2$) regular tilings and honeycombs are: all with $d < 3$, α_d, β_d and all 13 bipartite ones:
  γ_d, δ_d and 8, 2, 1 hyperbolic tilings with $d = 3, 4, 5$.
- So, for $d > 2$: all 3 series of polytopes (on $\mathbb{S}^d$), the unique series on $\mathbb{R}^d$ and all 11 bipartite tilings of $\mathbb{H}^d$.
- Four infinite series δ_d, γ_d, α_d and β_d embed into Z^d, H_d, $\frac{1}{2}H_{d+1}$ and (with scale $2t$, for $t = \lceil \frac{d}{4} \rceil$) H_{4t}, respectively.
- Existence of an Hadamard matrix and a finite projective plane have equivalents in terms of variety of those embeddings of β_d and α_d, respectively.
- The bipartite tilings are those with cells δ_m, γ_m and (6^3); all 11 such hyperbolic tilings embed into $\mathbb{Z}^\infty$.

Wythoff construction

- For a $(d-1)$-dimensional complex $\mathcal{K}$, a flag is a sequence (f_i) of faces with $f_0 \subset f_1 \subset \cdots \subset f_u$.
- The type of a flag is the sequence $dim(f_i)$.
- Given a non-empty subset S of $\{0, \dots, d-1\}$, the Wythoff (kaleidoscope) construction is a complex $P(S)$, whose vertex-set is the set of flags with fixed type S.
- The other faces of $\mathcal{K}(S)$ are expressed in terms of flags of the original complex $\mathcal{K}$.

Formalism of faces of Withoffian $\mathcal{K}(S)$

- Set $\Omega = \{\emptyset \neq V \subset \{0, \dots, d\}\}$ and fix an $S \in \Omega$.
  For subsets $U, U' \in \Omega$, we say that U' blocks U (from S) if, for all $u \in U$ and $v \in S$, there is an $u' \in U'$ with $u \leq u' \leq v$ or $u \geq u' \geq v$. This defines a binary relation on Ω (i.e., on subsets of $\{0, \dots, d\}$), denoted by $U' \leq U$.
- Write $U' \sim U$, if $U' \leq U$ and $U \leq U'$, and
  write $U' < U$ if $U' \leq U$ and $U \not\leq U'$.
- Clearly, $\sim$ is reflexive and transitive, i.e., an equivalence. $[U]$ is an equivalence class containing U.
- Minimal elements of equivalence classes are types of faces of $\mathcal{K}(S)$; vertices correspond to type S, edges to "next closest" type S' with $S < S'$, etc.

Properties of Wythoff construction

If $\mathcal{K}$ is a $(d-1)$-dimensional complex, then:

- $\mathcal{K}(\{0\}) = \mathcal{K}$ and $\mathcal{K}(\{d-1\}) = \mathcal{K}^*$ (dual complex).
- In general, $\mathcal{K}(S) = \mathcal{K}^*(\{d-1-s : s \in S\})$.
- $\mathcal{K}(\{1\})$ is median complex and $\mathcal{K}(\{0,1\})$ is (vertex) truncated complex.
- $\mathcal{K}$ admits at most $2^d - 1$ different Wythoff constructions.
- $\mathcal{K}(\{0,\dots,d-1\}) = \mathcal{K}^*(\{0,\dots,d-1\})$ is order complex.
  Its skeleton is bipartite and the vertices are full flags. Edges are full (maximal) flags minus some face.
  In general, flags with i faces correspond to faces of dimension $d-i$.

Archimedean polytopes

- An Archimedean d-polytope is a d-polytope, whose symmetry group acts transitively on its set of vertices and whose facets are Archimedean $(d-1)$-polytopes.
- They are classified into dimensions 2 (regular polygons), 3
  (Kepler: 5 (regular) $+13+m$-prisms $+m$-antiprisms) and 4 (Conway and Guy).
- If $\mathcal{K}$ is a regular polytope, then $\mathcal{K}(S)$ is an Archimedean polytope.
- Since $\mathcal{K}(S) = \mathcal{K}^*(\{d-1-s : s \in S\})$, it suffices to consider, for any non-empty subset S of $\{0,\dots,d-1\}$, only $\alpha_d(S)$, $\beta_d(S)$ and $Ico(S)$, 24-cell(S), 600-cell(S).
- A complex X embeds into H_m or $\frac{1}{2}H_m$ if its skeleton embeds into hypercube H_m with scale 1 or 2.

Archimedean l_1-Wythoffians with $d=2$

(non-regular) l_1-Wythoffian	n	Embedding
$(Cuboctahedron)^* = \alpha_3(\{0,2\})^*$	14	H_4
Rhombicuboctahedron= $\beta_3(\{0,2\})$	24	$J(10,5)$
tr Octahedron= $\alpha_3(\{0,1,2\}) = \beta_3(\{0,1\})$	24	H_6
tr Cuboctahedron= $\beta_3(\{0,1,2\})$	48	H_9
tr Icosidodecahedron= $Ico(\{0,1,2\})$	120	H_{15}
Rhombicosidodecahedron= $Ico(\{0,2\})$	60	$\frac{1}{2}H_{16}$
(Icosidodecahedron)$^* = Ico(\{1\})^*$	32	H_6
(tr Icosahedron)$^* = Ico(\{0,1\})^*$	32	$\frac{1}{2}H_{10}$
(tr Dodecahedron)$^* = Ico(\{1,2\})^*$	32	$\frac{1}{2}H_{26}$
(tr Cube)$^* = \beta_3(\{1,2\}^*$	14	$J(12,6)$
(tr Tetrahedron)$^* = \alpha_3(\{0,1\})^*$	8	$\frac{1}{2}H_7$

l_1-Wythoffians of regular d-polytopes

Conjecture: all such non-regular ones are 9 sporadic ones (600-cell$(\{0,1,2,3\})$, 24-cell$(\{0,1,2,3\})$, $Ico(\{0,1,2\})$; $Ico(\{0,2\})$, $Ico(\{1\})^*$, $Ico(\{0,1\})^*$, $Ico(\{1,2\})^*$, $\beta_3(\{1,2\}^*$, $\alpha_3(\{0,1\})^*$) and 6 following infinite series for $d \geq 2$.

1. $\alpha_d(\{k\}) = J(d+1,k+1)$ for $k = 1,\dots,d-2$.
2. $\alpha_d(\{0,d-1\})^* = Vor(A_d) \to H_{d+1}$ (all but 2 antipods).
3. $\alpha_d(\{0,\dots,d-1\}) = Vor(A_d^*) \to H_{\binom{d+1}{2}}$ (permutahedron). Moreover, $Vor(A_d) \to Z^{d+1}$ and $Vor(A_d^*) \to Z^{\binom{d+1}{2}}$.
4. $\beta_d(\{0,\dots,d-1\}) \to H_{d^2}$ (zonotope, not Voronoi).
5. $\beta_d(\{0,\dots,d-2\}) \to H_{d(d-1)}$ (idem, for $d \geq 4$).
6. $\beta_d(\{0,d-1\}) \to H_m$ with scale $2t \geq 2\lceil \frac{d}{4} \rceil$.

Cayley graph construction

- If a group G is generated by $g_1, \ldots, g_t$, then its Cayley graph is the graph with vertex-set G and edge-set:

$$(g, gg_i) \quad \text{for } g \in G \text{ and } 1 \le i \le t.$$

G is vertex-transitive; its path-distance is length of xy^{-1}.
- If P is a regular d-polytope, then its symmetry group is a Coxeter group with canonical generators $g_0, \ldots, g_{d-1}$ and its order complex is:

$$P(\{0, \ldots, d-1\}) = Cayley(G, g_0, \ldots, g_{d-1}).$$

- $Cayley(G, g_0, \ldots, g_{n-1})$ embeds into an H_m (moreover, a zonotope) for any finite Coxeter group G.

All Archimedean order complexes are zonotopes

$\mathcal{K}(\{0, \ldots, d-1\}) = \mathcal{K}^*(\{0, \ldots, d-1\})$	G	n	Embedding
$\alpha_d(\{0, \ldots, d-1\}) = Vor(A_d^*)$	A_d	$(d+1)!$	$H_{\binom{d+1}{2}}$
$\beta_d(\{0, \ldots, d-1\})$ (not Voronoi)	B_d	$2^d d!$	H_{d^2}
$D_d(\{0, 1, \ldots, d-1\})$	D_d	$2^{d-1} d!$	$H_{d(d-1)}$
$I_2(p)(\{0, 1\})$	$I_2(p)$	$2p$	H_p
$I\,co(\{0, 1, 2\})$ = tr Icosidodecahedron	H_3	120	H_{15}
24-cell$(\{0, 1, 2, 3\})$	F_4	1152	H_{24}
600-cell$(\{0, 1, 2, 3\})$	H_4	14400	H_{60}
$E_6(\{0, 1, \ldots, 5\})$	E_6	51840	H_{36}
$E_7(\{0, 1, \ldots, 6\})$	E_7	2903040	H_{63}
$E_8(\{0, 1, \ldots, 7\})$	E_8	696729600	H_{120}

IIIa. Fullerenes: *IQ*, Skyrmions and viruses

M. Deza, *Fullerenes: applications and generalizations*, Preprint 2005-38, Preprint Series of Com^{2}MaC, Pohang University of Science and Technology, 2005.

Fullerenes

- A fullerene F_n is a polyhedron (putative carbon molecule) with n 3-valent vertices and only pentagonal and hexagonal faces. Clearly, $p_5 = 12$ and $p_6 = \frac{n}{2} - 10$.
- F_n exist for all even $n \ge 20$ except $n = 22$.
1, 1, 1, 2, 5 ..., 1812, ... 214127713, ... isomers F_n, for $n = 20, 24, 26, 28, 30 \ldots, 60, \ldots, 200, \ldots$.
- Thurston,1998, implies: no. of F_n grows as n^9.
- **Conjecture** (Goldberg, 1933):
The polyhedron with $m \ge 12$ faces having maximal $IQ = 36\pi\frac{V^2}{S^3}$ is a fullerene (called "medial polyhedron").
IQ is abbreviation for Isoperimetric Quotient.
For solids (Schwarz,1890), it holds: $IQ = 36\pi\frac{V^2}{S^3} \le 1$ with equality only for sphere.

Skyrmions and fullerenes

Conjecture (Battye–Sutcliffe, 2002): any minimal energy Skyrmion (baryonic density isosurface for single soliton solution) with baryonic number (the number of nucleons) $B \ge 7$ is a fullerene F_{4B-8}.

Conjecture (true for $B < 107$; open from $(b, a) = (1, 4)$): there exist icosahedral fullerene as a minimal energy Skyrmion for any $B = 5(a^2 + ab + b^2) + 2$ with integers $0 \le b < a, gcd(a, b) = 1$ (not any icosahedral Skyrmion has minimal energy).

Skyrme, 1962, model is a Lagrangian approximating QCD (a gauge theory based on $SU(3)$ group). Skyrmions are special topological solitons used to model baryons.

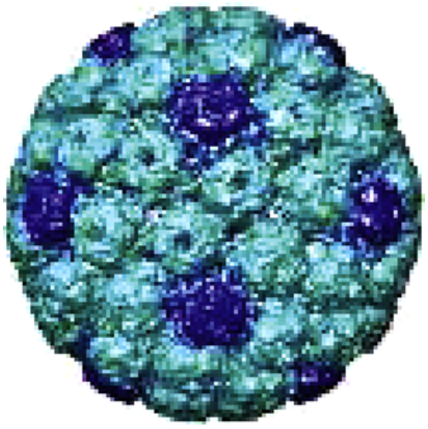
Icosahedral viruses as dual $F_n(I)$, $F_n(I_h)$

- Hippocrates of Kos, circa 400 BC: most diseases come from icosahedra (water) excess in body.
- Caspar and Klug, Nobel prize 1982: virion capsomers are $10T+2$ vertices of icosadeltahedron F^*_{20T}, where $T = a^2 + ab + b^2$ is triangulation number, since capsomers organized quasi-equivalently: in minimal number T of locations with non-equivalent bonding.
  But modern computers cannot evaluate capsid free energy by all-atom simulations. Is virion minimizing free energy and/or IQ-like functional on capsid?
- For icosahedral exceptions: *pseudo-equivalence* and Twarock, 2004, Janner, 2006, Chen et al., 2007. Non-icosahedral fullerene exceptions: retroviruses HIV, RSV and prolate shape of complex phages.

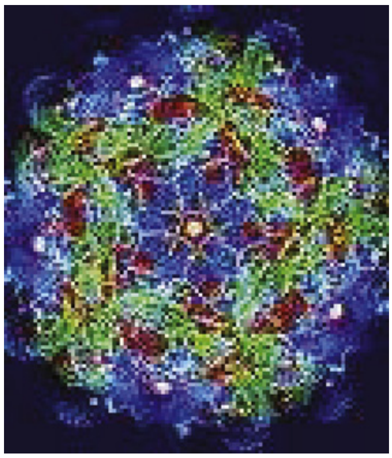
Capsids of icosahedral viruses

(a, b)	$T = a^2 + ab + b^2$	Fullerene	Examples of viruses
(1, 0)	1	$F^*_{20}(I_h)$	*B19 parvovirus, cowpea mosaic virus*
(1, 1)	3	$C^*_{60}(I_h)$	*picornavirus, turnip yellow mosaic virus*
(2, 0)	4	$C^*_{80}(I_h)$	*human hepatitis B, Semliki Forest virus*
(2, 1)	$7l$	$C^*_{140}(I)laevo$	*HK97, rabbit papilloma virus, Λ-like viruses*
(1, 2)	$7d$	$C^*_{140}(I)dextro$	*polyoma (human wart) virus, SV40*
(3, 1)	$13l$	$C^*_{260}(I)laevo$	*rotavirus*
(1, 3)	$13d$	$C^*_{260}(I)dextro$	*infectious bursal disease virus*
(4, 0)	16	$C^*_{320}(I_h)$	*herpes virus, varicella*
(5, 0)	25	$C^*_{500}(I_h)$	*adenovirus, phage PRD1*
(3, 3)	27	$C^*_{540}(I_h)$	*pseudomonas phage phiKZ*
(6, 0)	36	$C^*_{720}(I_h)$	*infectious canine hepatitis virus, HTLV1*
(7, 7)	147	$C^*_{2940}(I_h)$	*Chilo iridescent iridovirus* (outer shell)
(7, 8)	$169d$	$C^*_{3380}(I)dextro$	*Algal chlorella virus PBCV1* (outer shell)
(7, 10)	219	$C^*_{4380}(I)dextro?$	*Algal virus PpV01*

Examples



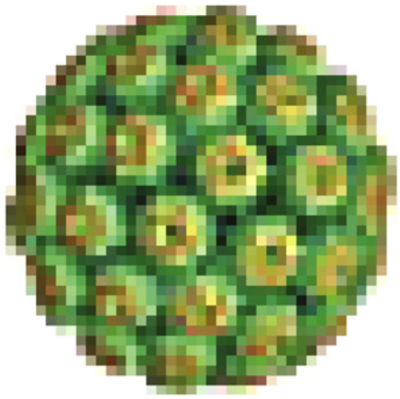
Satellite, $T = 1$, of TMV,
helical Tobacco Mosaic virus 1st
discovered (Ivanovski, 1892), 1st seen
(1930, EM)



Foot-and-Mouth virus,
$T = 3$

Human and simian papilloma viruses

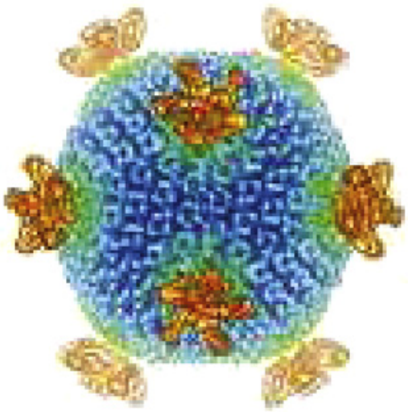
Polyoma virus,
$T = 7d$



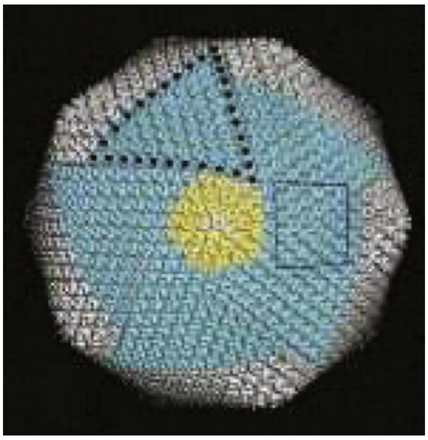
Simian virus 40,
$T = 7d$

TMV, foot-and-mouth virus and papilloma ($T = 7d$) violate quasi-equivalence: there are 72 capsomers (vertices of $C^*_{140}(I)$), but all are 5-mers; so, 360 subunits as for $T = 6$. Twarock, 2004, explained them as Penrose-like tilings of Icosahedron by rhombus and kite.

Large icosahedral viruses



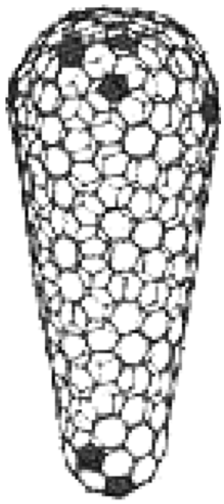
Archeal virus STIV, $T = 31$



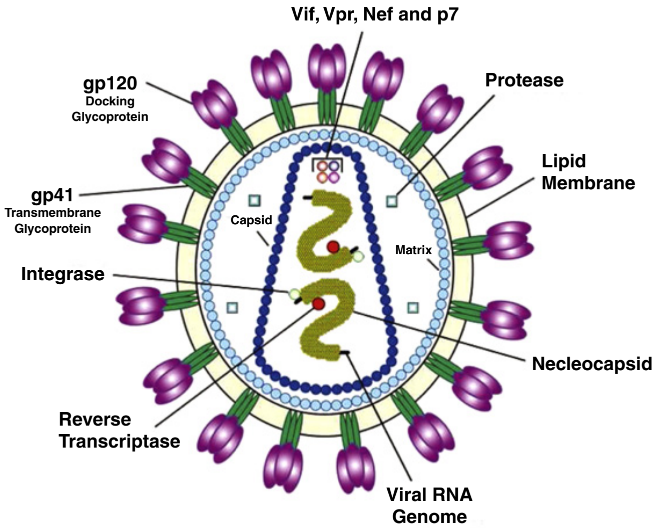
Algal chlorella virus PBCV1
(4th: ≃331.000 bp), $T = 169d$

- Sericesthis and Tipula iridescent viruses: $(12, 1)$, $(7, 7)$?
- Phytoplankton virus PpV01: $T = 219$, largest known T.
- Mimivirus (largest known virus): $1078 \le T \le 1371$; 1179?

HIV conic fullerene; which $F_n(G)$ it is?



Capsid core (7, 5)

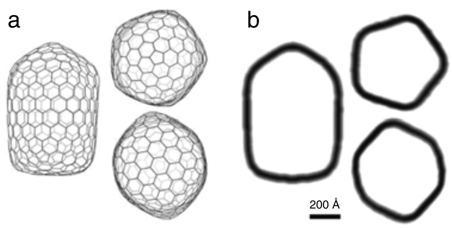


Icosahedral shape (spikes): $T \simeq 71$?

RSV fullerene coffin

Ganser et al., 1999: HIV capsids are conic (5, 7)-fullerenes mainly (but still not visualized at high resolution EM).

Butan et al., 2007: other *retrovirus* (DNA-replicating RNA), avian Rous sarcoma, is in fullerene coffins (5 + 1, 6 + 0 caps).



5+1 and 6+0 caps

IIIb. Space fullerenes

Space fullerenes

Frank–Kasper polyhedra are all four fullerenes with isolated hexagons: $F_{20}(I_h)$, $F_{24}(D_{6d})$, $F_{26}(D_{3h})$, $F_{28}(T_d)$.

FK space fullerene: a 4-valent 3-periodic combinatorial E^3-tiling

by them; space fullerene: such tiling by any fullerene. They occur in soap froths (foams, liquid crystals) and:

- tetrahedrally close-packed phases of metallic alloys,
- clathrates (compounds with 1 component, atomic or molecular, enclosed in the framework of another) incl. clathrate hydrates (cells are solutes, vertices are H_2O, hydrogen bonds) and zeolites (cells are H_2O, vertices are tetrahedra SiO_4 or $SiAlO_4$, oxygen bridges).

Main cases A_{15}, C_{15} correspond to: (a) alloys Cr_3Si, $MgCu_2$; (b) clathrate hydrates of type I, II; (c) zeolite topologies MEP, MTN and (d) clathrasils Melanophlogite, Dodecasil 3C.

24 known FK space fullerenes

t.c.p.	Clathrate, exp. alloy	Sp. group	$\bar{f}$	F_{20}:F_{24}:F_{26}:F_{28}	N
A_{15}	type I, Cr_3Si	$Pm\bar{3}n$	13.50	1, 3, 0, 0	8
C_{15}	type II, $MgCu_2$	$Fd\bar{3}m$	13.(3)	2, 0, 0, 1	24
C_{14}	type V, $MgZn_2$	$P6_3/mmc$	13.(3)	2, 0, 0, 1	12
Z	type III, Zr_4Al_3	$P6/mmm$	13.43	3, 2, 2, 0	7
σ	type IV, $Cr_{46}Fe_{54}$	$P4_2/mnm$	13.47	5, 8, 2, 0	30
H	complex	$Cmmm$	13.47	5, 8, 2, 0	30
K	complex	$Pmmm$	13.46	14, 21, 6, 0	82
F	complex	$P6/mmm$	13.46	9, 13, 4, 0	52
J	complex	$Pmmm$	13.45	4, 5, 2, 0	22
ν	$Mn_{81.5}Si_{8.5}$	$Immm$	13.44	37, 40, 10, 6	186
δ	MoNi	$P2_12_12_1$	13.43	6, 5, 2, 1	56
P	$Mo_{42}Cr_{18}Ni_{40}$	$Pbnm$	13.43	6, 5, 2, 1	56

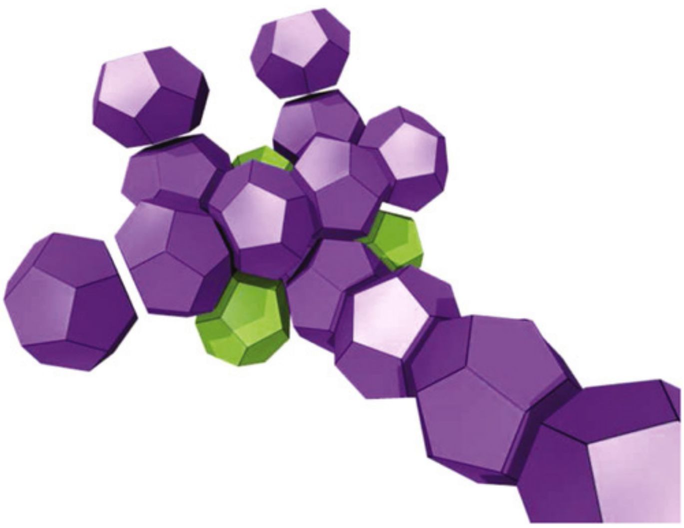
24 known FK space fullerenes

t.c.p.	Exp. alloy	Sp. group	$\bar{f}$	F_{20}:F_{24}:F_{26}:F_{28}	N
K	$Mn_{77}Fe_4Si_{19}$	$C2$	13.42	25,19, 4, 7	220
R	$Mo_{31}Cr_{51}Co_{18}$	$R\bar{3}$	13.40	27, 12, 6, 8	159
μ	W_6Fe_7	$R\bar{3}m$	13.39	7, 2, 2, 2	39
–	K_7Cs_6	$P6_3/mmc$	13.38	7, 2, 2, 2	26
$p\sigma$	$V_6(Fe, Si)_7$	$Pbam$	13.38	7, 2, 2, 2	26
M	$Nb_{48}Ni_{39}Al_{13}$	$Pnam$	13.38	7, 2, 2, 2	52
C	$V_2(Co, Si)_3$	$C2/m$	13.36	15, 2, 2, 6	50
I	$Vi_{41}Ni_{36}Si_{23}$	Cc	13.37	11, 2, 2, 4	228
T	$Mg_{32}(Zn, Al)_{49}$	$Im3$	13.36	49, 6, 6, 20	162
SM	$Mg_{32}(Zn, Al)_{49}$	$Pm\bar{3}n$	13.36	49, 9, 0, 23	162
X	$Mg_{45}Co_{40}Si_{15}$	$Pnmm$	13.35	23, 2, 2, 10	74
–	Mg_4Zn_7	$C2/m$	13.35	35, 2, 2, 16	110

FK space fullerene A_{15} (β-W phase)

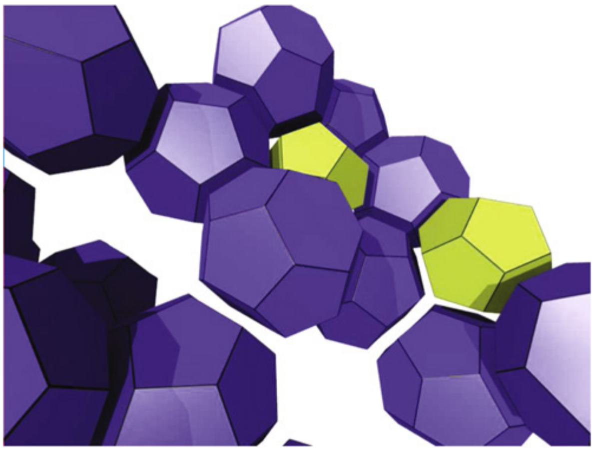
Gravicenters of cells F_{20} (atoms Si in Cr_3Si) form the bcc network A_3^*. Unique with its fractional composition (1, 3, 0, 0).

Oceanic methane hydrate (with type I, i.e., A_{15}) contains 500–2500 Gt carbon; cf. ∼230 for other natural gas sources.

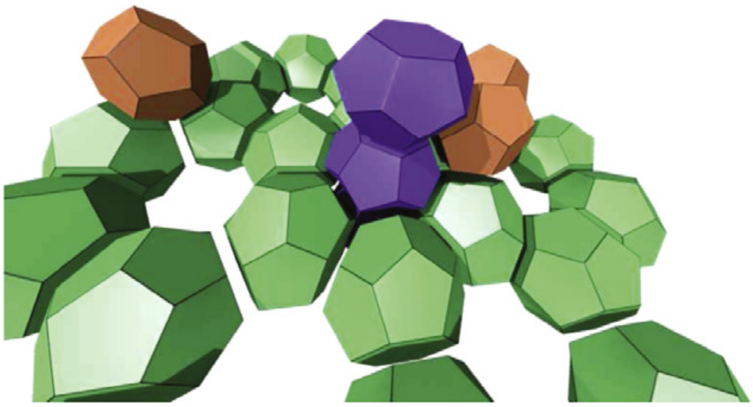


FK space fullerene C_{15}

Cubic $N = 24$; gravicenters of cells F_{28} (atoms Mg in $MgCu_2$) form diamond network (centered A_3). Cf. $MgZn_2$ forming hexagonal $N = 12$, variant C_{14} of diamond: lonsdaleite found in meteorites, 2nd in a continuum of (2, 0, 0, 1)-structures.



FK space fullerene Z



Z is also not unique with its fraction $(3, 2, 2, 0)$.

Computer enumeration

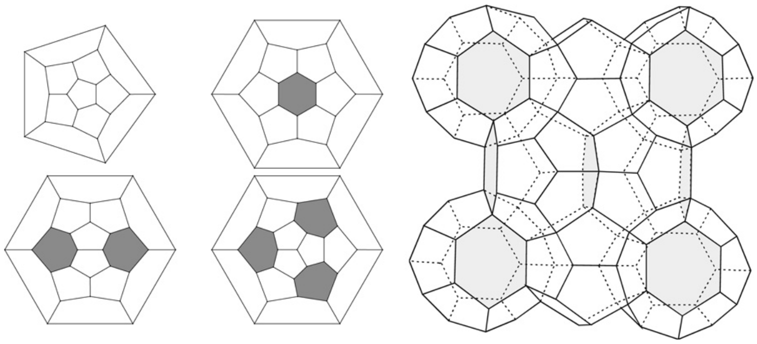
Dutour–Deza–Delgado, 2008, found 84 FK structures (including 13 of 24 known ones) with $N \leq 20$ fullerenes in reduced (i.e. by a Biberbach group) fundamental domain.

# 20	# 24	# 26	# 28	Fraction	N (nr. of)	n (known structure)
4	5	2	0	Known	11(1)	22(J complex)
8	0	0	4	Known	12(1)	6, 12(C_{14}), 24(C_{15} et al.)
7	2	2	2	Known	13(5)	26(−), 26($p\sigma$), 39(μ), 52(M)
6	6	0	2	New	14(3)	–
6	5	2	1	Known	14(6)	56(δ), 56(P)
6	4	4	0	Known	14(4)	7(Z)
7	4	2	2	Counterexample	15(1)	–
5	8	2	0	Known	15(2)	30(σ), 30(H)
9	2	2	3	New	16(1)	–
6	6	4	0	Counterexample	16(1)	–
4	12	0	0	Known	16(1)	8(A_{15})

Counterexamples to two old conjectures

- Yarmolyuk–Kripyakevich, 1974: for known FK structures, fractions $(x_{20}, x_{24}, x_{26}, x_{28})$ are linear combinations $a_1(1, 3, 0, 0)(A_{15}) + a_2(3, 2, 2, 0)(Z) + a_3(2, 0, 0, 1)(C_{15})$. So, $6x_{20} - 2x_{24} - 7x_{26} - 12x_{28} = 0$ and $(a_1, a_2, a_3) = (\frac{x_{24}-x_{26}}{3}, \frac{x_{26}}{2}, x_{28})$.
- Counterexamples: $(6, 8, 4, 0)$, $(6, 6, 4, 0)$, $(7, 4, 2, 2)$ with $(N, n) = (18, 18), (16, 32), (15, 60)$. See $(6, 8, 4, 0)$ below.
- Its mean number of faces per cell, $\bar{f} = 13.55\cdots > 13.5$ (A_{15}) disproving the conjecture of Rivier–Aste, 1996: $13.29 \leq \bar{f} \leq 13.5$.

Frank–Kasper polyhedra and A_{15}

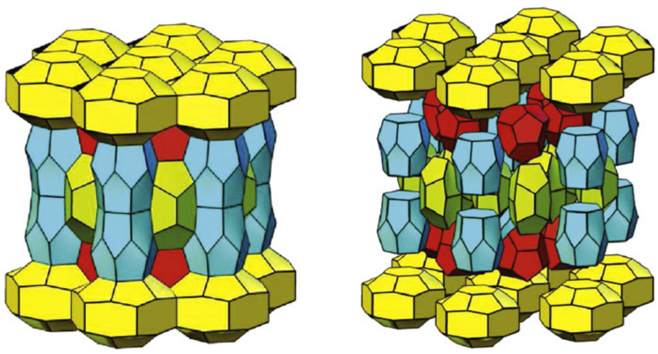


24 known *FK* structures have mean number $\overline{f}$ of faces per cell (mean coordination number) in $[13.(3)(C_{15}),\ 13.5(A_{15})]$ and their mean face-size is within $[5+\frac{1}{10}(C_{15}),\ 5+\frac{1}{9}(A_{15})]$.

Closer to impossible 5 or $\overline{f} = 12$ (120-*cell*, $\mathbb{S}^3$-tiling by F_{20}) means lower energy. Minimal $\overline{f}$ for *simple* (3, 4 tiles at each edge, vertex) $\mathbb{E}^3$-tiling by a *simple* polyhedron is 14 (tr.oct).

Non-FK space fullerene: Is it unique?

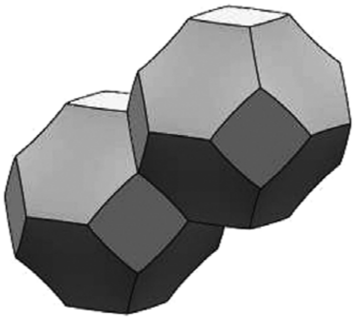
Deza–Shtogrin, 1999: unique known non-FK space fullerene, 4-valent 3-periodic tiling of E^3 by F_{20}, F_{24} and its elongation $F_{36}(D_{6h})$ in ratio 7:2:1; so, new record: mean face-size $\approx 5.091 < 5.1\,(C_{15})$ and $\overline{f} = 13.2 < 13.29$ (Rivier–Aste, 1996, conj. min.) $<13.(3)\,(C_{15})$.



Delgado, O'Keeffe: all space fullerenes with ≤ 7 orbits of vertices are 4 FK ($A_{15}, C_{15}, Z, C_{14}$) and this one (3, 3, 5, 7, 7).

Weak Kelvin problem

Partition $\mathbb{E}^3$ into *equal volume* cells D of minimal surface area, i.e., with maximal $IQ(D) = \frac{36\pi V^2}{A^3}$ (lowest energy form). Kelvin conjecture (about *congruent* cells) is still out.



Lord Kelvin, 1887: bcc $= A_3^*$
IQ(curved tr.Oct.) ≈ 0.757
IQ(tr.Oct.)
≈ 0.753

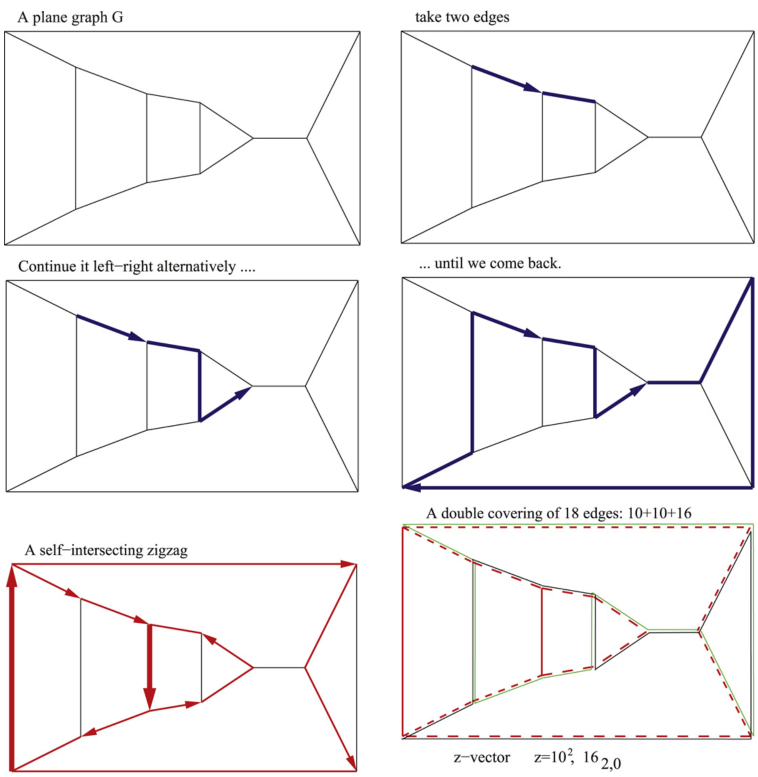
Weaire-Phelan, 1994: A_{15}
IQ(unit cell) ≈ 0.764
2 curved F_{20} and 6 F_{24}

In $\mathbb{E}^2$, the best is (Ferguson–Hales) graphite $F_\infty = (6^3)$.

IVa. Zigzags and railroads in fullerenes

M. Deza, M. Dutour and P.W. Fowler, *Zigzags, Railroads, and Knots in Fullerenes*, J. Chemical Information and Computer Science, **44** (2004) 1282–1293.

Zigzags



z-knotted fullerenes

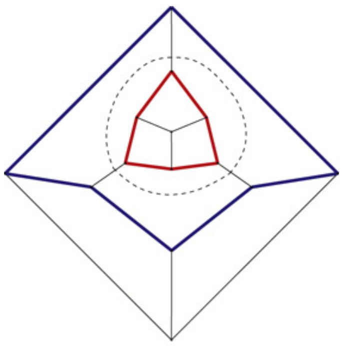
- A zigzag in a 3-valent plane graph G is a circuit such that any 2, but not 3 edges belong to the same face.
- Zigzags can self-intersect in the same or opposite direction.

- Zigzags doubly cover edge-set of G.
- A graph is z-knotted if there is unique zigzag.
- What is the proportion of z-knotted fullerenes among all F_n?

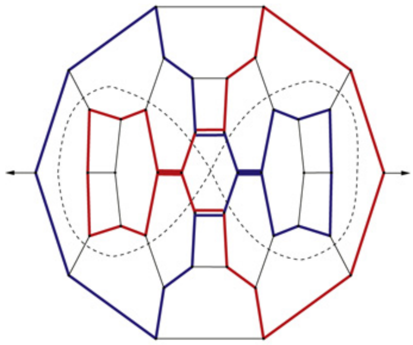
  Schaeffer and Zinn–Justin, 2004, implies: for any m, the proportion, among 3-valent n-vertex plane graphs of those having $\leq m$ zigzags goes to 0 with $n \to \infty$.
- **Conjecture**: all z-knotted fullerenes are chiral and their symmetries are all possible (among 28 groups for them) pure rotation groups: C_1, C_2, C_3, D_3, D_5.

Railroads

A railroad in a 3-valent plane graph is a circuit of hexagonal faces, such that any of them is adjacent to its neighbors on opposite faces. Any railroad is bordered by two zigzags.



$4_{14}(D_{3h})$

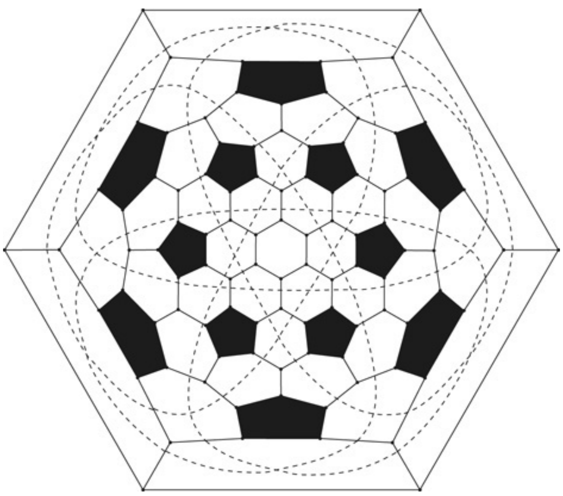


$4_{42}(C_{2v})$

Railroads (as zigzags) can self-intersect (doubly or triply).

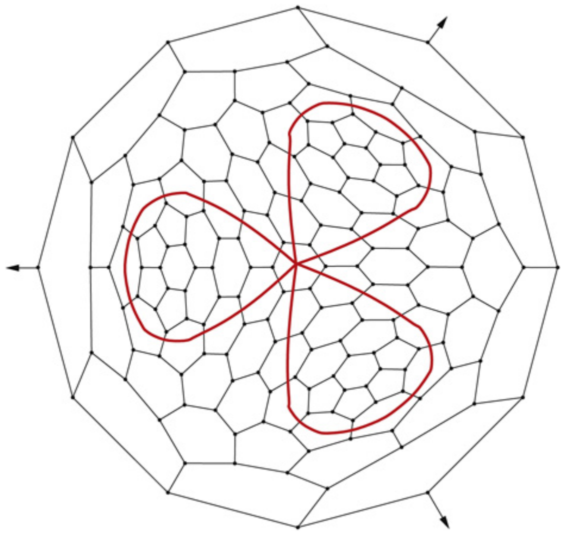
A 3-valent plane graph is tight if it has no railroad.

First IPR fullerene with self-intersecting railroad



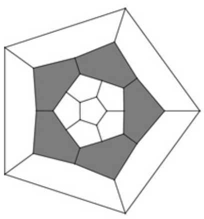
$F_{96}(D_{6d})$; realizes projection of Conway knot $(4 \times 6)^*$.

Fullerene with triply intersecting railroad



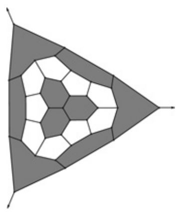
Conjecture: the above $F_{176}(C_{3v})$ is the smallest such fullerene.

Some special fullerenes

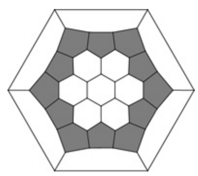


30, D_{5h}
all 6-gons
in railroad
(unique)

36, D_{6h}



38, C_{3v}
all 5-, 6-
in rings
(unique)



48, D_{6d}
all 5-gons
in alt. ring
(unique)

2nd one is the case $t = 1$ of infinite series $F_{24+12t}(D_{6d,h})$, which are the only ones with 5-gons organized in two 6-rings.

It forms, with F_{20} and F_{24}, unique known non-FK space fullerene tiling.

The skeleton of its dual is an isometric subgraph of $\frac{1}{2}H_8$.

Tight fullerenes

- Tight fullerene is one without railroads, i.e., pairs of "parallel" zigzags.
- Clearly, any z-knotted fullerene (unique zigzag) is tight.
- $F_{140}(I)$ is tight with $z = 28^{15}$ (15 simple zigzags).
  Conjecture: any tight fullerene has $\leq$ 15 zigzags.
- **Conjecture**: all tight fullerenes with simple zigzags are 9 known ones (holds for all F_n with $n \leq 200$).

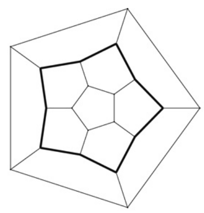
Tight F_n with only simple zigzags

n	Group	z-vector	Orbit lengths	Int. vector
20	I_h	10^6	6	2^5
28	T_d	12^7	3, 4	2^6
48	D_3	16^9	3, 3, 3	2^8
60, IPR	I_h	18^{10}	10	2^9
60	D_3	18^{10}	1, 3, 6	2^9
76	D_{2d}	$22^4, 20^7$	1, 2, 4, 4	4, 2^9 and 2^{10}
88, IPR	T	22^{12}	12	2^{11}
92	T_h	$22^6, 24^6$	6, 6	2^{11} and 2^{10}, 4
140, IPR	I	28^{15}	15	2^{14}

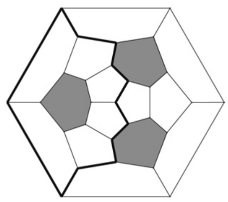
Conjecture: this list is complete (checked for $n \leq 200$).

It gives 7 Grünbaum arrangements of plane curves.

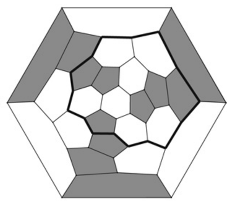
Tight F_n with simple zigzags



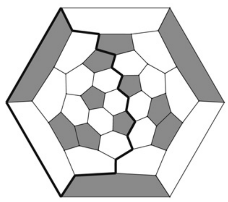
20 I_h, 20^6



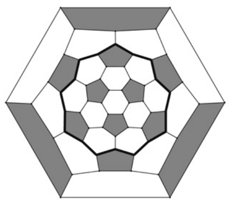
28 T_d, 12^7



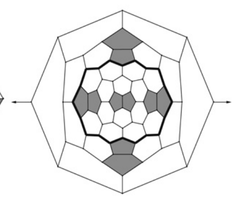
48 D_3, 16^9



60 D_3, 18^{10}

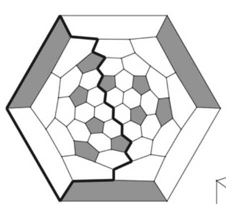


60 I_h, 18^{10}

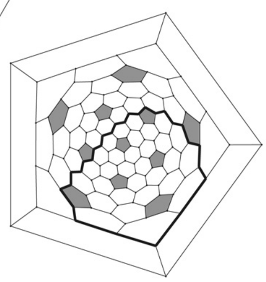


76 D_{2d}, $22^4, 20^7$

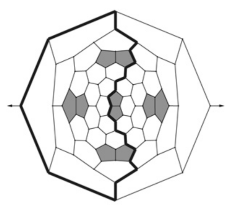
Tight F_n with simple zigzags



88 T, 22^{12}



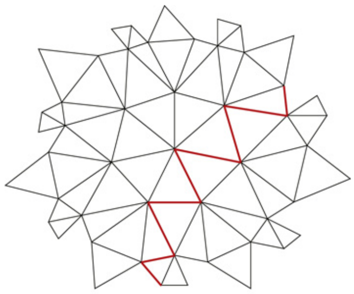
140 I, 28^{15}



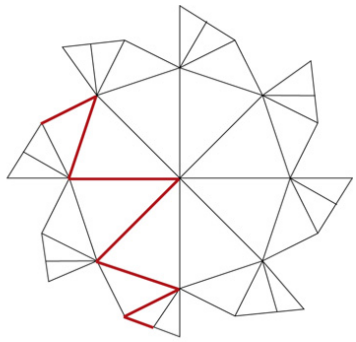
92 T_h, $24^6, 22^6$

IVb. Zigzags and Lins triality of maps

Zigzags on 2-complexes (surface maps)



Klein map: $z = 8^{21}$



Dyck map: $z = 6^{16}$

A zigzag, being a local notion, is defined on any surface, even on a non-orientable one.

Zigzags are also called left-right paths (Shank) or Petrie paths, from Petrie polygons of polytopes (Coxeter).

A map and its dual have the same zigzag vector z.

In an infinite graph, zigzags are circuits or infinite paths.

Zigzags of regular maps

A flag-transitive map is called regular.
Zigzags of regular maps are simple (not self-intersecting).

Map	n	Rot. group	z	$z(GC_{k,l})/(k^2+kl+l^2)$
Dod. $\{5^3\}$	20	$PSL(2,5)$	10^6	10^6 or 6^{10} or 4^{15}
Klein* $\{7^3\}$	56	$PSL(2,7)$	8^{21}	8^{21} or 6^{28}
Dyck* $\{8^3\}$	32	$(^1)$	6^{16}	6^{16} or 8^{12}
$\{11^3\}$	220	$PSL(2,11)$	10^{66}	10^{66} or 6^{110} or 12^{55}

$(^1)$ is a solvable group of order 96 generated by two elements R, S subject to $R^3 = S^8 = (RS)^2 = (S^2R^{-1})^3 = 1$.

Lins trialities

$(v,f,z) \rightarrow$	Notation in [3]	Notation in [1]	Notation in [2]
(v,f,z)	$\mathcal{M}$	**G**raph-**E**coded **M**ap	$\mathcal{M}$
(f,v,z)	$\mathcal{M}^*$	dual gem	$\mathcal{M}^*$
(z,f,v)	$phial(\mathcal{M})$	phial gem	$(s(\mathcal{M}^*))^*$
(f,z,v)	$(phial(\mathcal{M}))^*$	skew-dual gem	$s(\mathcal{M}^*)$
(v,z,f)	$skew(\mathcal{M})$	skew gem	$s(M)$
(z,v,f)	$(skew(\mathcal{M}))^*$	skew-phial gem	$(s(\mathcal{M}))^*$

Jones–Thornton, 1987: those are only “good” dualities.

1. S. Lins, *Graph-Encoded Maps*, J. Comb. Th. **B-32**, 1982.
2. K. Anderson and D.B. Surowski, *Coxeter–Petrie Complexes of Regular Maps*, Europ. J. of Comb. **23-8**, 2002.
3. M. Deza and M. Dutour, *Zigzag Structure of Complexes*, SEAMS Math. Bull. **29-2**, 2005; arXiv:math.CO/0405279.

Graph-encoded maps

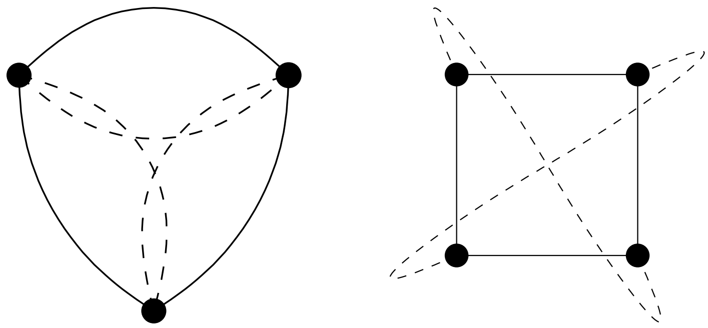
Given a set X and fixed-point-free involutions A, B, C on X with $AB = BA$ and $\langle A, B, C\rangle$ transitive on X, the quadruple $(X; A, B, C)$ defines a GEM (combinatorial map) M with sets $V(M)$, $E(M)$, $F(M)$, $Z(M)$ of vertices, edges, faces, zigzags being orbit-sets of (acting on X) groups $\langle A, C\rangle$, $\langle A, B\rangle$, $\langle C, B\rangle$, $\langle C, AB\rangle$, respectively.

For a map $M = (X; A, B, C)$, $[\langle A, B, C\rangle : \langle CA, CB\rangle] \leq 2$: M is orientable if this rank is 2 (orienting monodromy group).

Operations *dual*, *skew*, *phial* are reflexions.
Usual $dual(M)$ interchanges roles of A and B; so, vertices and faces leaving edges, zigzags. Petrie dual ($skew(M)$) interchanges B and AB; so, faces/zigzags leaving vertices.

The group $\langle dual,\ skew\rangle$ of trialities is $\simeq S_3 \simeq Sym_3$.

Example: Tetrahedron

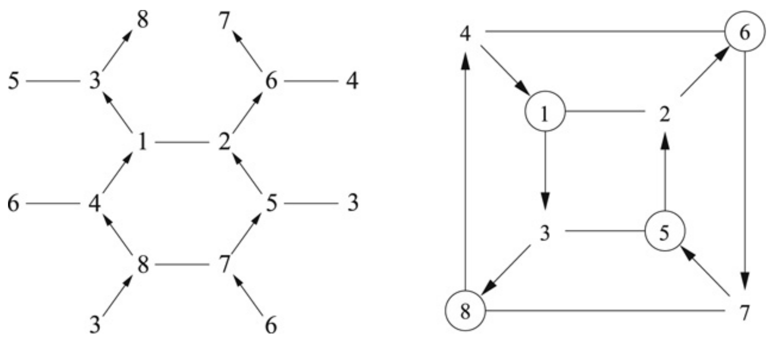


$phial(Tetrahedron)$ $skew(Tetrahedron)$

Two Lins maps on projective plane.

- Two above maps are *folded* (i.e. obtained by identifying opposite vertices) Octahedron and Cube.
- $skew(Cube)$ and $phial(Octahedron)$ are toric maps. $phial(Cube)$ and $skew(Octahedron)$ are maps on a non-oriented surface of genus 4, i.e., with $\chi = -2$.

Bipartite skeleton case



Two representation of $skew(Cube)$: on Torus and as a Cube with cyclic orientation of vertices (marked by ◯) reversed.
For bipartite graph embedded in oriented surface, the skew operation is, in fact, reversing orientation of one of the part of the bipartition.

Nedela–Skoviera–Zlatos, 2001: $skew(M)$ (Petrie dual) of orientable map M is orientable if and only if M is bipartite.

$\chi(skew(M)) = v - e + Z$; $\chi(phial(M)) = \chi((skew(M^*))^*) = f - e + Z$, where χ denotes the Euler characteristic and e, Z are the numbers of edges and zigzags of M.

Zigzags on d-dimensional complexes

A (maximal) flag $u = (f_0, \ldots, f_{d-1})$ is a sequence of i-dimensional faces f_i with $f_i \subset f_{i+1}$.
Given a flag u, there exists an unique flag $\sigma_i(u)$, which differs from u only in position i, i.e., in $f_i' \neq f_i$, $f_{i-1} \in f_i, f_i' \in f_{i+1}$.

A zigzag z is a circuit of flags $(u_j)_{0 \le j \le l}$, such that $u_0 = u, u_j = \sigma_n \ldots \sigma_1(u_{j-1})$; so, $u_1 = (f_0', \ldots, f_{n-1}')$.
The number of flags is called its length (it is even for odd d).

Zigzags partition the flag-set of the complex.
z-vector is a vector, listing zigzags with their lengths.

A complex is polytopal if it is the face-lattice of a polytope.

Problem: generalize Lins triality of maps on d-complexes.

Zigzags of regular/semiregular polytopes

d	d-polytope	z-vector
3	Dodecahedron	10^6
4	24-cell	12^{48}
4	600-cell	30^{240}
d	d-simplex $= \alpha_d$	$(n+1)^{n!/2}$
d	d-cross-polytope $= \beta_d$	$(2n)^{2^{n-2}(n-1)!}$
4	octicosahedric 4-polytope	45^{480}
4	snub 24-cell	20^{144}
4	$0_{21} = \mathrm{Med}(\alpha_4)$	15^{12}
5	1_{21} = Half-5-Cube	12^{240}
6	2_{21} = Schläfli polytope (in E_6)	18^{4320}
7	3_{21} = Gosset polytope (in E_7)	90^{48384}
8	4_{21} (240 roots of E_8)	$36^{29030400}$

Va. Three classes of exotic plane graphs

Self-dual spheric $\{4^4\}$'s

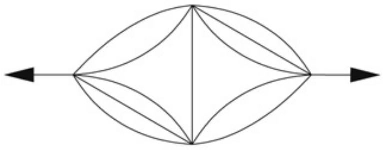
- A self-dual spheric $\{4^4\}$ (almost $\{4^4\}$ on $\mathbb{S}^2$) is a self-dual polyhedron with 3-, 4-valent vertices and 3-, 4-gonal faces only. Clearly, $v_3 = p_3 = 4$ (but $v_3 = p_3 = 0$ for such torus).
- Their medial (convex hull of midpoints of edges) are 4-valent polyhedra with 3-, 4-gonal faces. Clearly, $p_3 = 4$.
- **Example**: k-elongated square pyramid, $k \geq 1$. The medial of square pyramid ($k = 1$) is square antiprism.
- **Problem**: Characterize self-dual spheric $\{4^4\}$'s or, at least, their symmetries, growth as v^n, parametrization.
- The gyrobifastigum (one of 92 regular-faced polyhedra) also has $p = (p_3, p_4) = v = (v_3, v_4) = (4, 4)$ but it is not self-dual.

Spheric $\{3^6\}$'s

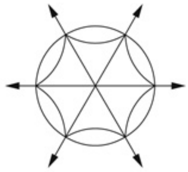
- A spheric $\{3^6\}$ (almost $\{3^6\}$ on $\mathbb{S}^2$) is a 6-valent plane graph with 2-, 3-gonal faces only. So, $p_2 = 6$, $v = 2 + \frac{p_3}{2}$.
- Such sphere exists for any $v \geq 2$ vertices, starting with *Bundle*$_6$ (2 vertices connected by 6 edges).
- Central circuit in an Eulerian (i.e., even-valent) plane graph is a circuit going only straight ahead.

- **Example**: consecutive, $t-1$ times, inscribing of *Bundle*$_4$ into *Bundle*$_6$, results in $2t$-vertex spheric $\{3^6\}$ with CC-vector $(2^t, (2t)^2)$, if t is odd, and $(2^t, 4t)$, otherwise.

4, D_{2d}, $(2^2, 8)$



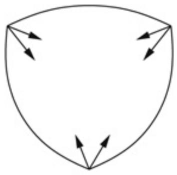
4, D_2, (12)



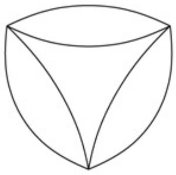
8, D_{6h}, $(4^3, 6^2)$

Three series of spheric $\{3^6\}$'s

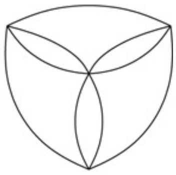
S_{ti}: $(3t+i-1)$-vertex spheric $\{3^6\}$ with CC$=$ $(3^t, (2t+i-1)^3)$, if $t+i \equiv 2 \pmod 3$, and CC $= (3^t, 3(2t+i-1))$, otherwise.



Incomplete

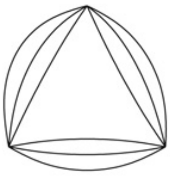


cap A



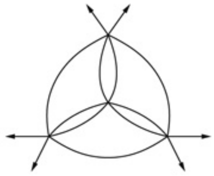
cap B

$i = 1, 2, 3$ if caps AA, AB, BB; first 2 members of 3 series:



3, D_{3h}, S_{11}

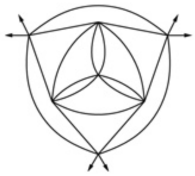
4, T_d, S_{12}



5, D_{3h}, S_{13}

6, D_{3d}, S_{21}

7, $C_{3\nu}$, S_{22}



8, D_{3d}, S_{23}

Problems for spheric $\{3^6\}$'s

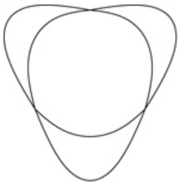
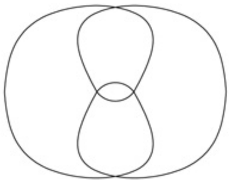
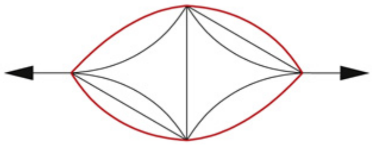
- Estimate, as v^n, the number of v-vertex spheric $\{3^6\}$'s and list their possible symmetries.
- Find all of them without self-intersecting central circuits.
- Is the number of central circuits of length ≥ 4 bounded?
- Extend, if possible, Goldberg–Coxeter construction for those 6-valent spheres.

Small t-knots

(Projection of) t-knot is a finite plane $2t$-valent graph (no loops but 2-gons permitted) having unique central circuit.

So, 1-knot is a knot; smallest 1-knot is trefoil 3_1.

Smallest t-knot if $t > 1$, is t-figure-of-eight: 4_1 if $t = 1$, and if $t > 1$, it comes from $(t-1)$-figure by adding 4-ring of 2-gons.

Problem: tabulate small t-knots for any t.
So, a program enumerating $2t$-valent plane graphs is needed.

V.I. Arnold, *Topology of Plane Curves, Wave Fronts, Legendrian Knots, Sturm Theory and Flattenings of Projective Curves*, Int. Math. Union Bulletin, 39, 1995.

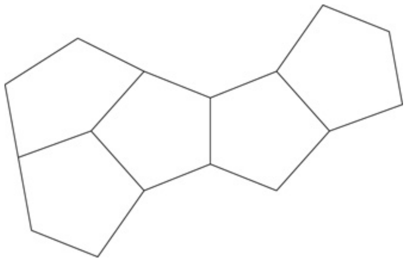
Vb. Ambiguous polycycle boundaries

M. Deza, M. Dutour and M. Shtogrin, *Filling of a given boundary by p-gons and related problems*, *Discrete Applied Mathematics*, **156** (2008) 1518–1535.

Polycycles

A $(p, 3)$-polycycle is a plane 2-connected finite graph with:

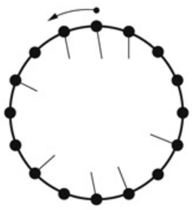
- all interior faces are (combinatorial) p-gons,
- all interior vertices are of degree 3,
- all boundary vertices are of degree 2 or 3.



In more general (p, q)-polycycle, interior vertices have degree q and boundary ones are of degree $2, \ldots, q$.

Boundary sequence of $(p, 3)$-polycycle

The boundary sequence is the sequence of degrees (2 or 3) of the vertices of the boundary.



Associated sequence is
3323223233232223

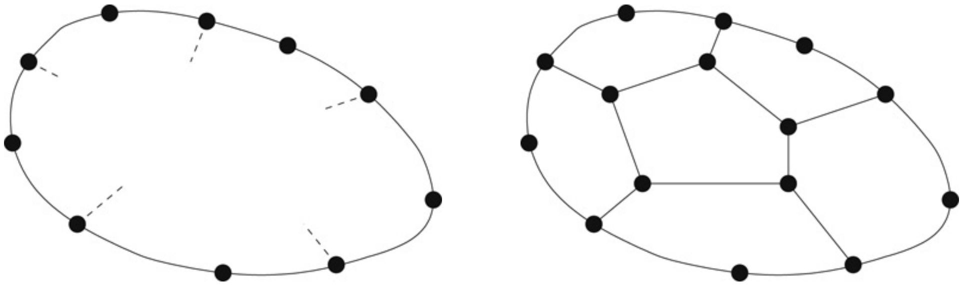
- The boundary sequence is defined only up to an action of D_n, i.e., the dihedral group of order $2n$ generated by cyclic shift and reflexion.
- The invariant given by the boundary sequence is the smallest (by the lexicographic order) representative of the all possible boundary sequences.

The filling problem

- Does there exist $(p, 3)$-polycycles with given boundary sequence?
- If yes, is this $(p, 3)$-polycycle unique?

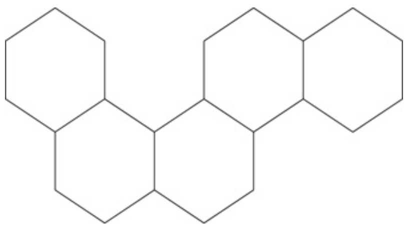
- The cases $p = 3$ or 4 are trivial:
  all (3, 3)-polycycles: Tetrahedron $= \alpha_3, \alpha_3 - e; \alpha_3 - v$.
  all (4, 3)-polycycles: Cube $= \gamma_3, \gamma_3 - e, \gamma_3 - v$ and
  the series $P_2 \times P_n, n \geq 2$.

  Let $p = 5$; consider, for example, the sequence 2323232323



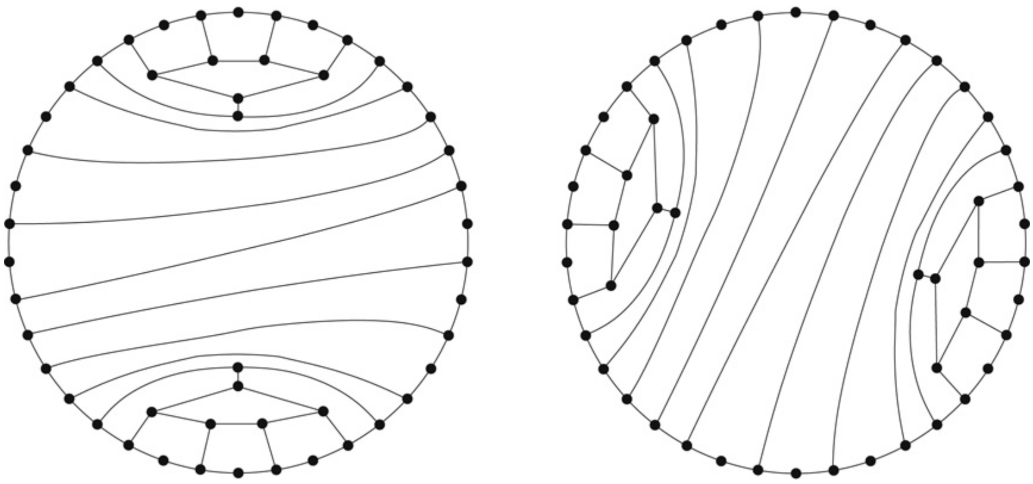
What boundary says about its filling(s?)

- The boundary of a $(p, 3)$-polycycle defines it if $p = 3, 4$.
- A (6, 3)-polycyle is of lattice type if its skeleton is a partial subgraph of the skeleton of the partition $\{6^3\}$ of the plane into hexagons. Such (6, 3)-polycycles are uniquely defined by their boundary sequence.



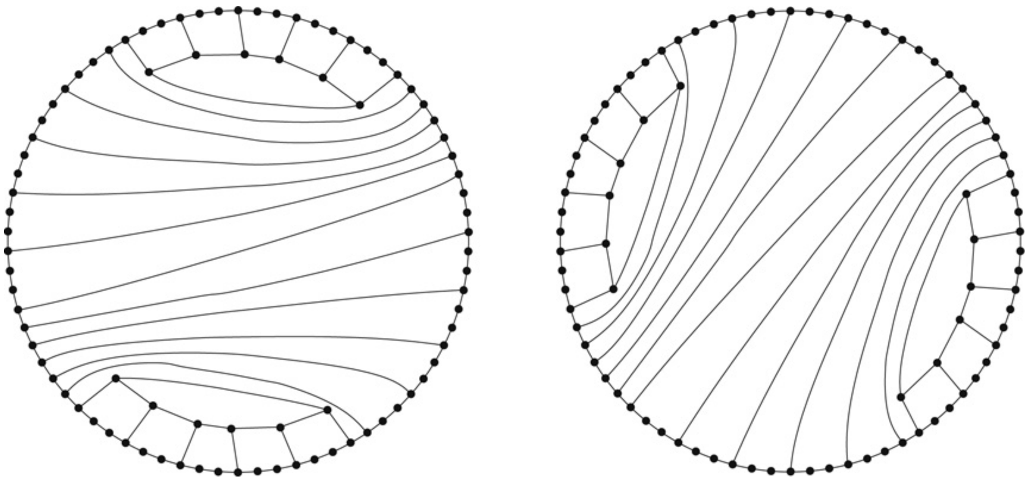
- From the Euler formula, the boundary sequence of any $(p, 3)$-polycycle, defines its number f_p of p-gons:
  If $p \neq 6$, then $f_p = \frac{v_2 - v_3 + 5}{p-6}$ and $v_{int} = \frac{2(v_2-p)-(p-4)v_3}{p-6}$.
  If $p = 6$, then f_6 is also defined uniquely and $v_2 = 6 + v_3$.

2 equi-boundary (5, 3)-polycycles



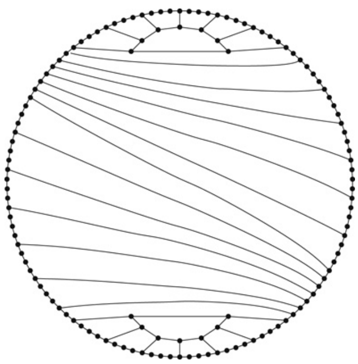
Boundary sequence: 12, 26 vertices of degree 2, 3, resp.
Symmetry groups: of boundary: C_{2v}, of polycycles: C_2.
Fillings: 20 pentagons, 12 interior vertices.
It is a unique ambiguous boundary with $f_5 \leq 20 = 4 \times 5$.

2 equi-boundary (6, 3)-polycycles



Boundary sequence: 40, 34 vertices of degree 2, 3, resp.
Symmetry groups: of boundary: C_{2v}, of polycycles: C_2.
Fillings: 24 hexagons, 12 interior vertices.
It is a unique ambiguous boundary with $f_6 \leq 24 = 4 \times 6$.

Ambiguous boundary for any $p \geq 6$



Boundary sequence is:
$b = u2^{p-1}u3^{p-6}u2^{p-1}u3^{p-6}$,
where $u = (23^{p-4})^{p-1}2$.
$6p-2$ vertices of degree 3
and $4p^2-18p+4$ of degree 2.

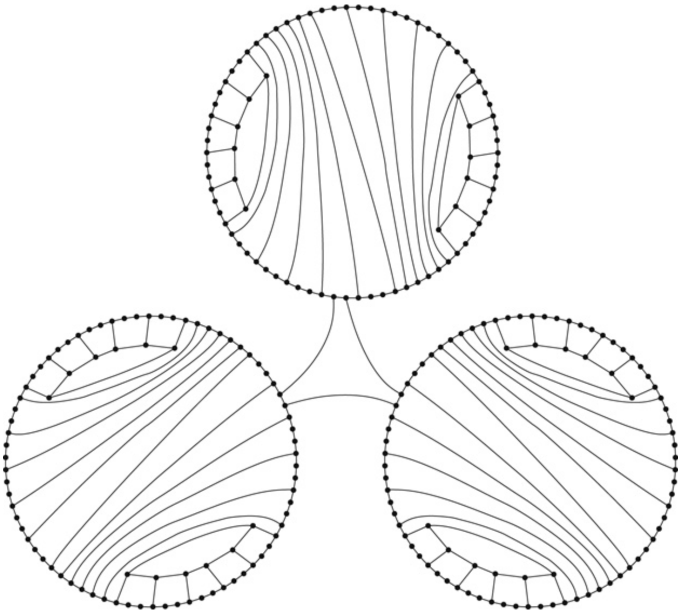
Symmetry groups are:
of boundary: C_{2v},
of polycycles: C_2.

Deza, Shtogrin and Dutour, 2005: it has two different (but isomorphic as maps) $(p, 3)$-fillings ($f_p = 4p$, $v_{int} = 2p$).

Conjecture: any $(p, 3)$-polycycle with $\leq 4p$ p-gons is uniquely defined by its boundary. It holds for $p = 6$ (Guo, Hansen and Zheng, 2002) and $p = 5$ (Deza and Shtogrin, 2006).

Many equi-boundary $(p, 3)$-fillings

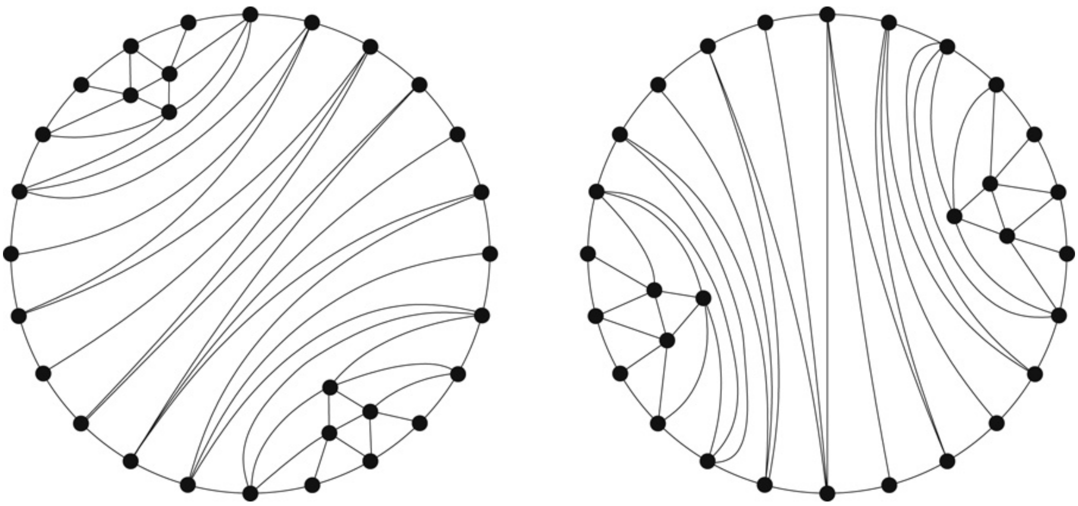
8 (6, 3)-fillings arises from two fillings of those 3 components; the same aggregation gives an arbitrarily large number for $p \geq 6$.



More ambiguity

- Boundaries, admitting two non-isomorphic $(p, 3)$-fillings, can be obtained by adding 1 p-gon to the general example.
- There exists a boundary admitting exactly N $(p, 3)$-fillings for any given number N.
  Example: boundary $223^{5n+1}223^{5n+3}223^{5n+1}223^{5n+3}$ has exactly $n+1$ $(5, 3)$-fillings ($f_5 = 20n+6$, $v_{int} = 20n+2$).
- Ambiguous boundaries exist for (p, q)-polycycles, i.e., with max. degree q and exactly q for int. vertices.
- Does Ramsey type results hold for large f_p or v_{int}?
  For example, is any (p, q)-polycycle a partial subgraph of a (p, q)-filling with the boundary having given "degree of ambiguity"?

Equi-boundary (3, 5)-fillings



Two non-isomorphic $(3, 5)$-fillings of the same boundary $(34345)^2 5^2 (34345)^2 5^2$ (by 34 triangles and 30 int. vertices).

Their symmetry is C_2, as of the boundary. This boundary might be minimal for the number f_3 of triangles and/or v_{int}.

VI. Extreme physical distances

Chapter 27 of E. Deza and M. Deza, *Dictionary of Distances*, Elsevier, 2006 and *Encyclopedia of Distances*, Springer, 2009.

The range of physical distances

- The distances having physical meaning range from 1.616×10^{-35} m (Planck length $l_P = \sqrt{\frac{\hbar G}{c^3}}$) to 7.4×10^{26} m (Hubble distance D_H, the estimated size of the observable Universe) $\approx 46 \times 10^{60}$ Planck lengths.
  So, $\sqrt{l_P D_H}$ is about 0.1 mm, size of a bacterium.
- Quantum Theory, Relativity Theory and Newton laws describe physical systems within 10^{-15}–10^{25} m.
- 10^{-15} =1 f: strong force, proton/neutron radius.
- Gigantic accelerators can register particles 10^{-19} m.
  10^{-18} =1 am: weak force range, quark/electron.
- Below, till 10^{-35}: 17 *Dark Magnitudes* of unknown (10^2–10^{19} GeV in energy terms).

Lower limit

10^{-34} m: length of a putative string in M-theory (all forces and elementary particles arises from their vibration).

Space is smooth till $\sim 10^{-14}$, roughness starts at $\sim 10^{-32}$.

At $\sim l_P \approx 1.6 \times 10^{-35}$: quantum foam: violent warping and turbulence of *spacetime*; it is not described by cartesian coordinates, position measurements fail to commute. The dominant structures: multiply-connected *wormholes* and *bubbles* popping into existence and back out of it.

Uncertainty principle with x, p_x being position, momentum along x-axis: $\triangle x \triangle (p_x) \geq \hbar = 1.054 \times 10^{-27}$ erg s.

Quantum Mechanics, General Relativity and all Theories of Everything (unify gravity, electroweak and strong nuclear forces) indicate the existence of minimal length, where the very notion of "distance" looses operational meaning.

Gravitation on extreme distances

- The gravitation is untested for extreme distances.
- Newton's law was tested till 56 μm (5.6×10^{-5} m); so, no extra dimension of ≥44 μm. It will be tested further at LHC (Large Hadron Collider, CERN).
  LHC and ILC (late 2010s) will measure the number, size and shape of TeV-scale ($\sim 10^{-18}$ m) extra dimensions.
- The existence of 2 extra dimensions of >8 microns (or 4 of $>10^{-12}$) will be tested via proportionality of the gravitational attraction in n-dimensional space to d^{1-n}.
- So, if the Universe have (compactified "large") 4th dimension, LHC will detect inverse proportionality to the cube of small inter-particle distance.
- General Relativity, more accurate than Newton's law, is untested on galactic and cosmological scales.

Appoaching to upper limit

10^{24} m = 1 Ym = 104.7 MLY = 32.4 Mpc: largest metric length unit.

200 MLY: width of the Great Wall and Lyman alpha blobs, largest observed superstructures in the Universe.

2.36×10^{24} m = 250 MLY: distance to the Great Attractor, a gravitational anomaly where our galaxy is going.

9.46×10^{24} m =1 hubble = 1 light-Gyr: largest distance unit.

Redshift $z \geq 1$ ($\geq$ 8 light-Gyr): cosmological distances.

$z = 6.43$ =12080 MLY: distance to farthest known quasar.

$z \approx 6.5$: the *Wall of Invisibility* for visible light.

$z \approx 20 \approx$ BB+400 MY: first stars formation (end of *Dark Age*)

1.3×10^{26} m = 13.7 light-Gyr = 4.22 Gpc ($z \approx 1089$): Hubble radius (the cosmic light horizon, age of the Universe), cosmic background radiation journey since the Big Bang.

The Cosmic Web

- On a typical scale of about 10–100 Mpc, the structure of the Universe is foamlike: near empty voids separated by sheetlike walls (filaments of galaxies), denser edges and esp. dense nodes (clusters of galaxies).
- Origin: gravitational growth of tiny initial density/velocity deviations. COBE/WMAP telescopes observed < a factor 10^{-5} disturbances in 379.000 years old Universe.
- Voids are expanding (from their centers — minima of Gaussian density fluctuation field). They are becoming more round and of about the same size of 30–50 Mpc. They merge or get destroyed by larger collapsing overdensity.
- In a void, mean inter-galactic distance increases. Galaxy reach a wall, move on it to an edge, then into a node.
- Voronoi tiling is the asymptotic ultimate matter distribution?

Upper limit

- 4.3×10^{26} m: the present (comoving: $(1 + z)d$) distance to the edge of the observable Universe; the size of the observable Universe is larger than Hubble radius, since the Universe is expanding.
- This number being of the order of the gravitational radius for the observable Universe mass ($\approx 10^{60}$ kg), some physicists see the Universe as a huge rotating black hole.
- If (the topology of) Universe is non-simply connected, then it is compact (finite in extent) and the estimated maximum length scale is only 5–15% of Hubble radius.
- On the other hand, the hypothesis of parallel universes estimates that one can find another identical copy of our Universe within the distance $10^{10^{118}}$ m.

Time limits

- In terms of time, Planck time $t_P = \sqrt{\frac{\hbar G}{c^5}} \approx 5.39 \times 10^{-44}$ s is the smallest observable unit of time and the time before which science cannot describe the Universe.
- The present time from the Big Bang is about 13.7 billion years $\approx 4 \times 10^{17}$ s. Cf. 155 trillion years (Hinduism).

  If protons decay, their half-life is at least 10^{35} years.
- Beyond 10^{1000} years in the *Heat Death* scenario, the Universe achieves low-energy state, so that quantum events became major phenomena and space–time loose usual meaning again, as below the Planck time or length.

  But now the Universe generates (by nuclear fusion in star cores) an yearly average power of 5 PW = 5×10^{15} W per cubic light-year ($\approx$300 times the human consumption in 2007).