Spherical Tilings by Congruent Quadrangles

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Spherical tilings

- edges are parts of great circles
- edge-to-edge tiling
- vertex degree ≥ 3

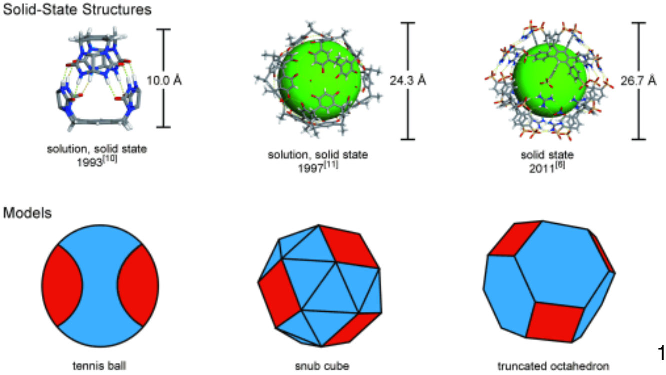
Spherical tilings by congruent polygons

all faces the same size

$$\Downarrow$$

only triangles, quadrangles or pentagons

Chemical applications



[1]

[1] Leonard R. MacGillivray, “Design Rules: A Net and Archimedean Polyhedra Score Big for Self-Assembly”, in: *Angewandte Chemie International Edition* 51.5 (2012), pp. 1110–1112, ISSN: 1521-3773, DOI: 10.1002/anie.201107282, URL: http://dx.doi.org/10.1002/anie.201107282.

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A molecular sphere of octahedral symmetry†

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Complexation of tridentate ligand 1 with $Pd(NO_3)_2$ leads to the quantitative self-assembly of M_6L_8 molecular sphere 2.

Synthesis of molecular architectures from organic ligands and transition metal ions through the self-assembly route, in contrast to the troublesome stepwise synthesis, has received much attention during the last decade.[1] Designed structures having predetermined structural and functional properties can sometimes be obtained by simply mixing the participating components under suitable conditions. Recently, the focus of several groups has been on the construction of self-assembled species possessing internal cavities.[2,3] There are handful of structures with a 3-D cavity within a tetrahedron,[4] hexahedron,[5] dodecahedron,[6] and similar shapes,[7] obtained by a metal-directed self-assembly route. There are also reports of 3-D cavities constructed by utilizing the principle of hydrogen-bond interactions.[8] Secondary building units, the metal ion containing self-assembled structures possessing lateral sites capable of H-bonding interactions, are used successfully to construct cuboctahedron and faceted polyhedra.[9] However, not many reports are available on closed cavities which are more or less

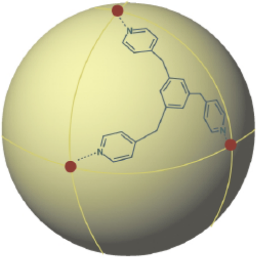


Fig. 1 Cartoon representation of a molecular sphere, conceptualized from eight tripodal tridentate ligands, and six metal ions that can provide a square planar coordination environment. All the 14 components are cooperatively embracing the surface of sphere.

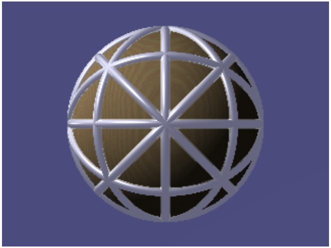
Angewandte
Chemie

Self-Assembly

Finite, Spherical Coordination Networks that Self-Organize from 36 Small Components**

*Masahide Tominaga, Keisuke Suzuki, Masaki Kawano, Takahiro Kusukawa, Tomoji Ozeki, Shigeru Sakamoto, Kentaro Yamaguchi, and Makoto Fujita**

Classification of spherical tilings by congruent triangles completed by Davies[2] and Ueno-Agaoka[3].



[2] H.L. Davies, "Packings of spherical triangles and tetrahedra", in: *Proc. Colloquium on Convexity (Copenhagen, 1965)*, Kobenhavns Univ. Mat. Inst., 1967, pp. 42–51.

[3] Y. Ueno and Y. Agaoka, "Classification of tilings of the 2-dimensional sphere by congruent triangles", in: *Hiroshima Math. J.* 32.3 (2002), pp. 463–540.

The next step:

classification of spherical tilings by congruent quadrangles

Types of quadrangles

aaaa

abab

aabb

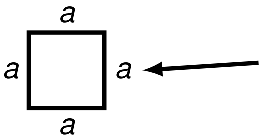
aaab

aabc

abac

abcd

Types of quadrangles



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Types of quadrangles

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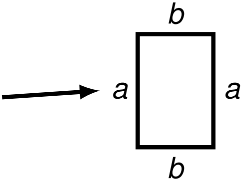
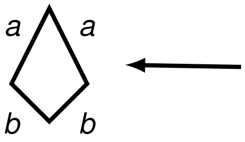


Types of quadrangles



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Types of quadrangles

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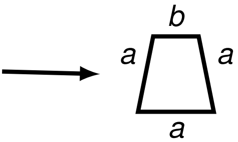
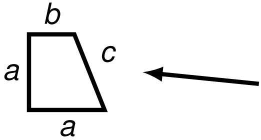


Types of quadrangles



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Types of quadrangles

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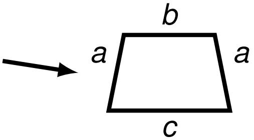

Types of quadrangles

aaaa

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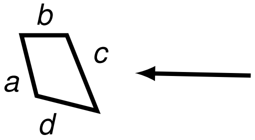
aabb

aaab

aabc

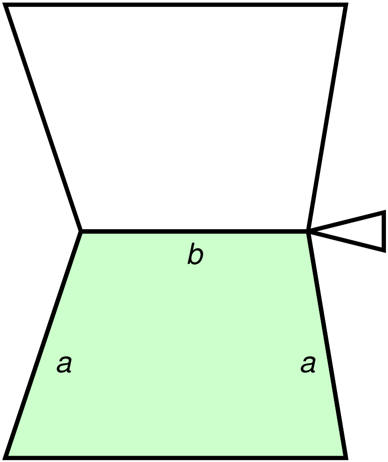
abac

abcd

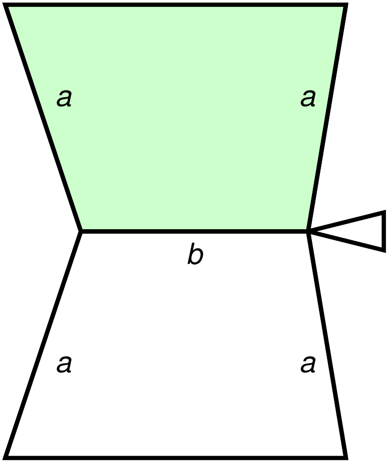


In every quadrangulation of the sphere,
there exists a vertex of degree 3.

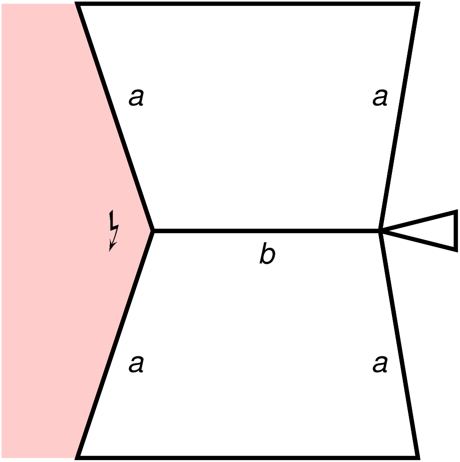
abab, *abac*



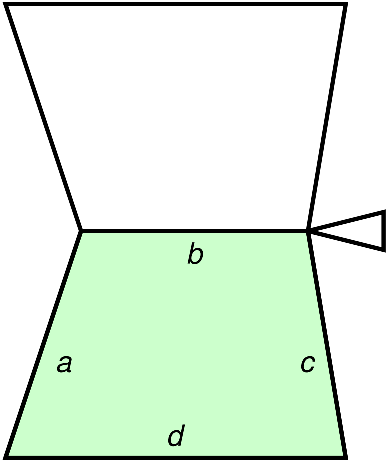
abab, *abac*



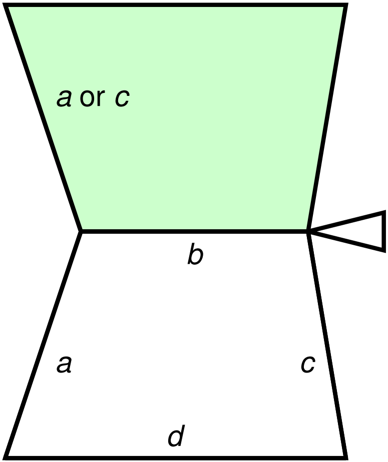
abab, *abac*



abcd



abcd



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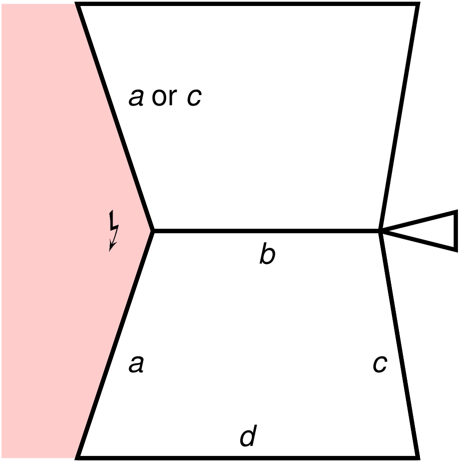


Types of quadrangles

aaaa

~~*abab*~~

aaab

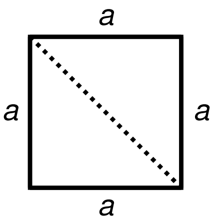
aabb

aabc

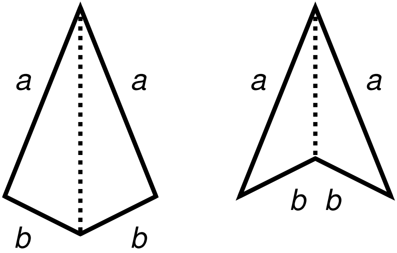
~~*abac*~~

~~*abcd*~~

aaaa



aabb



Classification of spherical tilings by congruent rhombi, kites and daggers completed by Akama-Sakano[4].

[4] Y. Akama and Y. Sakano, “Classification of spherical tilings by congruent rhombi (kites, darts)”, In preparation.

Types of quadrangles

aaaa

~~*abab*~~

aaab

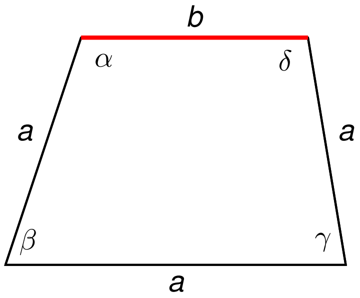
aabb

aabc

~~*abac*~~

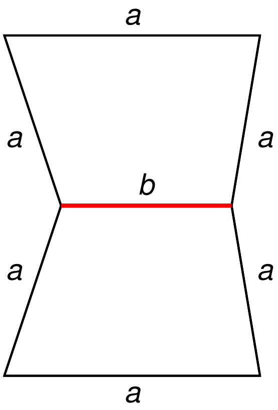
~~*abcd*~~

Type 2 quadrangles



Even number of tiles

Assignment of side lengths corresponds
to perfect matching in dual



Concave type 2 quadrangles

- Ambiguity of inner angles[5]
- Edge which is not a geodesic[5]

[5] Yohji Akama and K. Nakamura, “Spherical tilings by congruent quadrangles over pseudo-double wheels (II) the ambiguity of the inner angles”, Preprint, 2012.

Convex type 2 quadrangles

$$0 < \alpha, \beta, \gamma, \delta < \pi$$

Some restrictions on the angles

$$\alpha + \delta < \pi + \beta$$
$$\alpha + \delta < \pi + \gamma$$

$$\alpha = \delta \Leftrightarrow \beta = \gamma$$

$$(1-\cos\beta)\cos^2\alpha - (1-\cos\beta)(1-\cos\gamma)\cos\alpha\cos\delta + (1-\cos\gamma)\cos^2\delta$$
$$+\cos\beta\cos\gamma + \sin\alpha\sin\beta\sin\gamma\sin\delta = 1$$

Area of a tile

$$S = \alpha + \beta + \gamma + \delta - 2\pi$$

$$S = \frac{4\pi}{F}$$

Area of a tile

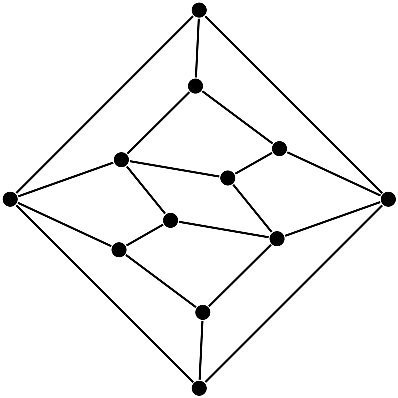
$$S = \alpha + \beta + \gamma + \delta - 2\pi$$

$$S = \frac{4\pi}{F}$$

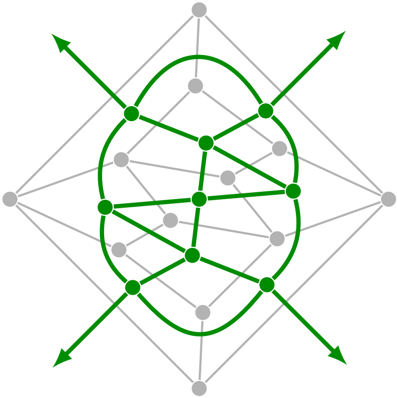
$$\alpha + \beta + \gamma + \delta - 2\pi = \frac{4\pi}{F}$$

Generation of spherical tilings by congruent convex quadrangles of type 2

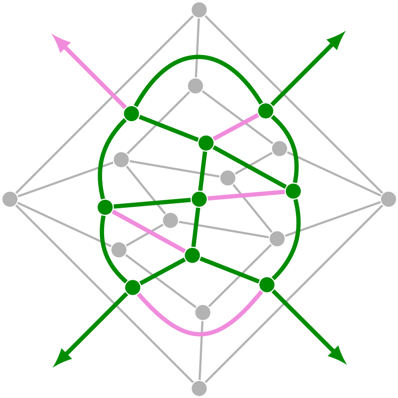
Generate quadrangulations of the sphere



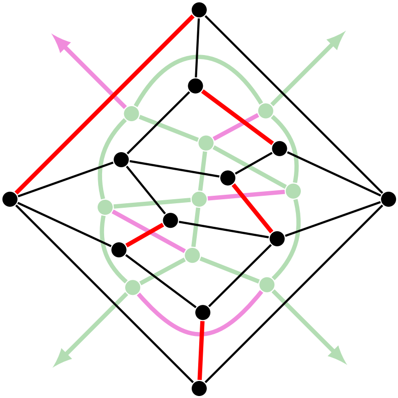
Generate perfect matchings for the dual of the quadrangulation



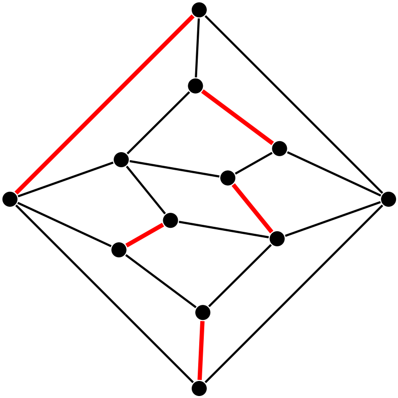
Generate perfect matchings for the dual of the quadrangulation



Generate perfect matchings for the dual of the quadrangulation



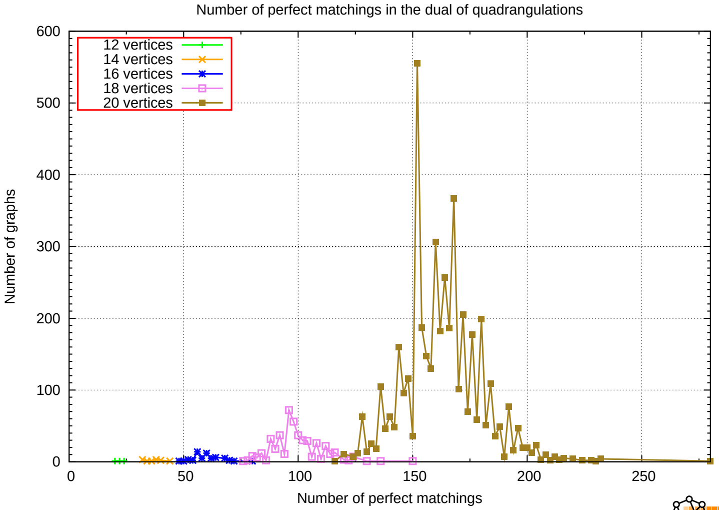
Generate perfect matchings for the dual of the quadrangulation



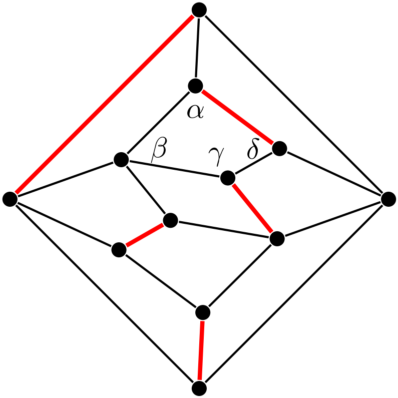
Filter out quadrangulations for which the dual has no perfect matching?

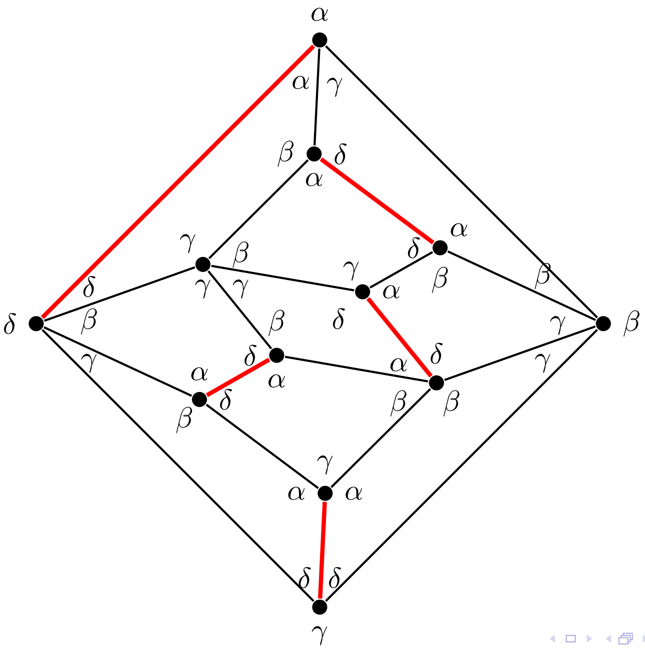
Every edge in the dual of a quadrangulation belongs to a perfect matching of the dual.[6]

[6] C. D. Carbonera and Jason F. Shepherd, *On the existence of a perfect matching for 4-regular graphs derived from quadrilateral meshes.* Tech. rep., UUSCI-2006-021, SCI Institute Technical Report, 2006.

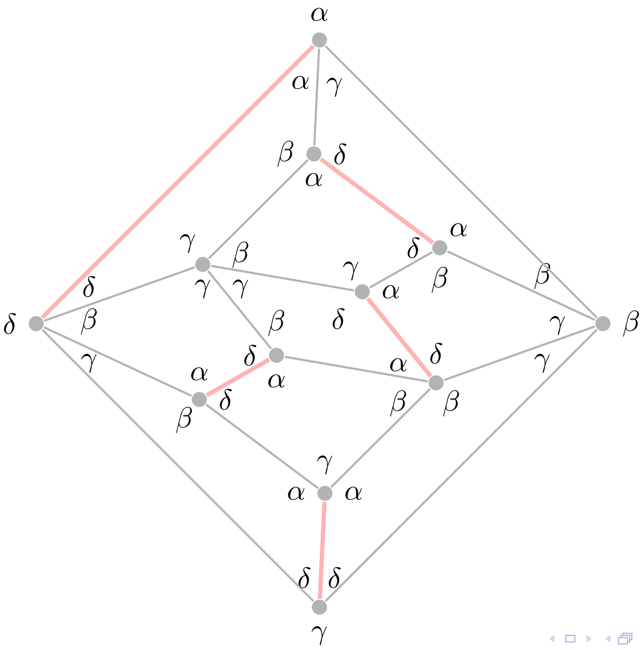

Number of perfect matchings in the dual of quadrangulations
12 vertices
14 vertices
16 vertices
18 vertices
20 vertices
Number of graphs
Number of perfect matchings
0
100
200
300
400
500
600
0
50
100
150
200
250

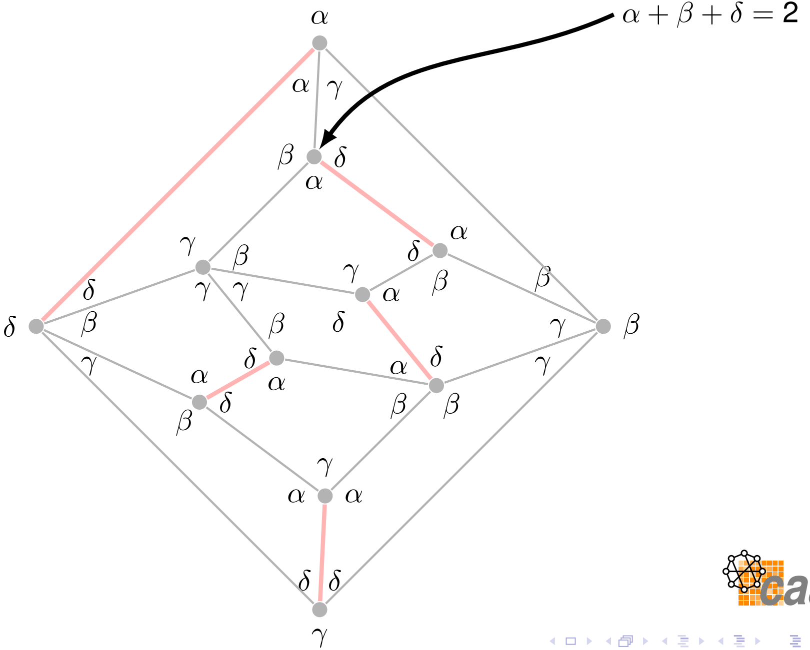
Generate angle assignments: 2^{F-1} possibilities

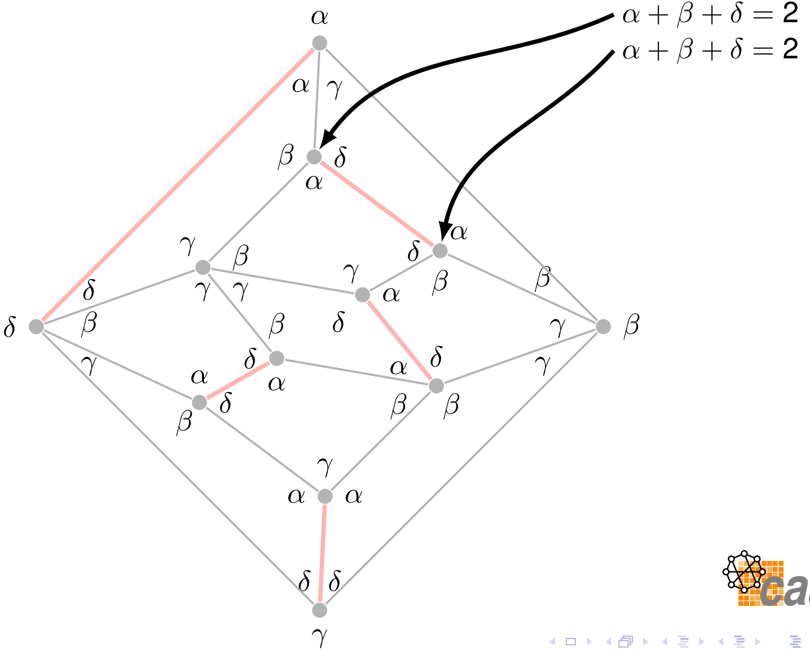




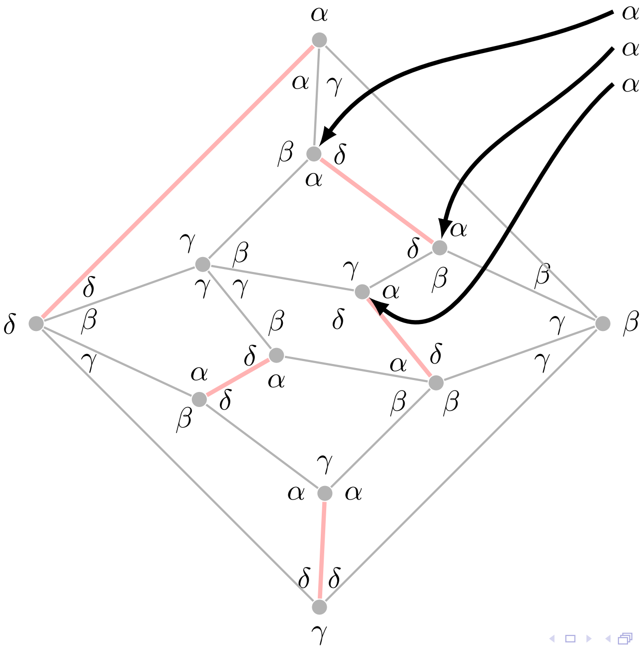
α
α γ
β δ
α
γ δ α
β γ β β
δ γ γ α
δ β β δ γ β
δ δ
γ γ α
α α
δ β β
β
γ
α α
δ δ
γ

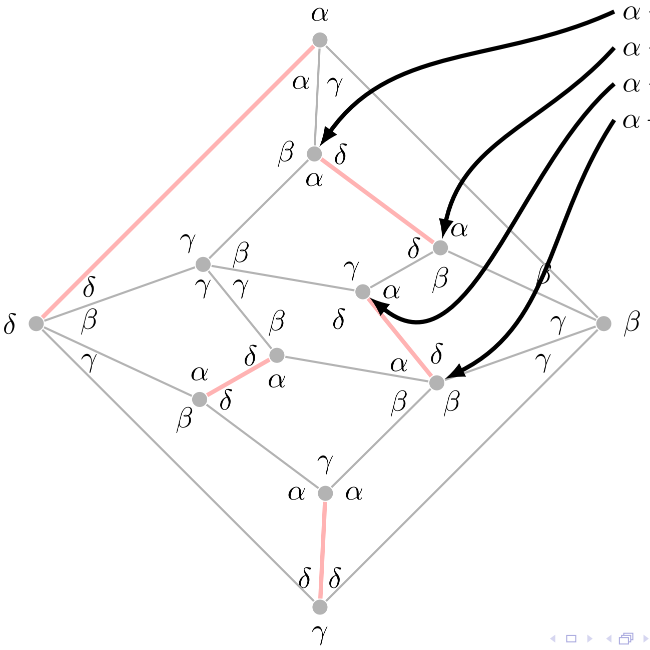



$\alpha + \beta + \delta = 2$


$\alpha + \beta + \delta = 2$
$\alpha + \beta + \delta = 2$

$\alpha + \beta + \delta = 2$
$\alpha + \beta + \delta = 2$
$\alpha + \gamma + \delta = 2$



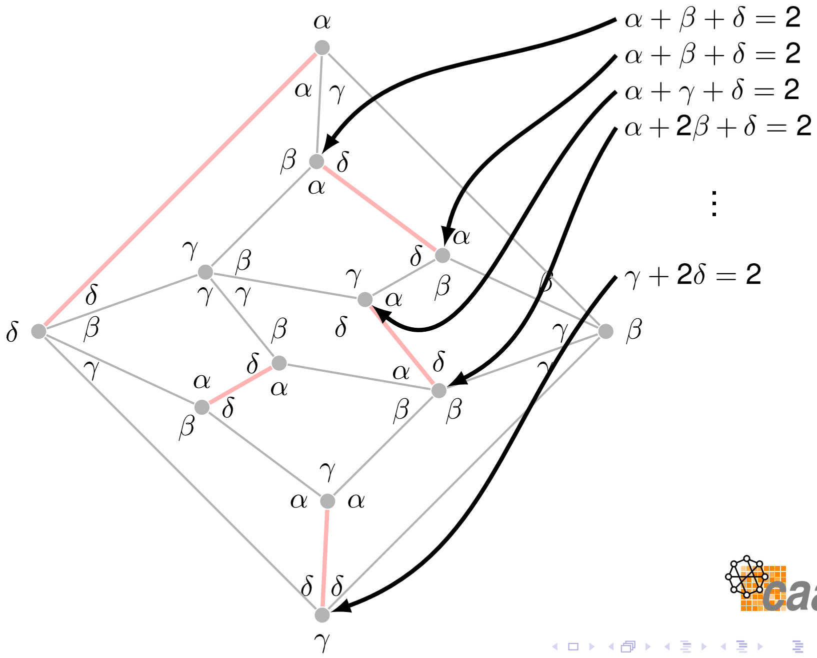


$\alpha + \beta + \delta = 2$

$\alpha + \beta + \delta = 2$

$\alpha + \gamma + \delta = 2$

$\alpha + 2\beta + \delta = 2$



$\alpha + \beta + \delta = 2$
$\alpha + \beta + \delta = 2$
$\alpha + \gamma + \delta = 2$
$\alpha + 2\beta + \delta = 2$
$\vdots$
$\gamma + 2\delta = 2$

System of at most V equations:

$$\alpha + \beta + \delta = 2$$
$$\alpha + \gamma + \delta = 2$$
$$\alpha + 2\beta + \delta = 2$$
$$\vdots$$
$$\gamma + 2\delta = 2$$

System of at most V equations:

$$\alpha + \beta + \delta = 2$$
$$\alpha + \gamma + \delta = 2$$
$$\alpha + 2\beta + \delta = 2$$
$$\vdots$$
$$\gamma + 2\delta = 2$$

$$\beta = 0$$

$$0 < \alpha, \beta, \gamma, \delta < 1$$
$$\alpha - \beta + \delta < 1$$
$$\alpha - \gamma + \delta < 1$$
$$\alpha + \beta + \gamma + \delta = 2 + \frac{4}{F}$$

System of vertex equations

$$\alpha = \delta \Leftrightarrow \beta = \gamma$$

$$(1-\cos\beta)\cos^2\alpha-(1-\cos\beta)(1-\cos\gamma)\cos\alpha\cos\delta+(1-\cos\gamma)\cos^2\delta$$
$$+\cos\beta\cos\gamma+\sin\alpha\sin\beta\sin\gamma\sin\delta = 1$$

Excluding some more systems

$$\alpha = \delta \Leftrightarrow \beta = \gamma$$

Theorem

There is no spherical tiling by isosceles spherical quadrangles of type 2.

In a quadrangulation we have that

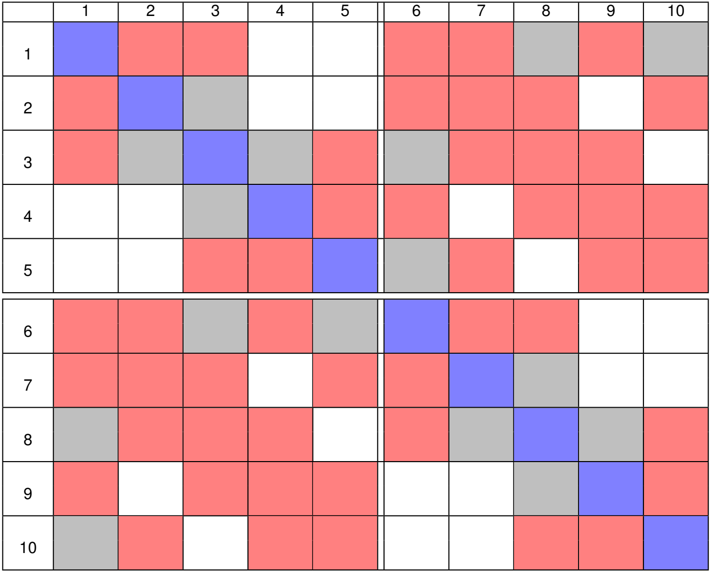
$$V_3 = 8 + V_5 + 2V_6 + 3V_7 + \cdots$$

	8	10	12	14	16	18	20	22	24	26
8	1	1	2	5	8	12	25	30	51	76
9				2	9	32	91	240	542	1 117
10			1	3	22	109	458	1 595	4 847	13 111
11					14	138	998	5 417	23 578	85 526
12				1	4	122	1 437	11 887	72 923	359 205
13						30	986	14 450	137 427	955 661
14					1	7	389	10 777	164 119	1 668 478
15							68	4 414	121 760	1 920 366
16						1	8	1 045	56 094	1 461 650
17								95	14 575	714 385
18							1	6	2 050	216 949
19									127	37 664
20								1	8	3 564
21										150
22									1	7
23										
24										1

The equation corresponding to a certain vertex v is called the **vertex type** of the vertex v.

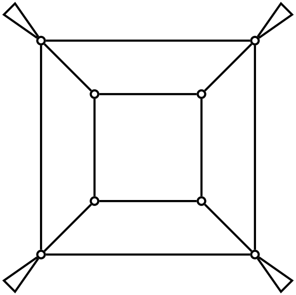
There are only 10 possible vertex types for a vertex of degree 3:

1. $3\beta = 2$
2. $2\beta + \gamma = 2$
3. $\alpha + \delta + \beta = 2$
4. $2\alpha + \gamma = 2$
5. $2\alpha + \beta = 2$
6. $3\gamma = 2$
7. $2\gamma + \beta = 2$
8. $\alpha + \delta + \gamma = 2$
9. $2\delta + \beta = 2$
10. $2\delta + \gamma = 2$


1 2 3 4 5 6 7 8 9 10
1 2 3 4 5 6 7 8 9 10

Theorem

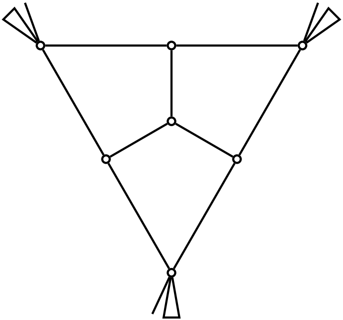
There is no spherical tiling by spherical quadrangles of type 2 which has 3 different vertex types for vertices of degree 3.



Theorem

A quadrangulation on more than 8 vertices that contains a cubic quadrangle does not admit a STCQ2.

n	Quadrangulations	Has cubic quadrangle	Percentage
8	1	1	100.00%
10	1	0	0.00%
12	3	1	33.33%
14	11	2	18.18%
16	58	18	31.03%
18	451	156	34.59%
20	4 461	1 627	36.47%
22	49 957	18 732	37.50%
24	598 102	229 110	38.31%
26	7 437 910	2 910 773	39.13%
28	94 944 685	37 994 819	40.02%
30	1 236 864 842	506 583 828	40.96%



Theorem

In a STCQ2, there is no cubic tristar for which the central vertex is incident to an edge of length b.

	10	12	14	16	18	20	22	24	26
0	1	2	7	31	212	1 998	21 753	254 606	3 091 505
1				6	68	722	8 302	100 217	1 251 608
2			2	3	15	110	1 118	13 508	174 776
3						3	51	652	9 113
4						1	1	9	134
5									1
0	100%	100%	78%	78%	72%	71%	70%	69%	68%
≥ 1	0%	0%	22%	22%	28%	29%	30%	31%	32%

The number of cubic tristars in quadrangulations that do not contain a cubic quadrangle.

Solving the remaining systems

Linear system of equations and inequalities solved with `lp_solve`.

- Freely available (LGPL)
- Easy to integrate in C program

V	No STCQ2	Possible STCQ2	Time
8	0	1	0.194 seconds
10	0	1	0.184 seconds
12	1	2	0.118 seconds
14	8	3	0.158 seconds
16	56	2	0.294 seconds
18	446	5	2.076 seconds
20	4 458	3	37.132 seconds
22	49 952	5	15 minutes
24	598 099	3	6 hours
26	7 437 898	12	7 days
28	94 944 683	2	179 days
30	1 236 864 834	8	14 years

And now...

- Can we exclude some more quadrangulations from the start?
- Can we exclude some more systems without using `lp_solve`?
- Can we find more forbidden substructures or forbidden properties?
- Can we include the remaining restriction?

$$(1-\cos\beta)\cos^2\alpha-(1-\cos\beta)(1-\cos\gamma)\cos\alpha\cos\delta+(1-\cos\gamma)\cos^2\delta$$
$$+\cos\beta\cos\gamma+\sin\alpha\sin\beta\sin\gamma\sin\delta=1$$