# Random generation of combinatorial structures

## Uniform random maps and graphs on surfaces using Boltzmann sampling

a survey by Gilles Schaeffer

CNRS / Ecole Polytechnique,
Palaiseau, France

# What is uniform random generation?

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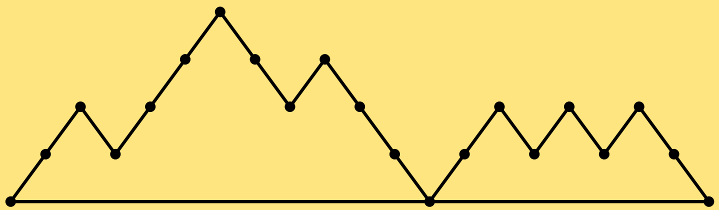
Ex: balanced parenthesis words ($n$ pairs) or ordered trees ($n$ edges)



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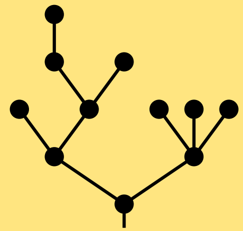

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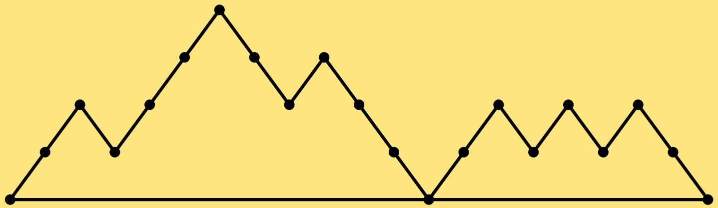

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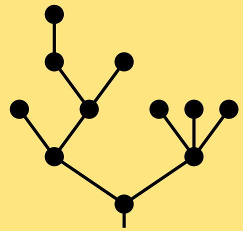

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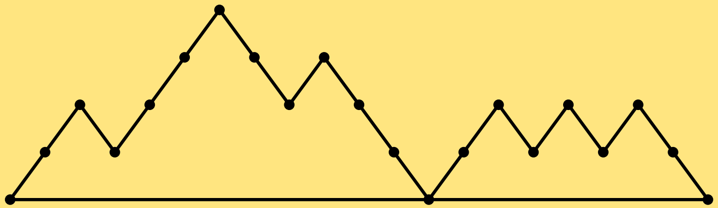

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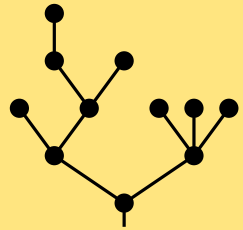

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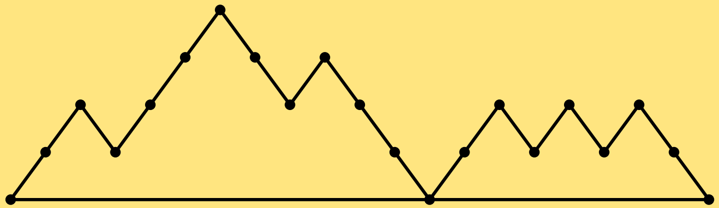

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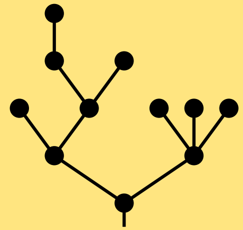

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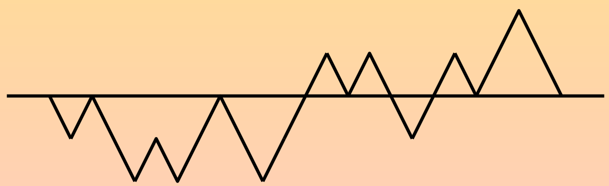

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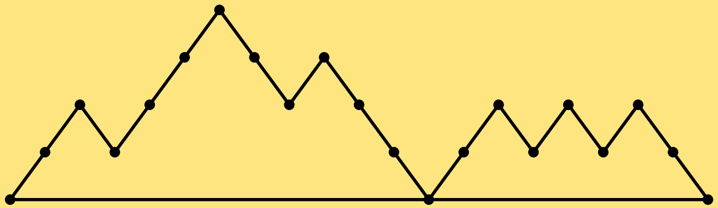

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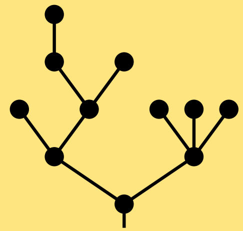

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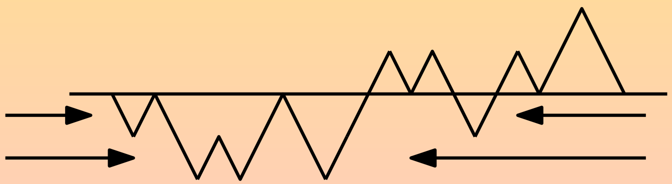

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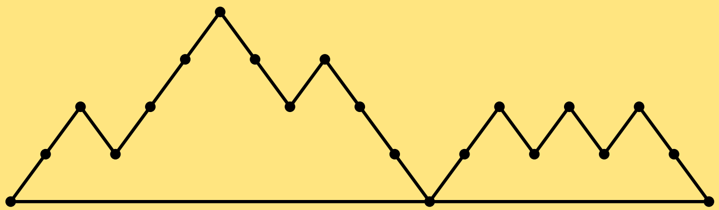

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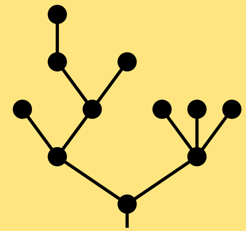

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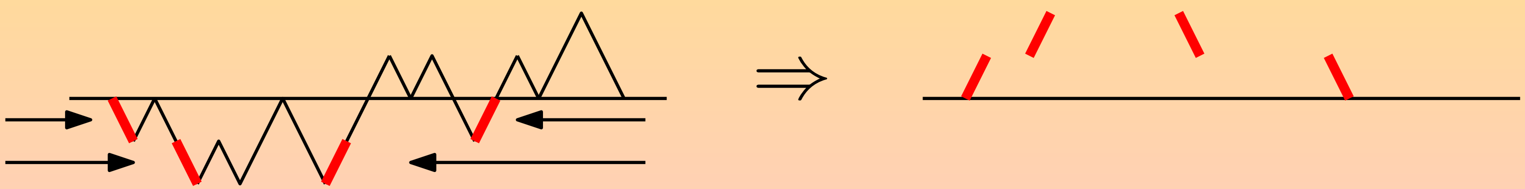

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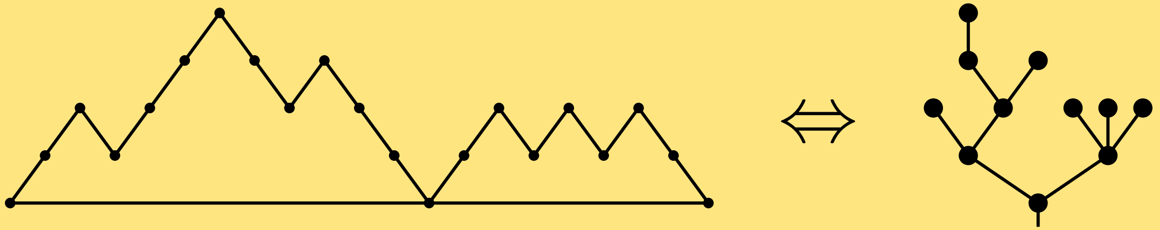

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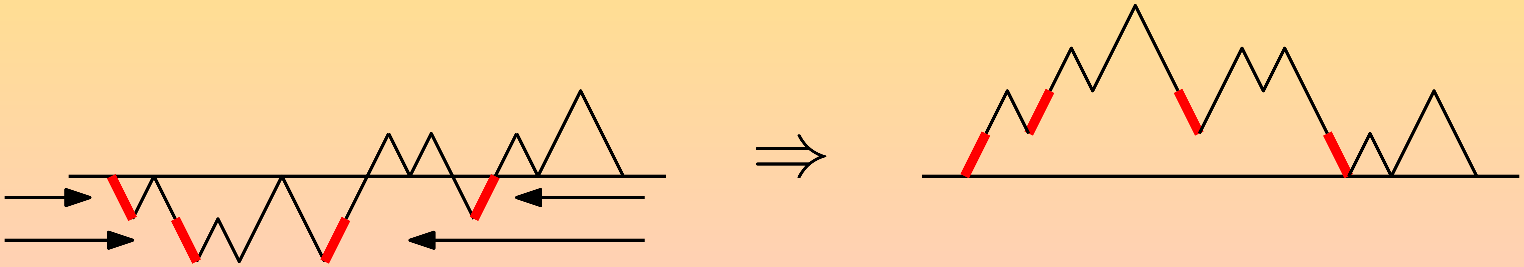

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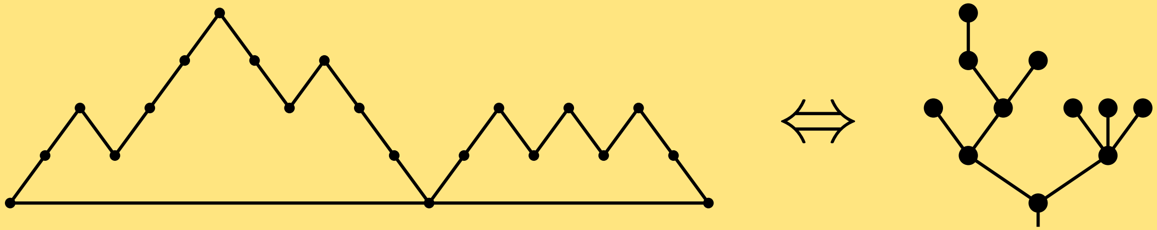

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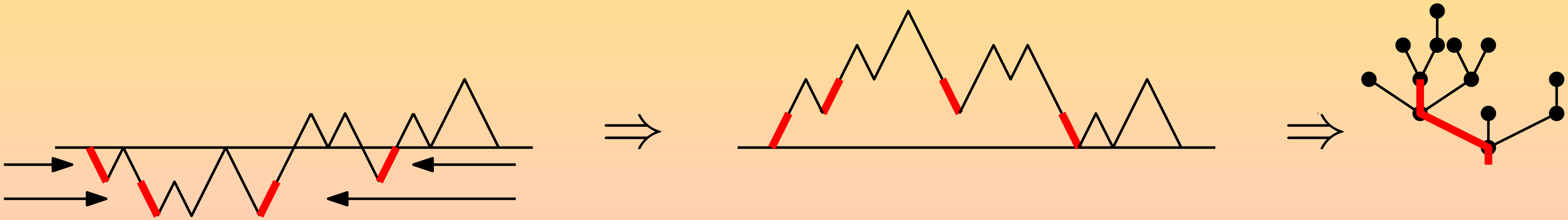

## Uniform random generation, what for?

In silico combinatorics, statistical physics and biology

too many people involved... Denise, Ponty

Experimental companion to average case analysis of algorithms

Flajolet, Zimmermann

Statistical test in model checking

Gaudel, Gouraud, Denise

Average drawing size analysis for planar drawing algorithms

Fusy, S.

## Random sampling paradigms

Markov chain simulations: venerable topic $\longrightarrow$ perfect sampling
$\Rightarrow$ versatile but slow in general (polynomial is good)

Recursive sampling: requires a "combinatorial" recurrence
$\Rightarrow$ optimal when nice bijections are available (linear is good)
$\Rightarrow$ ok for all "decomposable" structures (quadratic is good)

Boltzmann sampling: replace exact counting by GF evaluation
$\Rightarrow$ efficient for decomposable structures and more (linear/quad)

We concentrate on Boltzmann sampling...

## Boltzmann models, Boltzmann sampling

A combinatorial class $\mathcal{A} = (\mathcal{A}_n)_{n\geq 0}$

Its generating function $A(x) = \sum_{a\in A} x^{|a|} = \sum_n |\mathcal{A}_n| x^n$.

Let $x_0 > 0$ be such that $A(x_0)$ is finite (e.g. $x_0 < \rho_A$)

$\Gamma[\mathcal{A}](x_0)$ is a Boltzmann generator of parameter $x_0$ for $\mathcal{A}$ if

$$\Pr(\Gamma[\mathcal{A}](x_0) = a) = \frac{x^{|a|}}{A(x)} \text{ for all } x \in \mathcal{A}.$$

Boltzmann generators are compatible with the sum, product and composition of combinatorial classes.

$$\Gamma[\mathcal{A}+\mathcal{B}](x) := \texttt{if}\ \mathrm{Bern}\left(\frac{A(x)}{A(x)+B(x)}\right) \texttt{then}\, \Gamma[\mathcal{A}](x)\, \texttt{else}\, \Gamma[\mathcal{B}](x)$$

$$\Gamma[\mathcal{A}\times\mathcal{B}](x) := (\Gamma[\mathcal{A}(x)], \Gamma[\mathcal{B}(x)])$$

$$\Gamma[\mathcal{A}\circ\mathcal{B}](x) := \texttt{let}\, a = \Gamma[\mathcal{A}](B(x))\, \texttt{in}\, (a; (\Gamma[\mathcal{B}](x))^{|a|})$$

## Composition in Boltzmann sampling

$\Gamma[\mathcal{A} \circ \mathcal{B}](x) := \texttt{let}\, a = \Gamma[\mathcal{A}](B(x))\, \texttt{in}\, (a; (\Gamma[\mathcal{B}](x))^{|a|})$

Theorem: if $\Gamma[\mathcal{A}]$ and $\Gamma[\mathcal{B}]$ are Boltzmann so is $\Gamma[\mathcal{A} \circ \mathcal{B}]$.

Proof: Let $\gamma \in A \circ B$ with $\gamma = (a; b_1, \ldots, b_k)$ where $a \in \mathcal{A}$, $k = |a|$, $b_i \in \mathcal{B}$ for $i = 1, \ldots, k$, and $|\gamma| = |b_1| + \ldots + |b_k|$.

Then $\Pr\left(\Gamma[\mathcal{A} \circ \mathcal{B}](x) = \gamma\right)$

$$= \Pr\left(\Gamma[\mathcal{A}] = a\right) \cdot \prod_{i=1}^{|a|} \Pr\left(\Gamma[\mathcal{B}](x) = b_i\right)$$

$$= \frac{B(x)^{|a|}}{A(B(x))} \cdot \frac{\prod_i x^{|b_i|}}{B(x)^{|a|}} = \frac{x^{|b_1|+\cdots+|b_k|}}{A(B(x))} = \frac{x^{|\gamma|}}{(A \circ B)(x)}. \qquad \square$$

Theorem: if $\Gamma[\mathcal{A} \circ \mathcal{B}]$ is Boltzmann then so are Core$(\Gamma[\mathcal{A} \circ \mathcal{B}])$ and First$(\Gamma[\mathcal{A} \circ \mathcal{B}])$, where Core$(\gamma) = a$ and First$(\gamma) = b_1$.

# An example: Boltzmann for trees

Recall that $\mathcal{A}$ is the familly of ordered trees: a tree decomposes into a root and a sequence of subtrees attached by edges:

$$\mathcal{A} = \{\textsf{root}\} \times \mathrm{Seq}(\{\textsf{edge}\} \times \mathcal{A})$$

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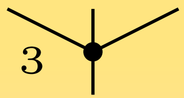
$\Gamma[\textsf{Seq}] = 3$ 

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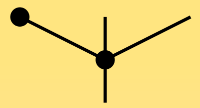

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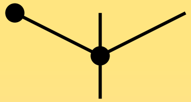

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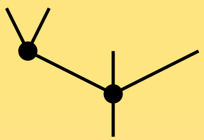

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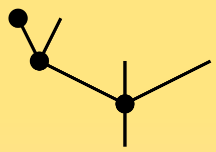

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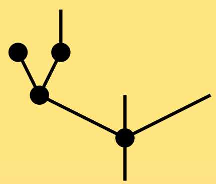

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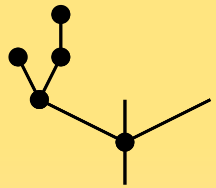

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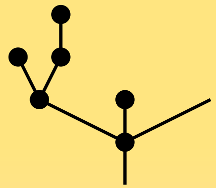

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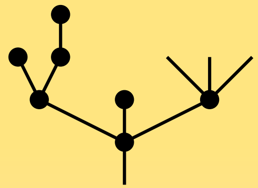

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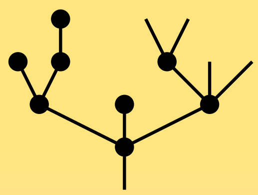

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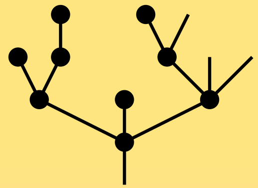

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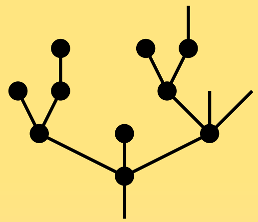

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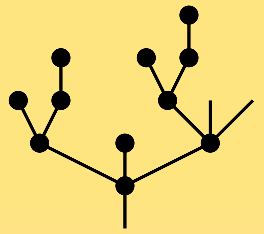

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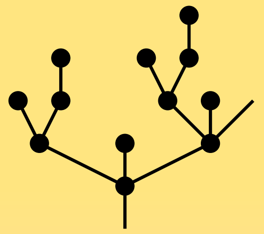

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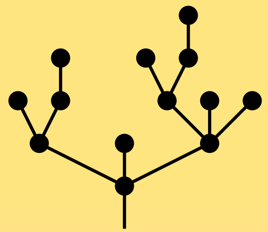

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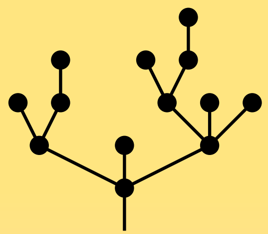

The generation finishes with proba 1.

The probability to get size $n$ depends on the choice of $x$, increasing near the singularity: if $x_n = \frac{1}{4}(1 - \frac{1}{n})$

$$\Pr\left(|\Gamma[\mathcal{A}](x_n))| = n\right) = \frac{|\mathcal{A}_n| \cdot x^n}{A(x)} \approx 4^n n^{-3/2} \left(\tfrac{1}{4}(1 - \tfrac{1}{n})\right)^n \approx n^{-3/2}$$

The expected size of a Boltzmann tree of parameter $x_n = \frac{1}{4}(1 - \frac{1}{n})$ is $\mathbb{E}(|\Gamma[\mathcal{A}](x_n)|) = \frac{A(x_n)'}{A(x_n)} \approx (1 - 4x_n)^{-1/2} = \sqrt{n}$

# Uniform sampling via Boltzmann

The probability to get $\Gamma[\mathcal{A}](x) = a$ depends only on the size of $a$.

Hence the uniform random generator:

$\mathsf{U}[\mathcal{A}(n)] :=$ `do let` $a = \Gamma[\mathcal{A}](x)$ **`until`** $|a| = n$; **`return`** $a$;

# Boltzmann in progress

Initial model: Labelled and rigid unlabelled structures

*Duchon, Flajolet, Louchard, Schaeffer (2002)*

Unlabelled structures and Polya theory

*Flajolet, Fusy, Pivoteau (2007)* and *Bodirsky, Fusy, Kang and Vigerske (2007)*

Efficient oracles for the evaluation of generating series

*Pivoteau, Salvy, Soria (2008)*

Graphs properties via Boltzmann models

*Bernasconi, Panagiotou, Steger, Weißt (2006)*

Complex structures: Apollonian structures, XML documents

*Darasse, Soria (2007), Darasse (2008)*

Complex structures: plane partitions, colored objects

*Bodini, Fusy, Pivoteau (2006), Bodini, Jacquot (2008)*

Complex structures: deterministic automata

*Bassino, NIcaud (2006), Bassino, David, Nicaud (2008)*

Complex structures: planar graphs

*Fusy (2006)*

# Planar graphs, planar maps, and surfaces

A planar graph: there exists an embedding in the plane

A planar map: the (combinatorial) embedding in the plane is fixed

# Planar graphs, planar maps, and surfaces

A planar graph: there exists an embedding in the ~~plane~~
sphere

A planar map: the (combinatorial) embedding in the ~~plane~~ is fixed
sphere

Surfaces: let $\mathcal{S}_g$ be the compact orientable surface of genus $g$: $\mathcal{S}_0$ is the sphere, $\mathcal{S}_1$ the torus; in general $\mathcal{S}_g$ is a "sphere" with $g$ handles.

A map of genus $g$: an embedding of a graph on $\mathcal{S}_g$ (faces must be simply connected): Euler's formula: $v + f = e + 2 - 2g$.

A graph of genus $g$: $g$ is the minimum genus of a surface on which the graph can be embedded.

# Random planar maps

Maps are somewhat easier to deal with.

Start with maps

1-c planar maps = Closure(well labelled ordered trees)

2-c planar maps = Core(1-c planar maps)

3-c planar maps = Core(2-c planar maps) = Closure (binary trees)

3Core(2Core(Closure($\Gamma[\mathcal{A}^3](x)$))) is Boltzmann

# Random planar graphs (rough idea of Eric Fusy's algorithm)

10 steps to planar graphs (title from Liskovets and Walsh, 87)
Decomposition for planar graphs have been available from decades: the equations were partially written several times until the asymptotic was done by Gimenez and Noy, and efficient random generation by Fusy

labelled planar graphs = sets of 1-connected planar graphs

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Illustration:

# Random planar graphs and maps: some remarkable properties

the decomposition tree: iterate the decomposition

the decomposition is "symmetric": the starting point does not matter

there is a unique giant node in the tree

Bender-Richmond-Wormald, Gao-Wormald, Banderier-Flajolet-Schaeffer-Soria, Gimenez-Noy, Panagiotou-Stenger

the distance between two vertices is of order $n^{1/4}$

the graph/map/giant component converge to the continuum brown

Recall that *emphasised statements* are conjectures

## Random graphs on surfaces

the same picture remains true "almost surely":

the genus is a.s. concentrated in the giant component

proved for maps (Chapuy, Kang, Schaeffer), not yet for graphs

Uniform on the set of graphs that can be embedded in $\mathcal{S}_g$:

have a.s. minimum genus $g$, concentrated in one 3-connected component with unique embedding

at fixed genus $g$, distances are of order $n^{1/4}$ and the limit is the continuum random map of genus $g$.

The problem (should) boils down to sampling maps of genus $g$

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# Random graphs on surfaces

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# Combinatorics

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Combinatorial objects

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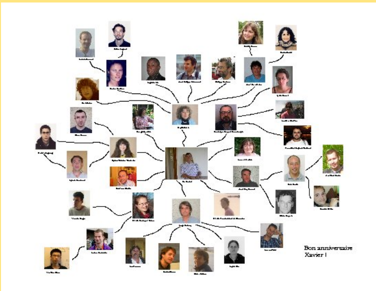
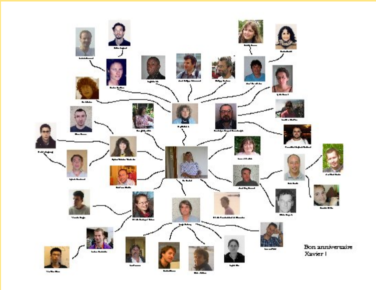
Combinatorial objects

tree like structures

# Combinatorics

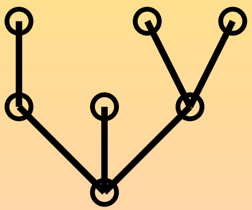
Combinatorial objects





tree like structures

concept of graph



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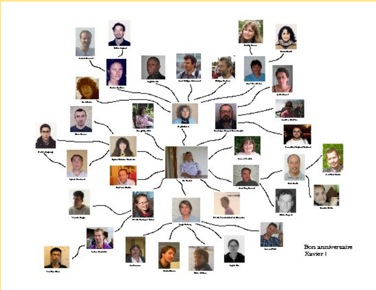

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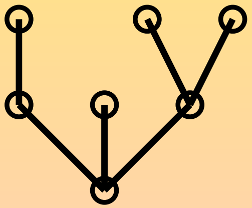

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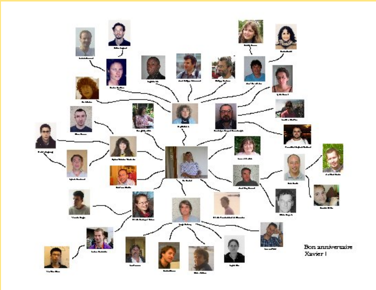

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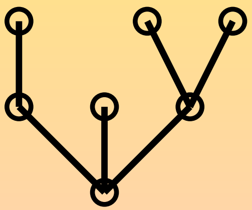

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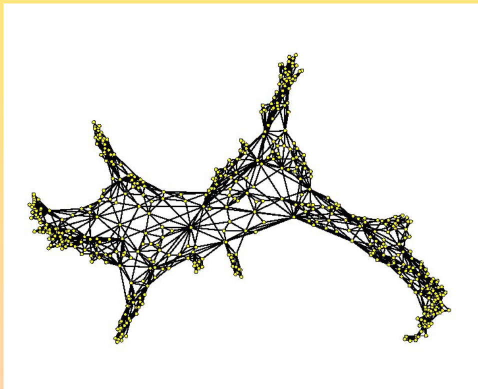
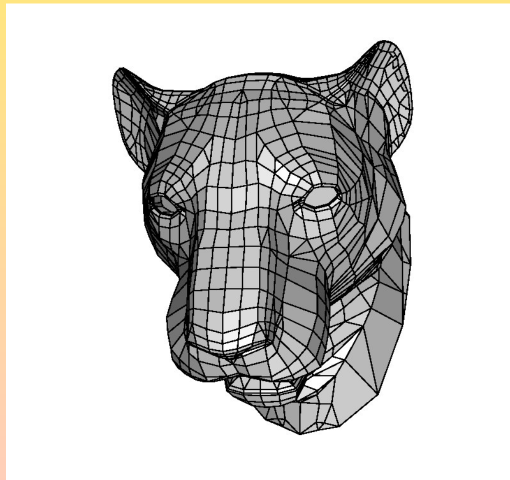
2d discrete structures

(discretized surfaces, meshes,...)



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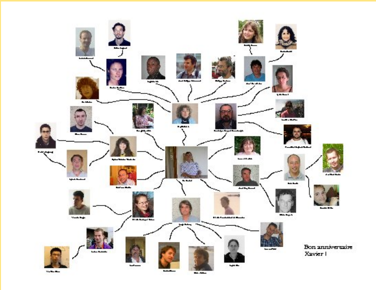


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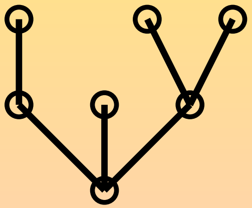

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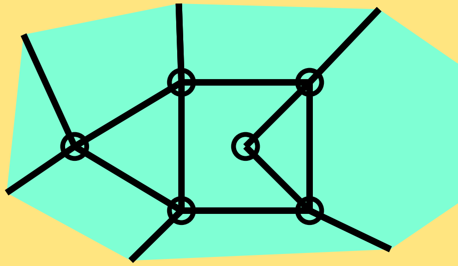

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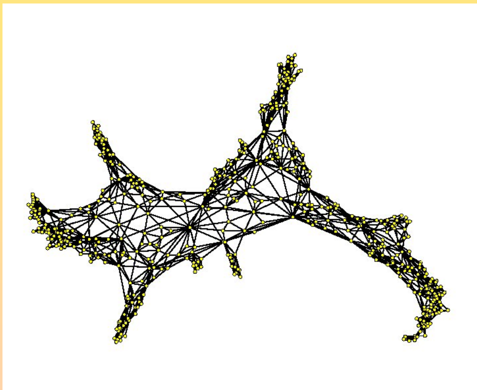

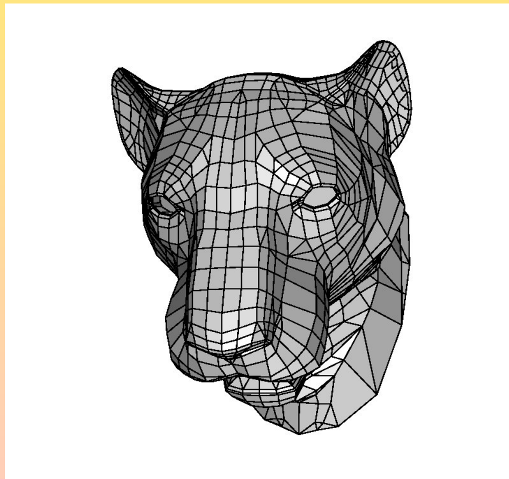

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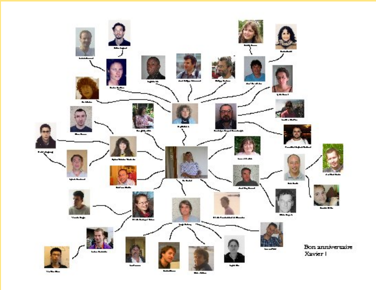


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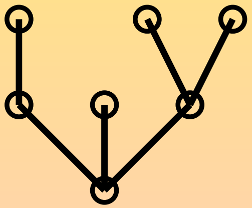

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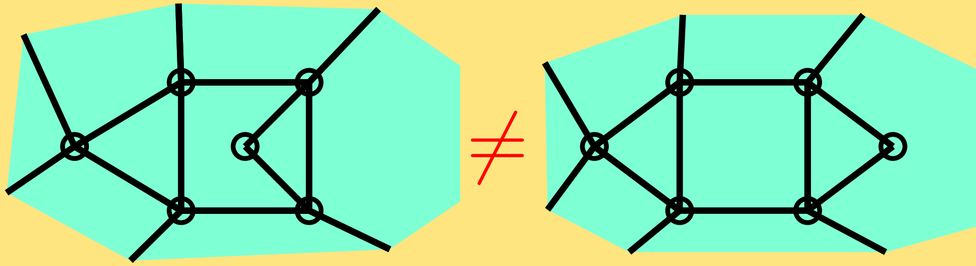
concept of *map*



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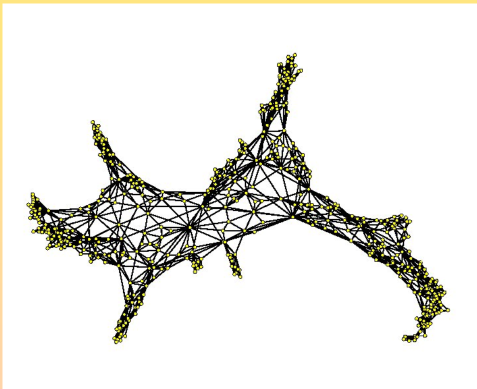
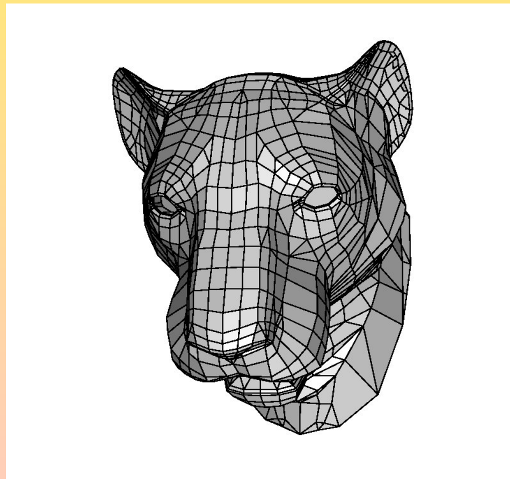
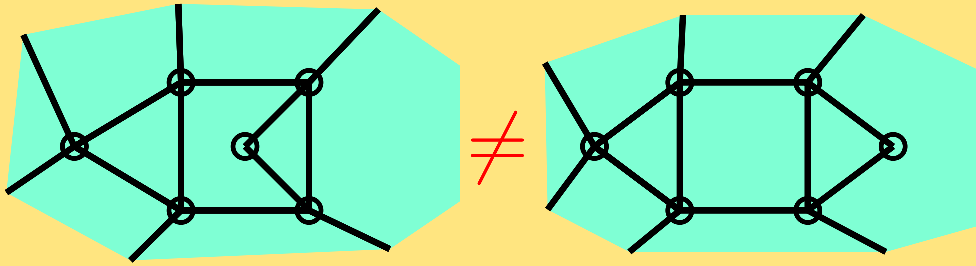




# Combinatorics

Combinatorial objects = discrete abstractions of fundamental structures

concept of *map*



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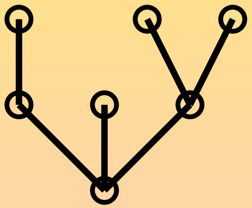

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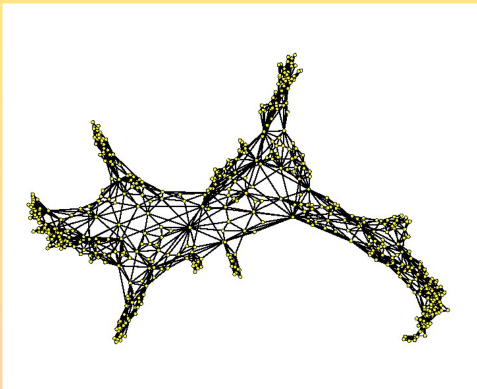

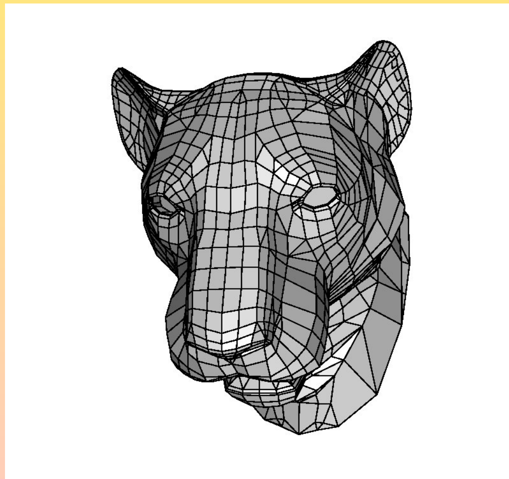

## My idea of combinatorics

Elucidate the properties of those fundamental discrete structures that are common to various scientific fields (CS/math/physics/bio).

# Algorithmic combinatorics

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## and, more specifically of "algorithmic combinatorics"

concentrate on constructive properties and on the algorithmic point of view on structures

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concentrate on constructive properties and on the algorithmic point of view on structures

## The example of trees...

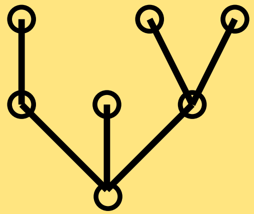
mathematical pt of view: connected graphs without cycle

algorithmic pt of view: recursive description (root; subtrees)
$\Rightarrow$ concept of breadth first or depth first search,
links with context free languages

(... Schützenberger's methodology...)

# Exploration algorithms

## Tree exploration



breadth first

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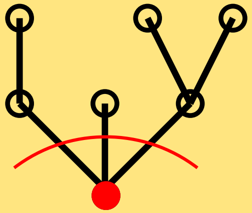

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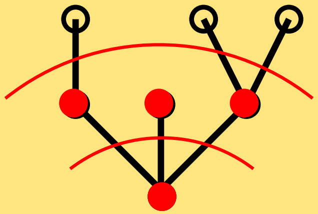

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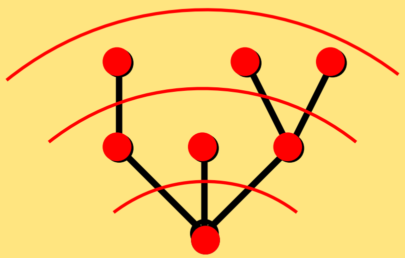

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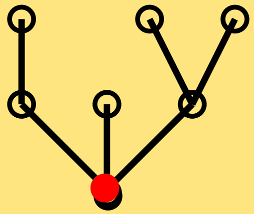

breadth first

depth first

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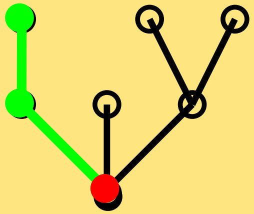

breadth first

depth first

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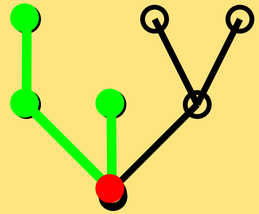

breadth first

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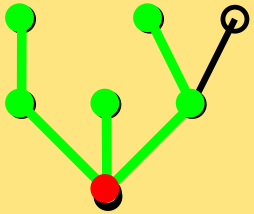

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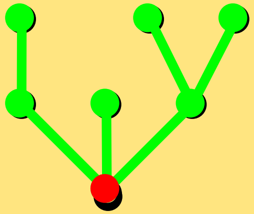

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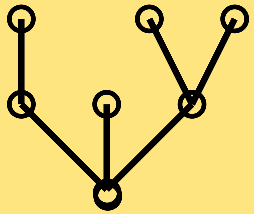

breadth first

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fundamental tools

for instance to encode trees

# Exploration algorithms

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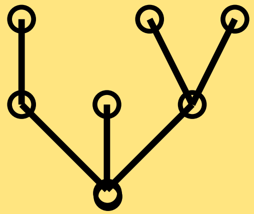

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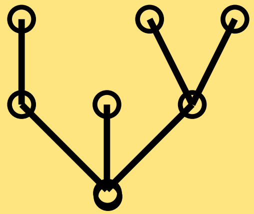

breadth first

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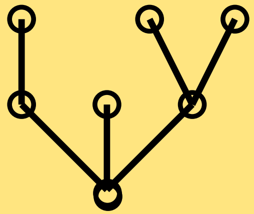
3 1 0 2 0 0 0 (breadth first)

3 1 0 0 2 0 0 (depth first)

# Exploration algorithms

## Tree exploration



breadth first

depth first

fundamental tools

for instance to encode trees

$\Rightarrow$ the prefix code of a tree

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**Statement.** The set of code words is easy to describe.

More precisely: the language of prefix codes of ordered trees is *context-free*.

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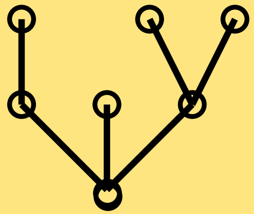

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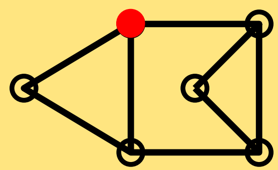

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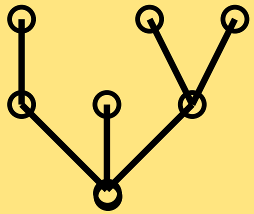

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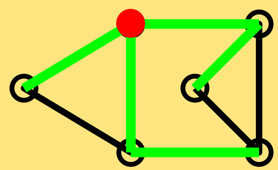

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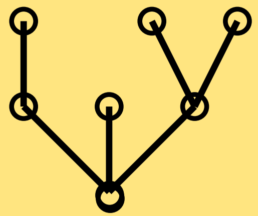

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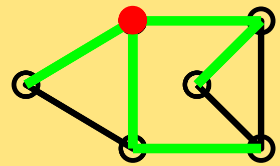

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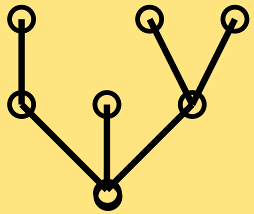

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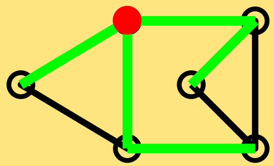

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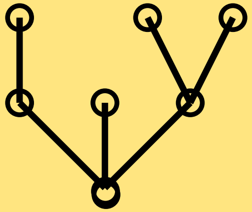

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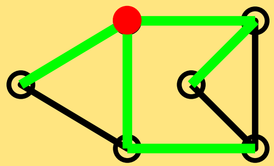

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No good analog of the previous "statement".

## Exploration of a map and surface surgery

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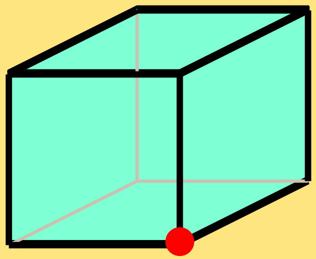

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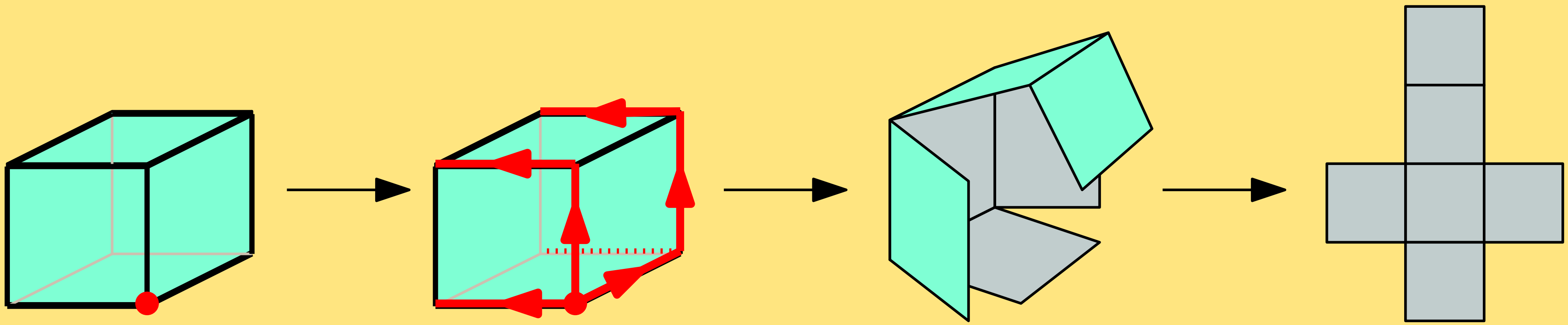

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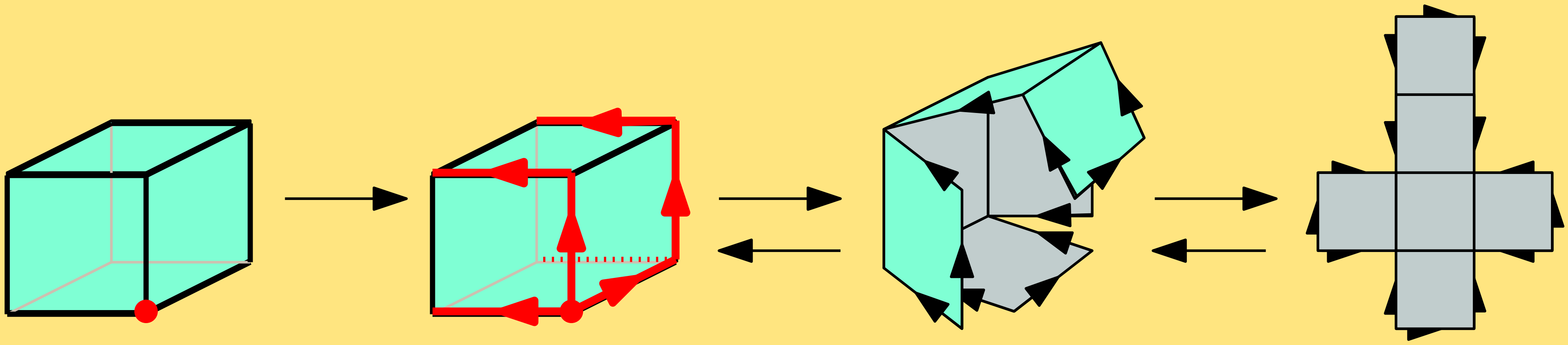

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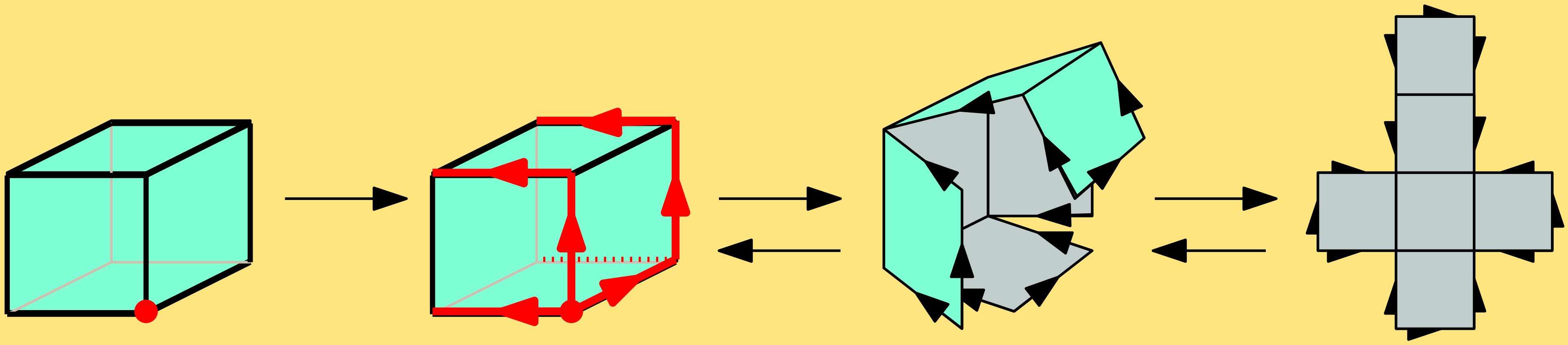

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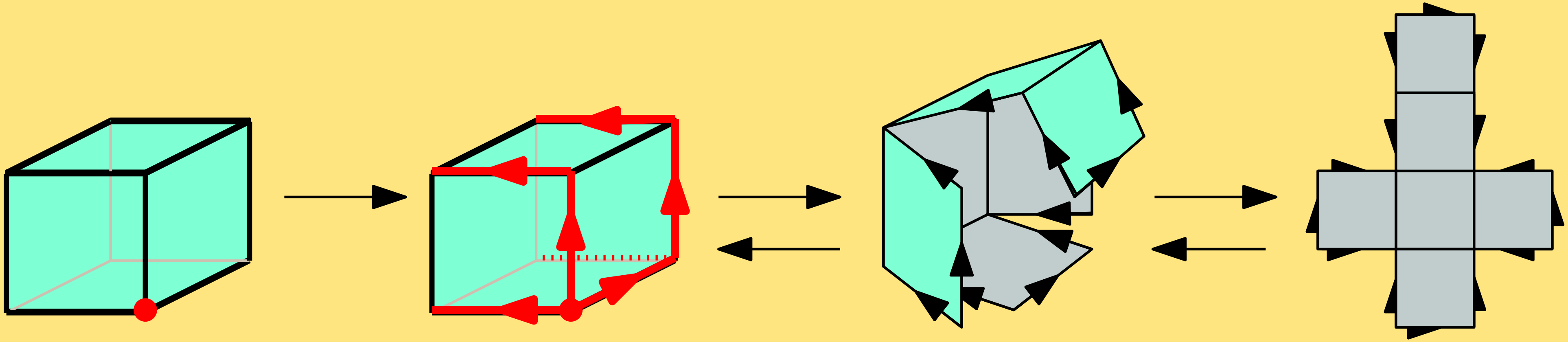

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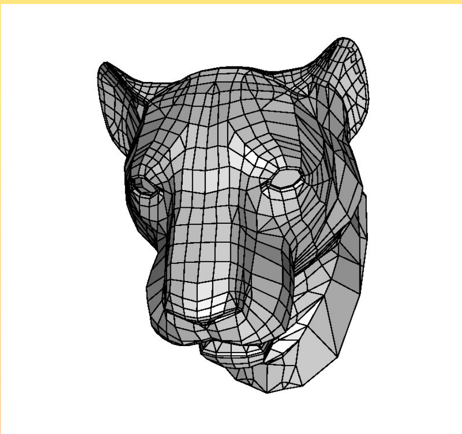
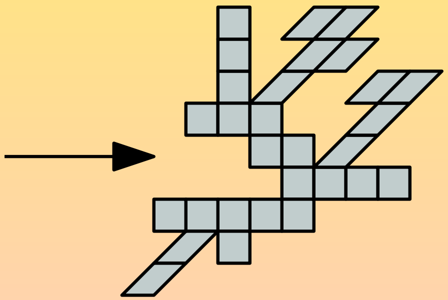


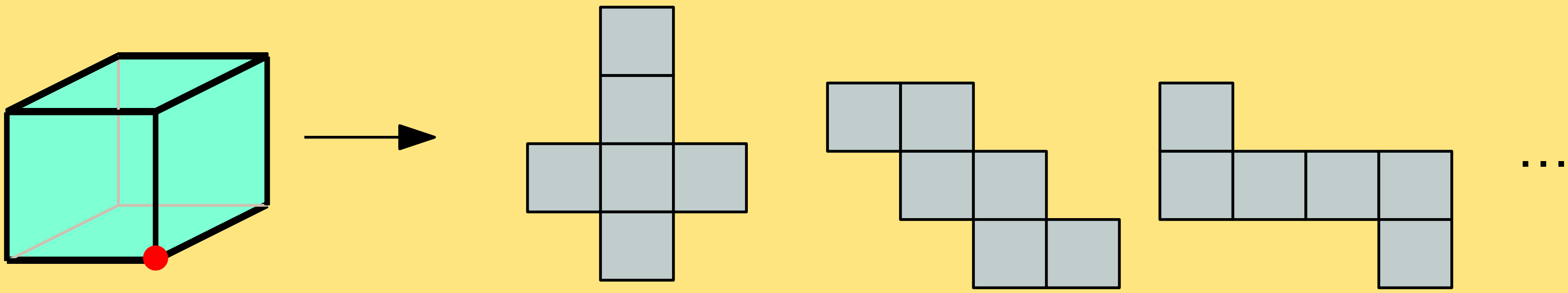


Nets are always trees of polygons

(as long as the surface has no handle)

# Exploration algorithms

To a map are associated many different nets



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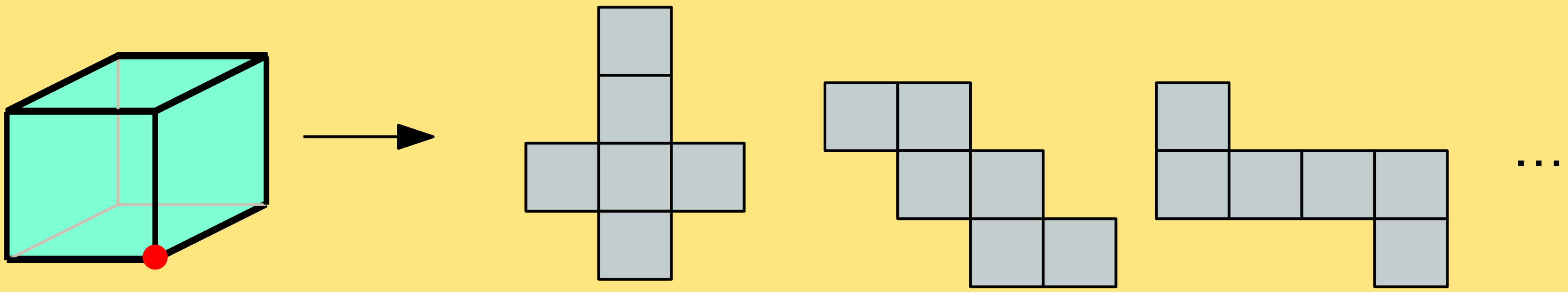

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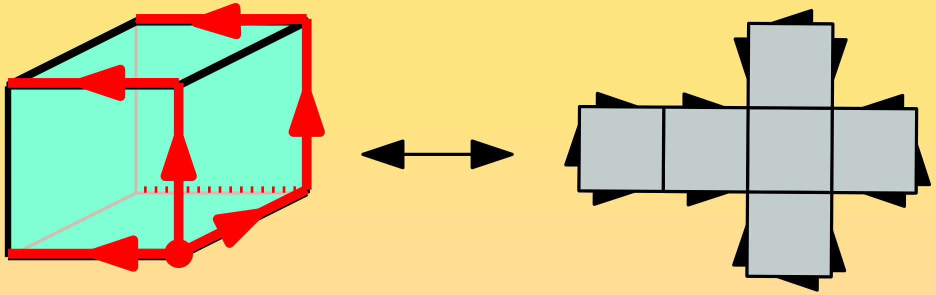

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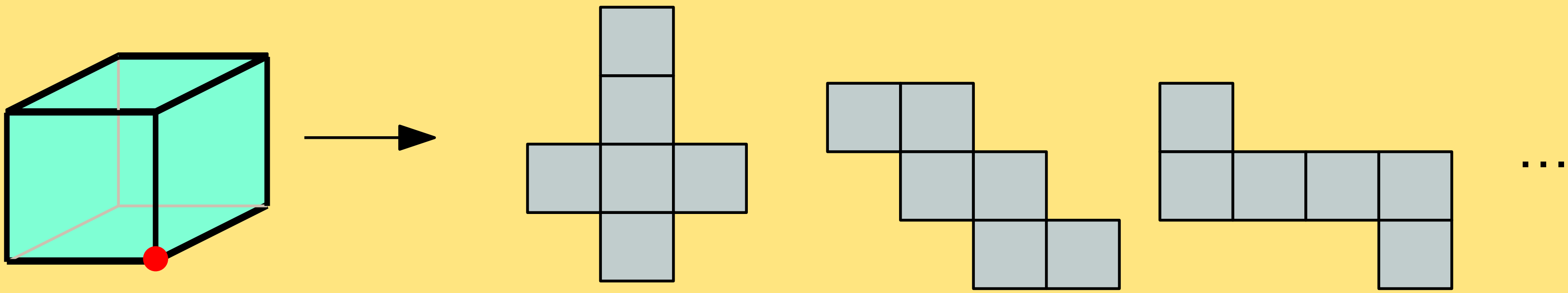

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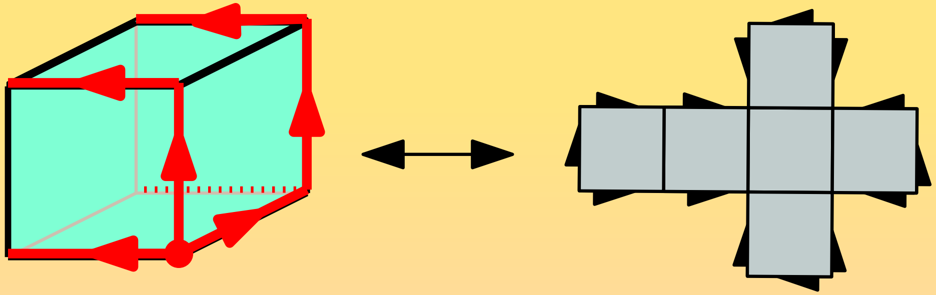

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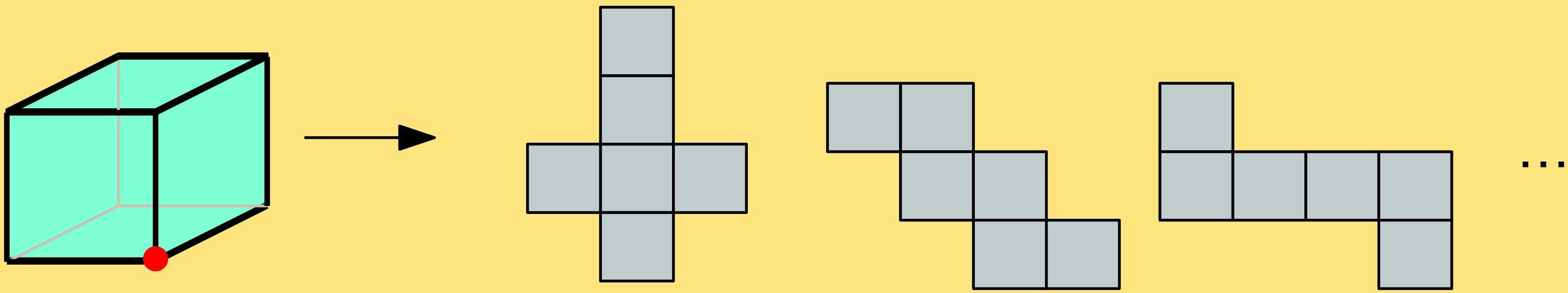

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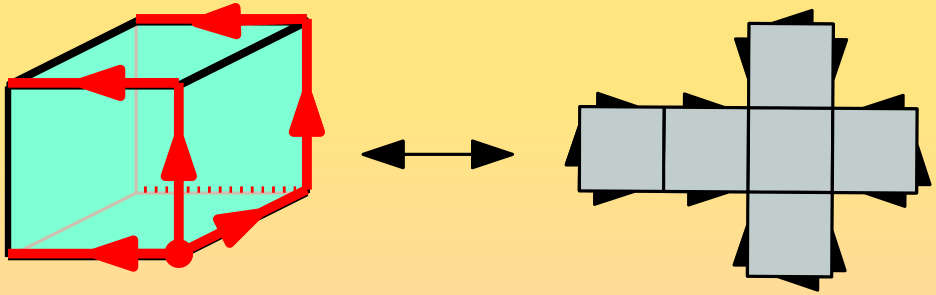

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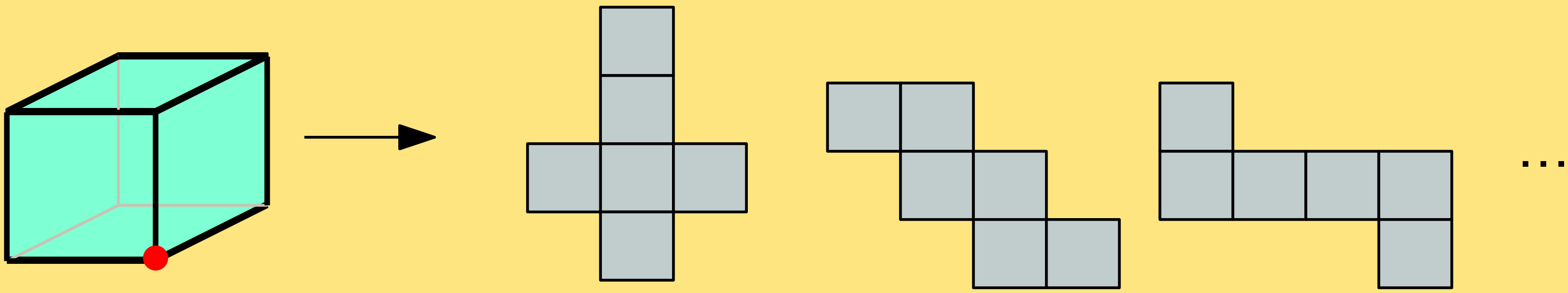


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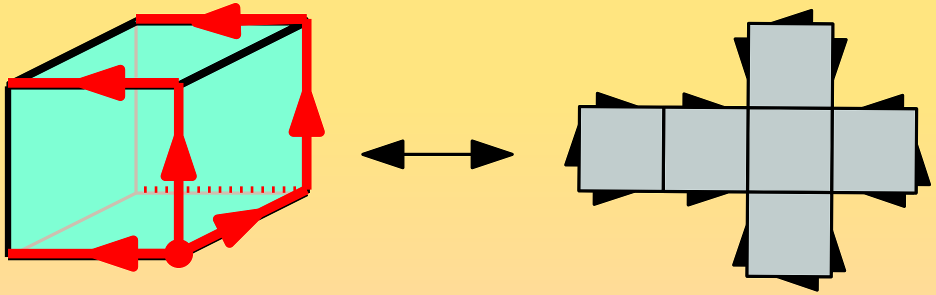

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Valid nets are easier to describe than exploration trees!

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To many natural families of maps is associated a standard exploration algorithms (breadth first, depth first, Schnyder,...) such that the cut yields *context-free* nets.

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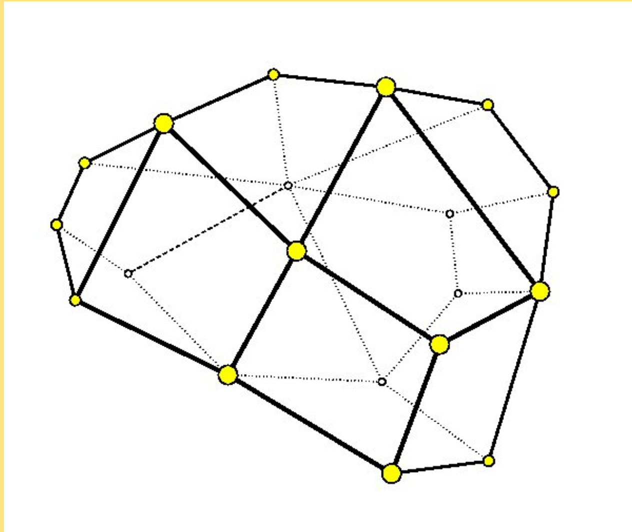
### with various types of applications

- optimal encodings and compact data structures for meshes
- random sampling and automatic drawing of graph and map
- enumeration: maps, ramified coverings, alternating knots...
- random discrete surfaces

# Application to discrete random surfaces

Planar quadrangulations (quads) as a model of discretized spheres



Let $|Q_n|$ be the set of quads with $n$ faces and $X_n$ be a uniform random quad of $Q_n$:

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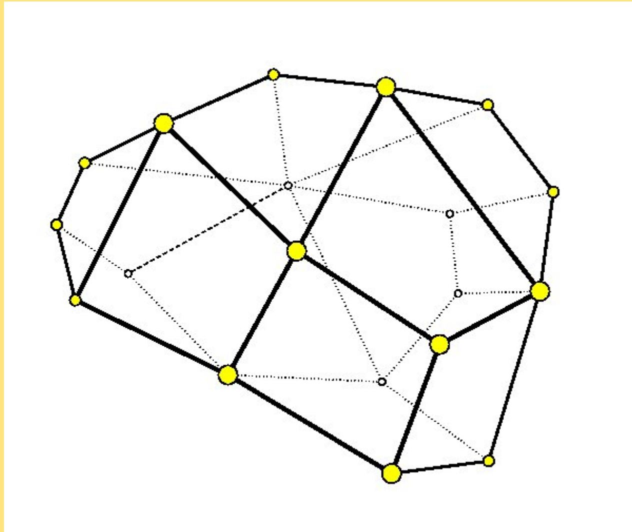

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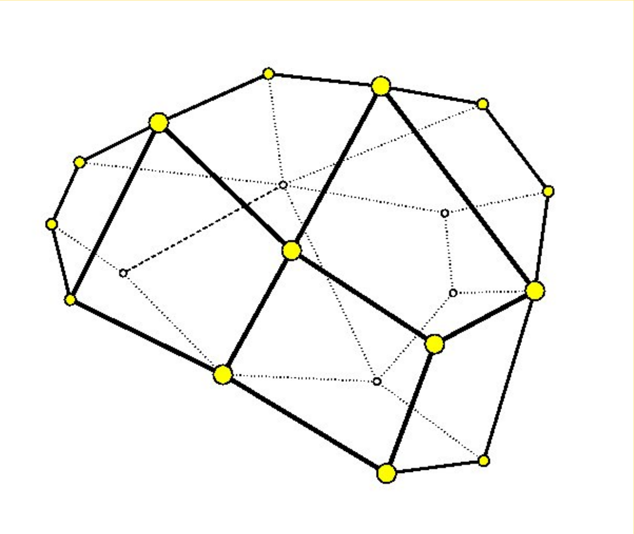

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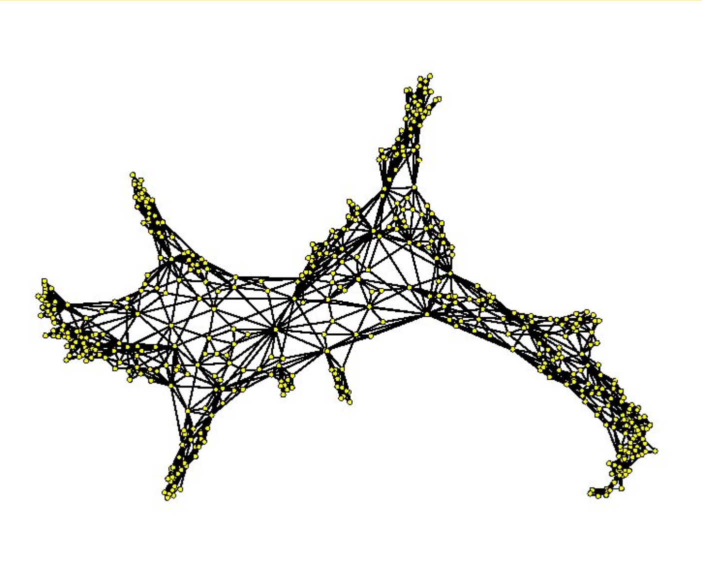

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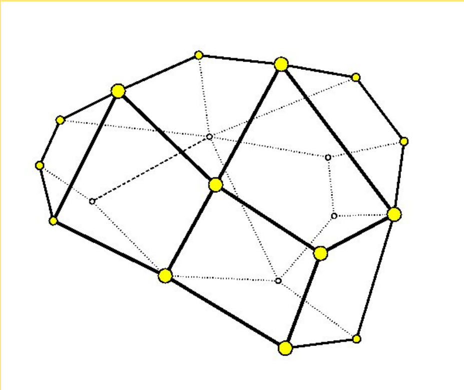
But this approach does not allow to study the intrinsec geometry of these surface!

# Quadrangulations via breadth first search

Consider a planar quadrangulation



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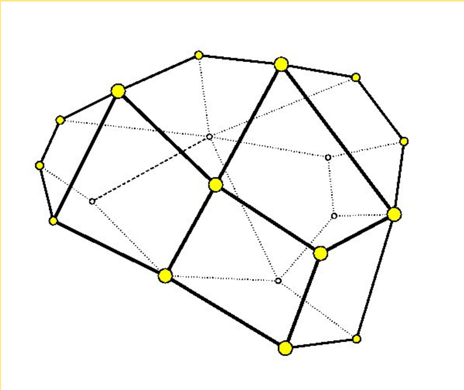

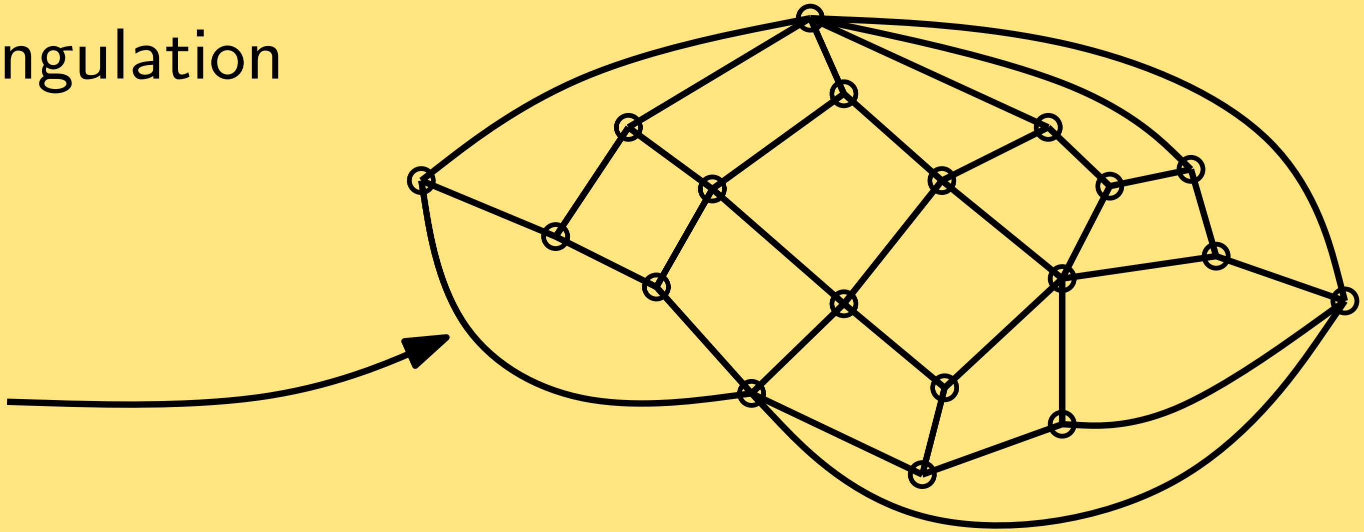

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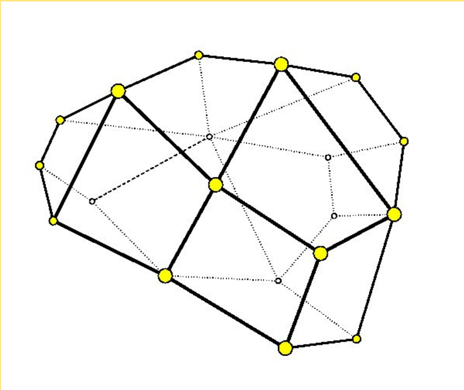

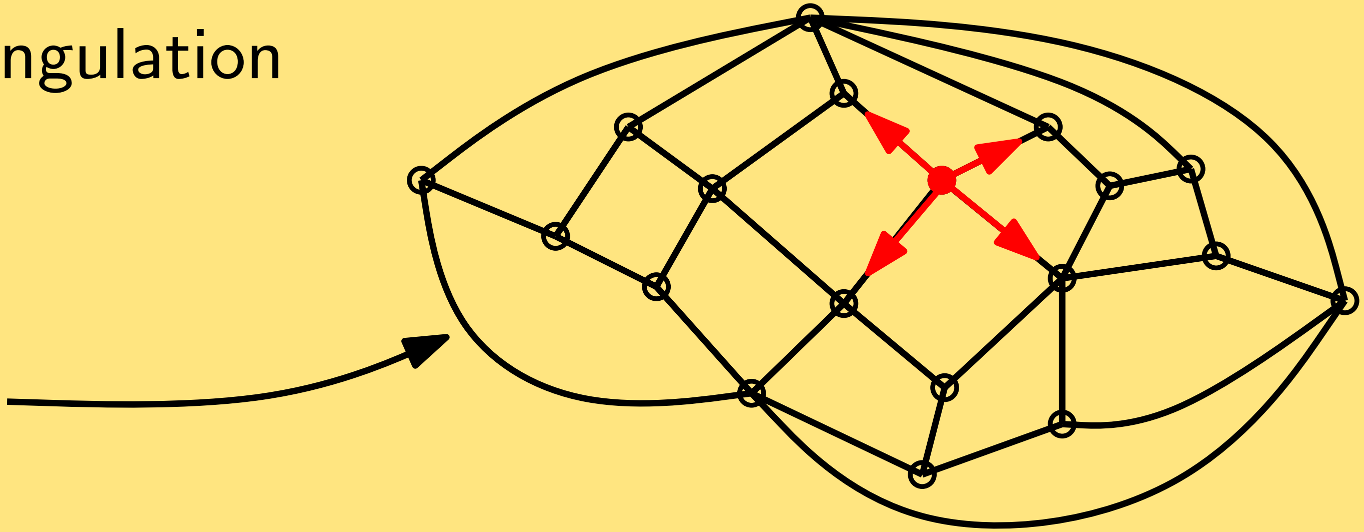

Apply bfs with the rotatoria rule
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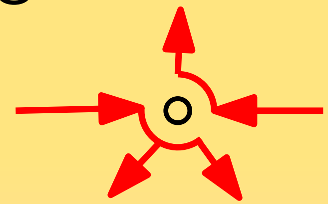

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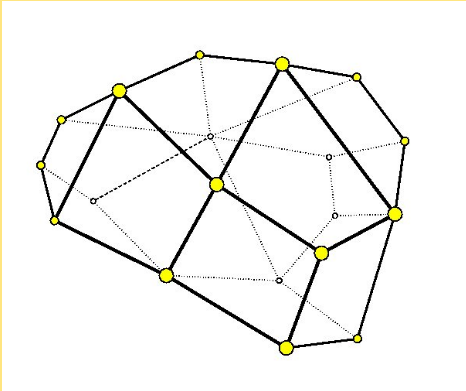

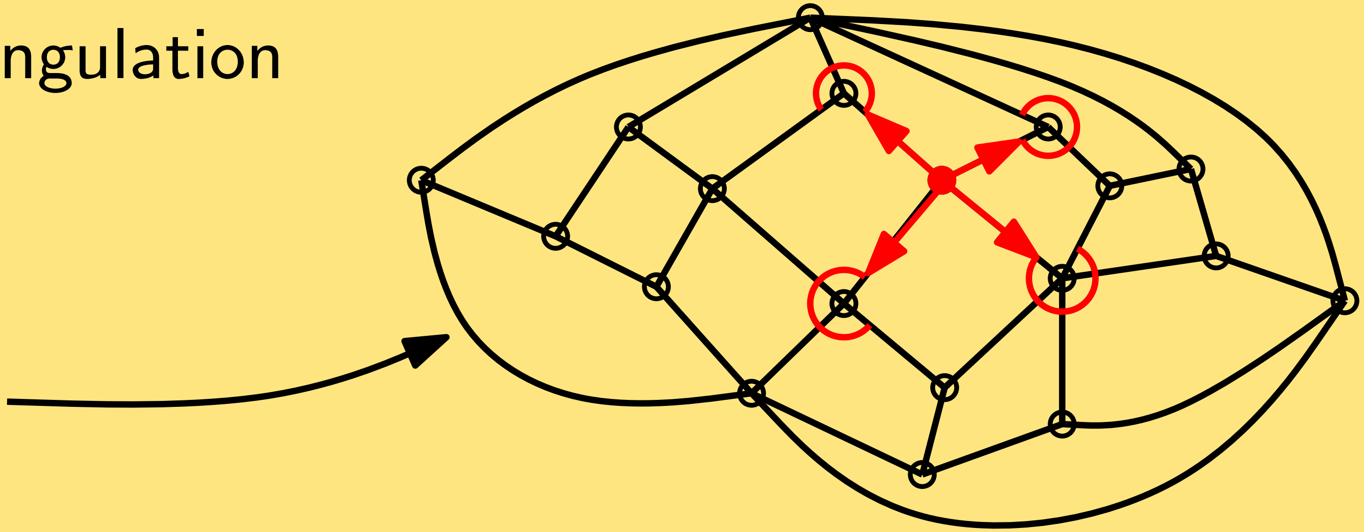

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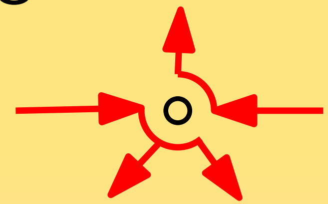

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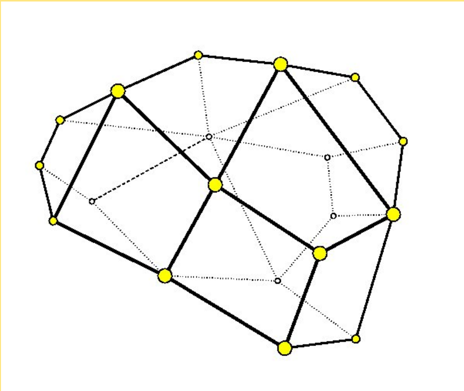

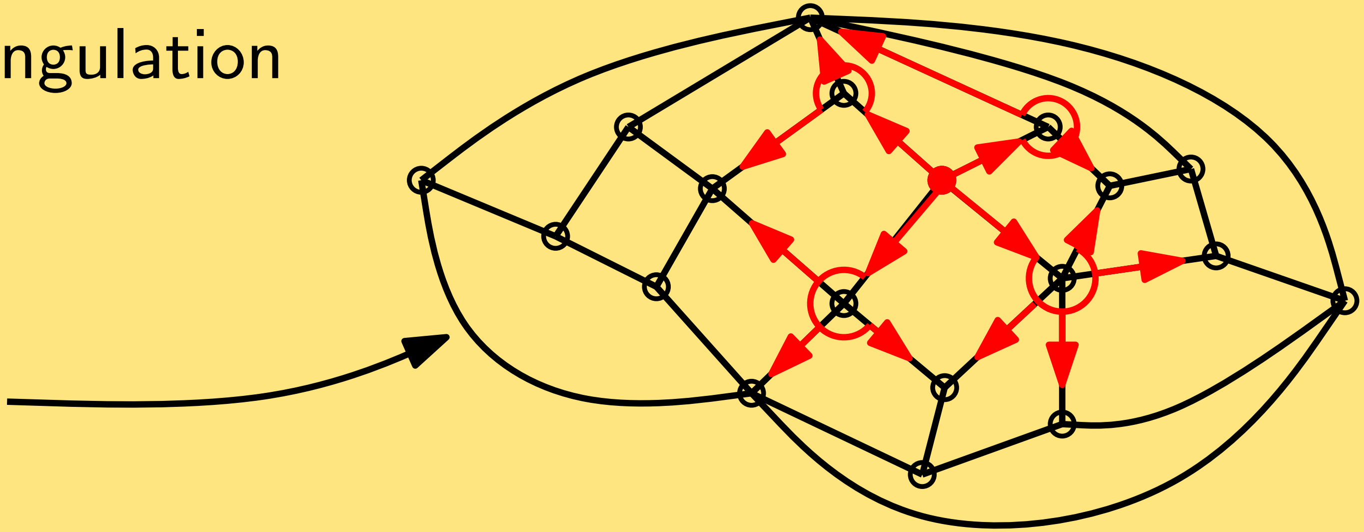

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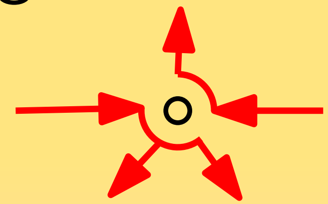

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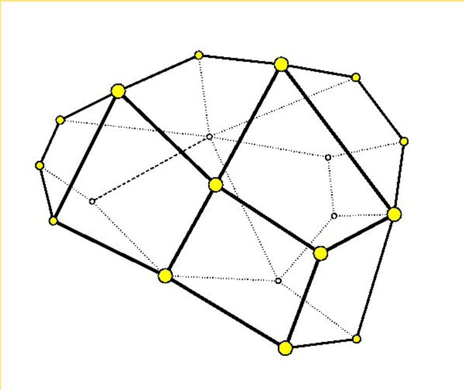

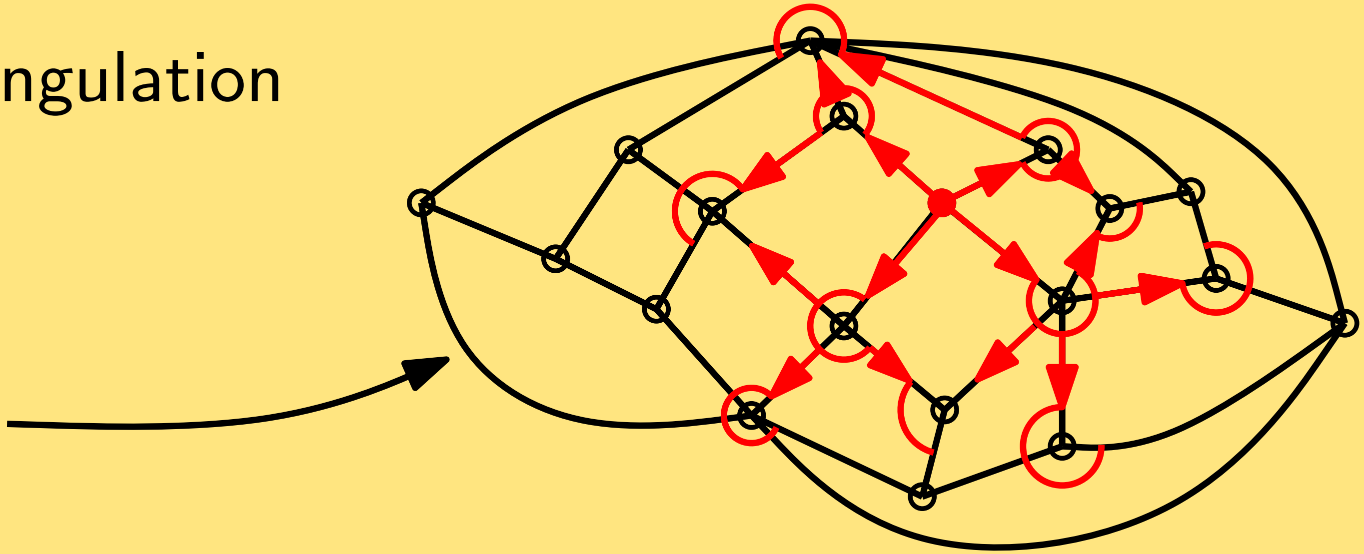

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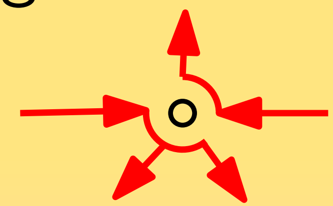

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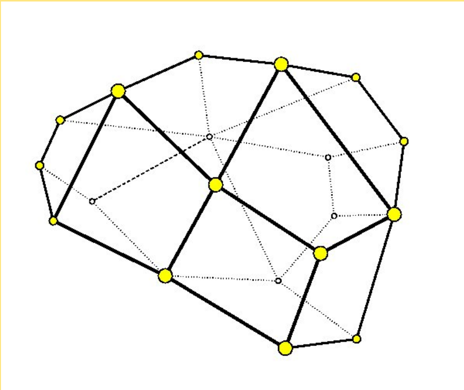

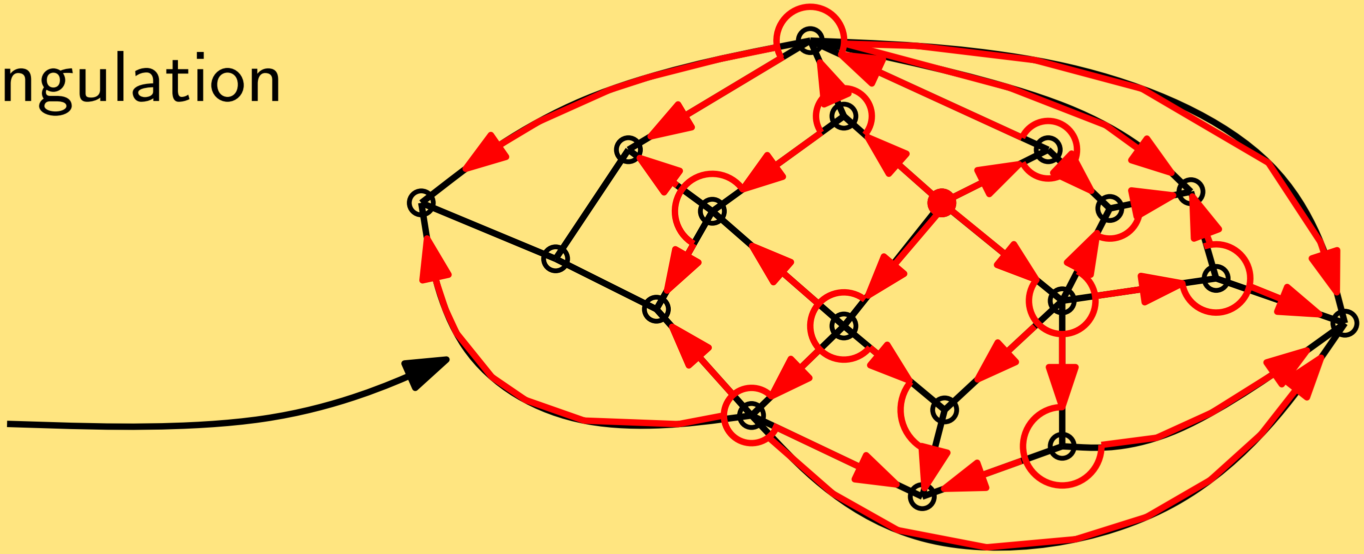

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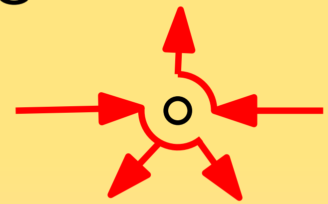

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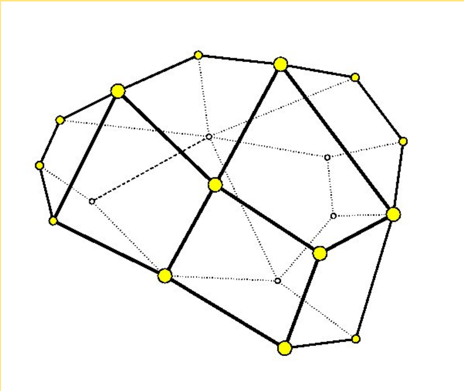

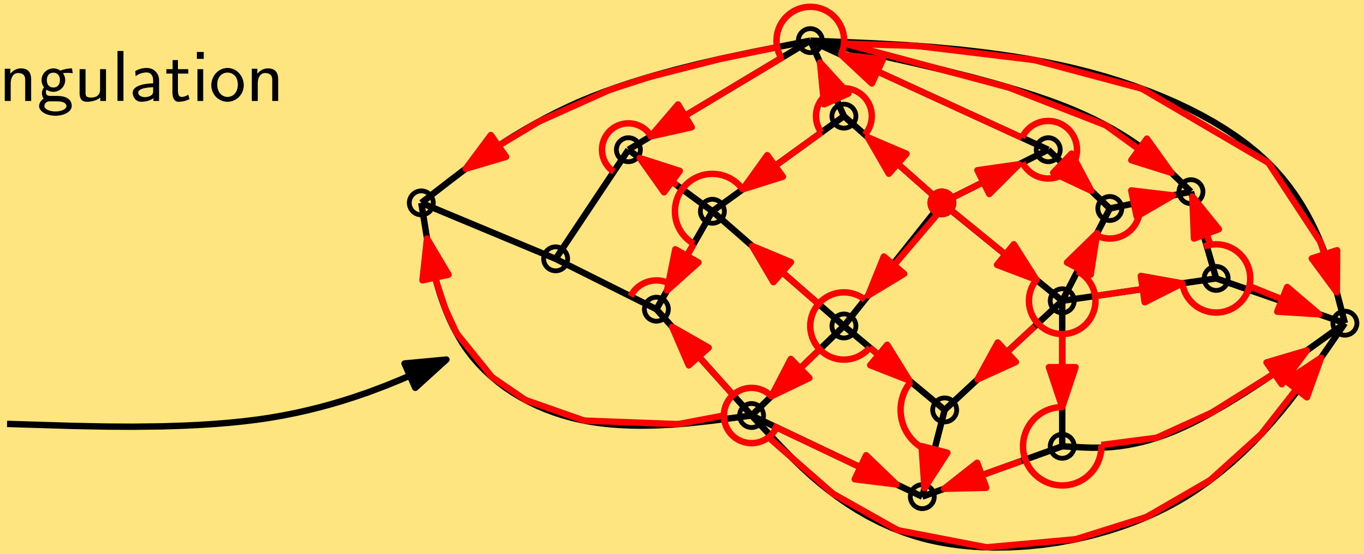

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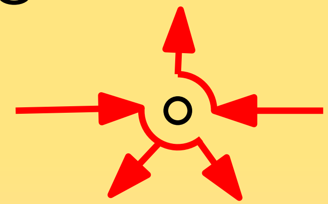

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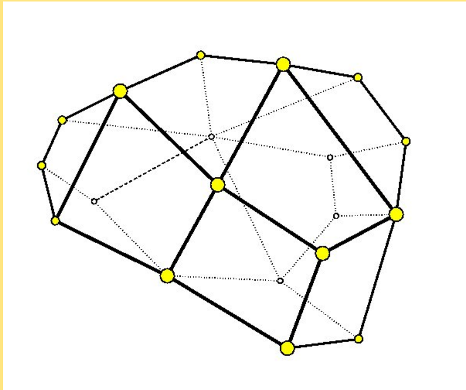

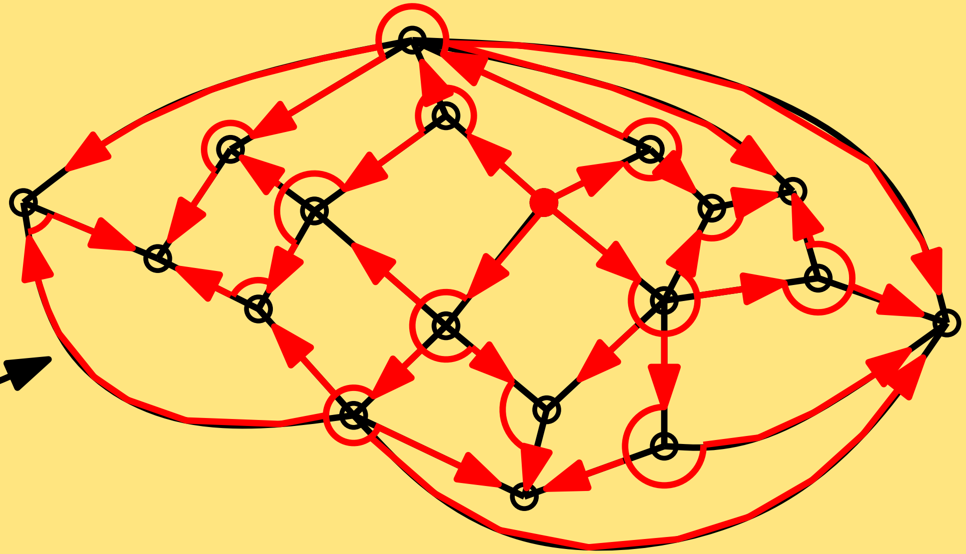

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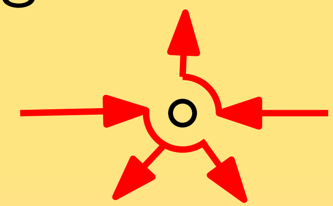

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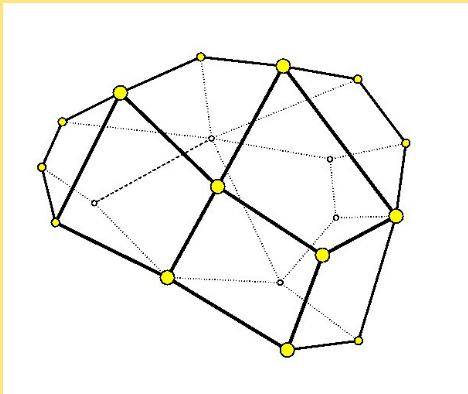

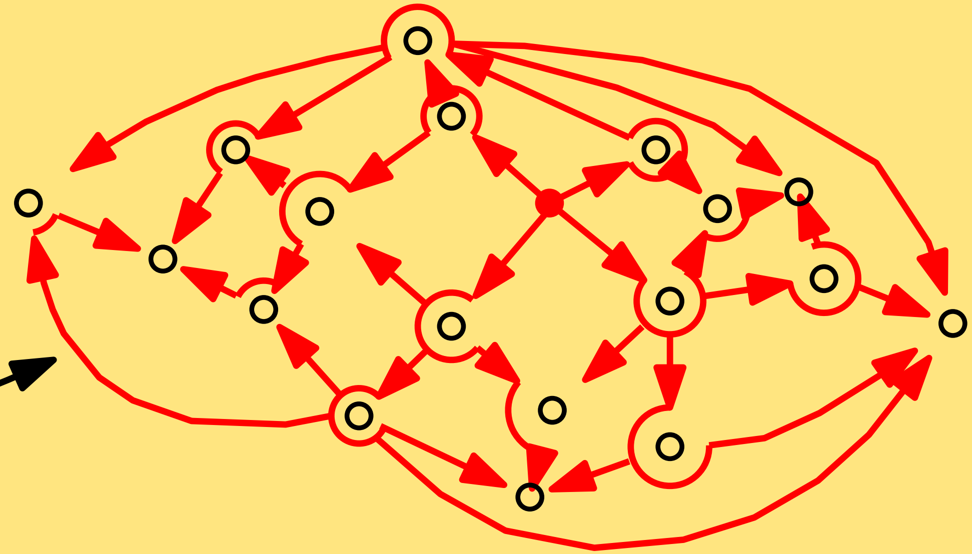

Apply bfs with the rotatoria rule
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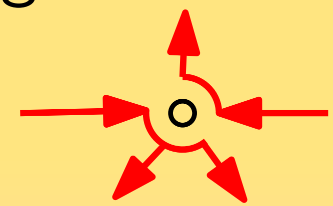

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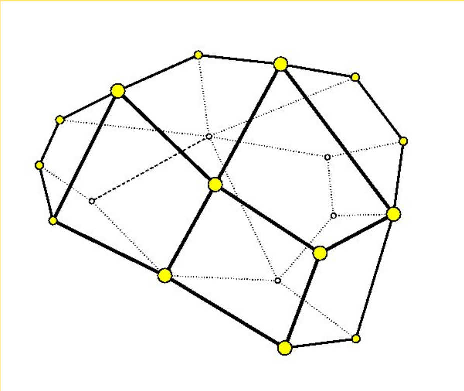

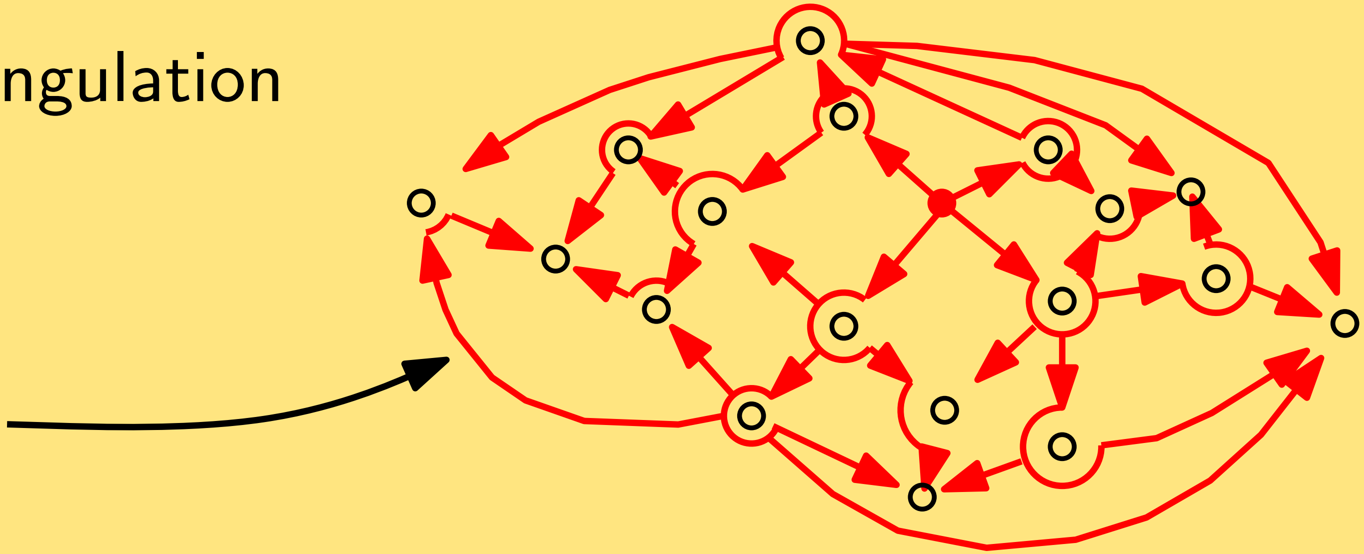

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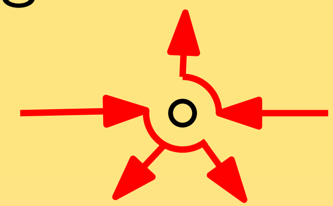
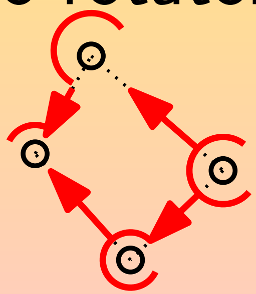


Each face sees exactly two rotatoria



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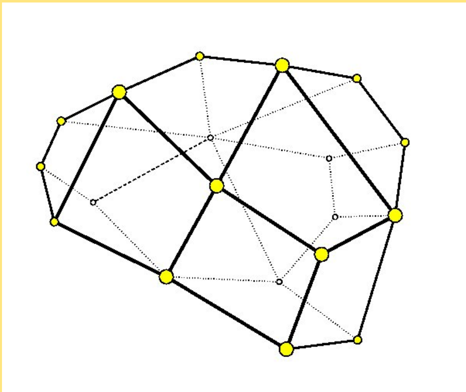

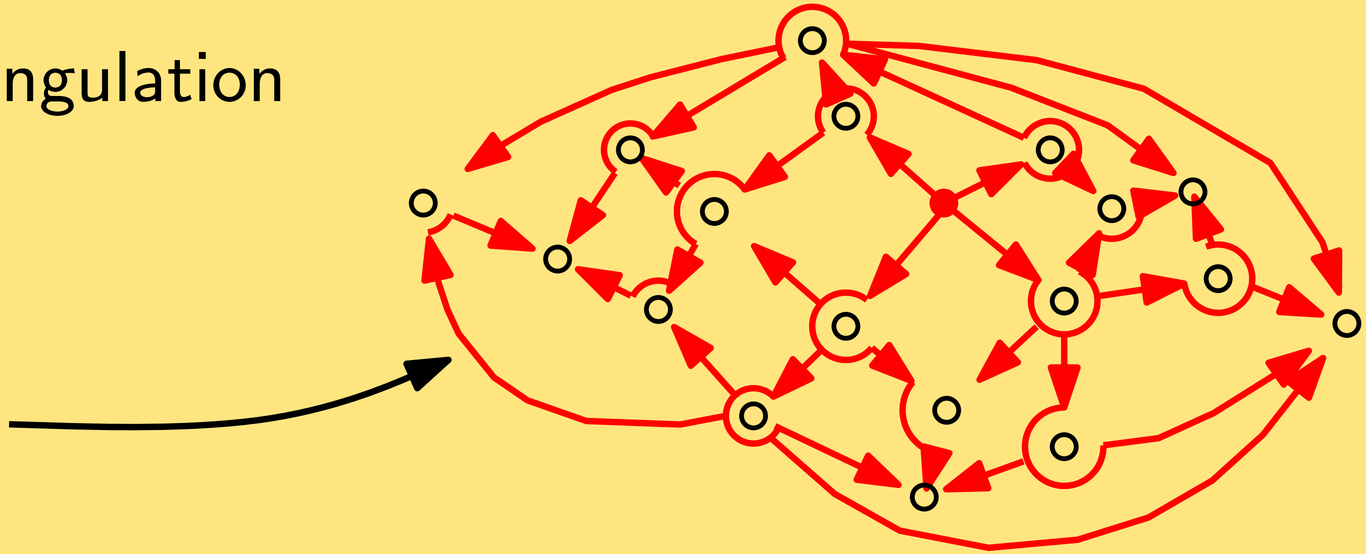

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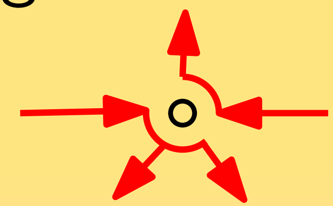

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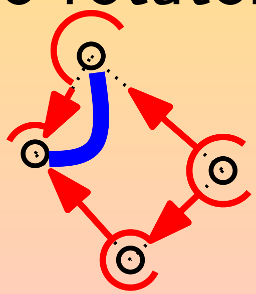

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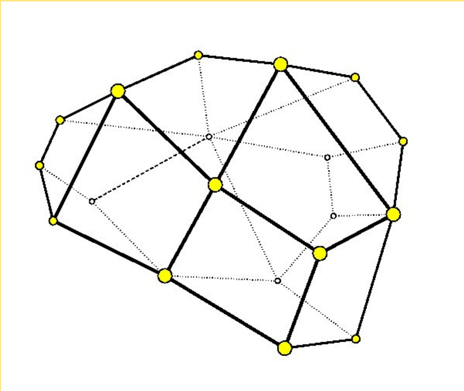

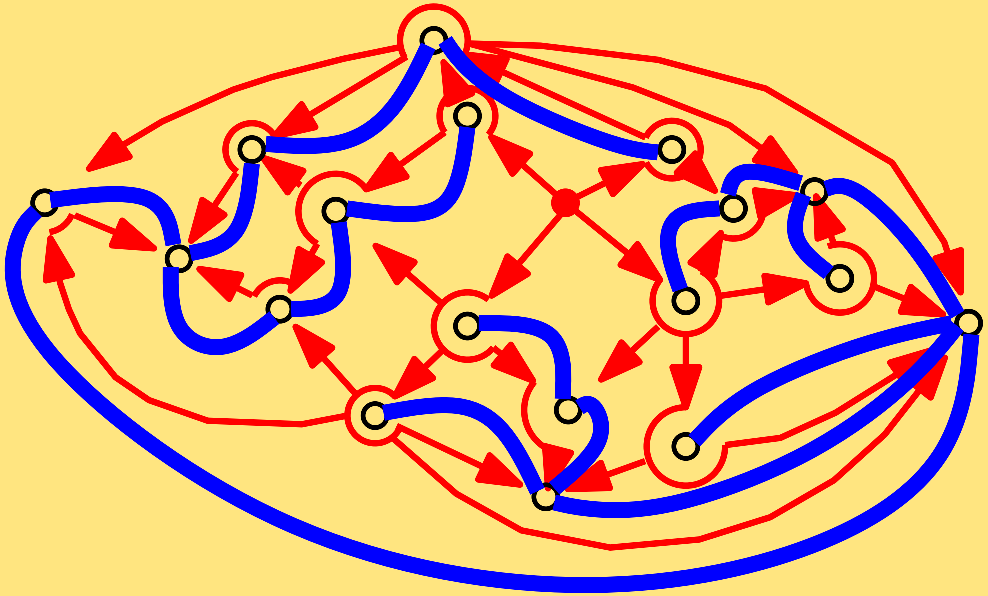

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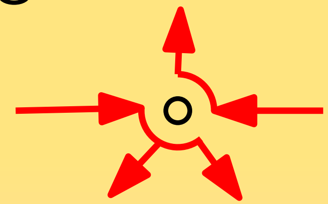

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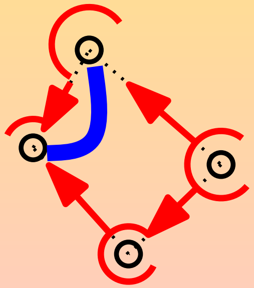

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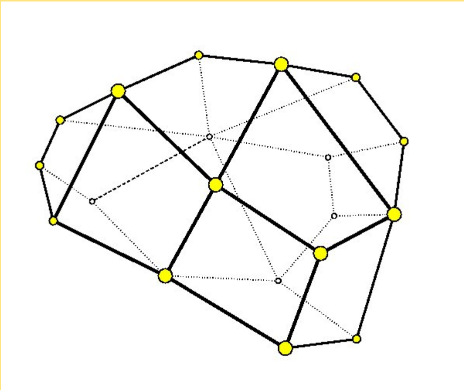

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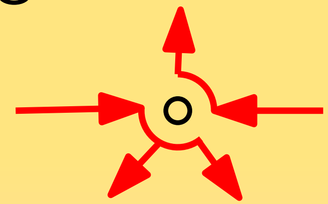

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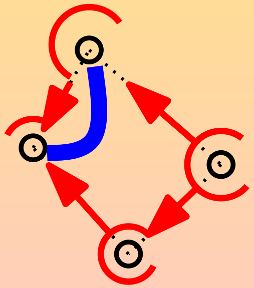

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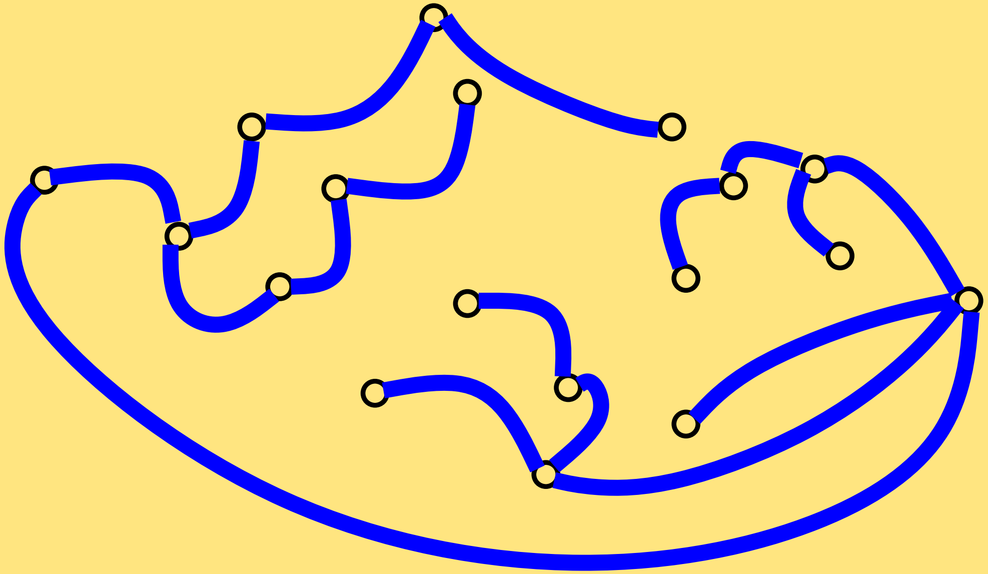

The result is **tree**.

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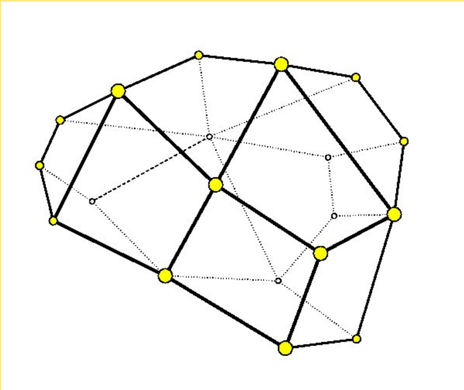

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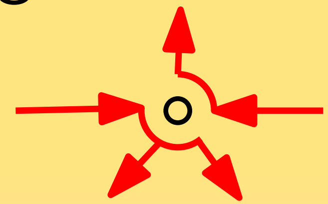

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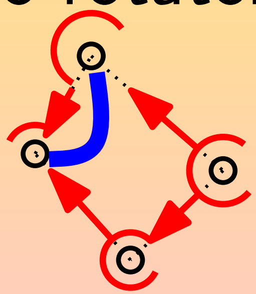

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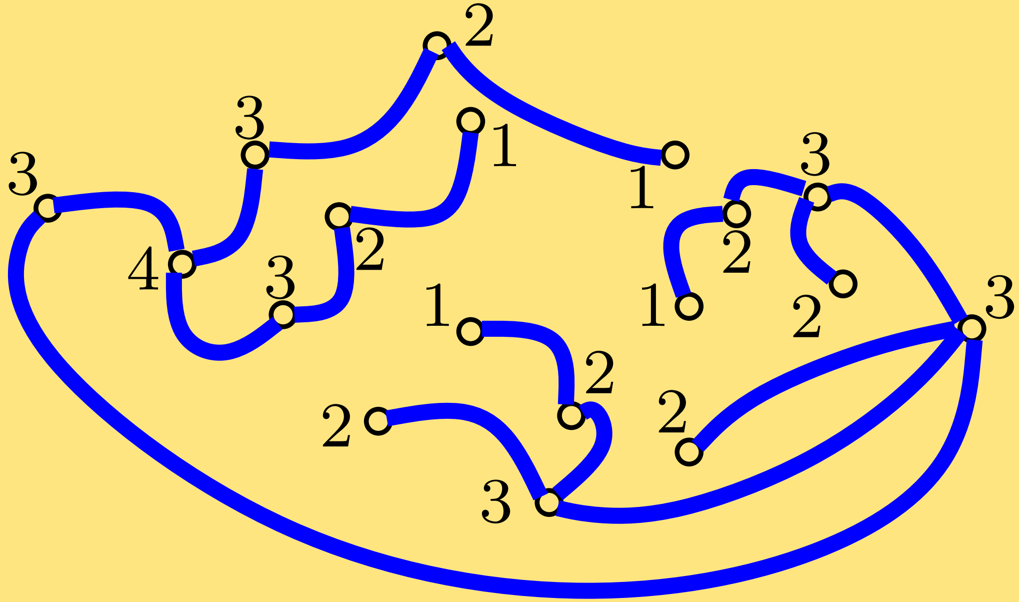

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Label vertices by the round at which they were visited by bfs.

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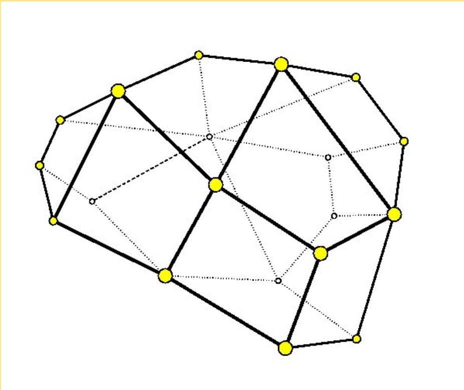

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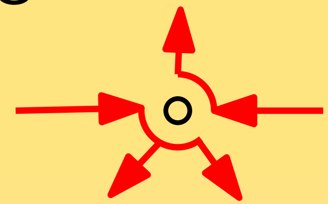

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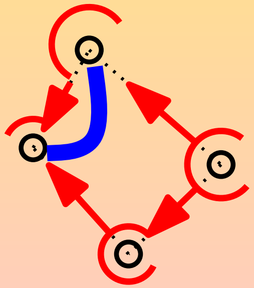

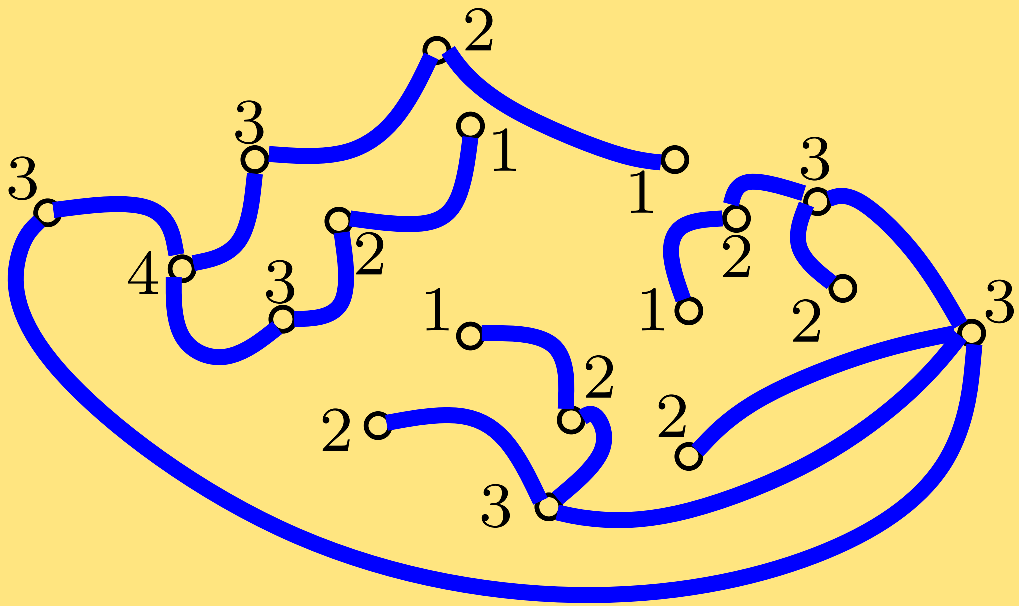


The result is a well labeled **tree**.

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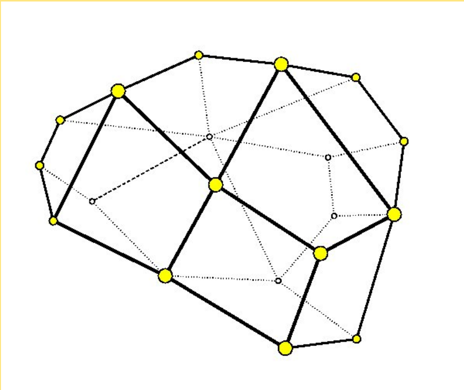

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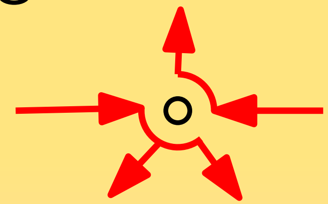

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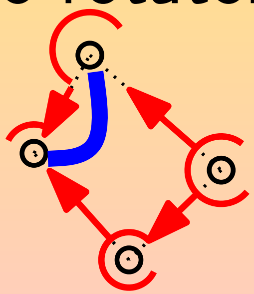

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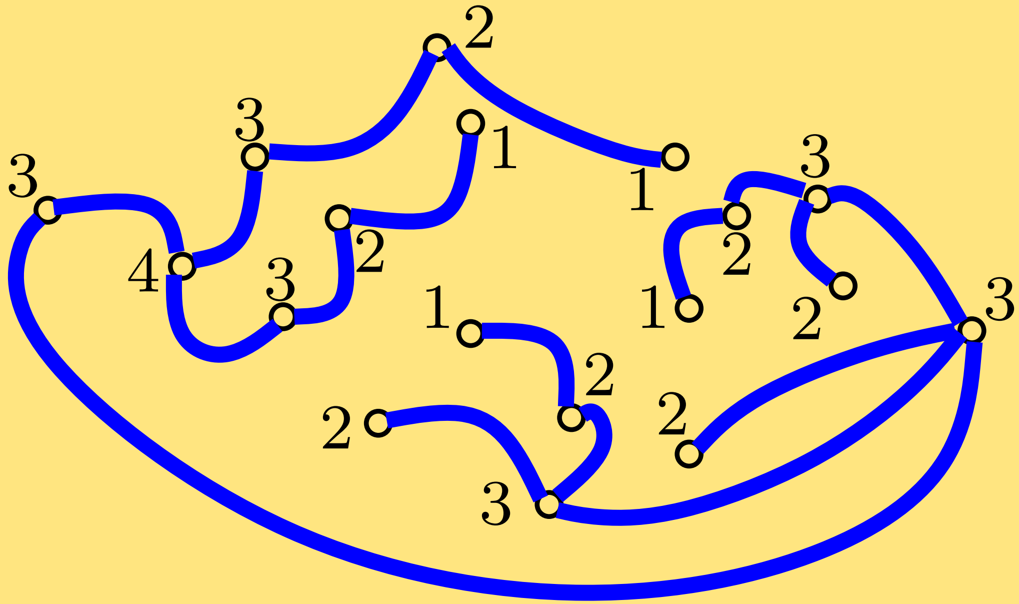

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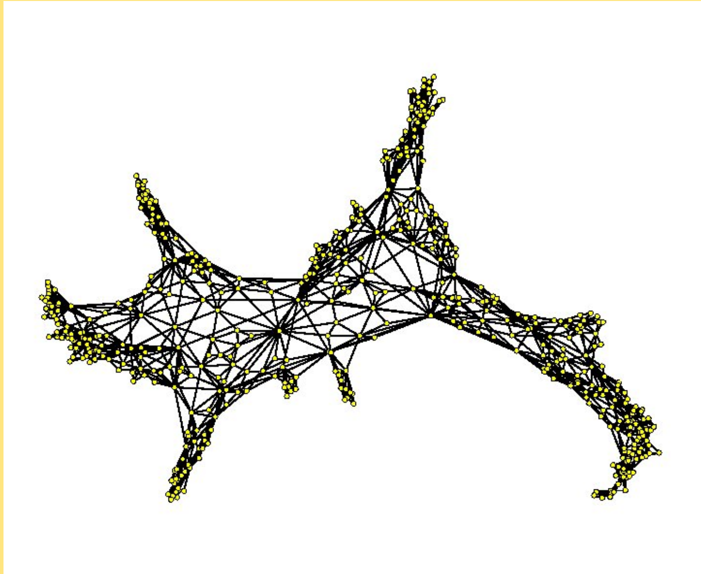
**Theorem**. This is a bijection.

$X_n$: pointed quads, $n$ faces

$\wr$

$T_n$: well labeled trees, $n$ vtx

# Quadrangulations via breadth first search



## use breadth first search to study the geometry

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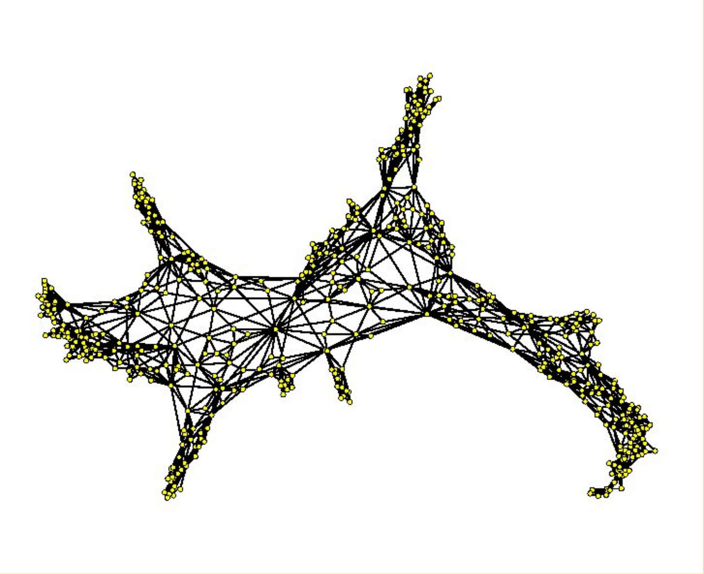

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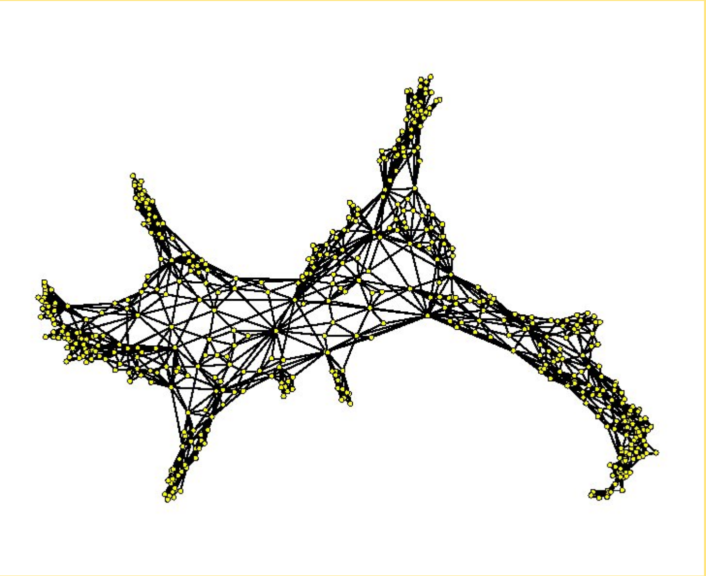

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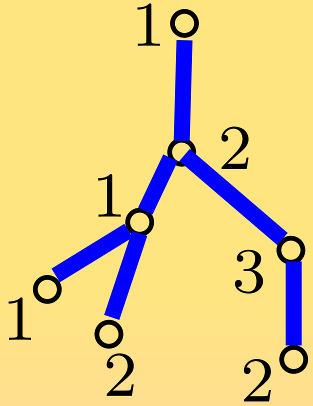

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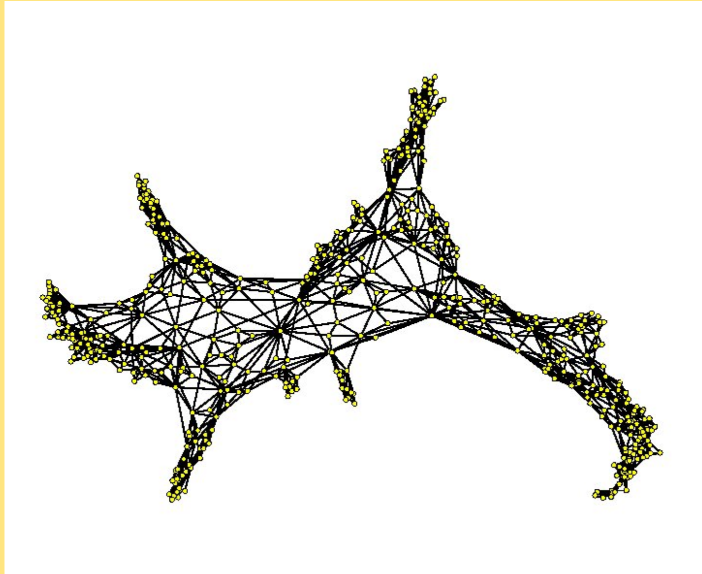

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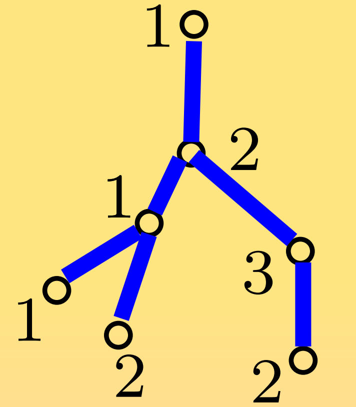
- the height of a random tree of size $n$ is $n^{1/2}$
- the random walk of labels on a branch of length $\ell$ has max about $\ell^{1/2}$

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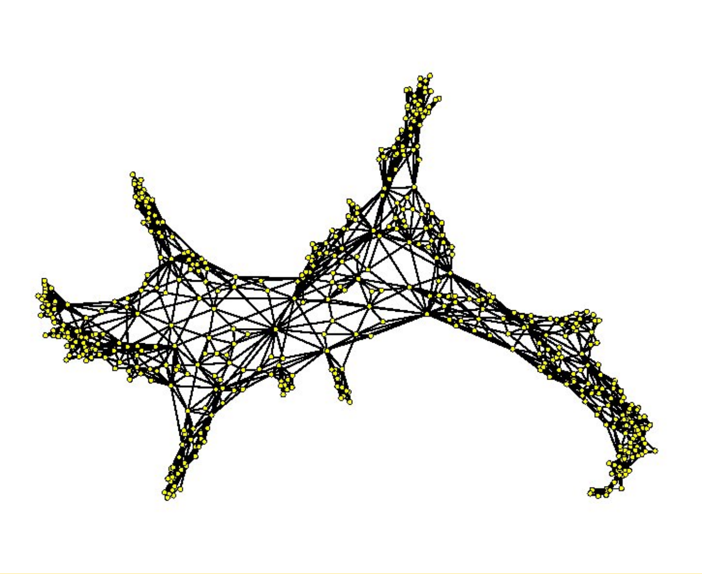

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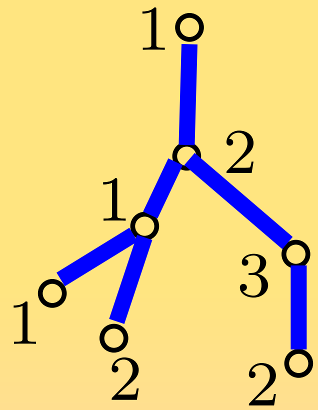


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**Theorem** (Chassaing-S, 2004).
The distance between 2 random vertices of $X_n$ is of order $n^{1/4}$.

## Some properties of random discrete surfaces

This approach was pursued by Chassaing-Durhuus (2005), Marckert-Mokkadem (2004), Miermond (2005), Weill (2006)... culminating with

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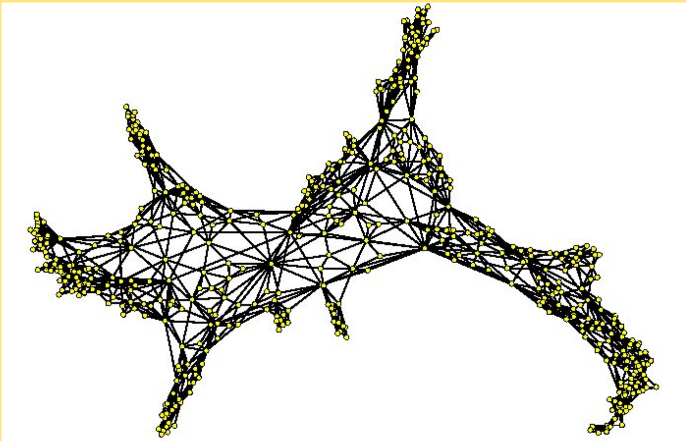

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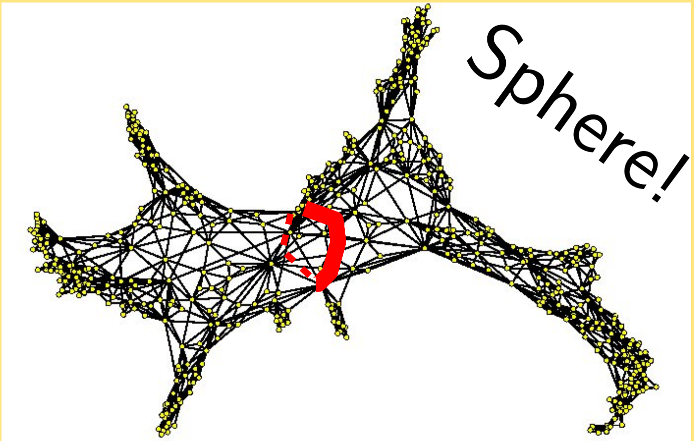


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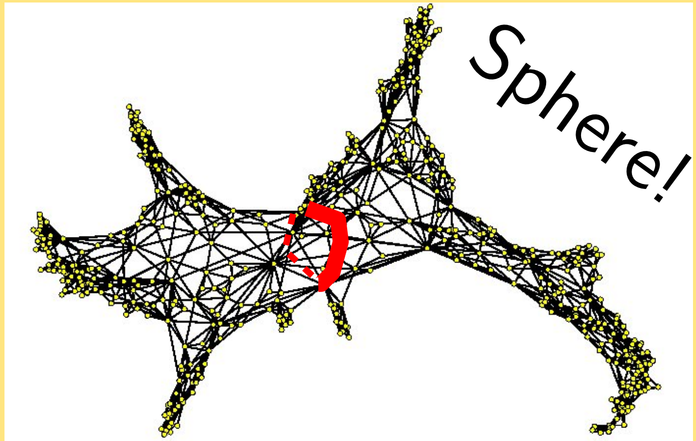


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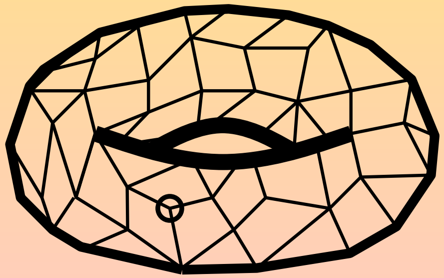
The bfs exploration works also for higer genus surfaces:
**Theorem** (Chapuy-Marcus-S. 2006) The distance between 2 random vertices of a random quad $X_n^g$ of genus $g$ is of order $n^{1/4}$.



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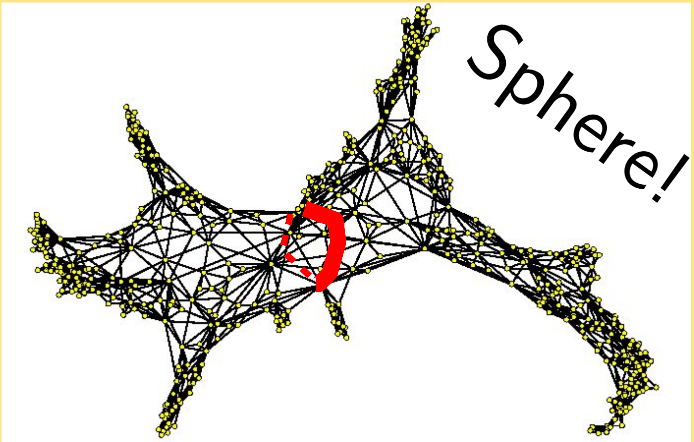


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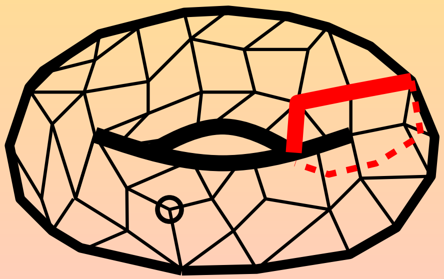
**Conjectures.**
There is no non-contractible cycles with size $\ll n^{1/4}$.
The rescaled continuum limit exists and has genus $g$.



## A conjecture on random graphs with low genus

Let $Y_n^g$ be a uniform random connected labelled graphs with $n$ vertices that can be embedded on a surface of genus $g$.

For instance $Y_n^0$ is a random connected planar graph with $n$ vertices.

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**Conjecture.** The graph $Y_n^g$ is a.s. composed of a 3-connected graph $Core(Y)$ of size $\Theta(n)$ with edges replaced by small planar networks and with small pending planar components.

Moreover $Core(Y)$ a.s. has minimal genus $g$ and has a unique minimal embedding. The small parts have size $O(n^{2/3})$.

In the rescaled limit, $Y_n^g$ converge to the same continuum random map of genus $g$ as $X_n^g$.

Cf. McDiarmid, Noy, Steger's talks for proofs...

Many thanks for your attention !

Many thanks to my collaborators!