Self-assembled Tilings

Thomas Fernique

Moscow, Spring 2011

1. Self-assembly
2. Forced self-assembly
3. Defects as seeds
4. Weighted self-assembly

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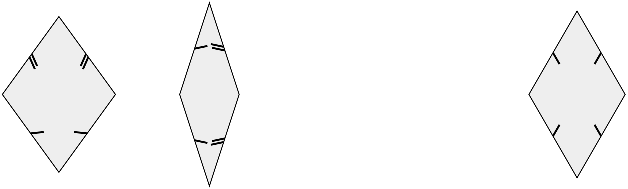
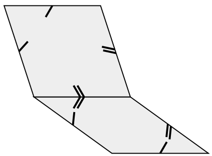
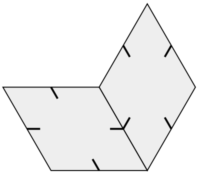
Principle



Add one tile at time, with matching rules being satisfied.
Physically: minimize the free energy $F = E - TS$ at $T = 0$.

Principle





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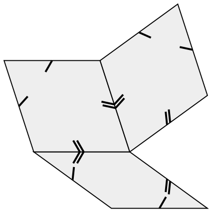

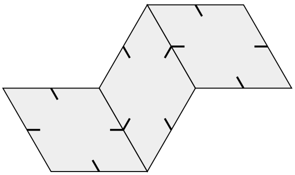

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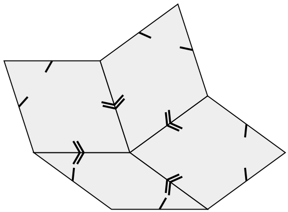

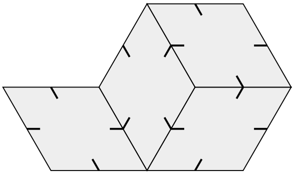

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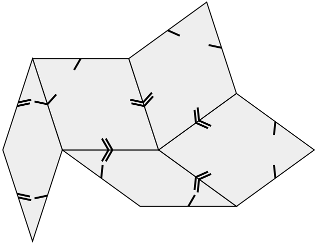

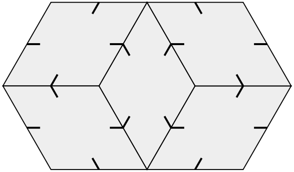

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Physically: minimize the free energy $F = E - TS$ at $T = 0$.

Deceptions

Fix a tile set τ. A τ-patch is *correct* if it appears in some τ-tiling.

Definition (Deception)

A *deception of order r* is a τ-patch homeomorphic to a closed ball, with only correct size r subpatches, but which is itself not correct.

Deceptions

Fix a tile set τ. A τ-patch is *correct* if it appears in some τ-tiling.

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A *deception of order r* is a τ-patch homeomorphic to a closed ball, with only correct size r subpatches, but which is itself not correct.

Theorem (Dworkin-Shieh, 1995)

An aperiodic plane tile set has deceptions of arbitrarily large order.

Proof (by contradiction):
Assume that r bounds the order of deceptions. We make 3 steps.

Step 1: remind quasiperiodicity

Definition (Quasiperiodic tiling)

A tiling is *quasiperiodic* if, for any $r > 0$, there is $R > 0$ such that any patch of size r appears in any patch of size R.

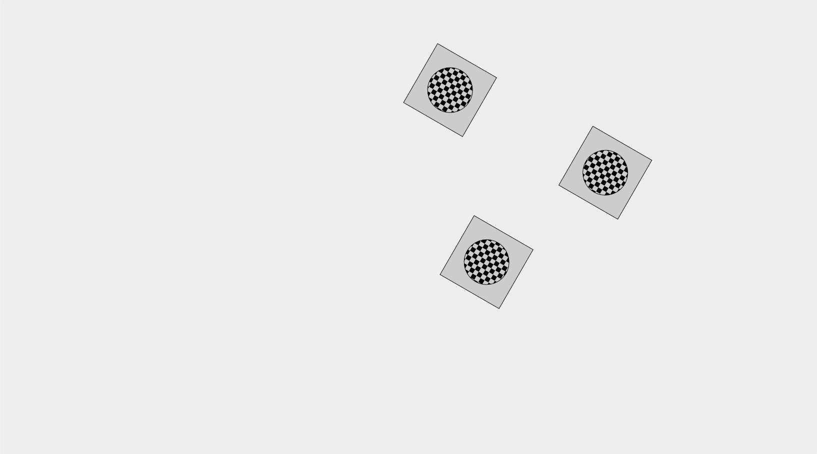
Theorem (Birkhoff, 1912)

If a tile set admits a tiling, then it admits a quasiperiodic tiling.

Proof (following Durand, 1998):

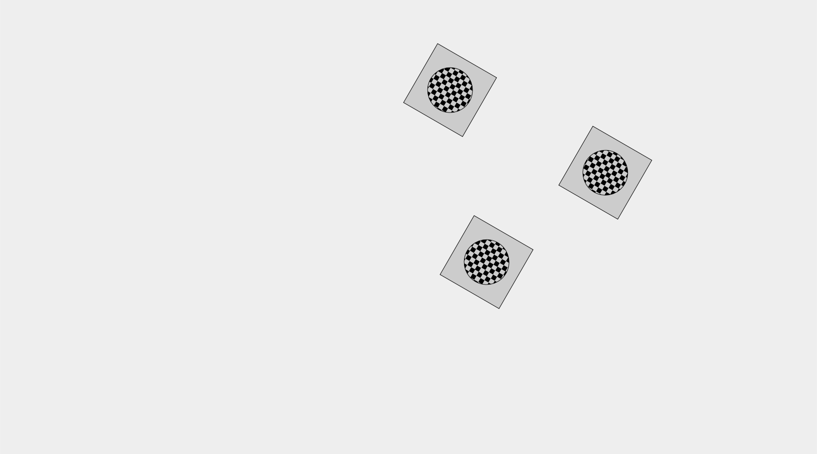
- write $T' \prec T$ if any finite (sub)patch of T' appears in T;
- show that the minimal tilings for $\prec$ are the quasiperiodic ones;
- $f(T) := \arg\min(T' \mapsto \inf\{\mathrm{Diam}(P) \mid P \not\prec T' \prec T,\ P \prec T\})$;
- diagonal extraction on $(f^n(T))_{n\geq 0} \rightsquigarrow$ quasiperiodic tiling.

Step 2: find three siblings



We want a tiling with three patches containing a ball of radius r, which are equal up to translation and not aligned (*siblings*).

Step 2: find three siblings

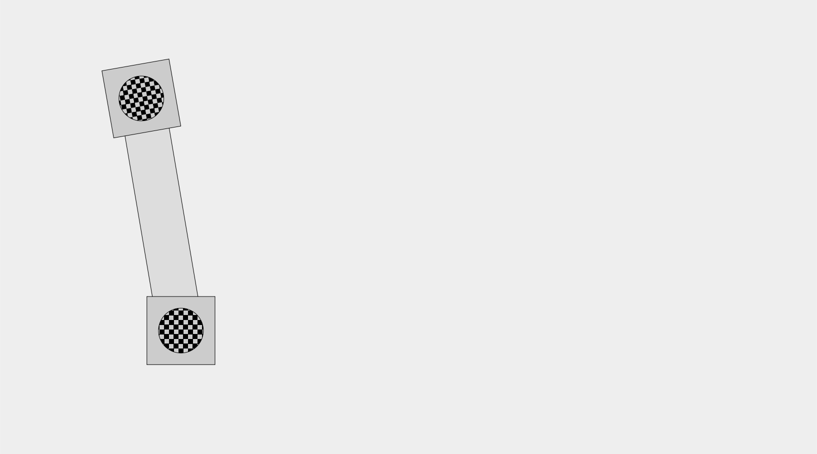


Quasiperiodic tiling $\rightsquigarrow$ patches equal up to isometries everywhere.
This suffices if tiles can take only finitely many different orientations.

Step 2: find three siblings

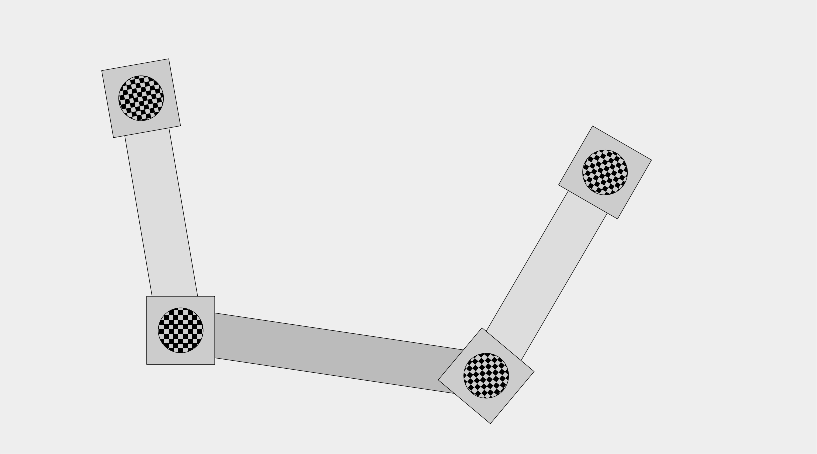
In any case, some tiling has two patches equal up to an isometry.

Step 2: find three siblings



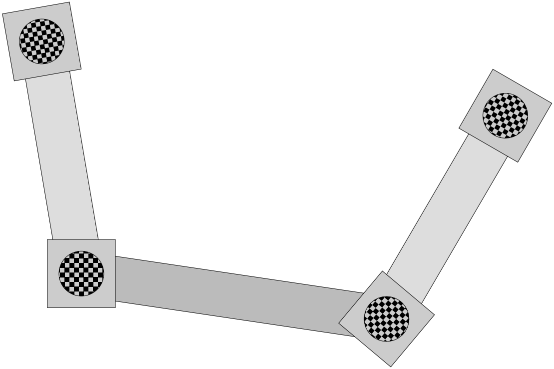
In this tiling, link these patches by a “bone” of diameter r.
This form a new patch which appears everywhere up to an isometry.

Step 2: find three siblings



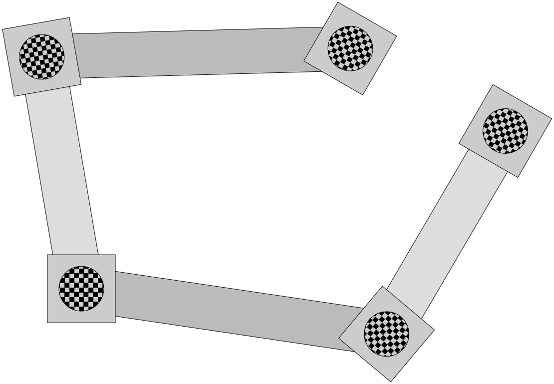
In the tiling, link two such occurences by a new bone (of diameter r).

Step 2: find three siblings



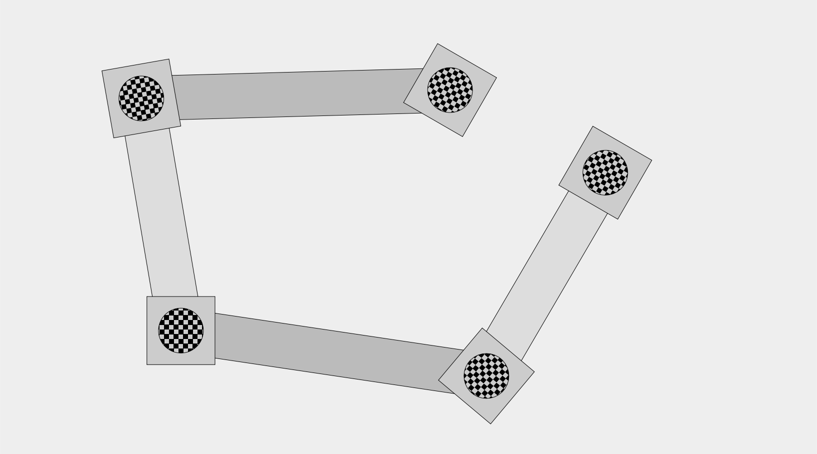
This form a new patch. Let us forget the tiling where it appears.

Step 2: find three siblings



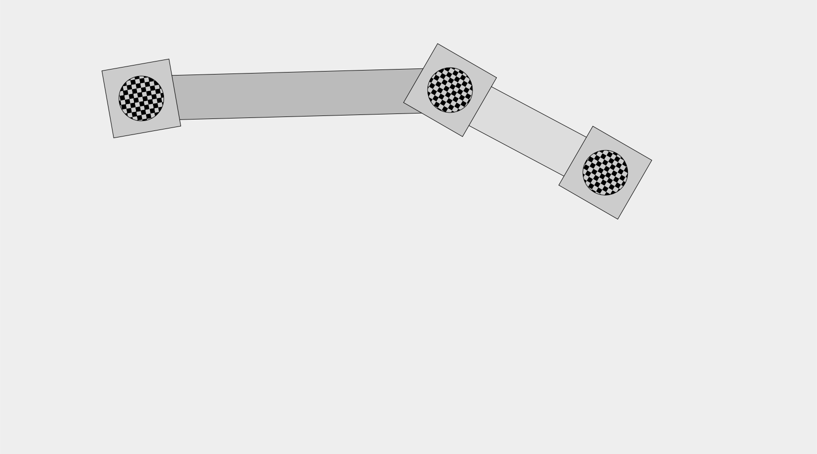
The new bone and its “patella” can be duplicated without creating incorrect subpatches of diameter r (for a thick enough “cartilage”).

Step 2: find three siblings



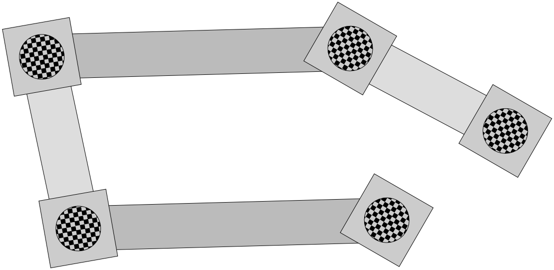
No deceptions of order $r \rightsquigarrow$ this new patch appears in some tiling.

Step 2: find three siblings



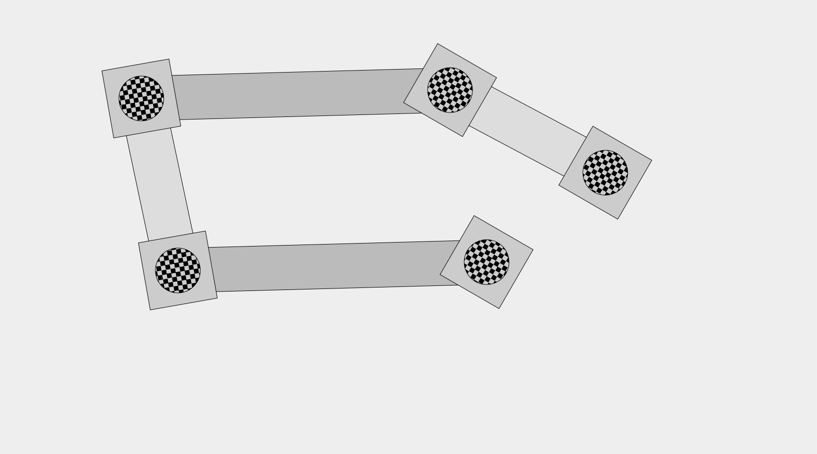
Forget some bones and patellae, link the two siblings by a bone.

Step 2: find three siblings



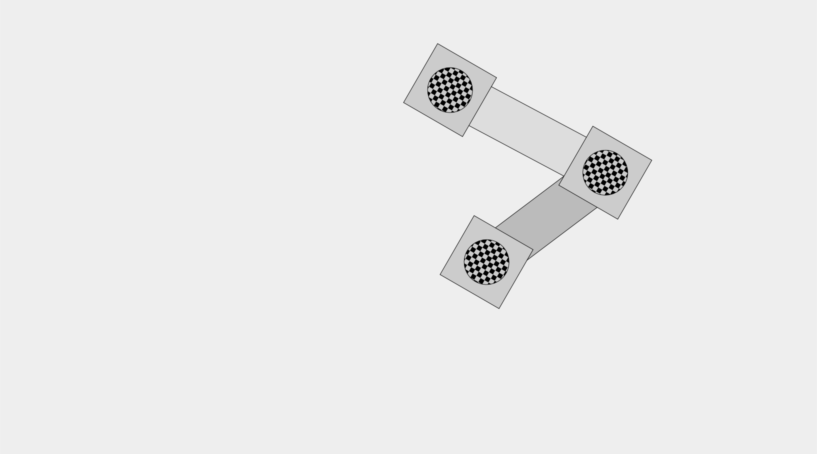
Forget the tiling. The patch can be extended without creating incorrect subpatches of diameter r, so that it contains three siblings.

Step 2: find three siblings



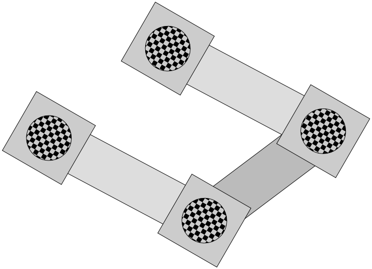
No deceptions of order r $\rightsquigarrow$ this new patch appears in some tiling.

Step 3: build a periodic tiling



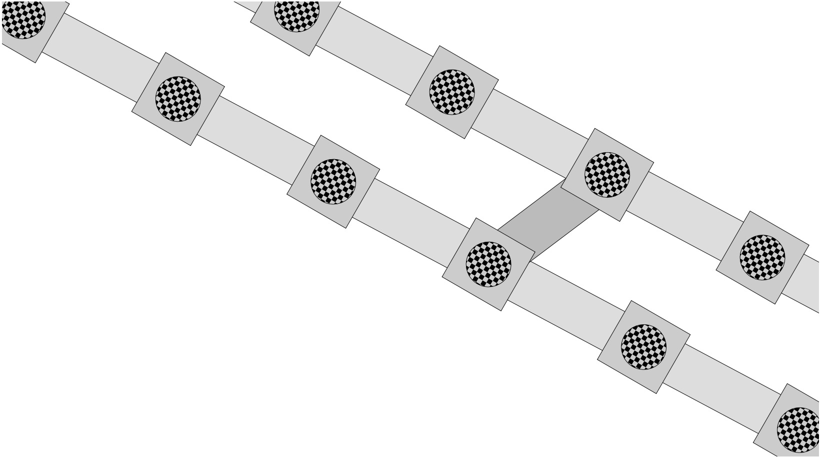
Consider these three siblings, with two bones linking them.

Step 3: build a periodic tiling



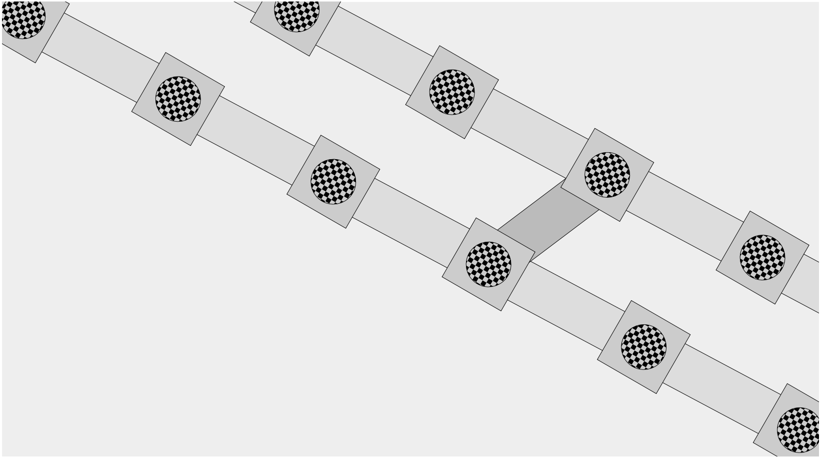
Forget the tiling, extend the patch without incorrect subpatches.

Step 3: build a periodic tiling



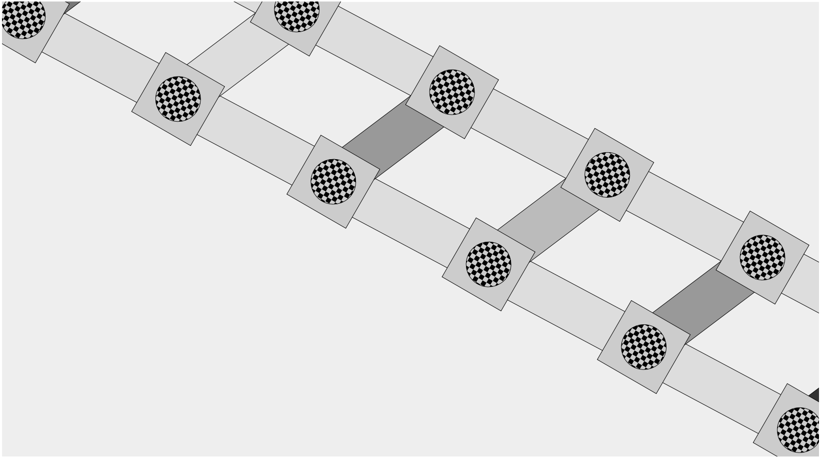
Extend further to form a sufficiently stretched H-shaped patch.

Step 3: build a periodic tiling



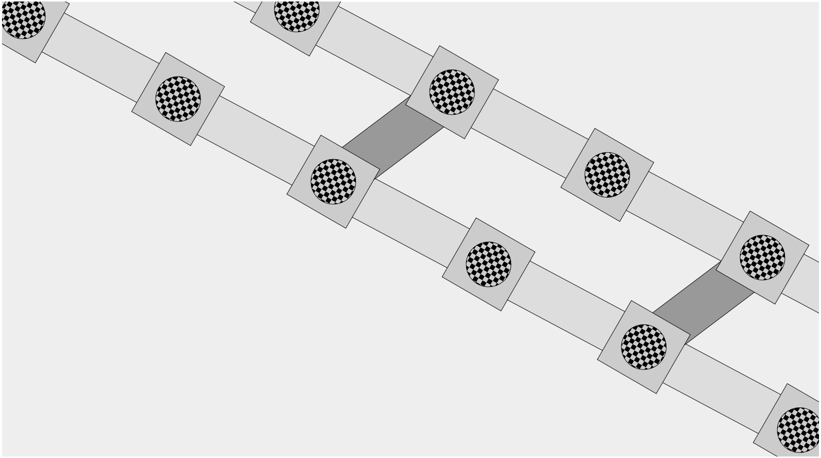
No deceptions of order $r \rightsquigarrow$ this new patch appears in some tiling.

Step 3: build a periodic tiling



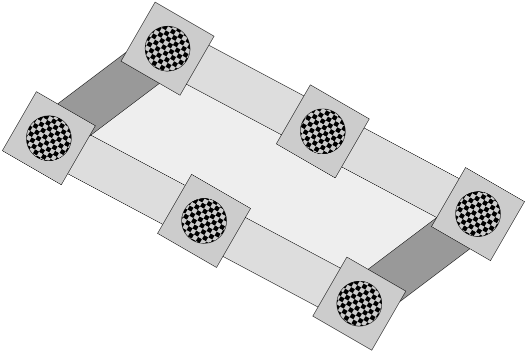
Link patellae by parallel bones $\rightsquigarrow$ rungs of a ladder-shaped patch.

Step 3: build a periodic tiling



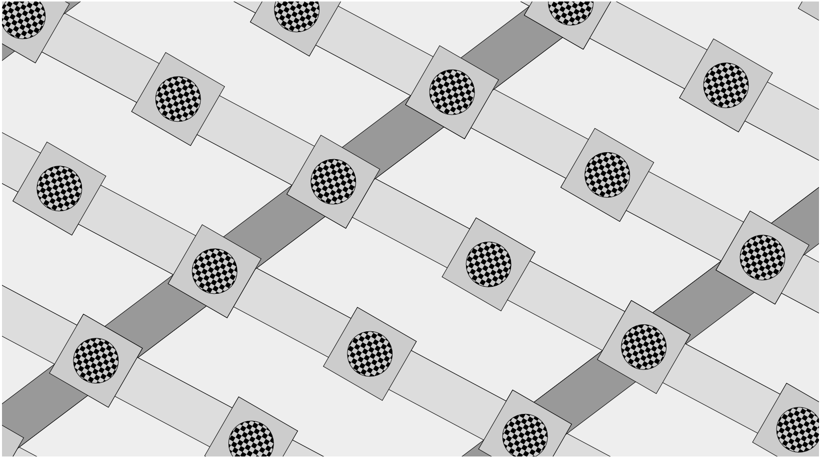
Stretched enough H-shaped patch $\rightsquigarrow$ two identical rungs.

Step 3: build a periodic tiling



This forms a patch which periodically tiles $\rightsquigarrow$ wanted contradiction!

Step 3: build a periodic tiling



This forms a patch which periodically tiles $\rightsquigarrow$ wanted contradiction!

Some comments

If deceptions can have holes and tiles have finitely many different orientations, then the proof is much simpler (exercice).

In the previous proof, deceptions are very artificial (stretched H). What if deceptions are assumed to be, *e.g.*, (roughly) convex?

Which proportion of the patches of a given size are deceptions?

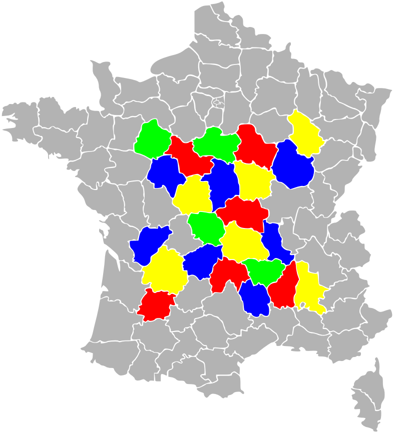
Can we play with the order tiles are added to avoid deceptions?

1. Self-assembly
2. Forced self-assembly
3. Defects as seeds
4. Weighted self-assembly

Let's play!

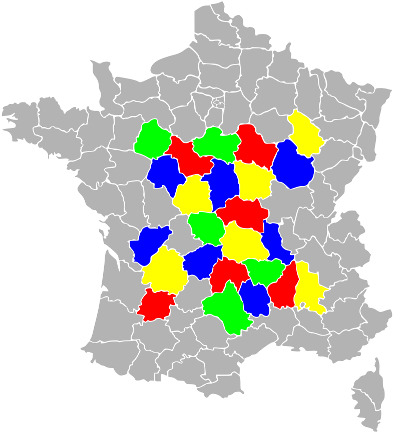
How to color french *departements* with only four different colors?

Let's play!



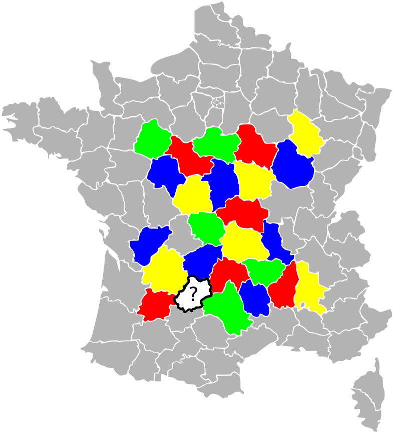
Assume some *departements* have already been coloried.

Let's play!



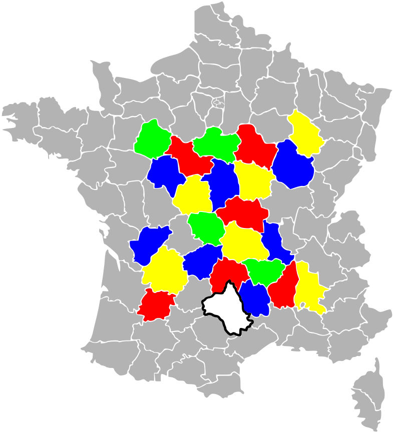
Let us choose, *e.g.*, green for Aveyron.

Let's play!



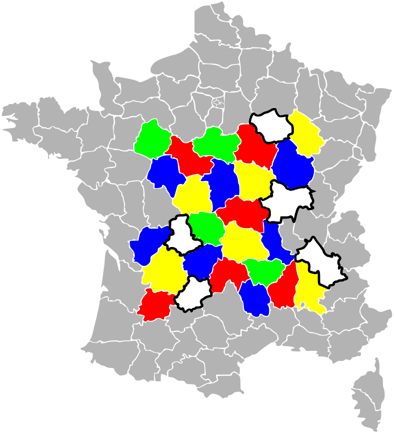
No more free color for Lot!

Let's play!



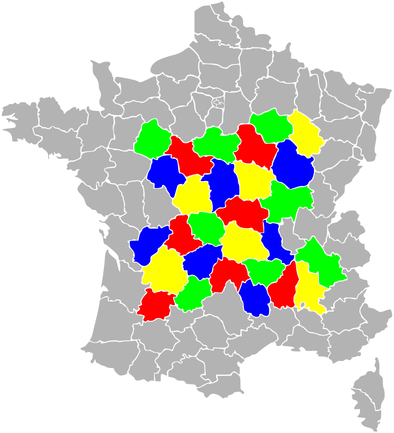
Aveyron can be green or yellow $\rightsquigarrow$ choice $\rightsquigarrow$ risk!

Let's play!



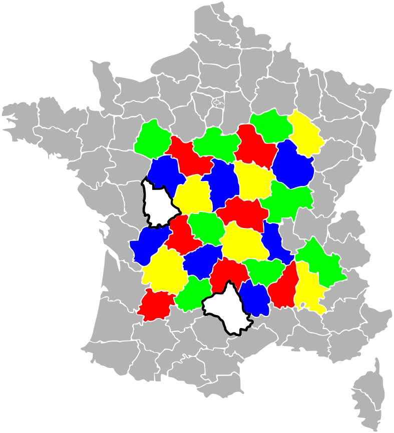
No choice for Lot, Haute-Vienne, Aube, Saône-et-Loire and Isère.

Let's play!



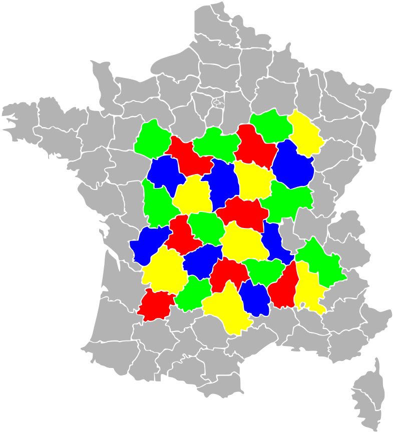
Color them “for free”: it does not reduce further possibilities!

Let's play!



No more choice for Aveyron and Vienne $\rightsquigarrow$ color them.

Let's play!



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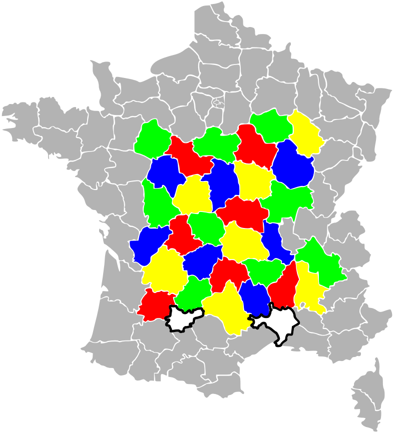
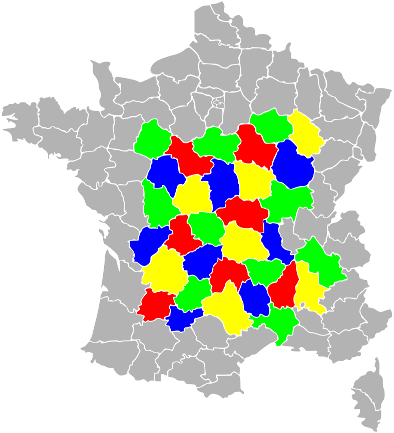
Let's play!



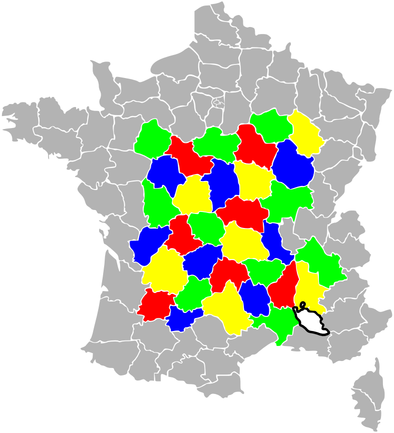
No more choice for Gard and Tarn-et-Garonne $\rightsquigarrow$ color them.

Let's play!



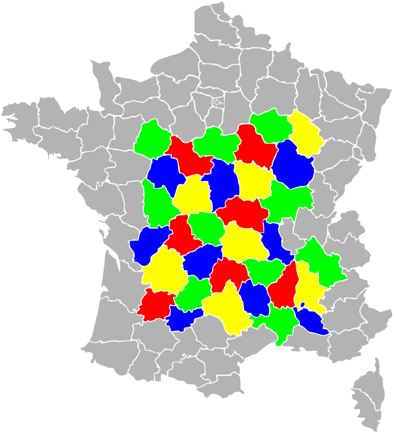
No more choice for Gard and Tarn-et-Garonne $\rightsquigarrow$ color them.

Let's play!



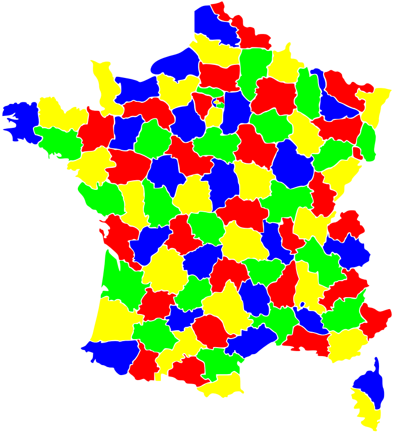
No more choice for Vaucluse $\rightsquigarrow$ color it.

Let's play!



At least two possible colors for each *departement* $\rightsquigarrow$ good luck!

Let's play!



Theory guarantees that this is possible (Appel-Haken, 1976).

Principle

Fix a tile set τ. Let $A(e)$ be the number of different ways one can add a τ-tile along a boundary edge e of some τ-patch P.

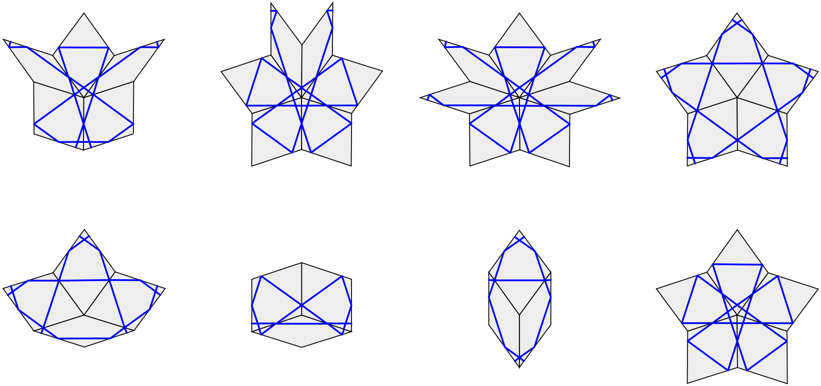
- if $A(e) = 0$, then e is a *dead edge* of P;
- if $A(e) = 1$, then e is a *forced edge* of P;
- if $A(e) \geq 2$, then e is a *free edge* of P.

Starting from a correct patch (*e.g.*, a single tile), repeat:

- complete forced edges until obtaining a *free patch*;
- add a suitable tile, so that the patch remains correct.

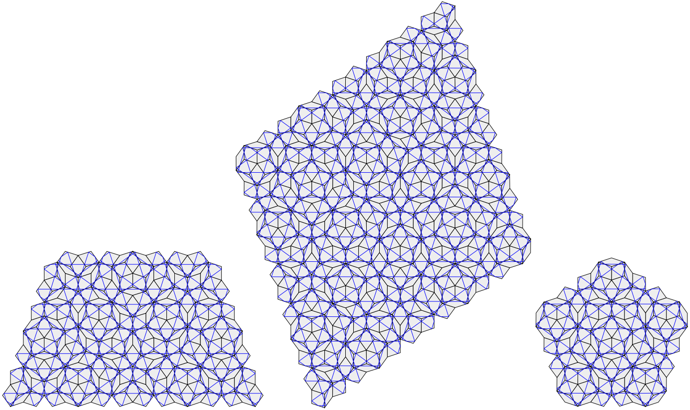
How to choose suitable tiles?

The Penrose case: forced edges



Forced edge: only one tile s.t. endpoints match the vertex atlas.

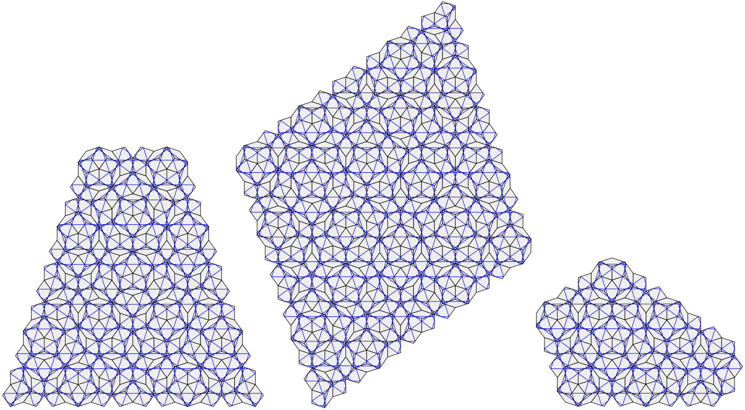
The Penrose case: free patches



Theorem (Onoda-Steinhardt-DiVincenzo-Socolar, 1988)

Complete classification of the free patches (via grouping/deflating).

The Penrose case: free patches



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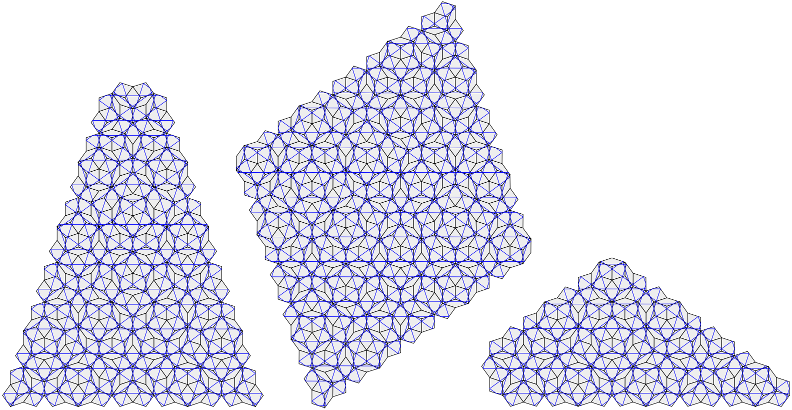

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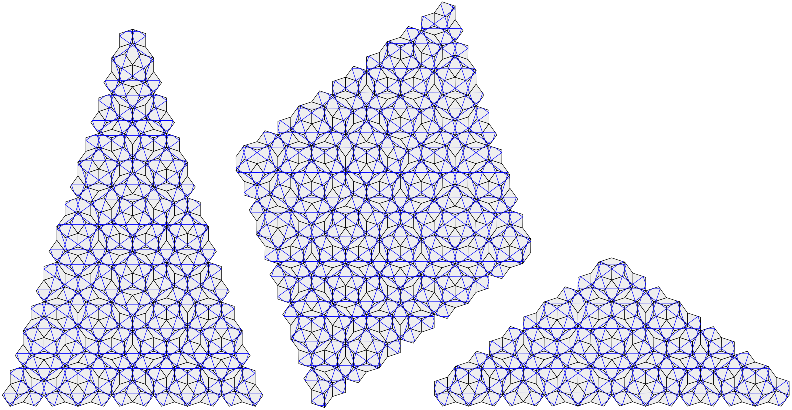

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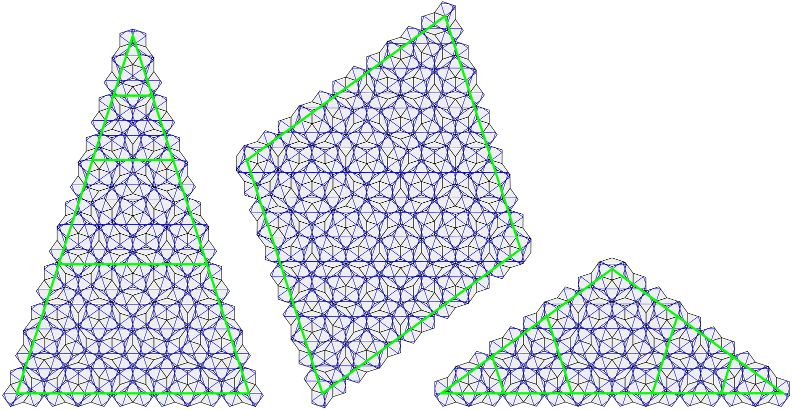

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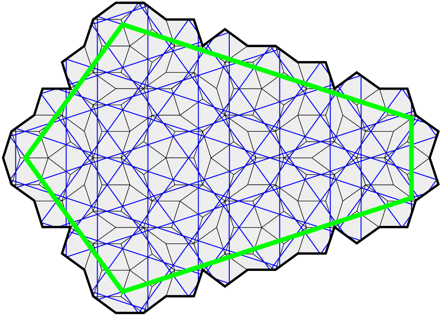
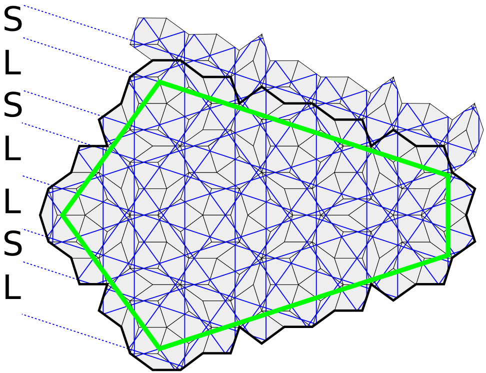
The Penrose case: Conway worms & Fibonacci sequences



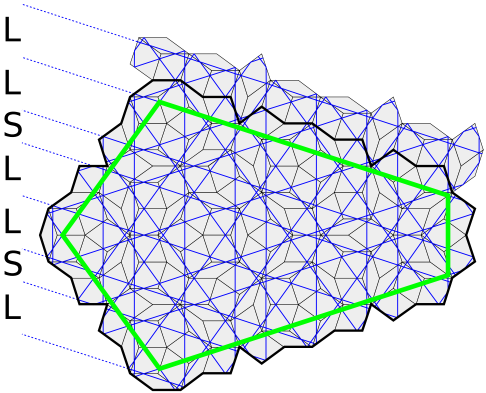
Free patches have facets directed by Ammann bars.

The Penrose case: Conway worms & Fibonacci sequences



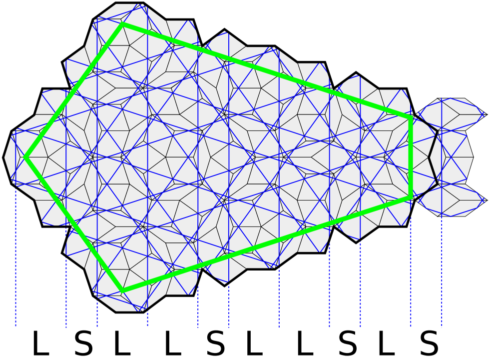
Along each facet can be added, in two ways, a *Conway worm*.

The Penrose case: Conway worms & Fibonacci sequences



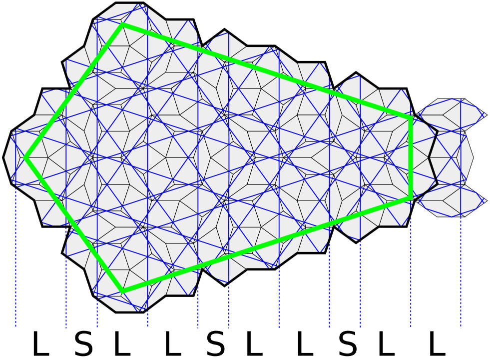
It forms a S(hort) or L(ong) space between parallel Ammann bars.

The Penrose case: Conway worms & Fibonacci sequences



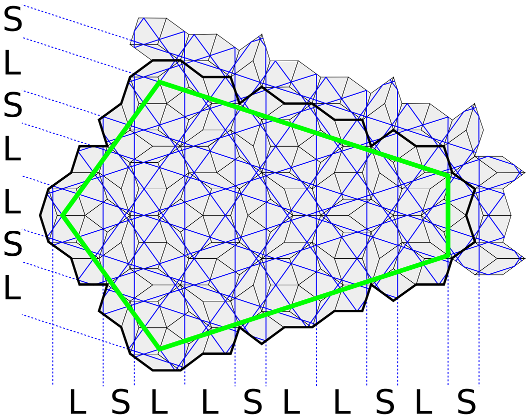
In any Penrose tiling, S and L spaces form a *Fibonacci sequence*.

The Penrose case: Conway worms & Fibonacci sequences



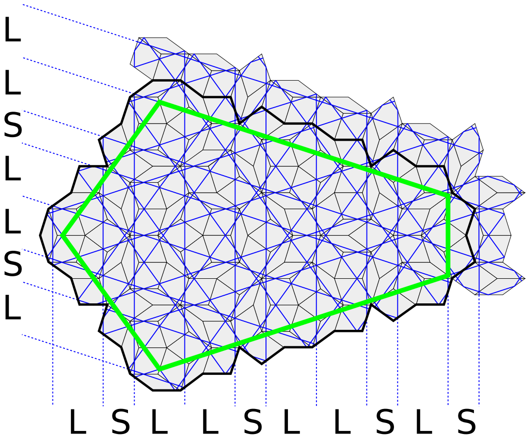
Non-local properties of this sequence can forbid one of the worms.

The Penrose case: Conway worms & Fibonacci sequences



It is remarkable that the 2D structure of Penrose tiling conspires to make this information available at the corners of dangerous faces.

The Penrose case: Conway worms & Fibonacci sequences



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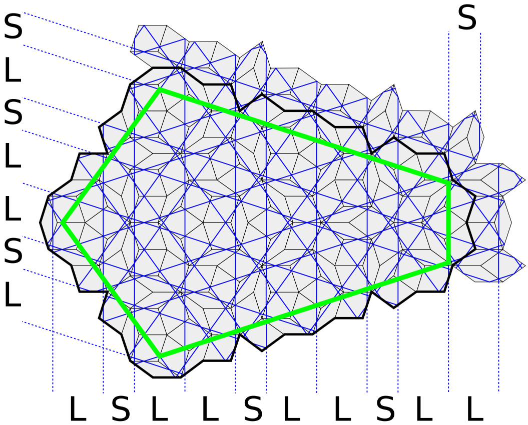
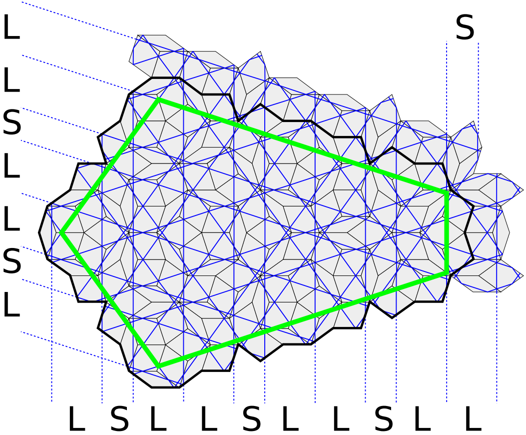


It is remarkable that the 2D structure of Penrose tiling conspires to make this information available at the corners of dangerous faces.

The Penrose case: Conway worms & Fibonacci sequences



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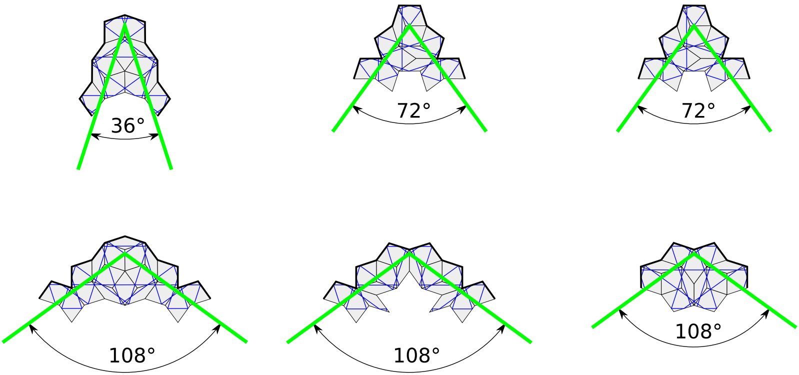
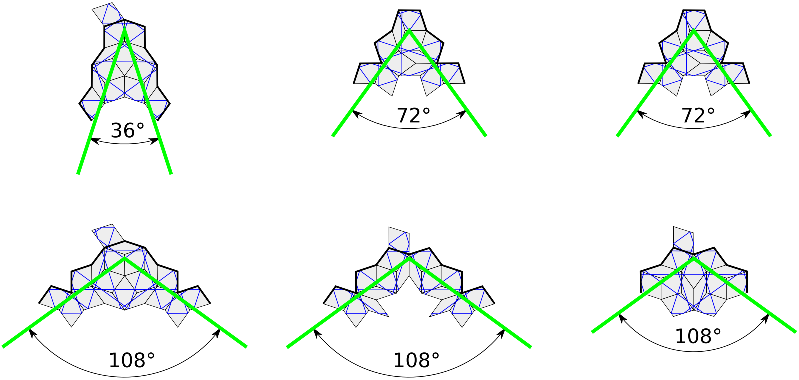
The Penrose case: OSDS rules



Theorem (Onoda-Steinhardt-DiVincenzo-Socolar, 1988)

Adding a fat tile on a 36° or 108° corner yields a correct tiling.

The Penrose case: OSDS rules



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The Penrose case: local or non-local growth?

Check if a patch is free $\rightsquigarrow$ check each boundary edge $\rightsquigarrow$ non-local.

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Trick:

- choose at each step a boundary edge at random;
- forced edge $\rightsquigarrow$ add the only possible tile;
- 36° or 108° corner $\rightsquigarrow$ add a fat tile with probability $\varepsilon > 0$;
- other cases $\rightsquigarrow$ go to the next step.

This converges to the previous process when $\varepsilon \to 0$.

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This converges to the previous process when $\varepsilon \to 0$.

Drawbacks:

- the growth is stucked $\sim |\partial P|/\varepsilon$ steps on a free patch P;
- the probability to get a dead patch increases with ε.

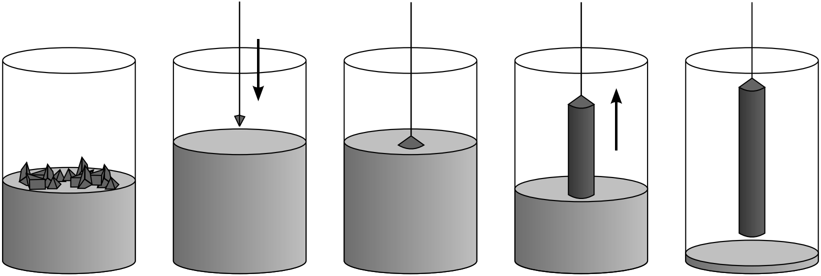
1 Self-assembly

2 Forced self-assembly

3 Defects as seeds

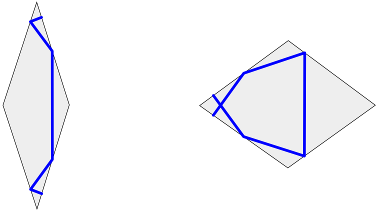
4 Weighted self-assembly

The Czochralski method



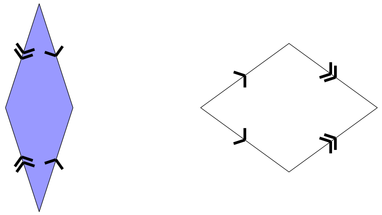
A seed initiates the growth; the crystal is pulled out while growing.

The Penrose case: patch charge



Penrose tiles can be equally decorated with Ammann bars or arrows.

The Penrose case: patch charge



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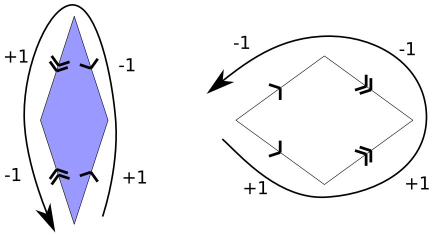
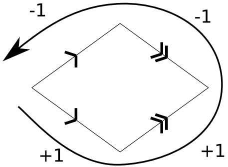


Unit *charge* on edges $\rightsquigarrow$ *charge* of tiles and patches (circulation).

The Penrose case: patch charge



The charge of a simply connected patch is always equal to zero.

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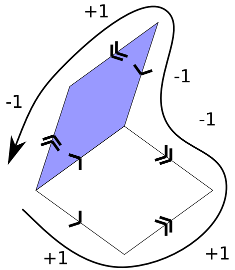

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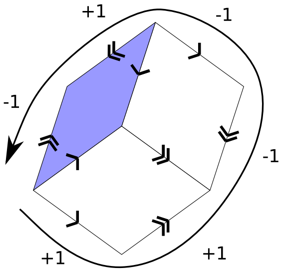

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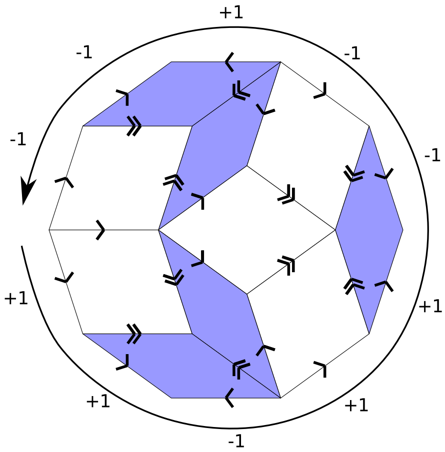
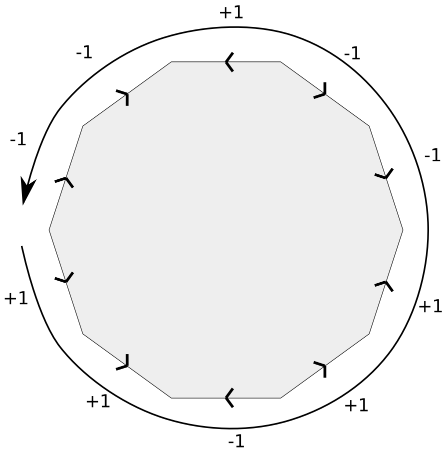


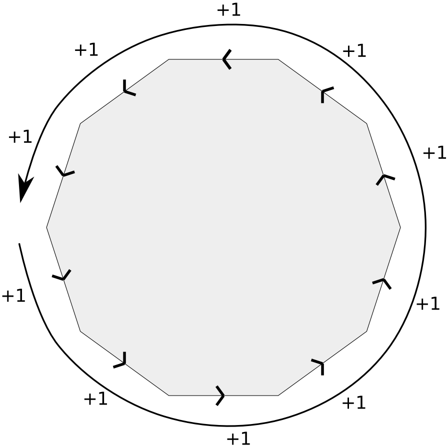
The charge of a simply connected patch is always equal to zero.

The Penrose case: holes/defects charge



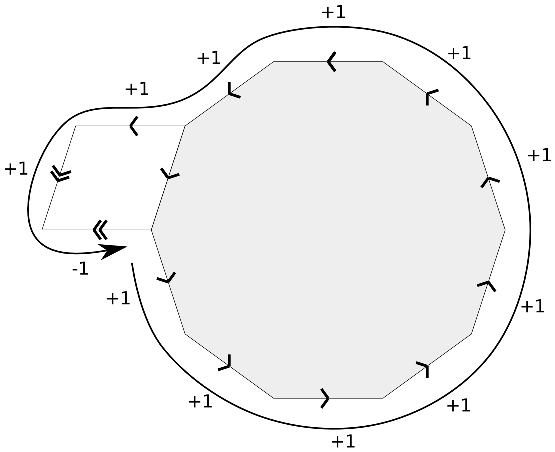
This extends to arrowed closed curves, seen as holes or *defects*.

The Penrose case: holes/defects charge



The charge of a defect can be non-zero.

The Penrose case: holes/defects charge



Adding tiles then yields defectuous patches with the same charge.

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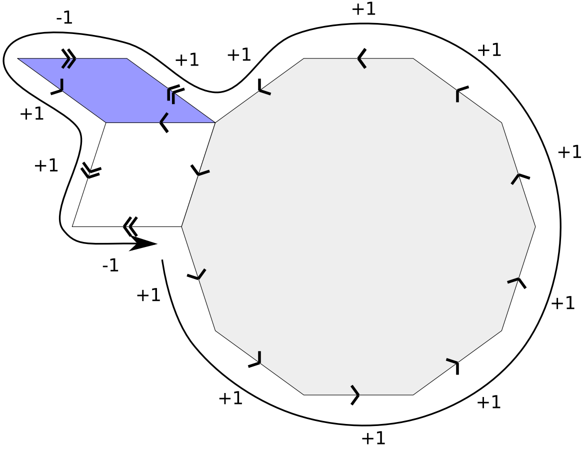

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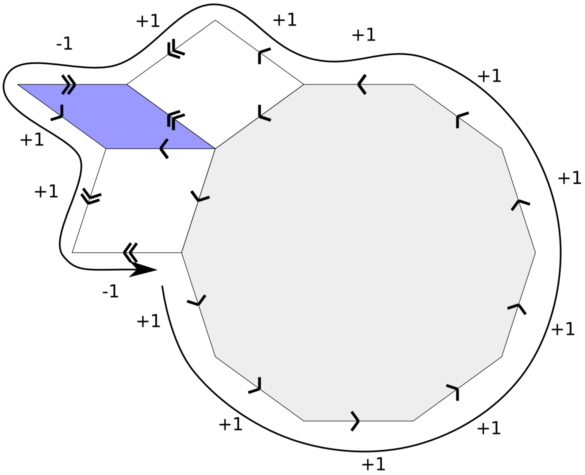
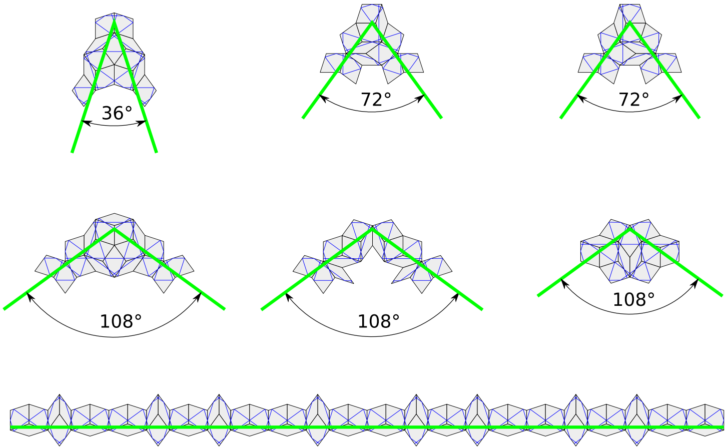


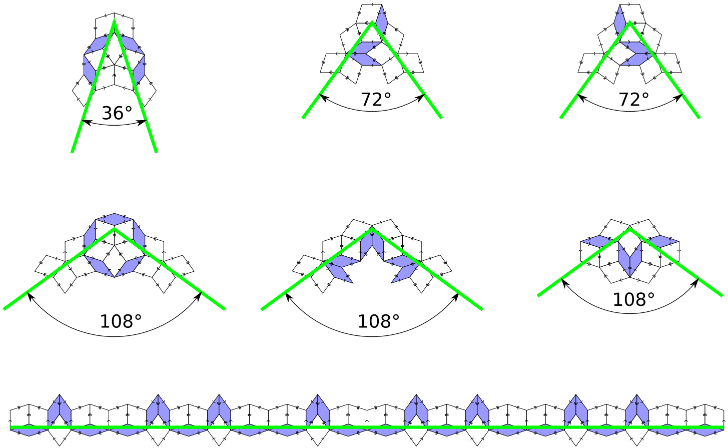
Adding tiles then yields defectuous patches with the same charge.

The Penrose case: free patch charge



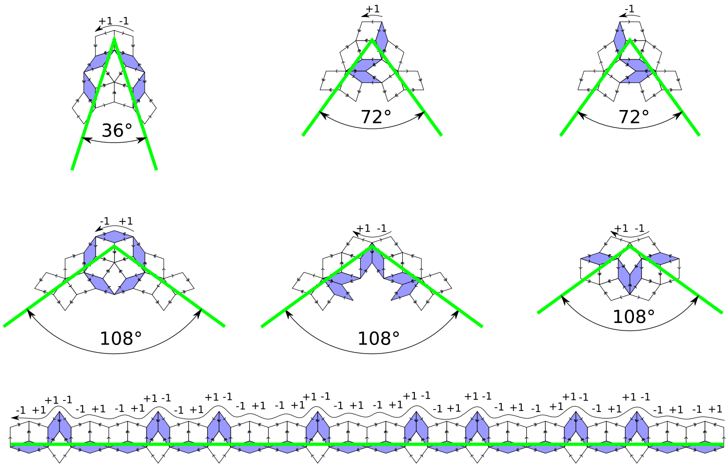
Free patch: boundary delimited by Conway worms, six corner types.

The Penrose case: free patch charge



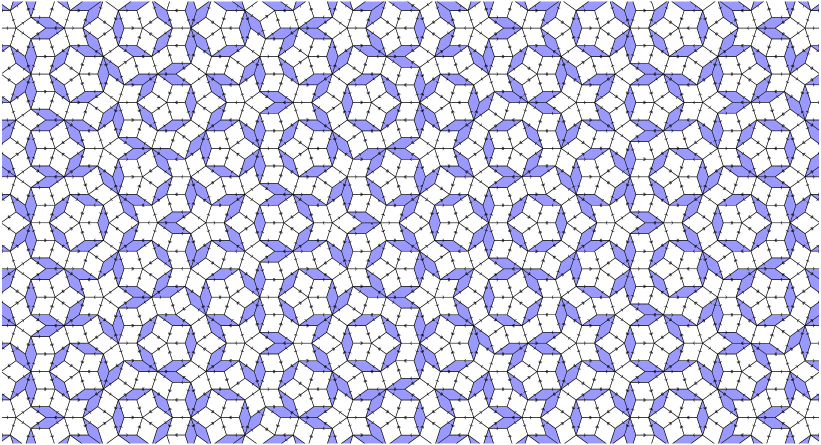
Ammann bars form a convex polygon with at most two 72° corners.

The Penrose case: free patch charge



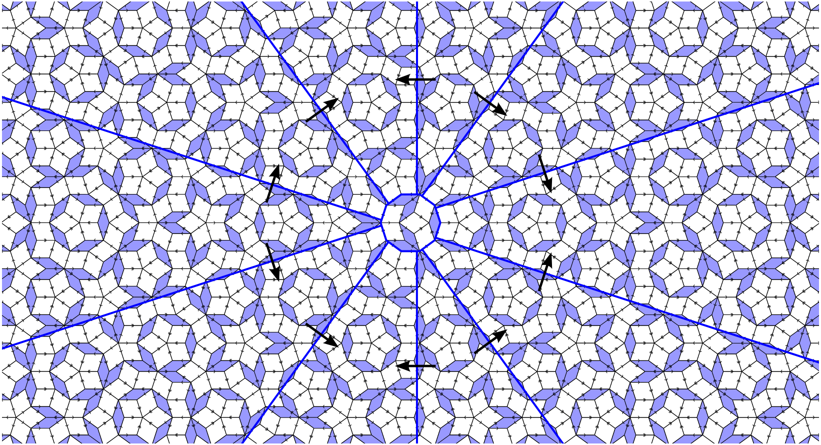
Only 72° corners have a non-zero charge $\rightsquigarrow$ total charge in $[-2, 2]$.

The Penrose case: the cartwheel tiling



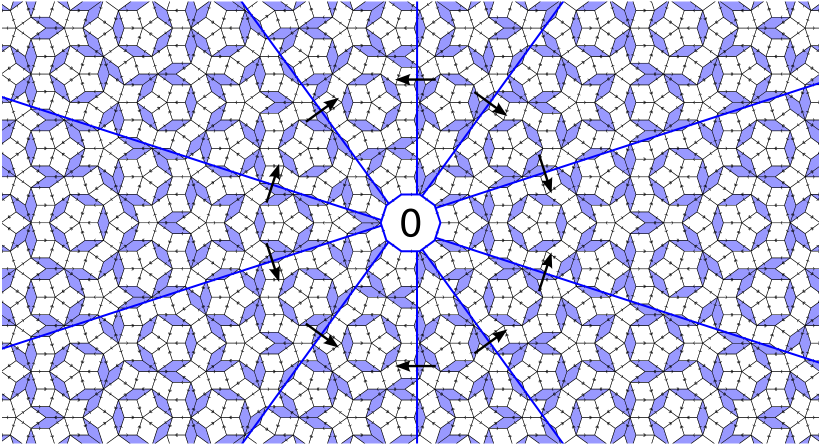
Among all the Penrose tilings, consider the so-called *cartwheel* tiling.

The Penrose case: the cartwheel tiling



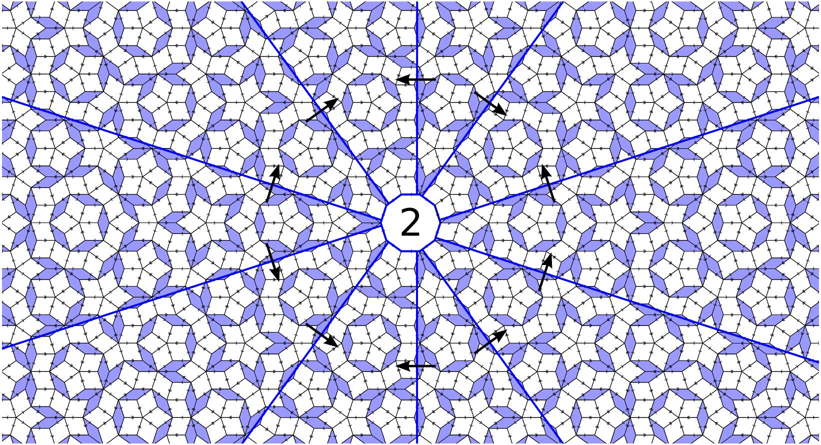
Ten semi-infinite Conway worms radiate out from a central *decapod*.

The Penrose case: the cartwheel tiling



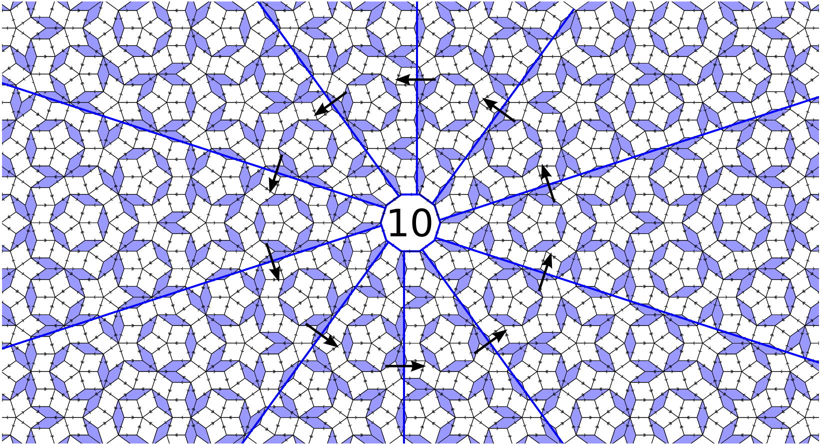
Removing this decapod yields a hole whose charge is equal to zero.

The Penrose case: the cartwheel tiling



By flipping a semi-infinite Conway worm, this charge changes by ± 2.

The Penrose case: the cartwheel tiling



This yields some correct holes which cannot belong to a free patch.

Some comments

This shows that a suitable seed allows to easily grow a tiling which matches almost everywhere with a Penrose tiling ($\rightsquigarrow$ non-periodic).

Can this be generalized to other tilings by aperiodic tile sets?

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This shows that a suitable seed allows to easily grow a tiling which matches almost everywhere with a Penrose tiling ($\rightsquigarrow$ non-periodic).

Can this be generalized to other tilings by aperiodic tile sets?

But remind the completion problem: it is very easy to find a tile set which is aperiodic once a tile is forced (exercice: find yours!).

$\rightsquigarrow$ in a certain sense, growing a tiling from a seed is “cheating”...

1 Self-assembly

2 Forced self-assembly

3 Defects as seeds

4 Weighted self-assembly

Principle

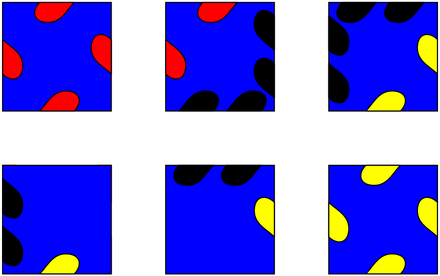
Assign weights to tile edges; introduce a temperature parameter.

A tile can be added to a patch iff the sum of weights of its edges which match edges of the patch is greater than the temperature.

$\rightsquigarrow$ yields some control on the order tiles are added.

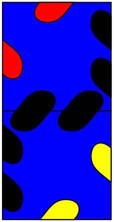
Can some non-periodic tilings be grown in this framework?

A simple example (Becker-Rémila-Schabanel)



Weight: number of colored disc. Temperature: 2. Only translations.

A simple example (Becker-Rémila-Schabanel)



Initially: tiles can be glued only along weight 2 black edges.

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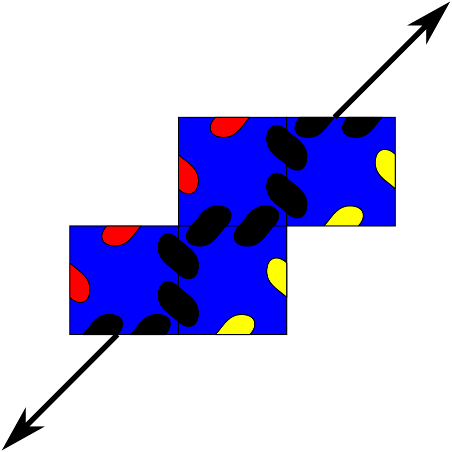
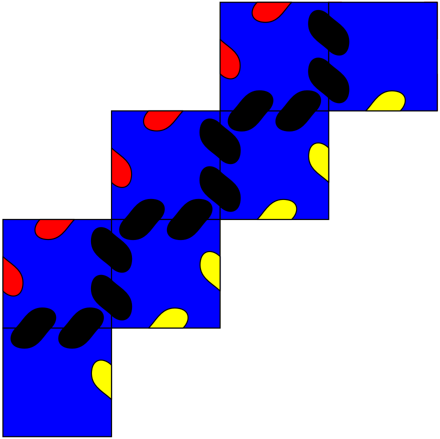


A diagonal of arbitrary length can then be grown.

A simple example (Becker-Rémila-Schabanel)



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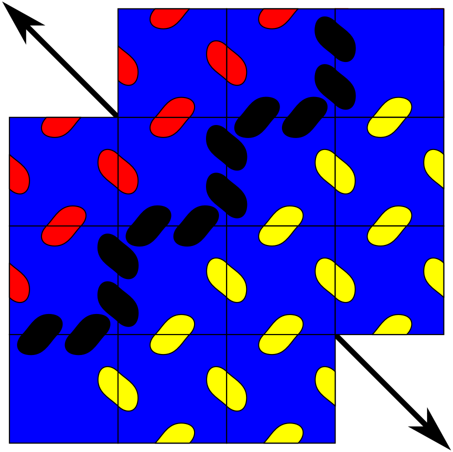
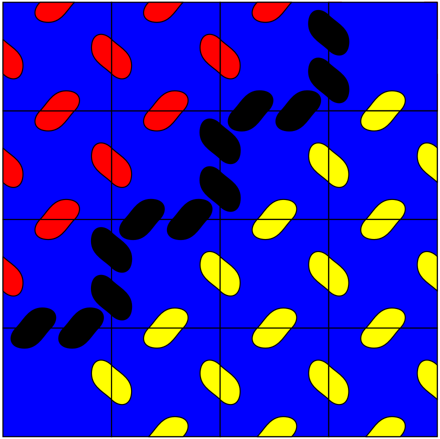


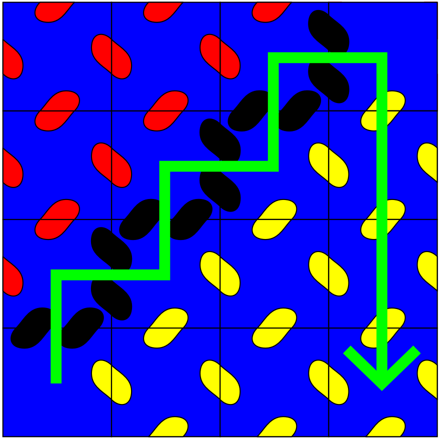
On the same time, red or yellow tiles can be added.

A simple example (Becker-Rémila-Schabanel)



This forces a square whose size $n \times n$ is determined by the diagonal.

A simple example (Becker-Rémila-Schabanel)



As many as possible tiles at each step $\rightsquigarrow$ assembly time $O(3n-2)$.

Some references for this lecture:

- Joshua Socolar, *Growth rules for quasicrystals*, in Quasicrystals: The State of the Art, 1991.
- Steven Dworkin, Jiunn-I Shieh, *Deceptions in quasicrystal growth*, Commun. Math. Phy. **128** (1995).
- Florent Becker, Éric Rémila, Nicolas Schabanel, *Time optimal self-assembly for 2D and 3D shapes: the case of squares and cubes*, in proc. DNA'08 (2008).

These slides and the above references can be found there:

`http://www.lif.univ-mrs.fr/~fernique/qc/`