Quasicrystallization by Flips

Thomas Fernique

CNRS, Marseille

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Part of a project STOCHASFLIP, also involving:

- O. Bodini (LIP6, Paris);
- Ch. Mercat (I3M, Montpellier);
- D. Regnault (LIP, Lyon);
- É. Rémila (LIP, Lyon);
- M. Sablik (LATP, Marseille).

Goal: study a toy-model for quasicrystal growth and stabilization.

Let $\vec{v}_1, \ldots, \vec{v}_d$ be non-colinears vectors of $\mathbb{R}^n$, $d > n \geq 1$.

For $1 \leq i_1 < \ldots < i_n \leq d$, one defines the proto-tile:

$$T_{i_1,\ldots,i_n} = \{ \sum_{1 \leq j \leq n} \lambda_{i_j} \vec{v}_{i_j} \mid \lambda_{i_j} \in [0,1] \}.$$

A $d \to n$ tiling is a tiling of $\mathbb{R}^n$ by translated copies of proto-tiles.

Let $(\vec{e}_1, \ldots, \vec{e}_d)$ be the canonical basis of $\mathbb{R}^d$.

Lift of a $d \to n$ tiling: image by the linear map $\phi : \vec{v}_i \mapsto \vec{e}_i$.

$$\rightsquigarrow n\text{-dim. “stepped” hypersurface of } \mathbb{R}^d.$$

A $d \to n$ tiling has thickness at most k if its lift lies into a “slice”

$$V + [0, k]^d,$$

where V is a n-dim. affine subspace of $\mathbb{R}^d$.

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A tiling of thickness at most 1 is called a V-cut.

Canonical tilings: widely spread theoretical model for quasicrystals.
(Tile $\simeq$ stable microscopic cluster)

Known: V-cuts have pure point diffraction (perfect quasicrystals).

How such complicated structures can be physically formed?

General physical principle:

$$\boxed{\text{Stability} \Leftrightarrow \text{minimal free energy } F = E - TS}$$

where

- E: (internal) energy; (local interactions)
- S: entropy; (phase space size)
- T: temperature. (local excitation)

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Low T approach: minimizing E (matching rules)
High T approach: maximizing S (random tilings).

Very general definition:

Definition (Matching rules)

Decoration of a proto-tile: real function defined over its boundary.
Two tiles match if, at any intersecting point, decorations sum to 1.

Decoration of boundaries $\simeq$ bumps & dents of jigsaw puzzles.

Slightly less general definition:

Definition (Matching rules)

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Two tiles match if, at any intersecting point, decorations sum to 0.

Decoration of boundaries $\simeq$ colors of jigsaw puzzles.

Idea: energy is proportional to the ratio of unmatched tiles.
$\rightsquigarrow$ decorations ensuring quasicrystalline ground states are known.

However, this does not help a lot to tile:

Theorem (Dworkin)

For any aperiodic tileset and for any $R > 0$, there is a deception of order R, i.e., a valid finite tiling of radius at least R which do not appears in any valid tiling of the plane.

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Self-assembly approach (Onoda-Steinhardt-Vicenzo-Socolar): promising, rises many questions, *e.g.* about the growth rate.

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Phase space of a finite tiling: all the tilings which are accessible by "elementary moves", *e.g.*, local reconfiguration of tiles.

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Example: some phase spaces of $2 \to 1$ tilings of size 4:

$$\{1111\}, \quad \{1112, 1121, 1211, 2111\},$$

$$\{1122, 1212, 1221, 2112, 2121, 2211\}.$$

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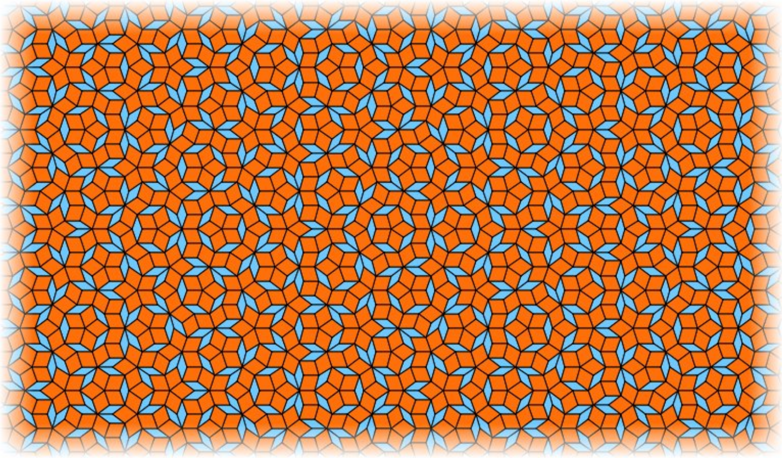
Entropy seems to be maximal for phase spaces containing quasicrystalline tilings (partial theoretical results).

Hybrid approach:

1. At high T, minimizing $F = E - TS \simeq$ maximizing S.
   $\rightsquigarrow$ tiling whose phase space contains a quasicrystalline tiling.
2. When T decreases, the effect of E overcomes the one of S.
   $\rightsquigarrow$ local transformations decreasing E become favoured.
3. At $T = 0$: local transformations are frozen.
   $\rightsquigarrow$ How far from the quasicrystalline tiling are we?

Note: looks like the *relaxation process* briefly described by Janot.

V-cuts with $\vec{V}$ directed by $(\cos(\frac{2k\pi}{5}))_{1\leq k\leq 5}$ and $(\sin(\frac{2k\pi}{5}))_{1\leq k\leq 5}$:



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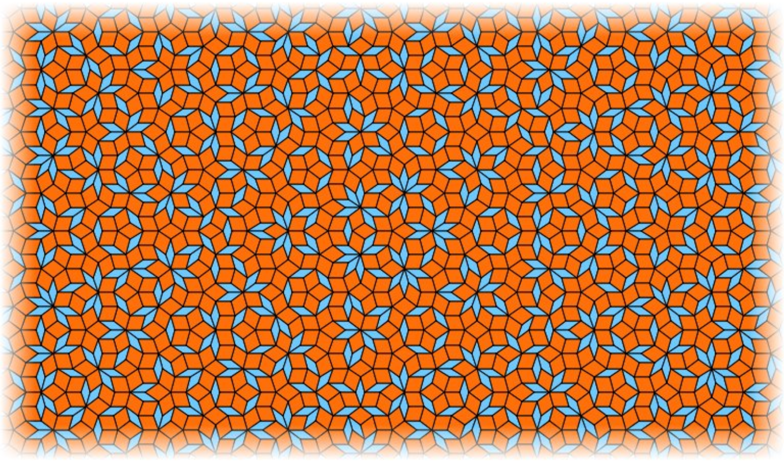

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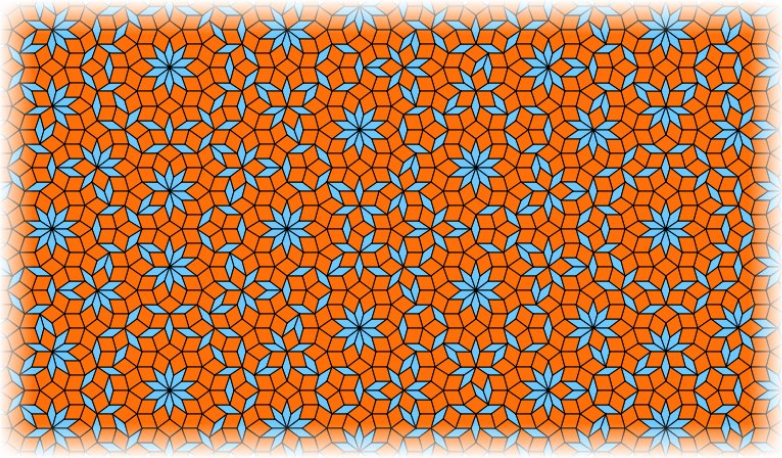
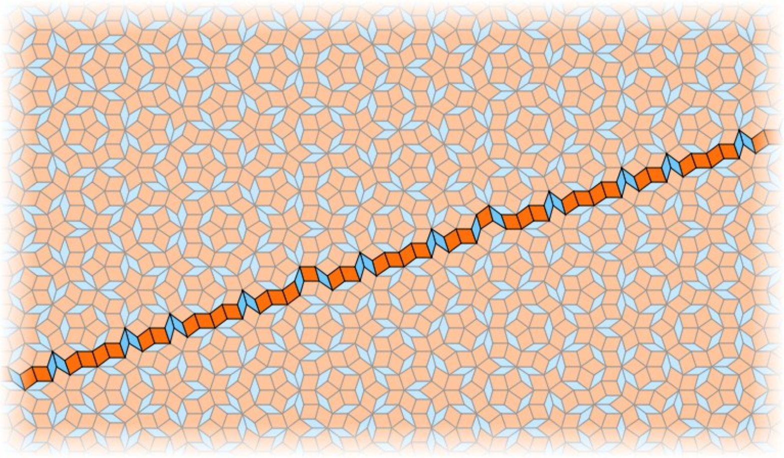


They are characterized by the Socolar's alternation condition (AC):



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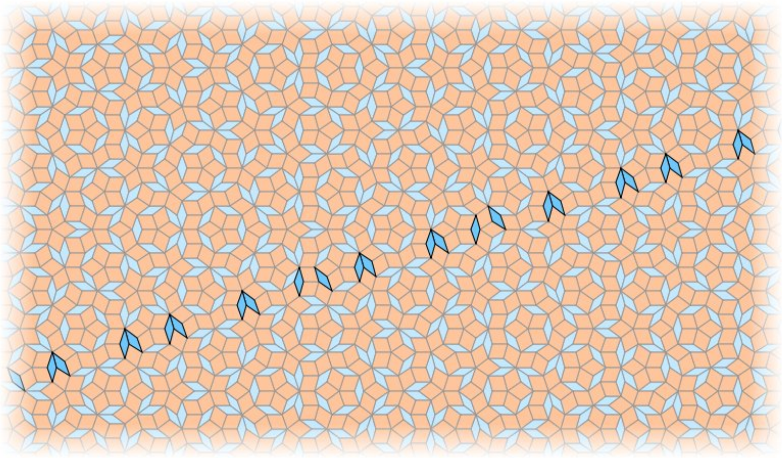

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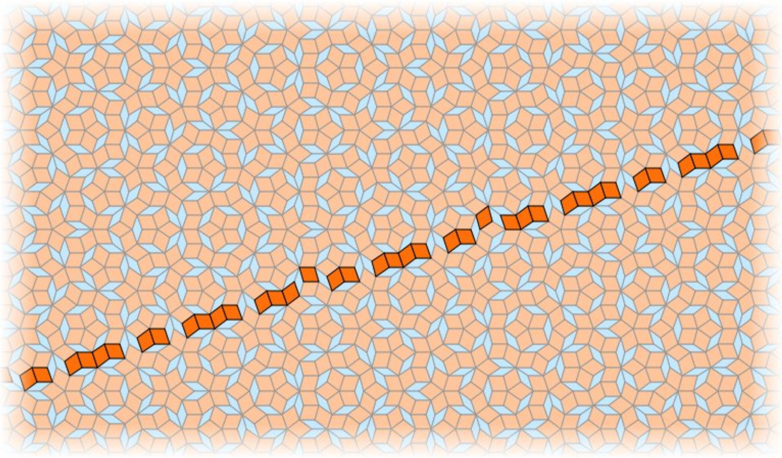

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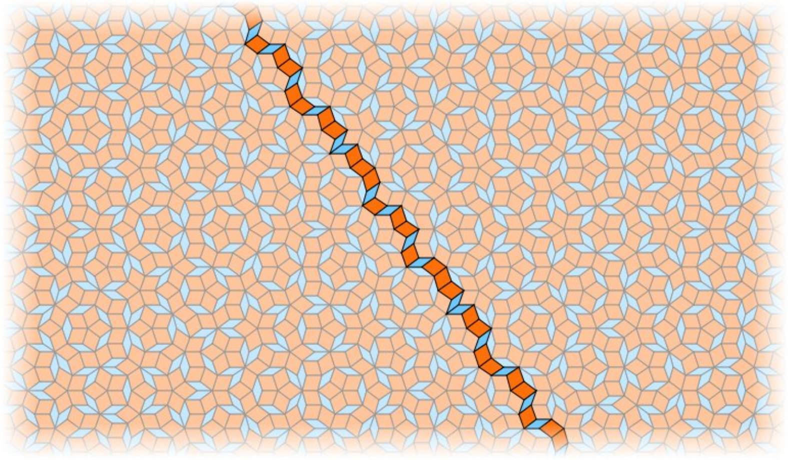

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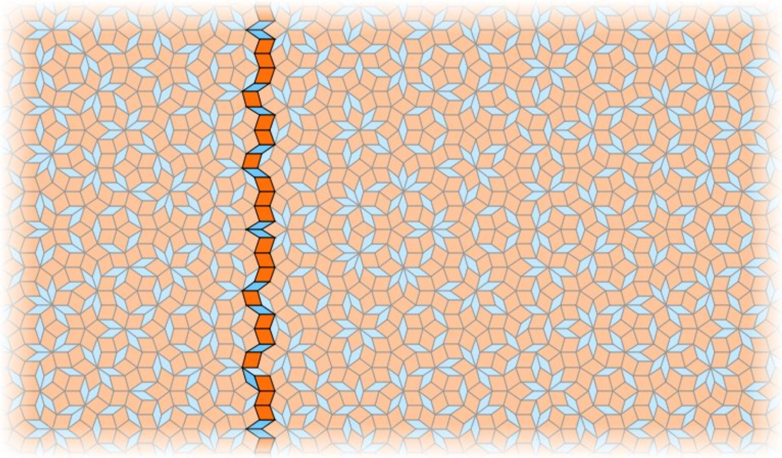

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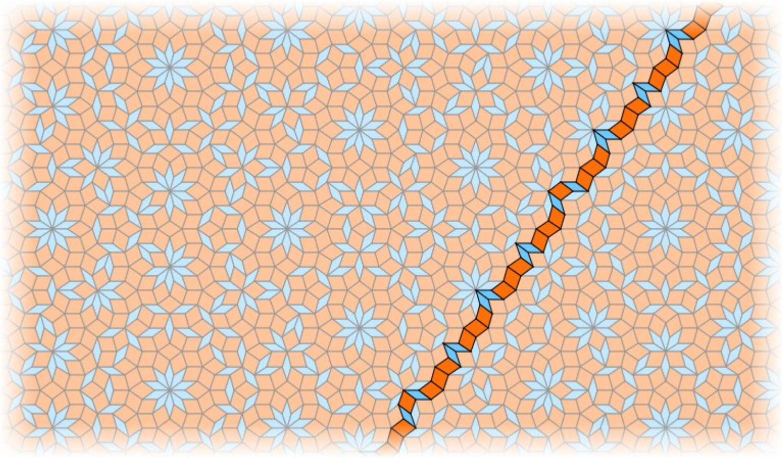

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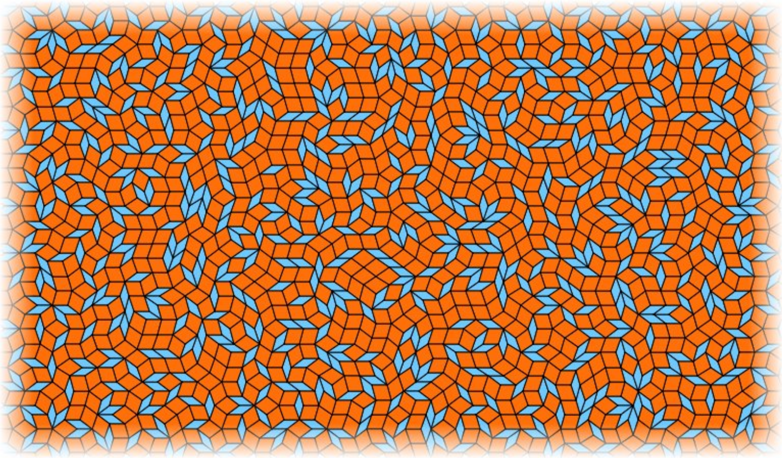

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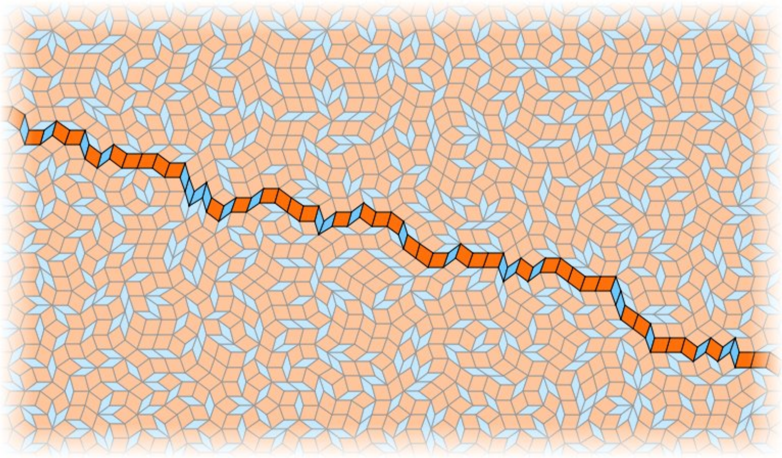

Flip: rotation by π of a hexagon tiled by three tiles:

The AC is affected only in the stripe of the two symmetric tiles:

- *good* flip: $T\dots T\overline{T}\dots\overline{T}\to T\dots\overline{T}T\dots\overline{T}$;
- *bad* flip: $T\dots\overline{T}T\dots\overline{T}\to T\dots T\overline{T}\dots\overline{T}$;
- *neutral* flip: $T\dots T\overline{T}\dots T\to T\dots\overline{T}T\dots T$.

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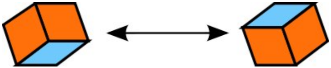

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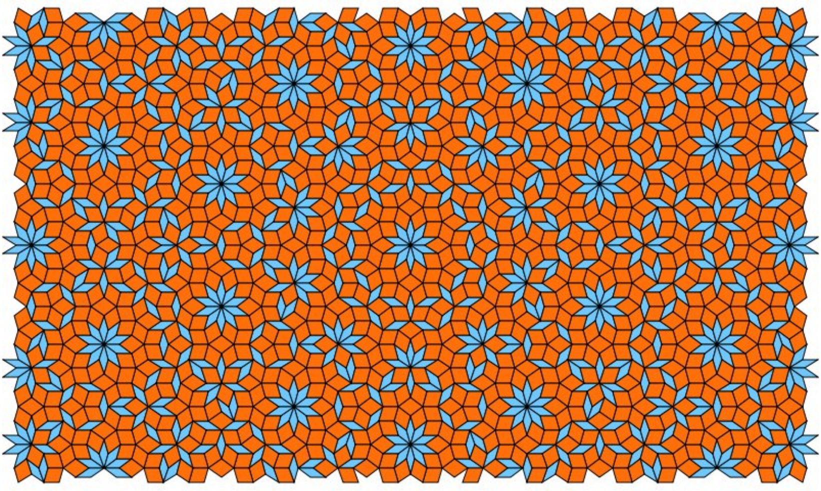
- *neutral* flip: $T \ldots T\overline{T} \ldots T \rightarrow T \ldots \overline{T}T \ldots T$.

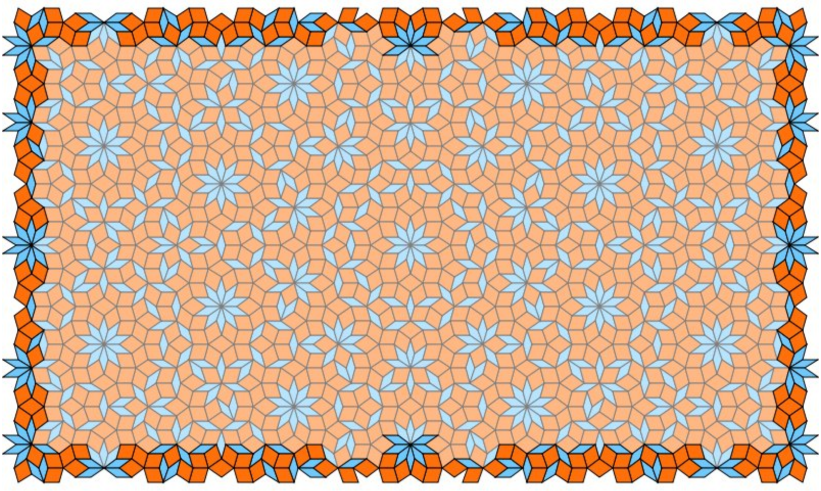
Process: at each step, each possible flip is performed with a probability depending whether it is good, bad or neutral.

The AC is satisfied when only bad flips can be performed (video).

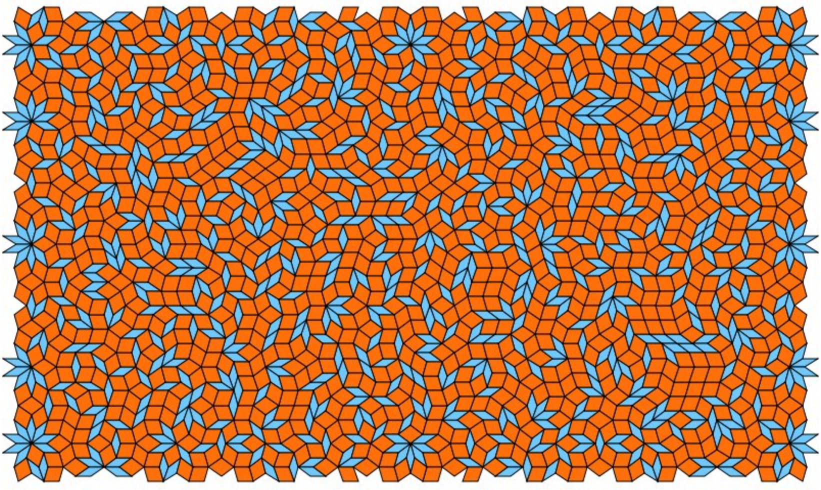
We start from a patch of a generalized Penrose tiling:



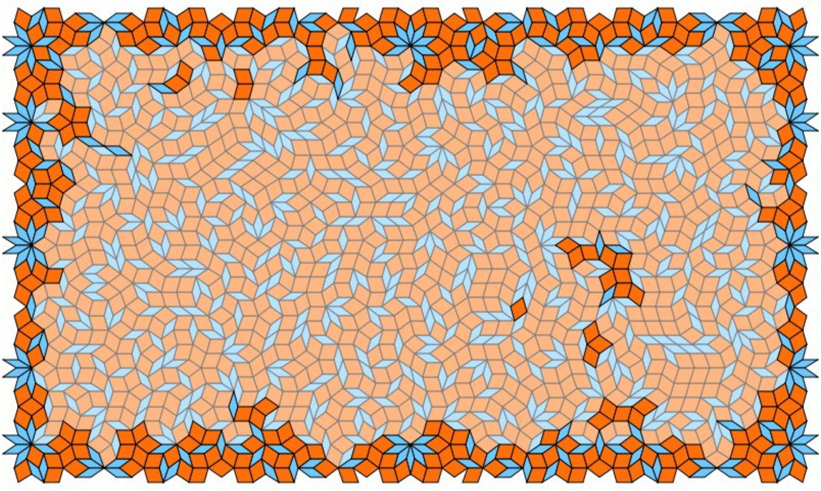
We “freeze” some boundary tiles to ensure possible AC-checking:



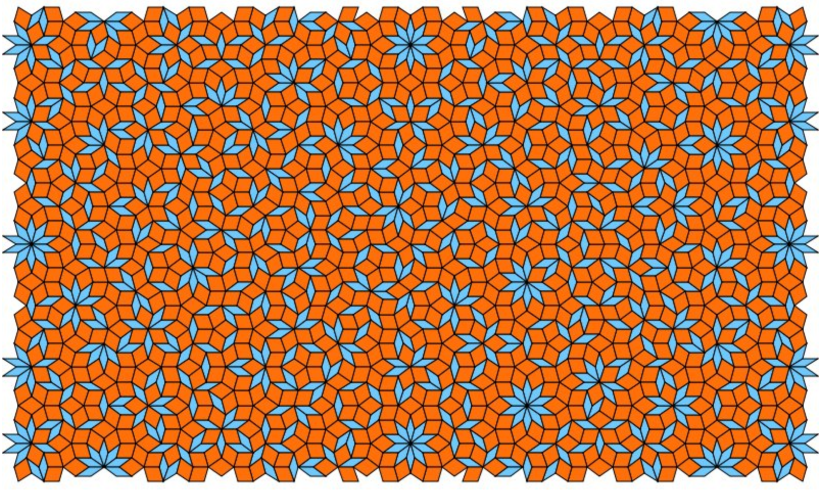
We perform "many" context-free flips (here 100 millions):



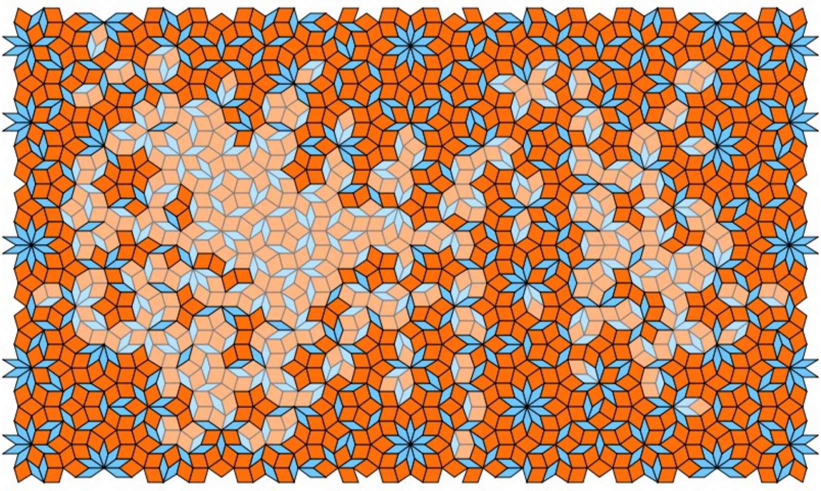
The result should have almost nothing to do with the initial tiling:



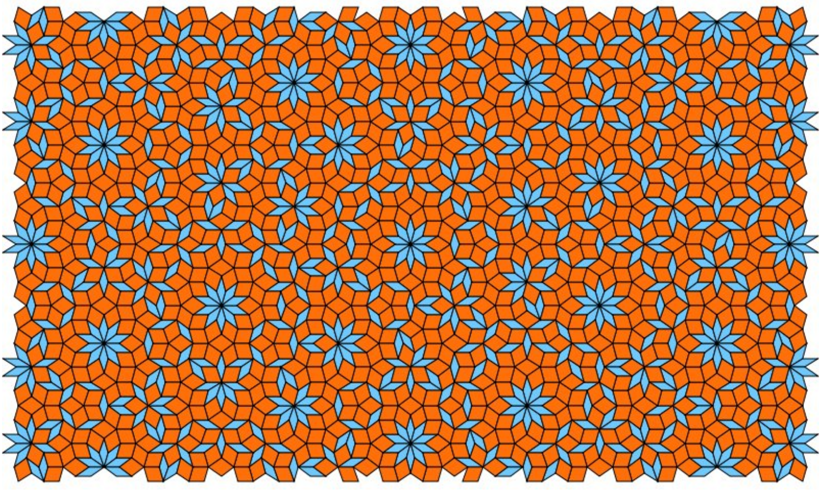
After 40 of the 307 steps ($\simeq$ 40% of the context-sensitive flips):



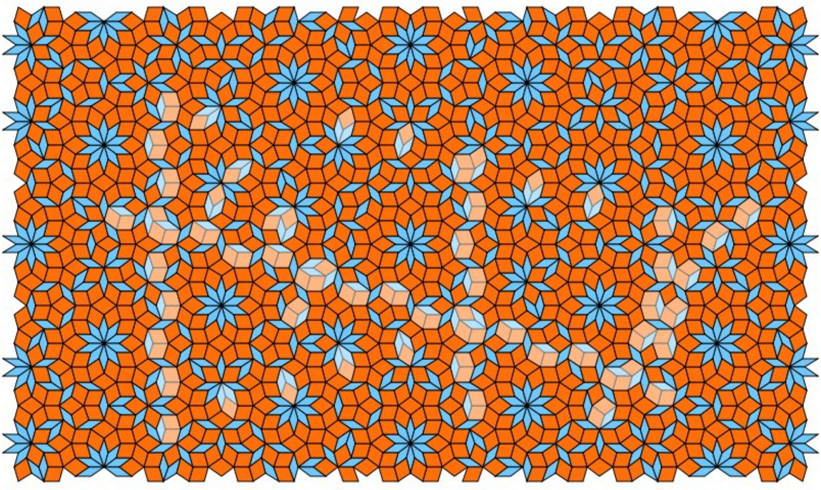
The result already partially agree with the generalized Penrose tiling:



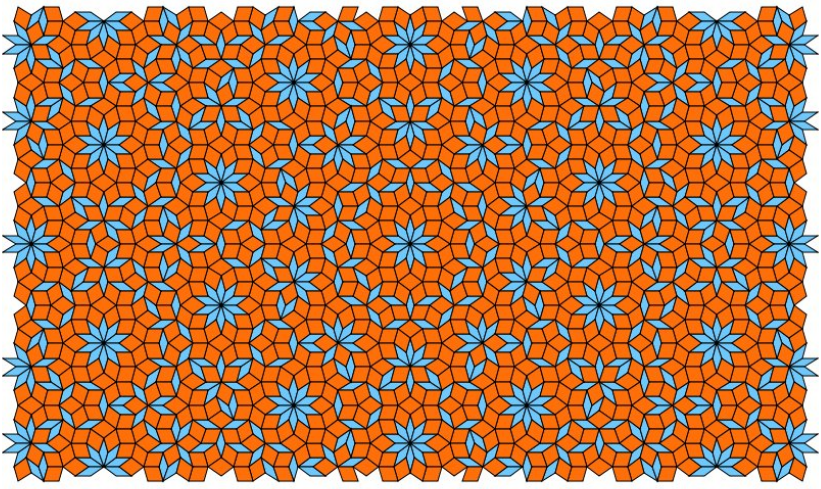
After half of the 307 steps ($\simeq 80\%$ of the context-sensitive flips):



The result almost totally agree with the generalized Penrose tiling:

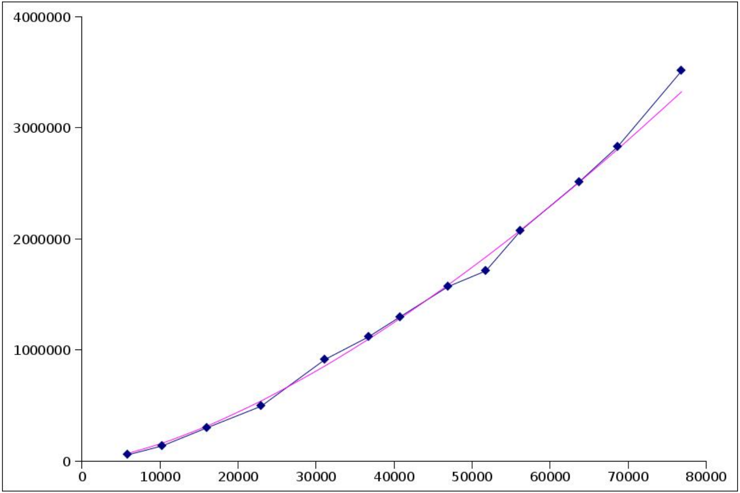


The initial tiling is reached in 307 steps (6797 flips):



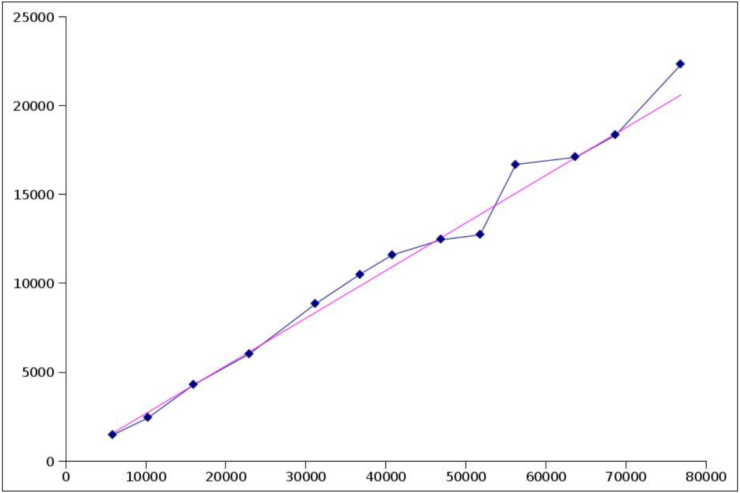
Some statistics...

In blue: x tiles, y flips. In pink: $y \simeq 0.156x\sqrt{x}$.



Some statistics. . .

In blue: x tiles, y steps. In pink: $y \simeq 0.268x$.



$2 \longrightarrow 1$ case: tilings of the line, or two-letter words.

AC characterizes the periodic tiling $\ldots 121212 \ldots$.

Flip: $12 \leftrightarrow 21$. As in the previous example:

- *good* flip: $xxyy \longrightarrow xyxy$;
- *bad* flip: $xyxy \longrightarrow xxyy$;
- *neutral* flip: $xxyx \longrightarrow xyxx$.

Process: perform a uniformly chosen good or neutral flip (.ml).

Consider a stochastic process $(X_t)_{t>0}$ in X.
Assume that there is $\psi : X \to \mathbb{R}^+$ such that:

$$\forall t > 0, \quad \mathbb{E}(\psi(X_{t+1}) - \psi(X_t)|X_t) \leq -\varepsilon < 0.$$

Then:

$$\mathbb{E}(\min\{t \mid \psi(X_t) = 0\}) \leq \frac{\psi(X_0)}{\varepsilon}.$$

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Here, by defining a suitable ψ, we get:

Theorem

The expected number of random good or neutral flips to stabilize a configuration is at most cubic in the size of this configuration.

More precisely, we introduce Dyck Factors:

Then, for $0 < \alpha < 1$, define:

$$\psi_\alpha(w) = \sum_{v \in DF(w)} (1 + |v|_1)^\alpha.$$

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Using the concavity of $x \to x^\alpha$, we show (with $n = |X_t|$):

$$\mathbb{E}(\psi_\alpha(X_{t+1}) - \psi_\alpha(X_t) | X_t) \leq -\alpha(1-\alpha)n^{\alpha-2} \quad \text{and} \quad \psi_\alpha(X_t) \leq n^{1+\alpha}.$$

Note: ψ_α maximal for 1^n2^n and 2^n1^n.
But these tilings are only special cases.

Expected value of ψ_α for a random uniformly chosen tiling?

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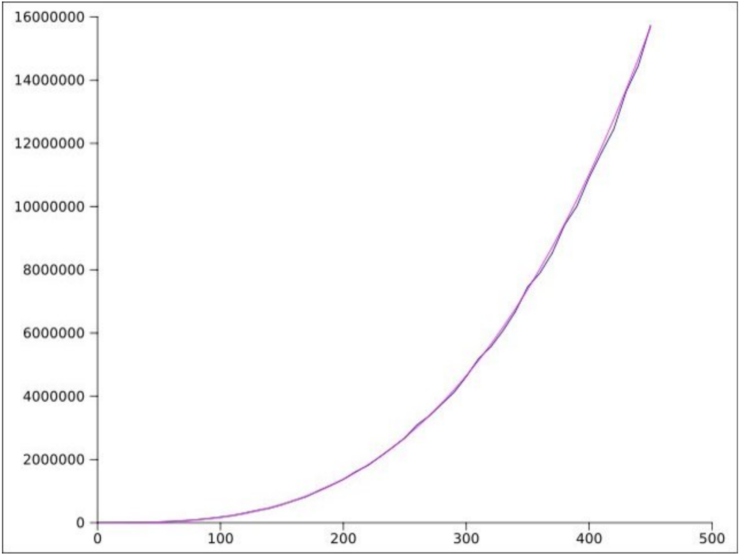
Expected value of ψ_α for a random uniformly chosen tiling?

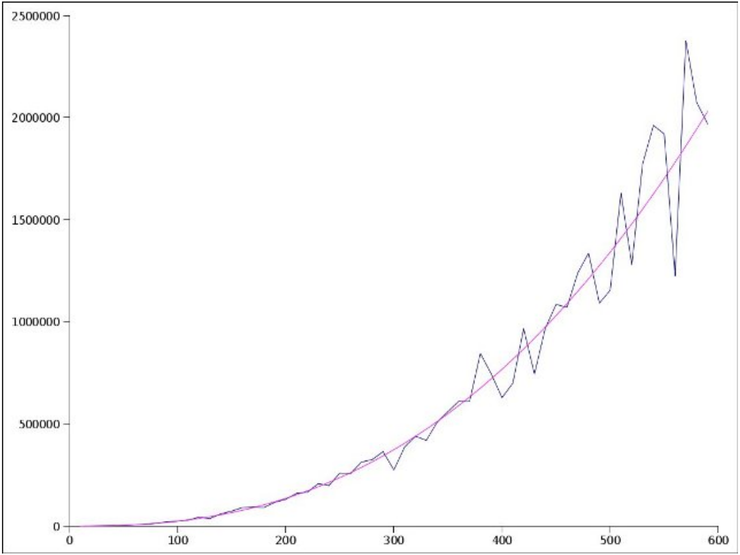
For $\alpha \to 1$, this tends to the average area below a Dyck path.
Using this yields a slightly better bound: $\mathcal{O}(n^{2,5+\delta})$, for $\delta > 0$.

In blue: x tiles, y flips (worst case). In pink: $y \simeq 0.17x^3$.



Experimental result

In blue: x tiles, y flips (average case). In pink: $y \simeq 0.24x^2\sqrt{x}$.



We defined a stochastic process which "straighten" tilings and stabilizes a V-cut, provided that tiles densities are suitable.

Does it make sense in physics?

Surprisingly, the convergence seems to be much better in the $5 \to 2$ case as in the $2 \to 1$. It is however harder to study.

We are first studying intermediate cases:

- $d \to 1$ (codimension effect);
- $d \to d - 1$ (dimension effect).