Quasicrystal Cooling

(Introductory talk)

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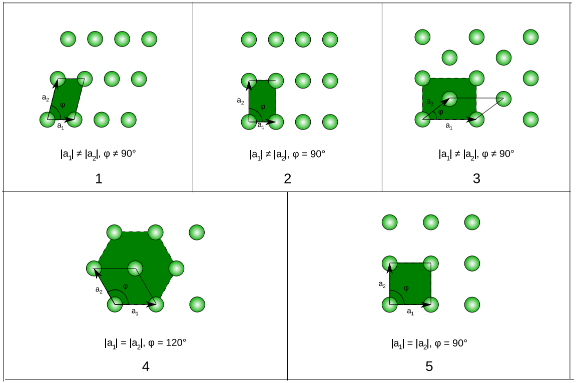
CNRS & Univ. Paris 13

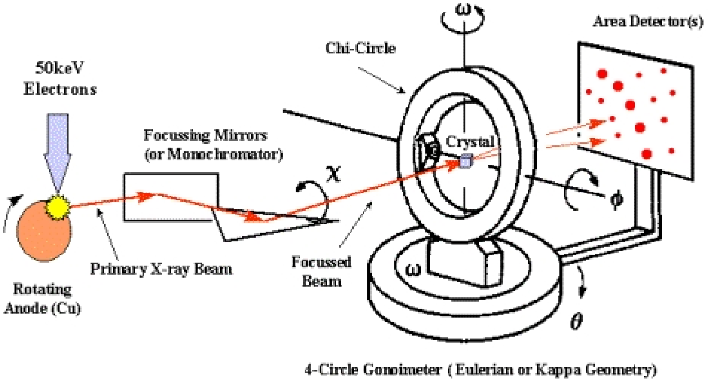
Univ. Roma 3, Januar 10th 2012

Quasicrystals



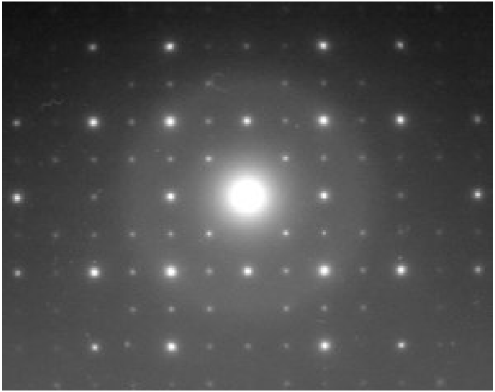
Crystal = ordered material = periodic structure (19th).

Quasicrystals



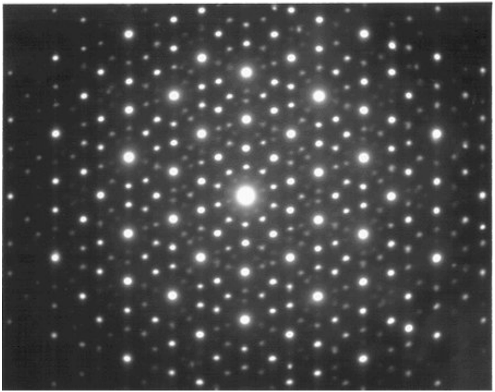
Examination by diffraction of X-rays (Von Laue, 1912).

Quasicrystals



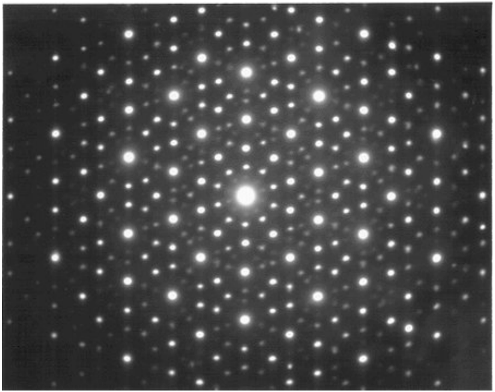
Physical effect: at least the symmetries of its causes (Curie, 1894).

Quasicrystals



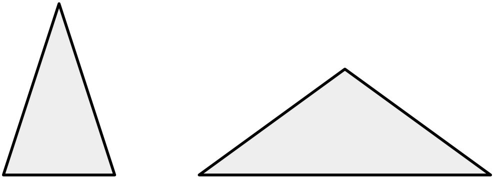
Discovering of non-periodic ordered materials (Shechtman, 1982).

Quasicrystals



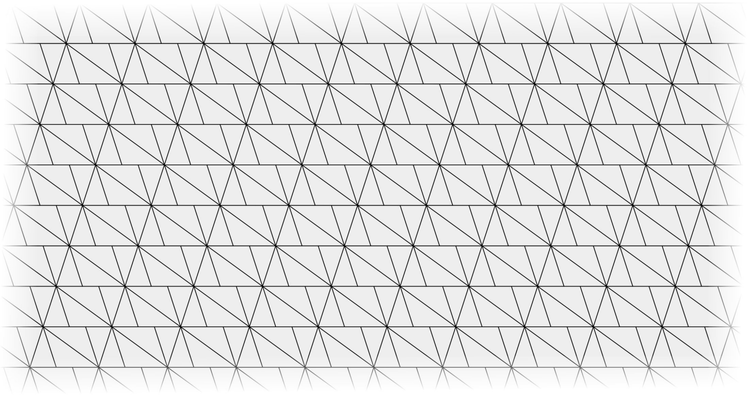
Crystal = ordered material = discrete diffraction (IUCr, 1992).

Aperiodicity



Tile set: finite set of compact homeomorphic to closed balls of $\mathbb{R}^n$.

Aperiodicity



Tiling: covering of $\mathbb{R}^n$ without overlap by isometric copies of tiles.

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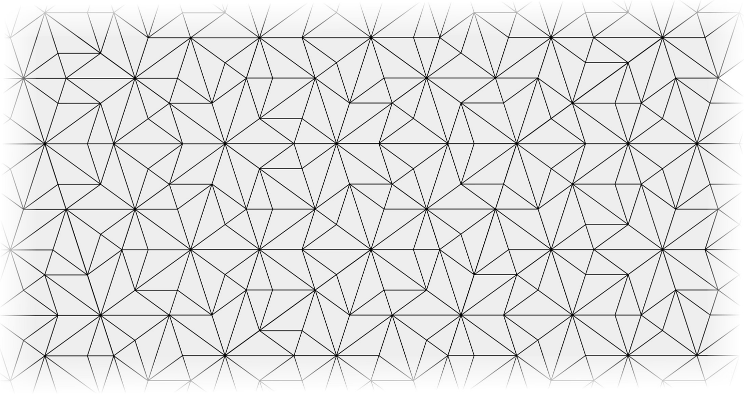

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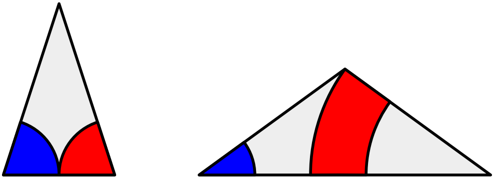
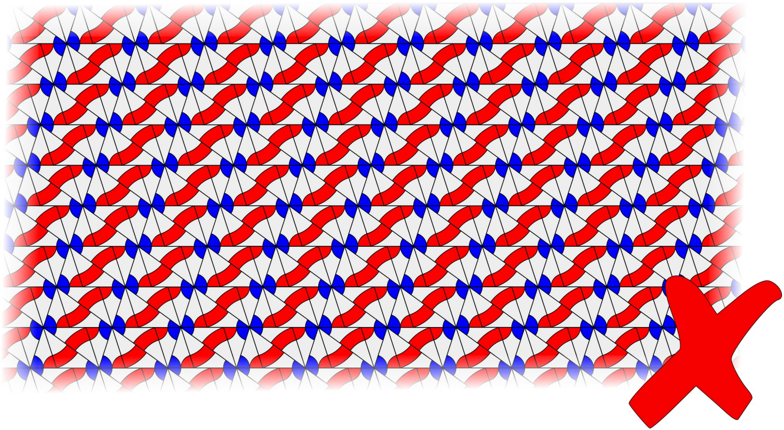


Local constraint: specification of the way tiles can be adjacent.

Aperiodicity



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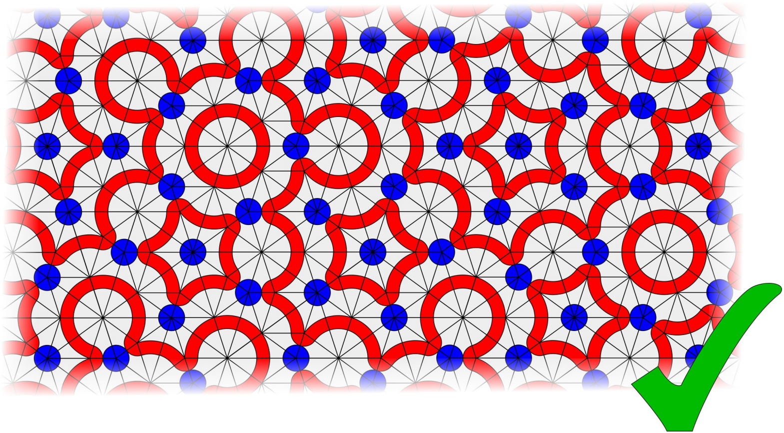

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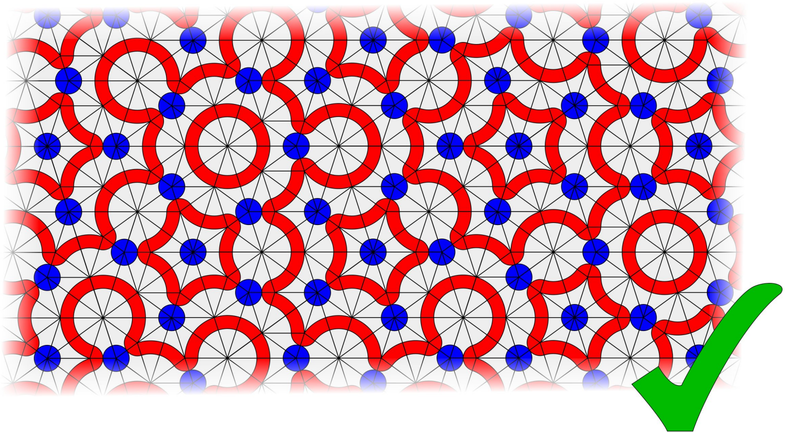
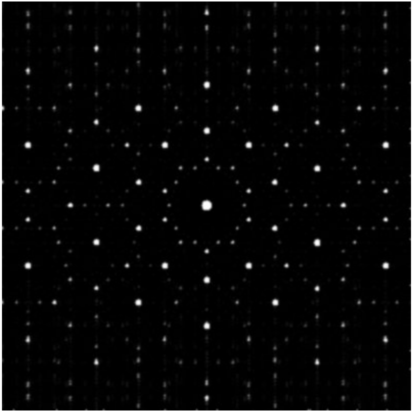


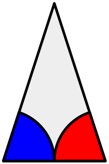
Aperiodic tile set: admits tilings of $\mathbb{R}^n$, but only non-periodic ones.

Aperiodicity



Tiles $\sim$ atom clusters, local constraints $\sim$ finite range interactions.

Energetically-driven growth



Randomly add one tile at time, with local constraint being satisfied.

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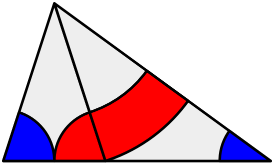

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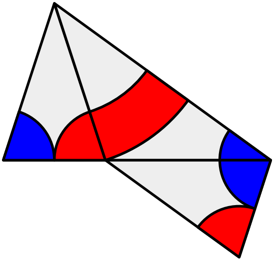

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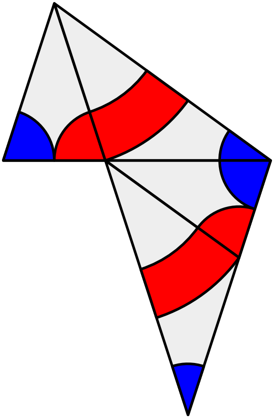

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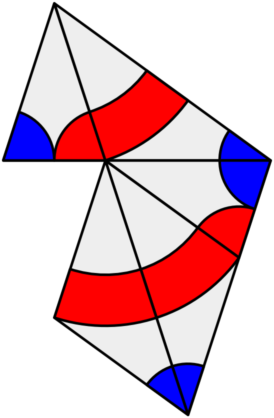

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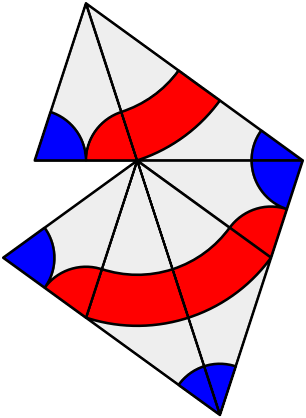
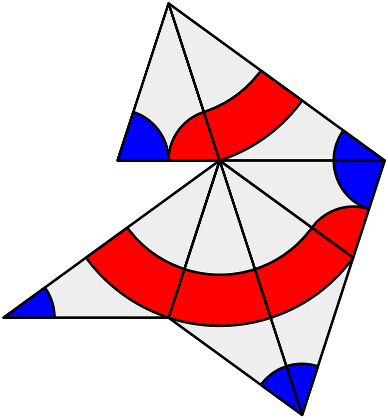


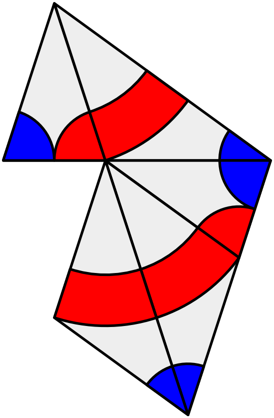
Often leads to *deceptions* (which can always be arbitrarily large).

Energetically-driven growth



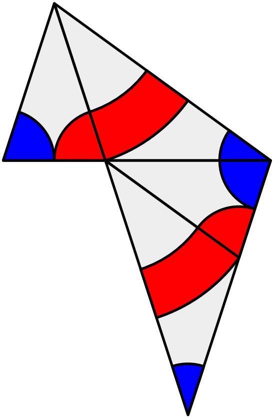
Connected with the intrinsic non-determinism of aperiodic tile sets.

Energetically-driven growth



Endless backtracking (try yourself!) $\rightsquigarrow$ Unrealistic growth.

Energetically-driven growth



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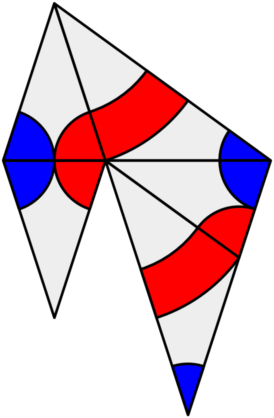

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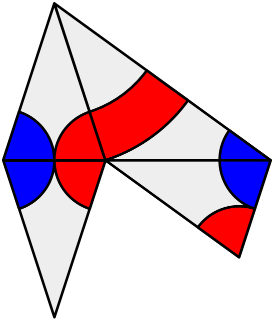

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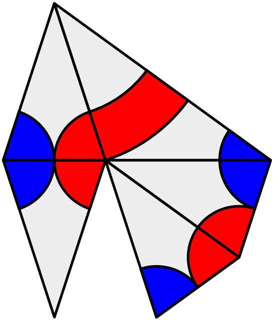

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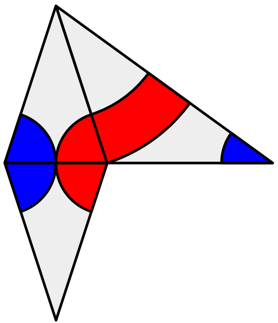

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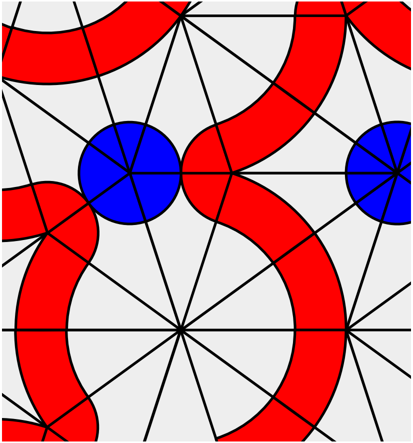

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A bit of thermodynamics

Thermodynamical principle

Stability at temperature $T \Leftrightarrow$ minimal free energy F

$$F = E - TS,$$

where E is the internal energy and S the entropy.

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In terms of tilings

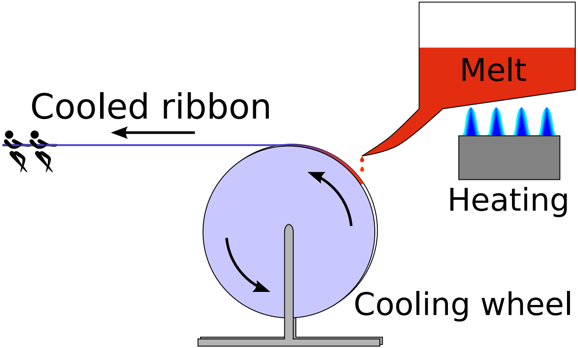
Given finitely many tiles and local constraints,
the energy and the entropy of a finite tiling are defined by:

- $E :=$ number of violated local constraints;
- $S :=$ logarithm of the number of *congruent* tilings.

Example

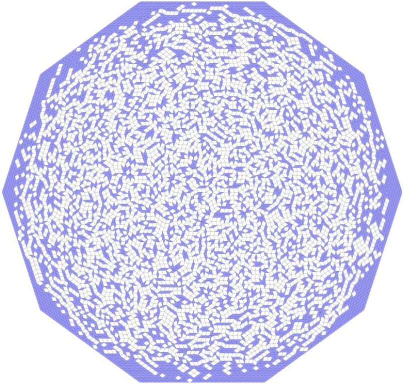
Most stable tilings of $\{a, b\}^N$ when $\{ab, ba\}$ are forbidden?

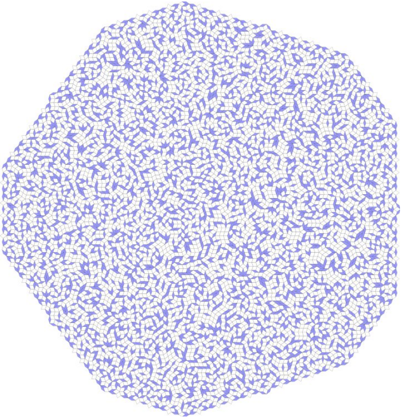
Random tilings



First quasicrystals have been obtained by *quenching*.

Random tilings





Which tilings do maximize the entropy? What is their *typical look*?

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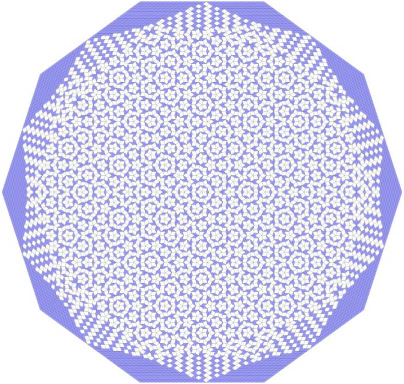

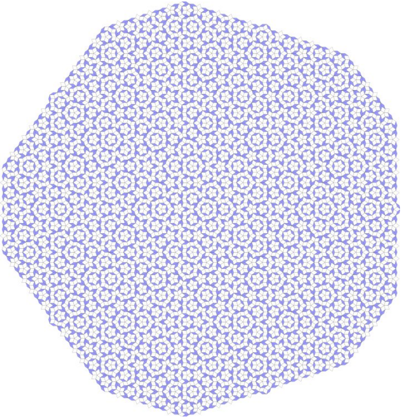

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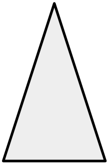

The growth can only be easier when local constraint are neglected!

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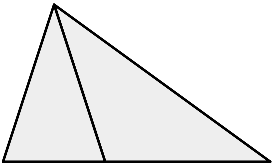

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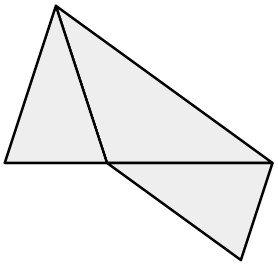

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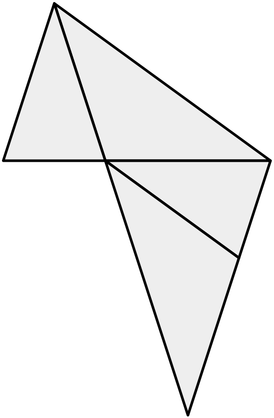

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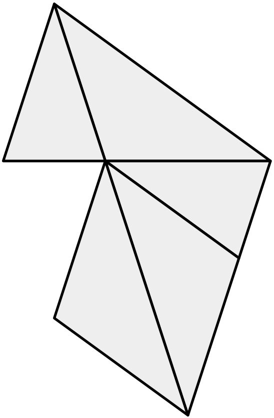

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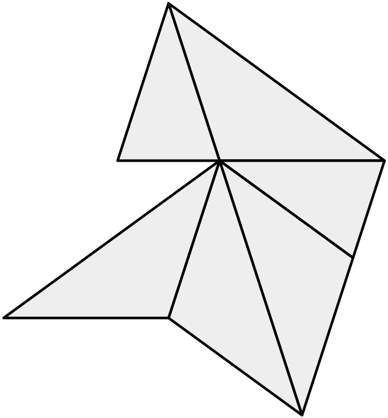

Deceptions (and backtracks) are still possible. . . but we have time!

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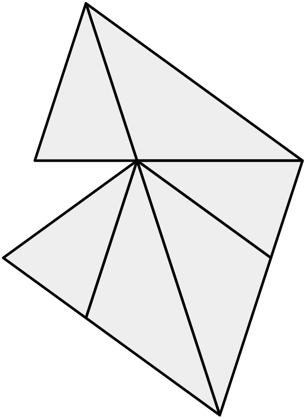

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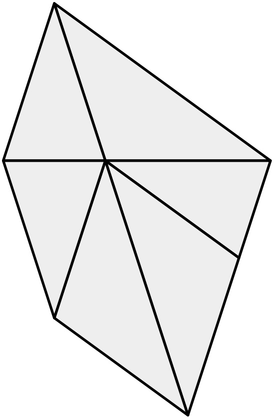

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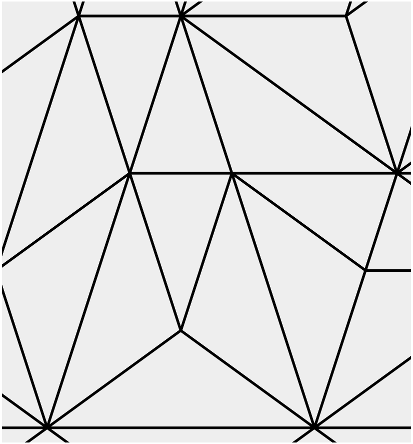

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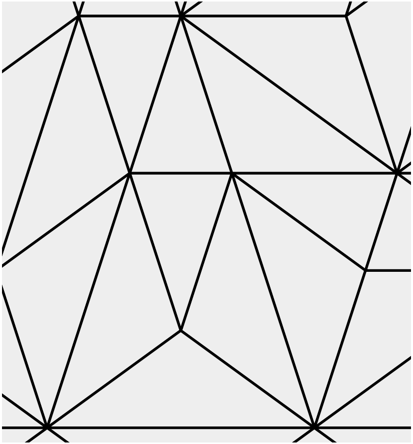
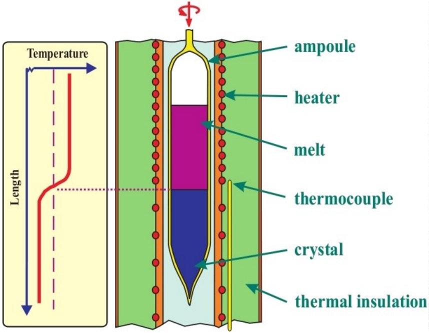
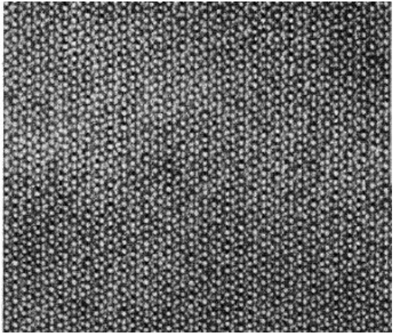


Does it yields S-maximizing tilings?

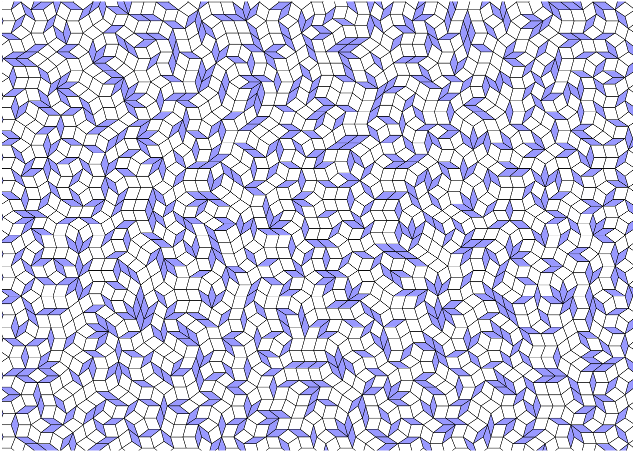
Cooling





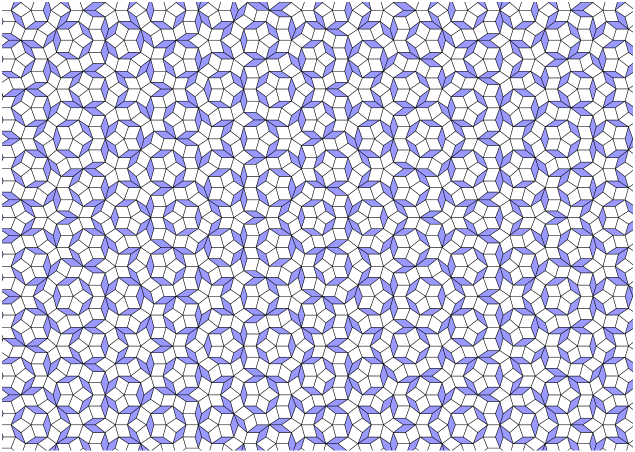
Recent quasicrystals: slow cooling produces quasiperfect structures.

Cooling



How S-maximizing tilings can transform into E-minimizing ones?

Cooling



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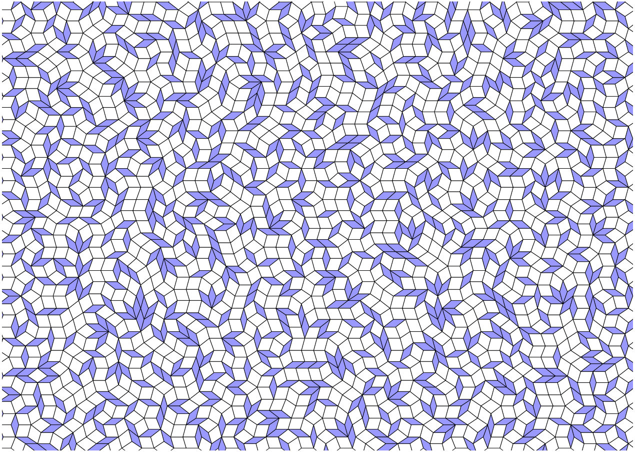
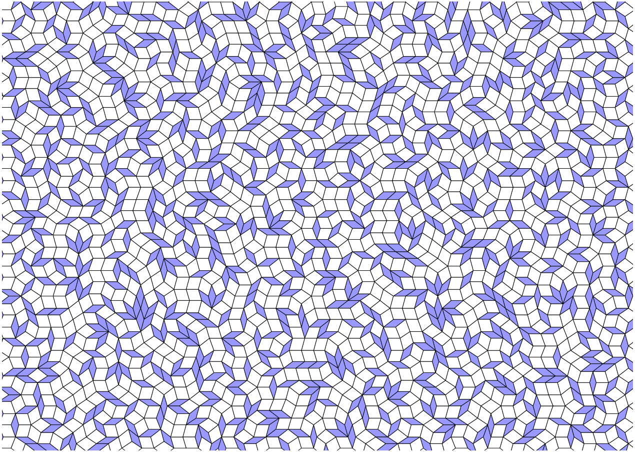


Model: local transformations performed with prob. $\exp(-\Delta E/T)$.

Cooling



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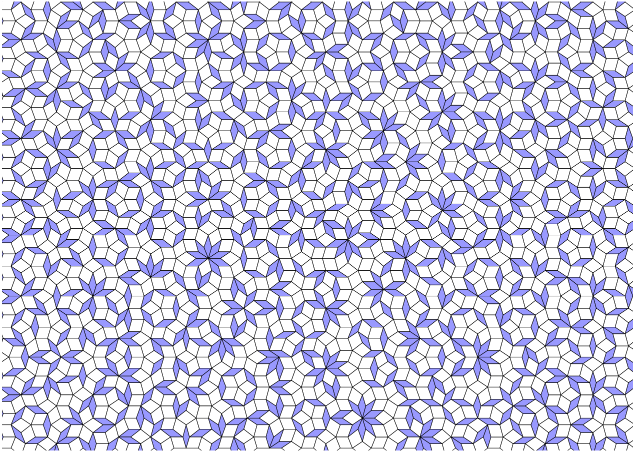
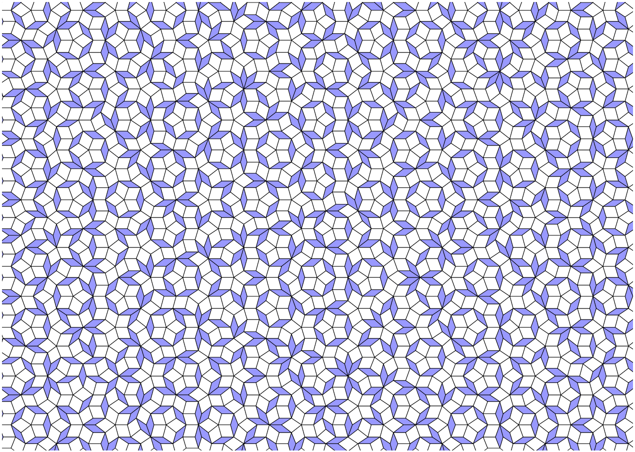


Ergodicity? Convergence rate? Optimal cooling schedule?

Cooling



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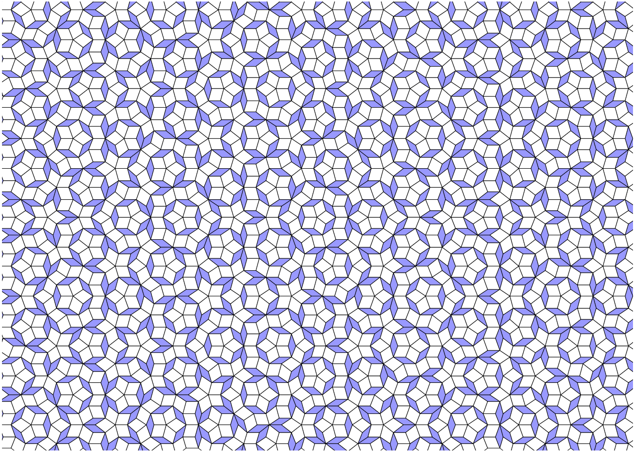

Ergodicity? Convergence rate? Optimal cooling schedule?

Thank you for your attention

and let us now turn towards precise specific cases!