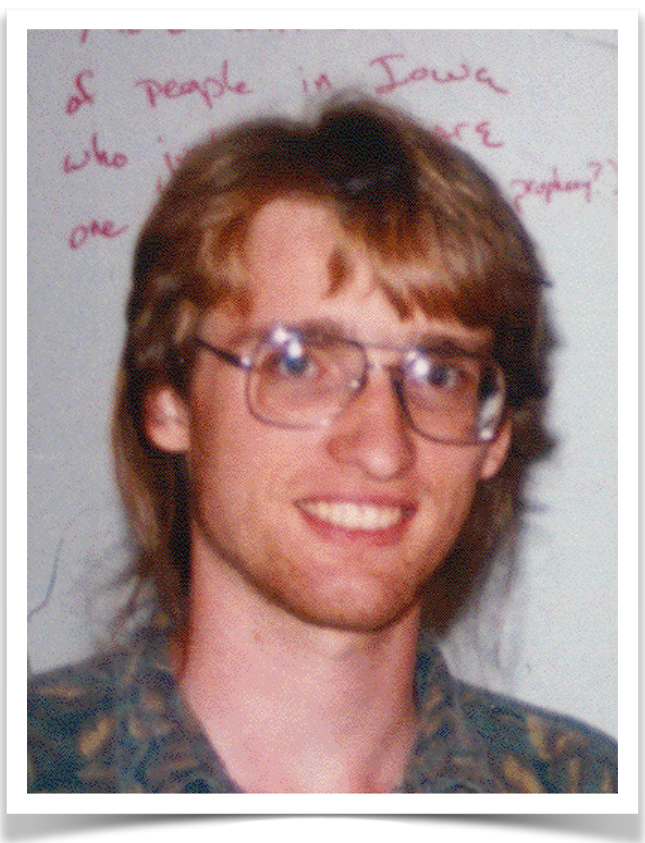
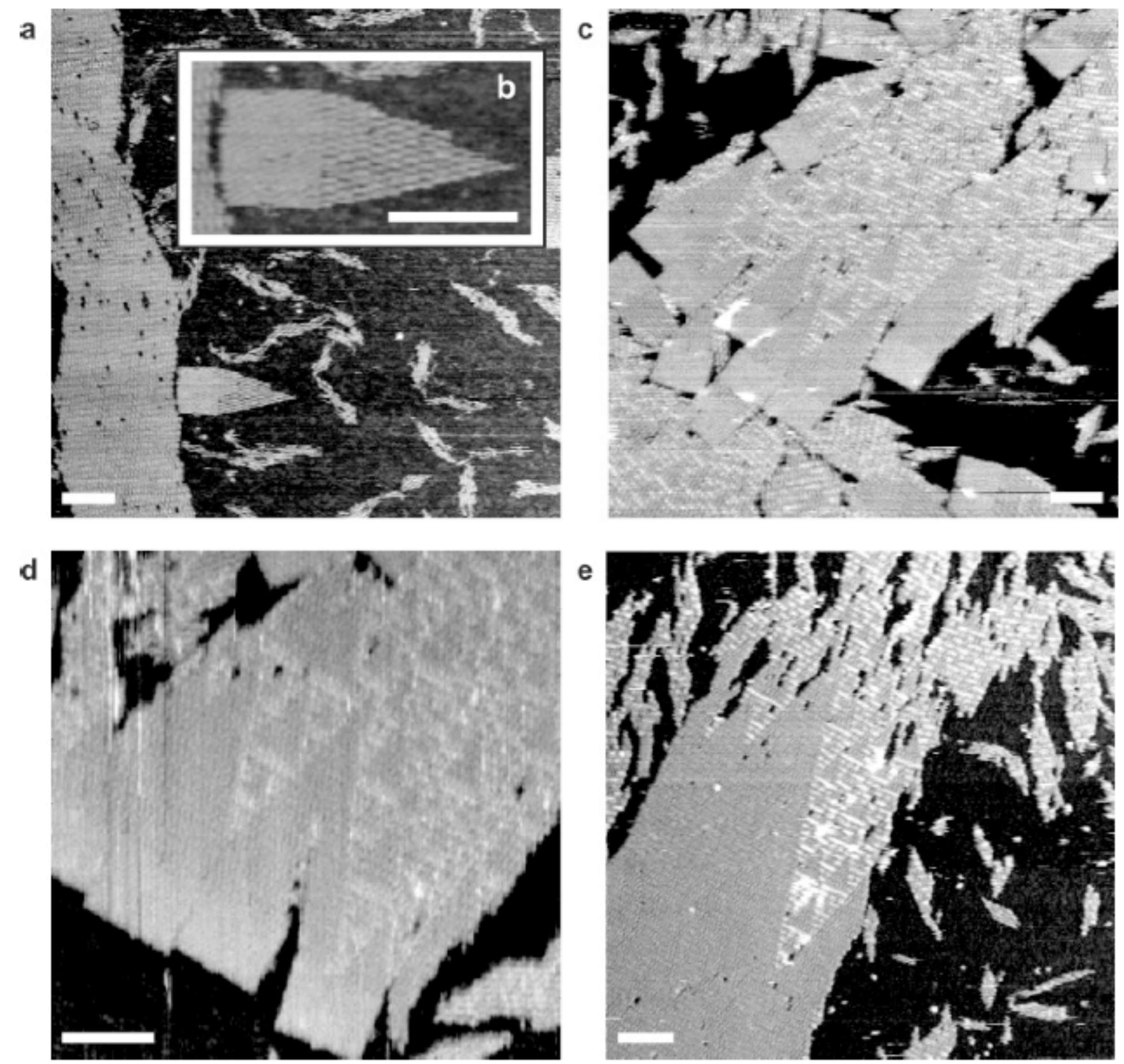
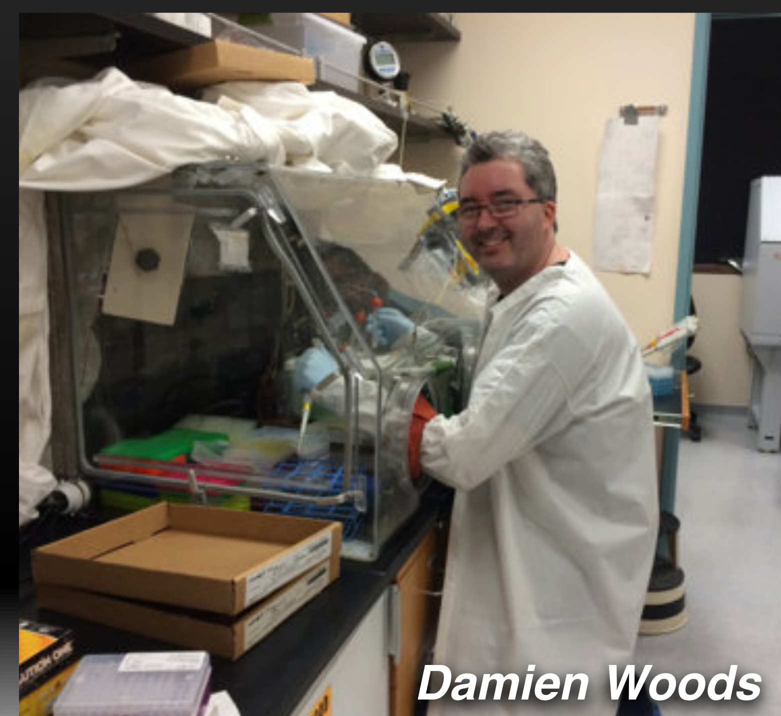
Part I:
Tile assembly

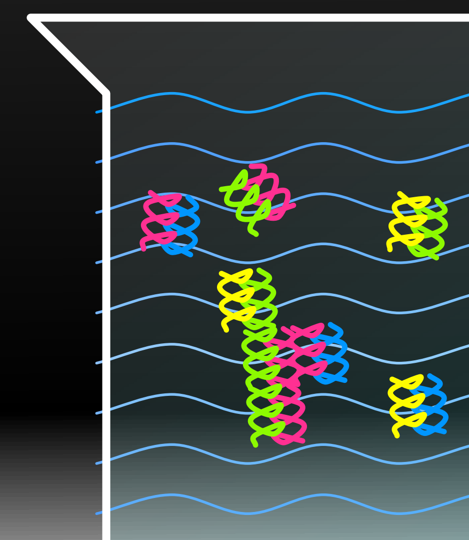
Erik **Winfree** (1998-):
DNA algorithmic self-assembly





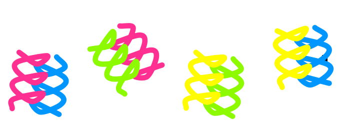
Principle of DNA algorithmic self-assembly





1. Thermal cycler

Hot / less hot cycles for exponential duplication of the DNA strands by Polymerase Chain Reaction (PCR)

⇒ the tiles ..

2. One-pot reaction

Mixing the tiles at 90°C and letting the solution cool down to room temperature for few hours

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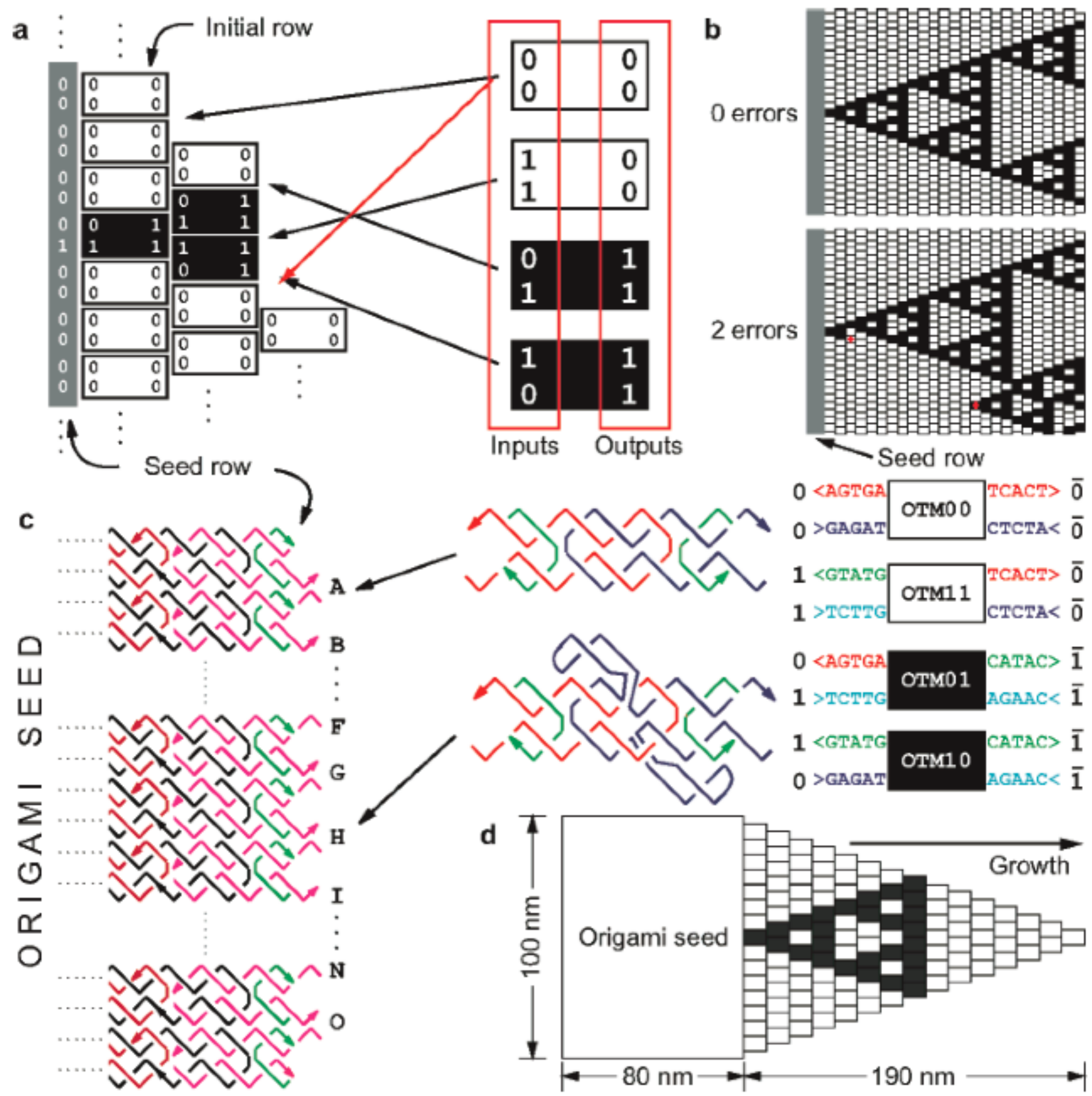

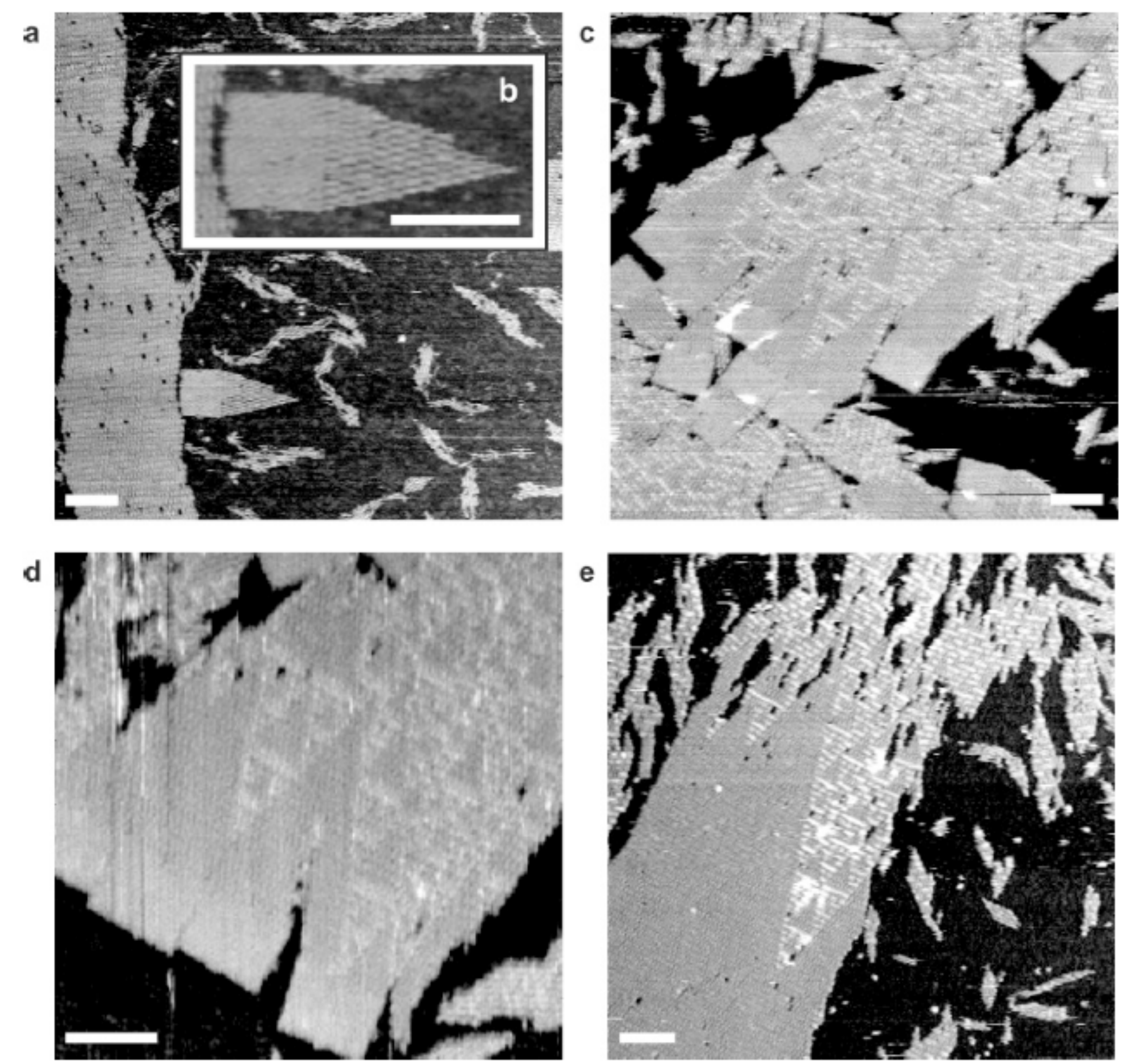

<u>Credits</u>: K. Fujibayashi, R. Hariadi, S.H. Park, E. Winfree & S. Murata

Calculer =

Transformer l’information

Triangles de Sierpiński

Règles de substitutions:

0 **1** → **1**   **1** 0 → **1**   0 0 → 0   **1** **1** → 0

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 **1** 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 **1** **1** 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 **1** 0 **1** 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 **1** **1** **1** **1** 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 **1** 0 0 0 **1** 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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0 0 0 0 0 0 0 0 0 0 0 0 **1** 0 **1** 0 **1** 0 **1** 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 **1** **1** **1** **1** **1** **1** **1** **1** 0 0 0 0 0 0 0 0 0 0 0 0 0
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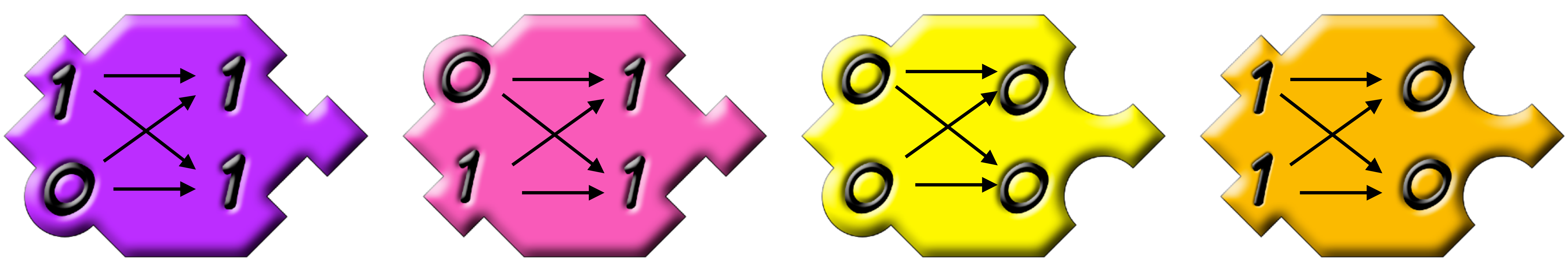
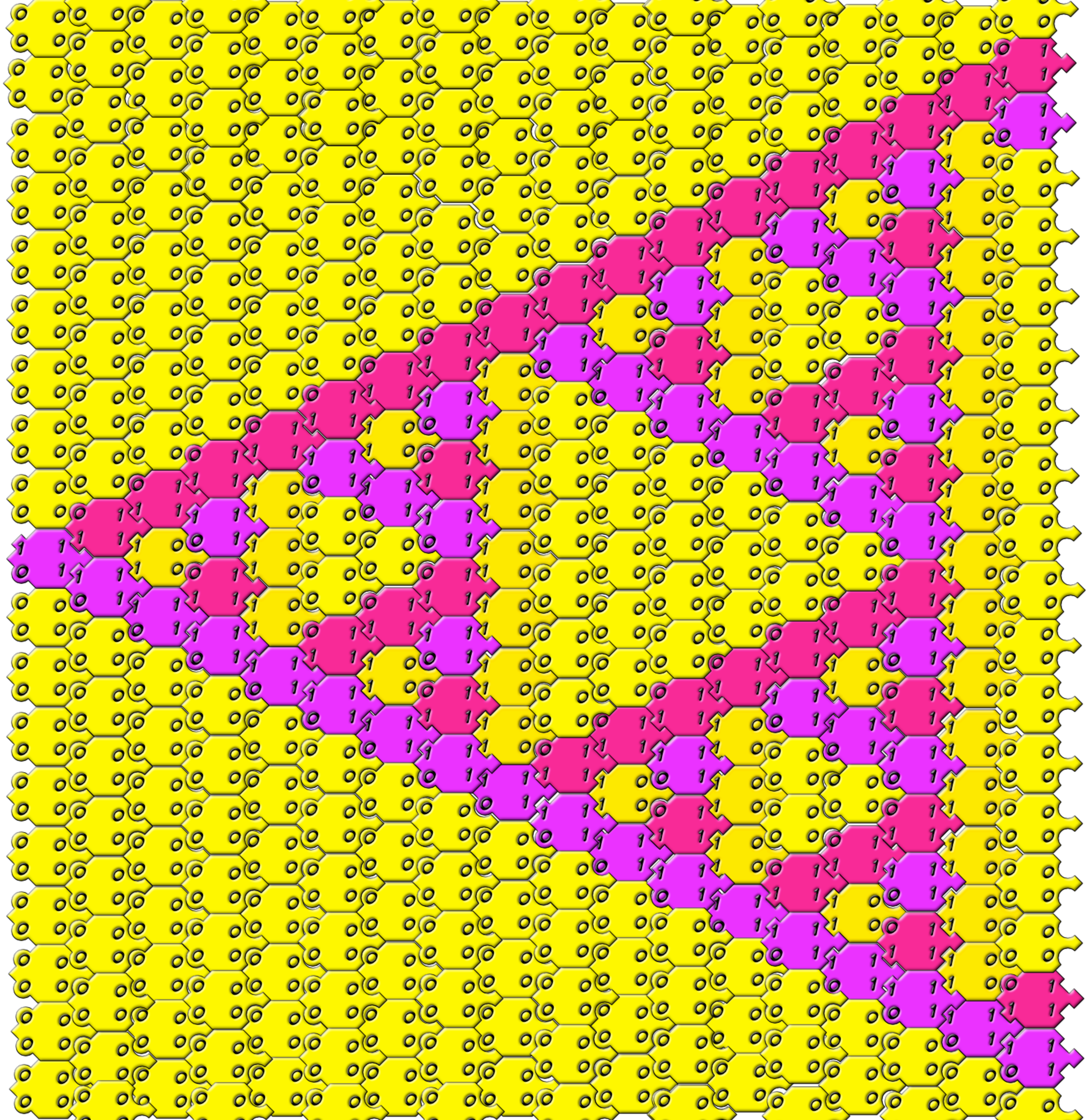
Triangles de Sierpiński

Règles de substitutions:

0 **1**	**1** 0	0 0	**1** **1**
1	**1**	0	0





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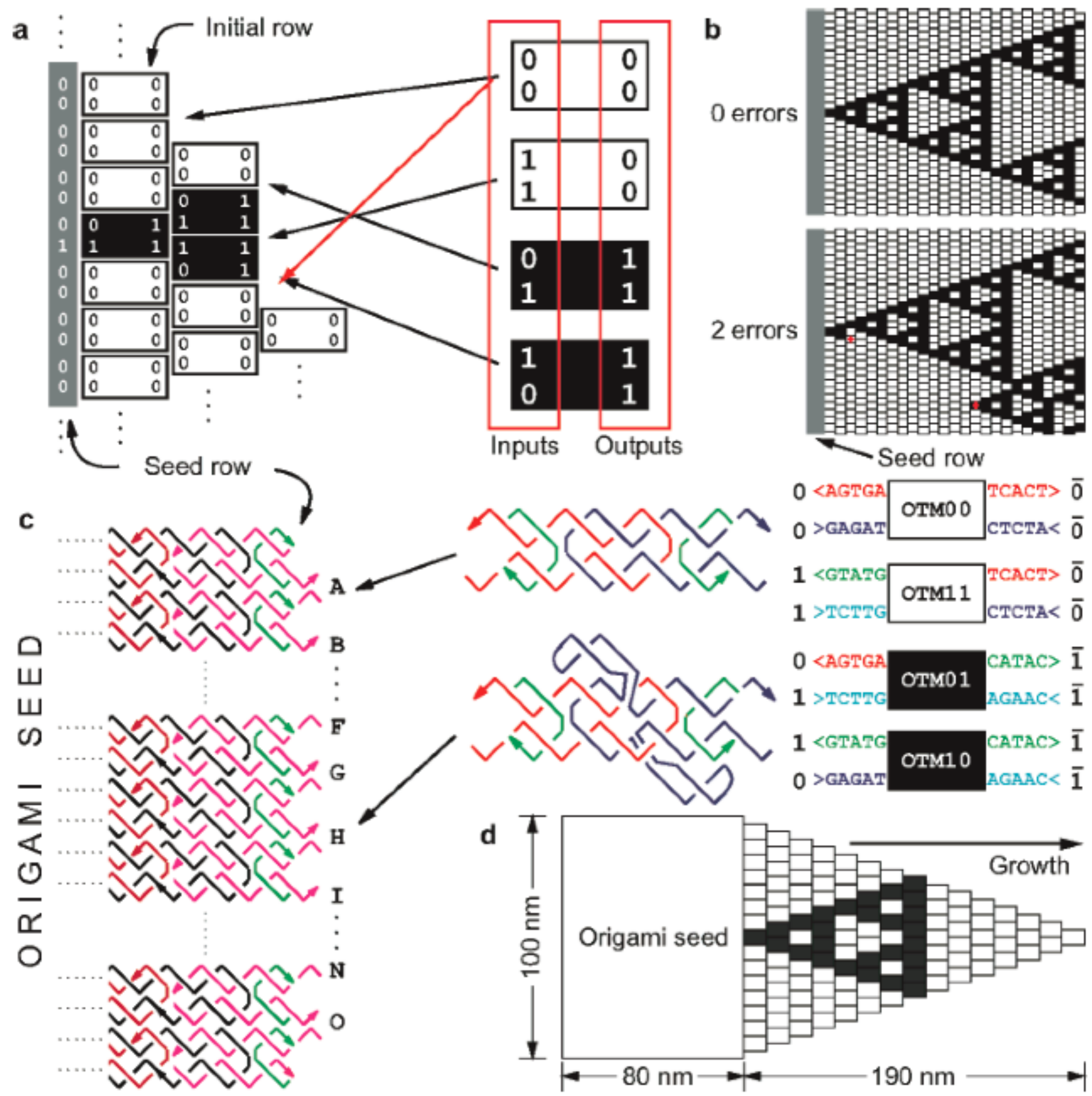

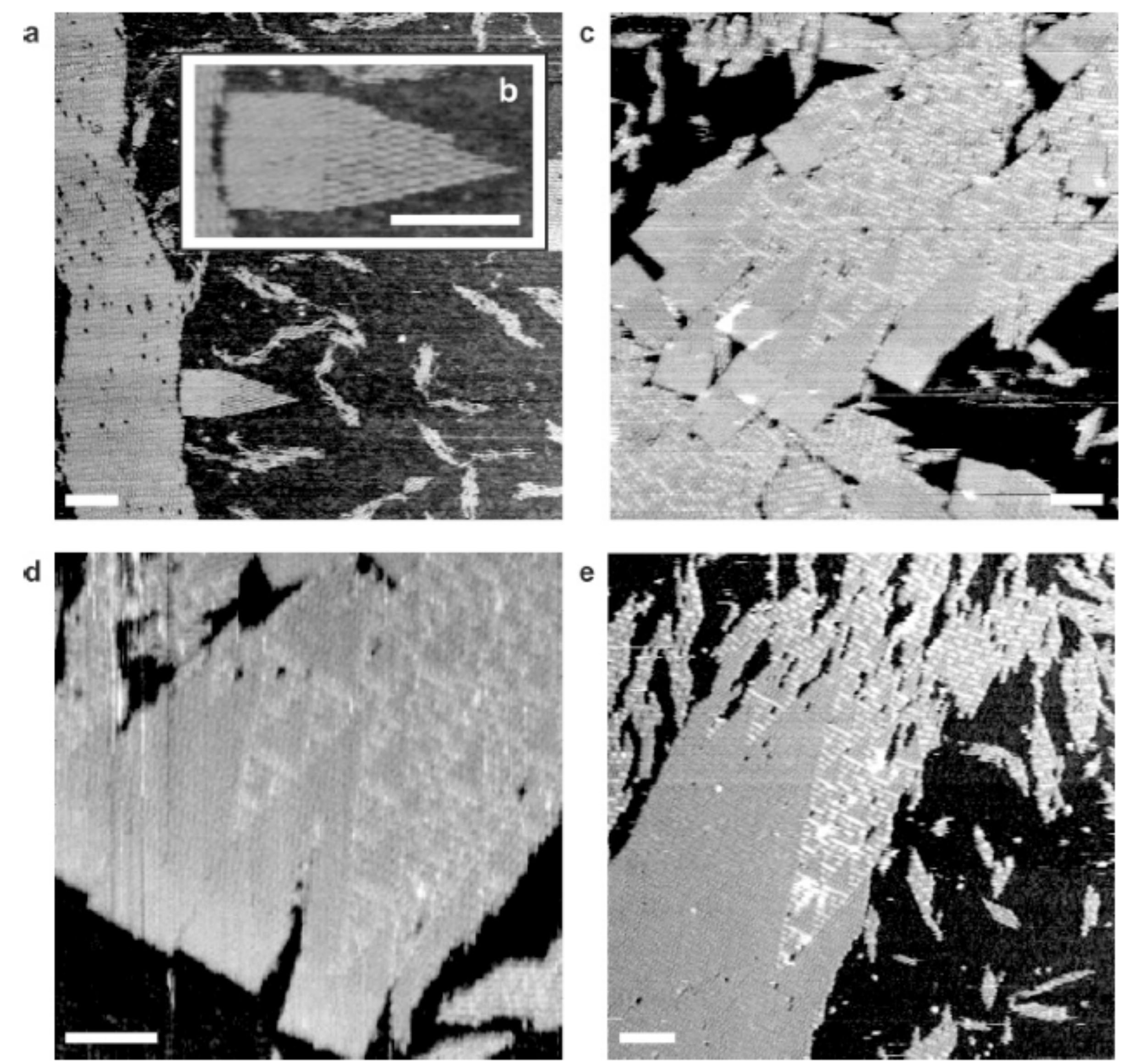

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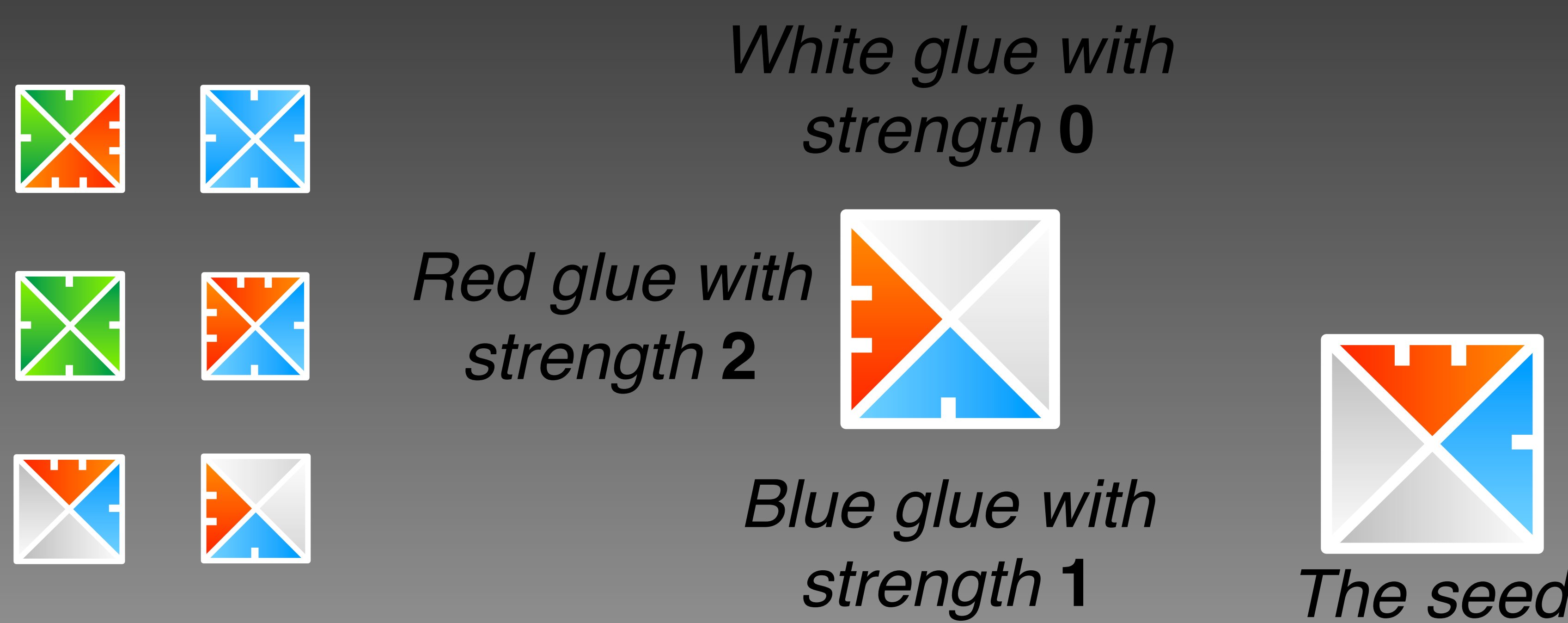
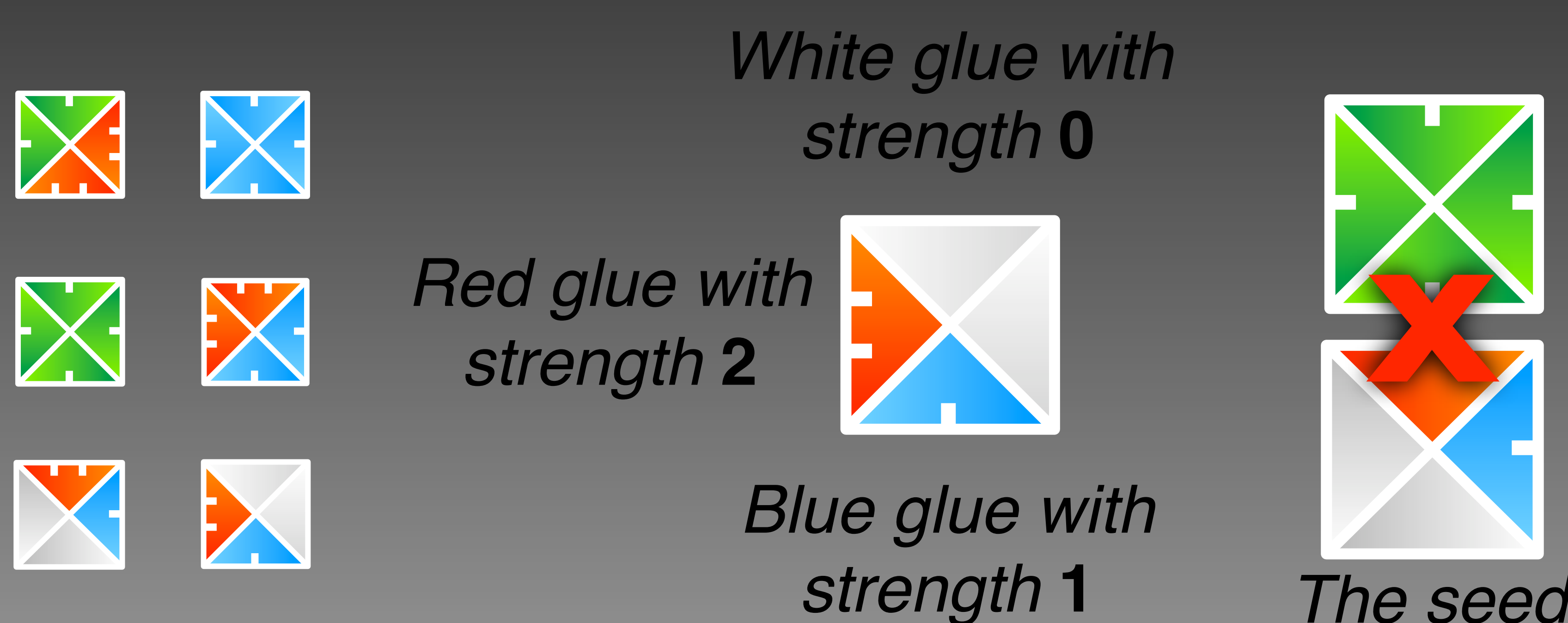
Algorithmic model



- A seed tile
- A temperature (= **2** in pratice)

Algorithmic model



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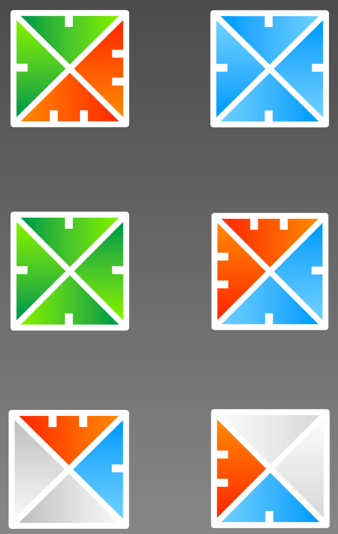
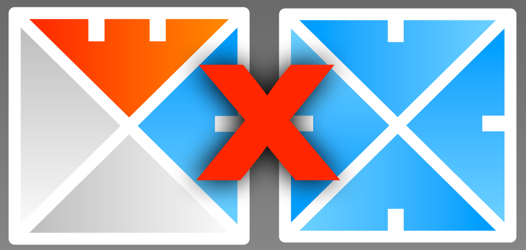


White glue with strength **0**

Red glue with strength **2**

Blue glue with strength **1**

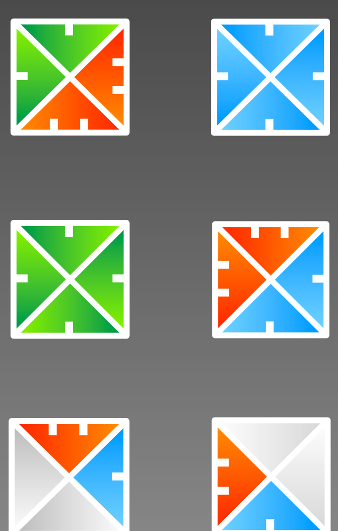


The seed

#bonds < T° = 2

- A seed tile
- A temperature (= **2** in pratice)

Algorithmic model



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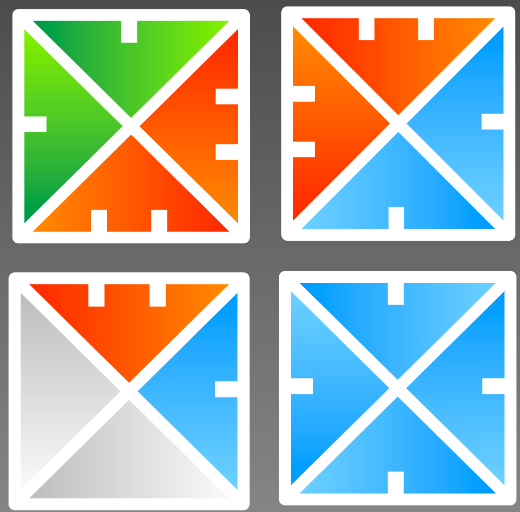
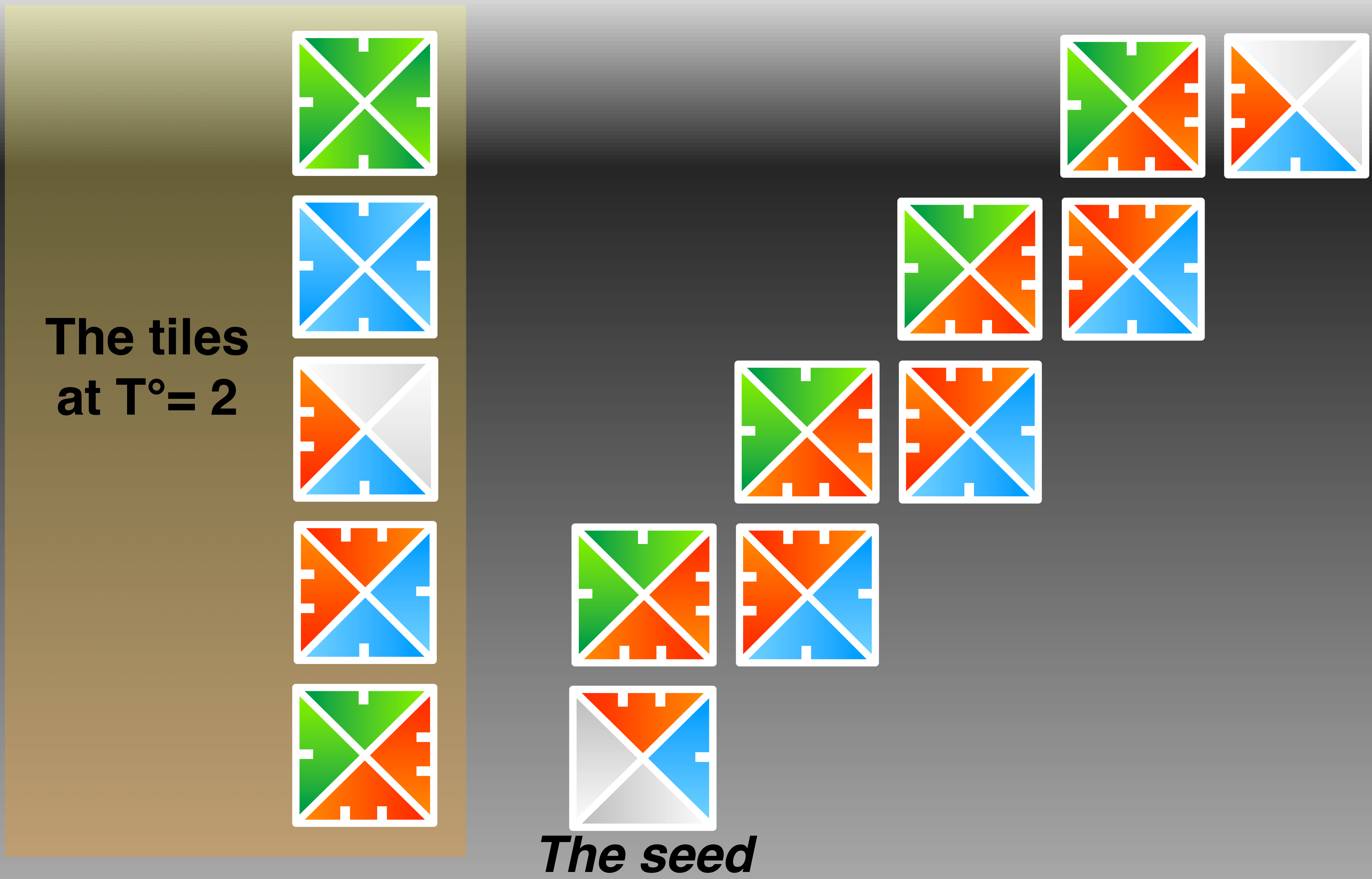


The seed

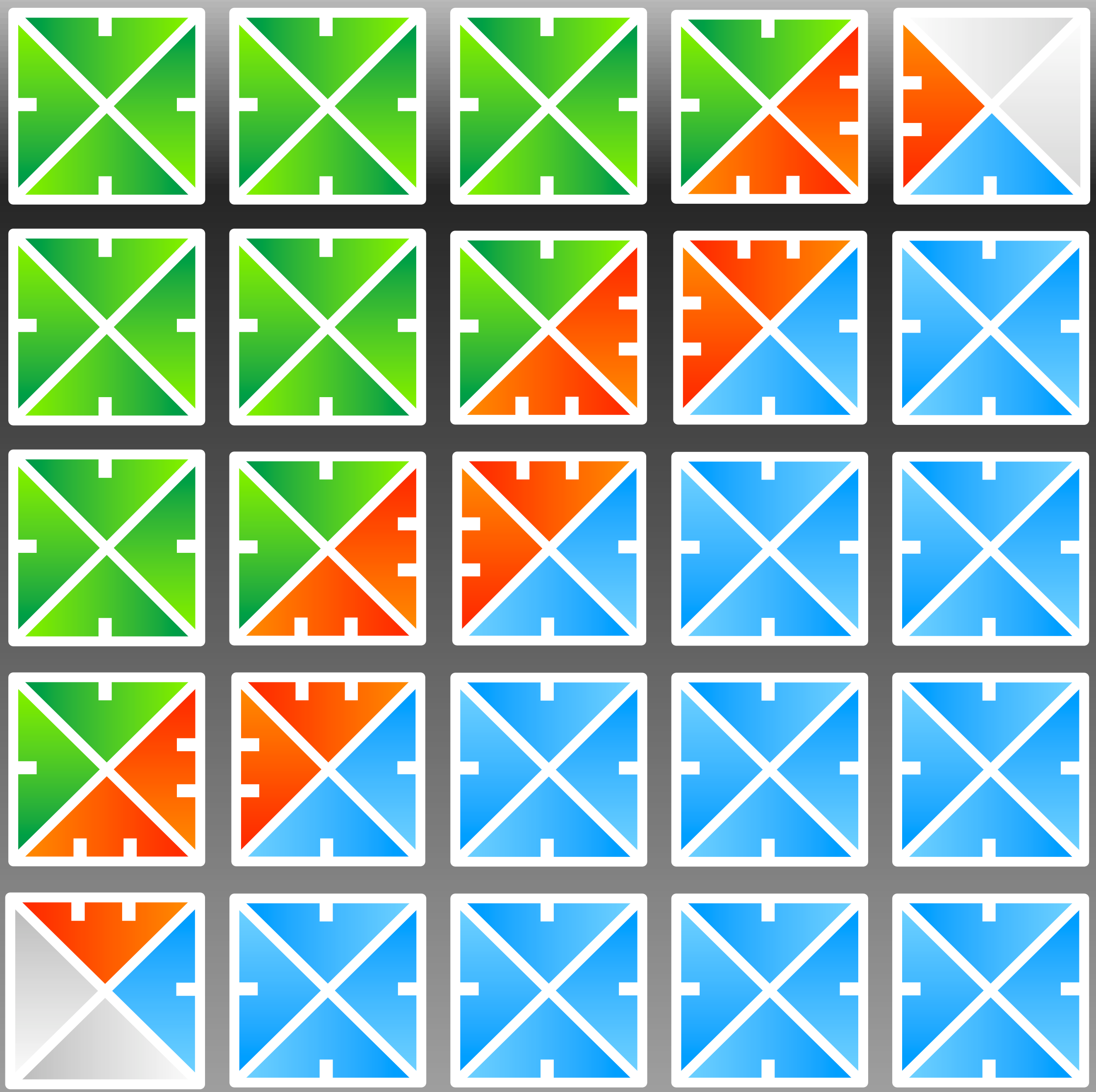
- A seed tile
- A temperature (= **2** in pratice)

Assembling a square



Assembling a square

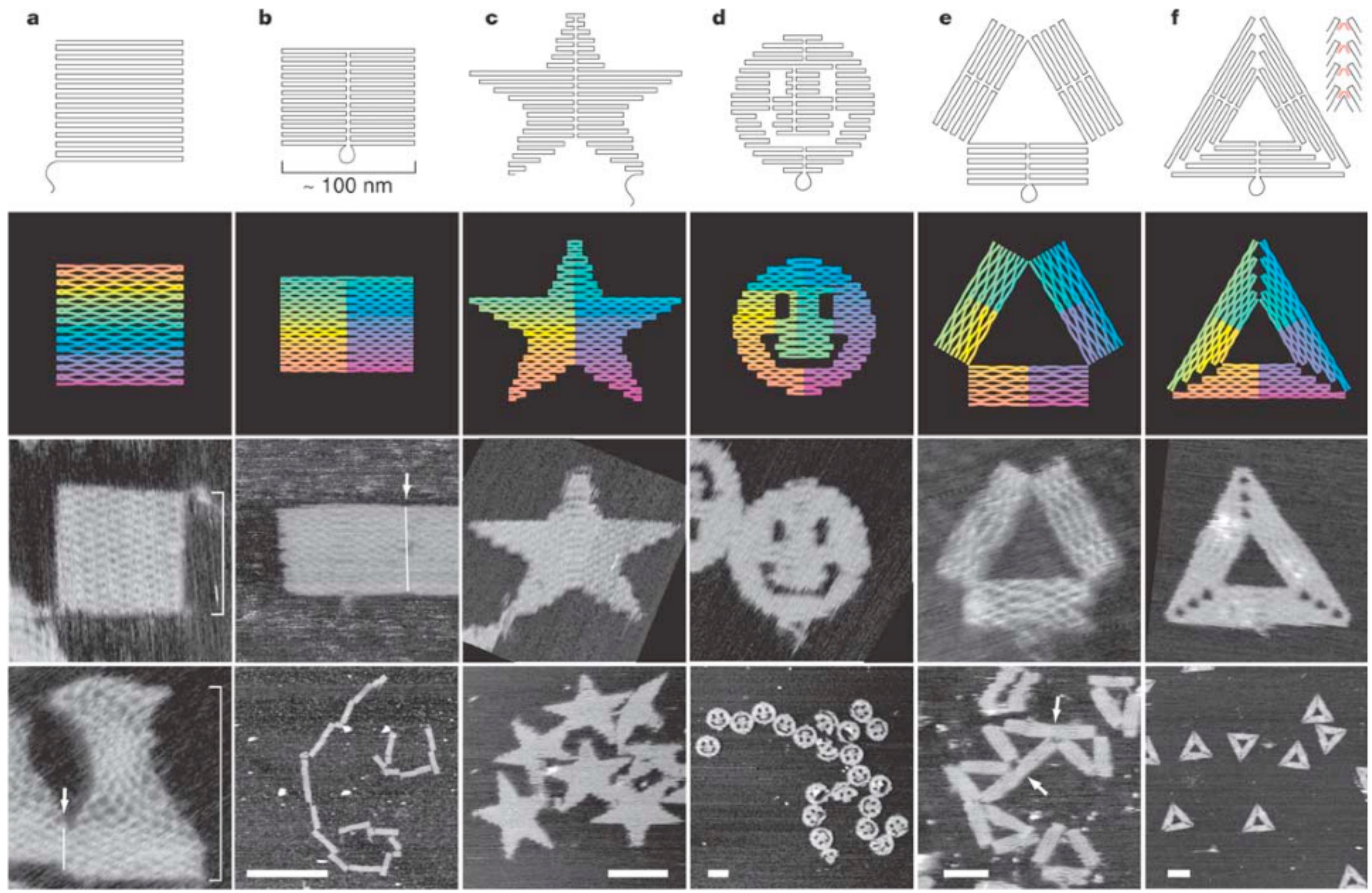
The tiles at T°= 2



The seed

No more tile can be added

Paul **Rothemund** (2001-): DNA Origami



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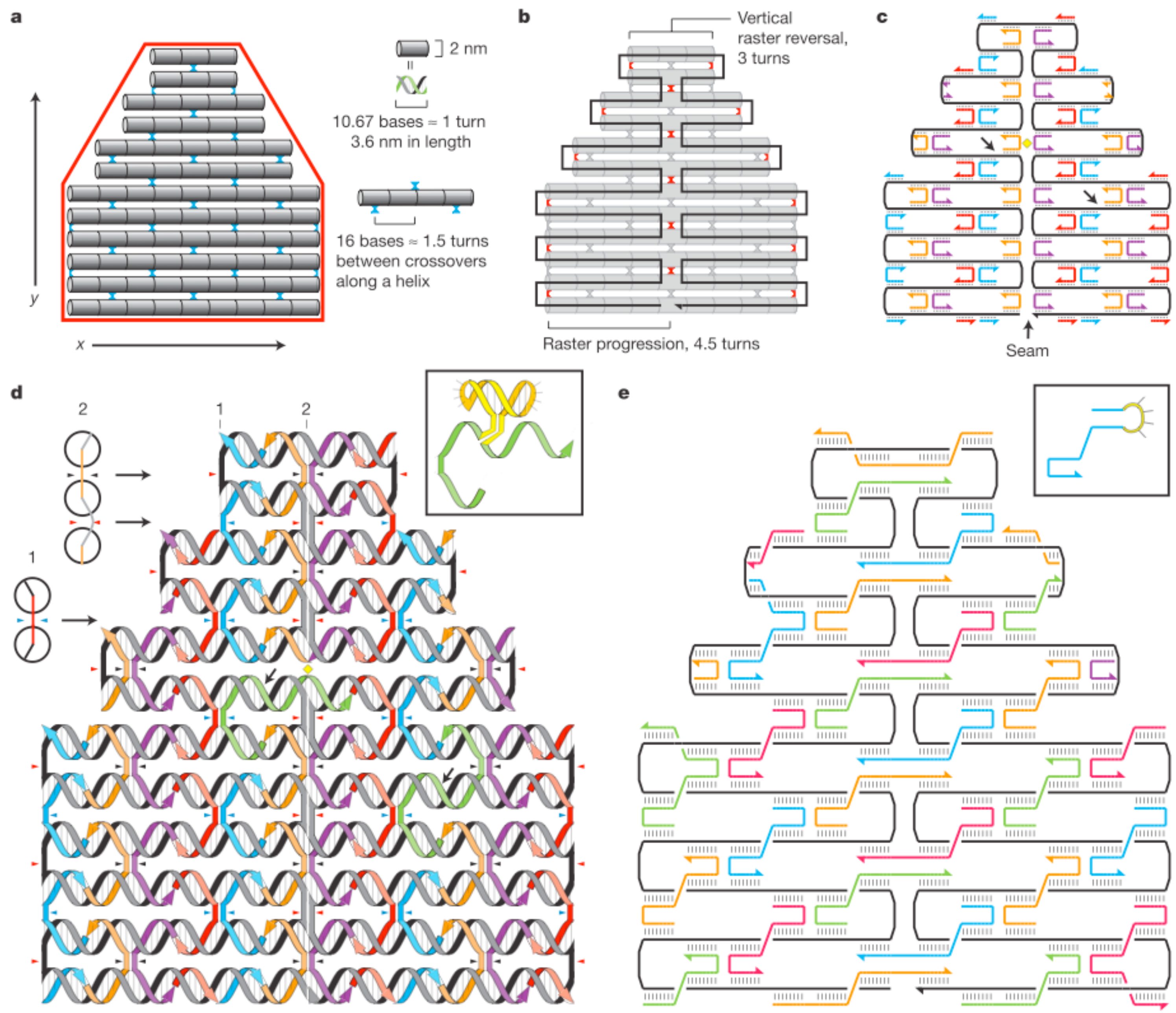
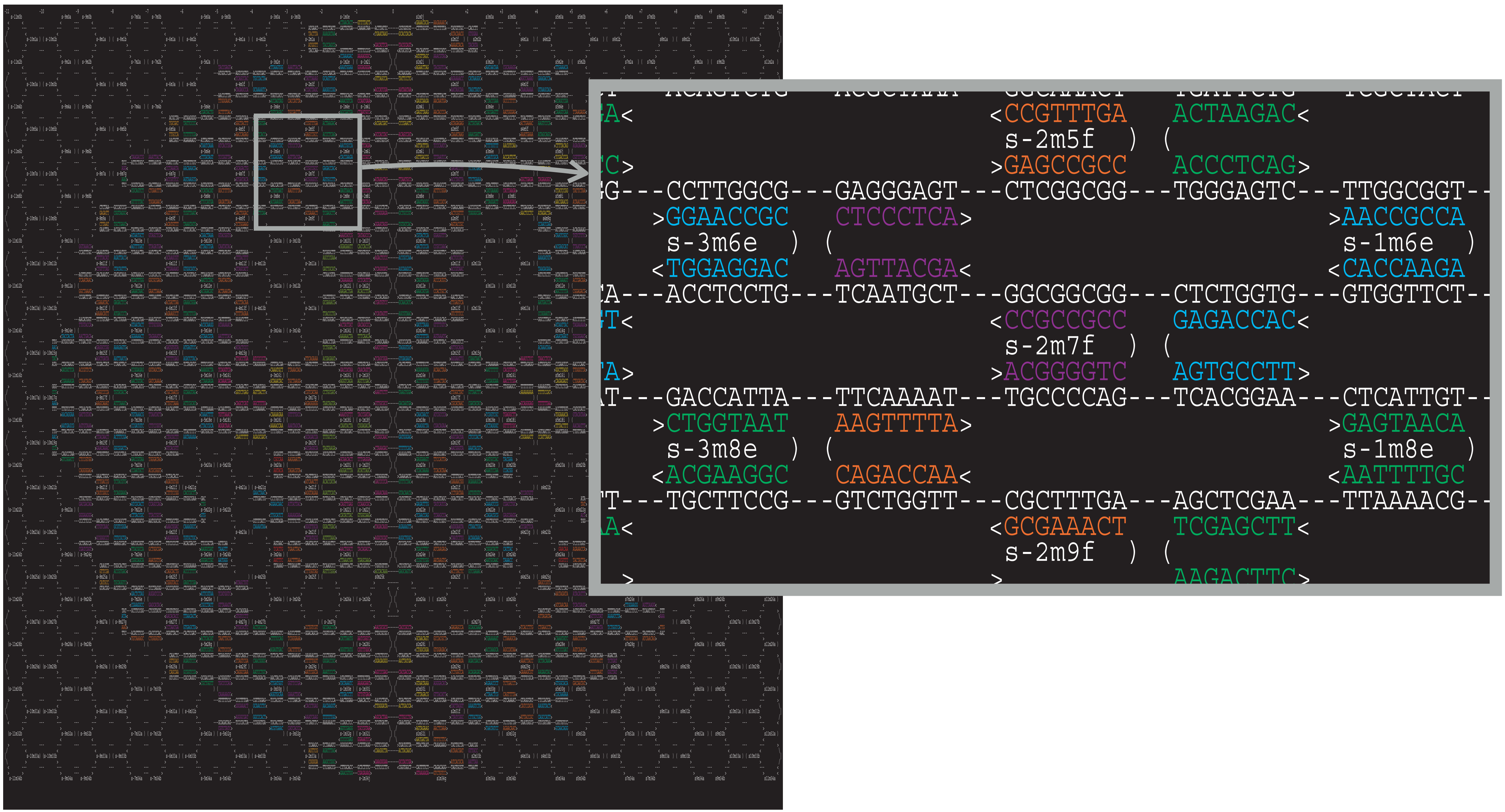


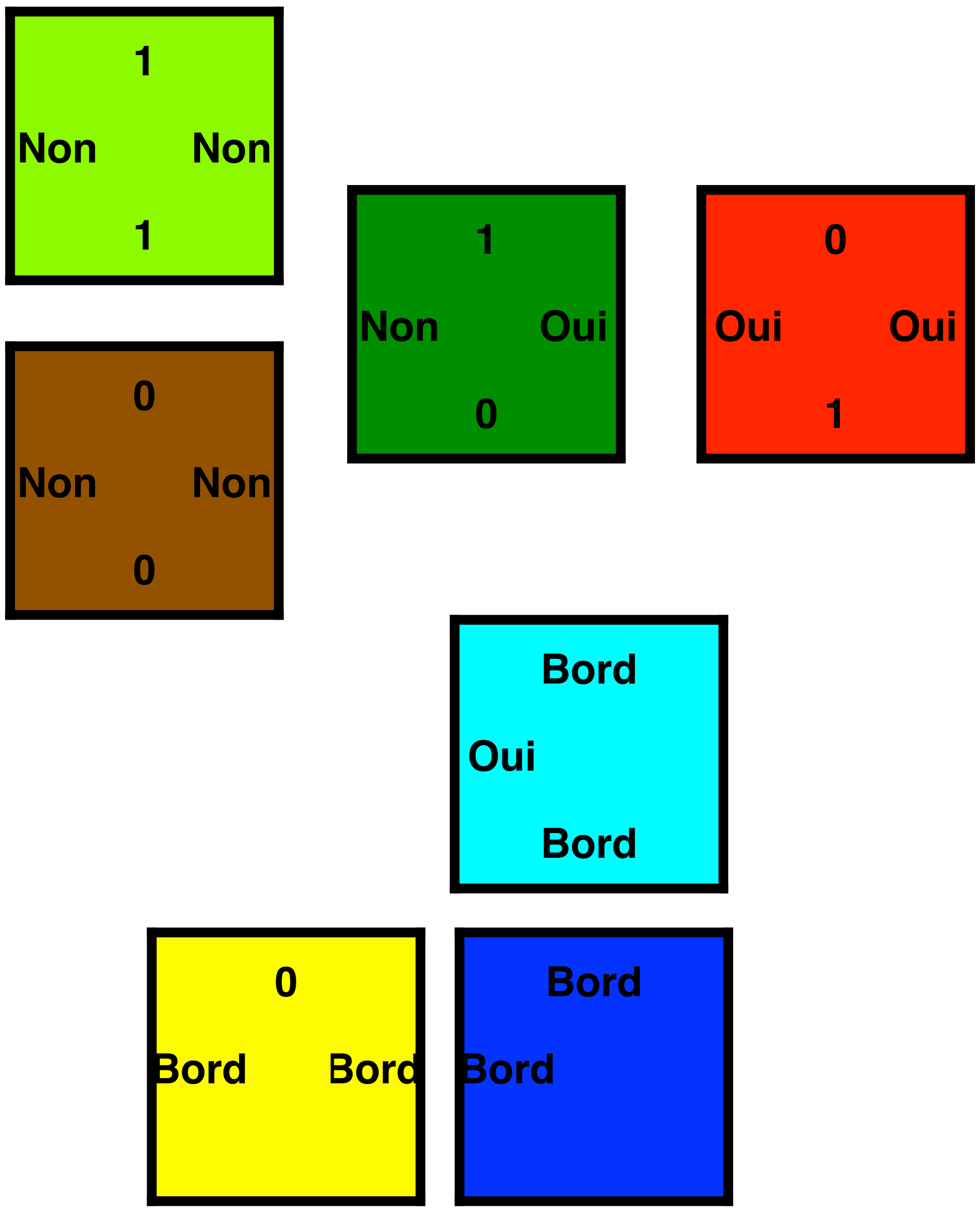
The DNA of a virus is folded by stapples!

Paul **Rothemund** (2001-): DNA Origami

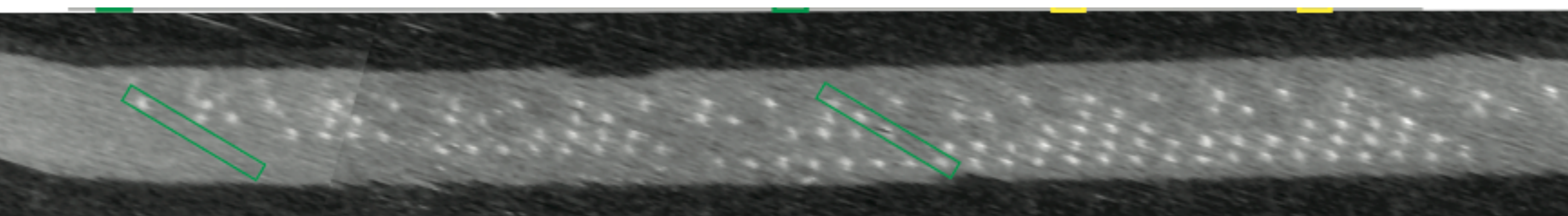


How to control the growth ?

With a binary counter!



State of the art in experiments



0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1
0	0	1	1	0	0	1	1	0	0	1	1	0	0	1	1	0	0	1	1	0	0	1	1	0	0	1	1	0	0	1	1	0	0	1	1	0	0	1	1	0	0
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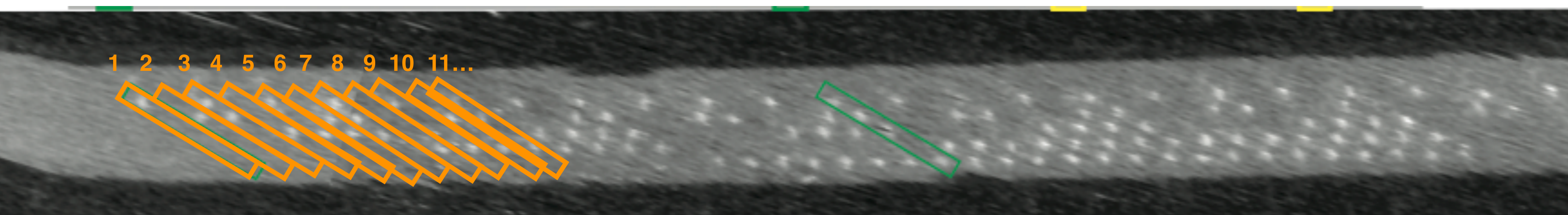
Constantine Evans, PhD Thesis, Caltech 2014

State of the art in experiments



0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1
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0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	1	1	1

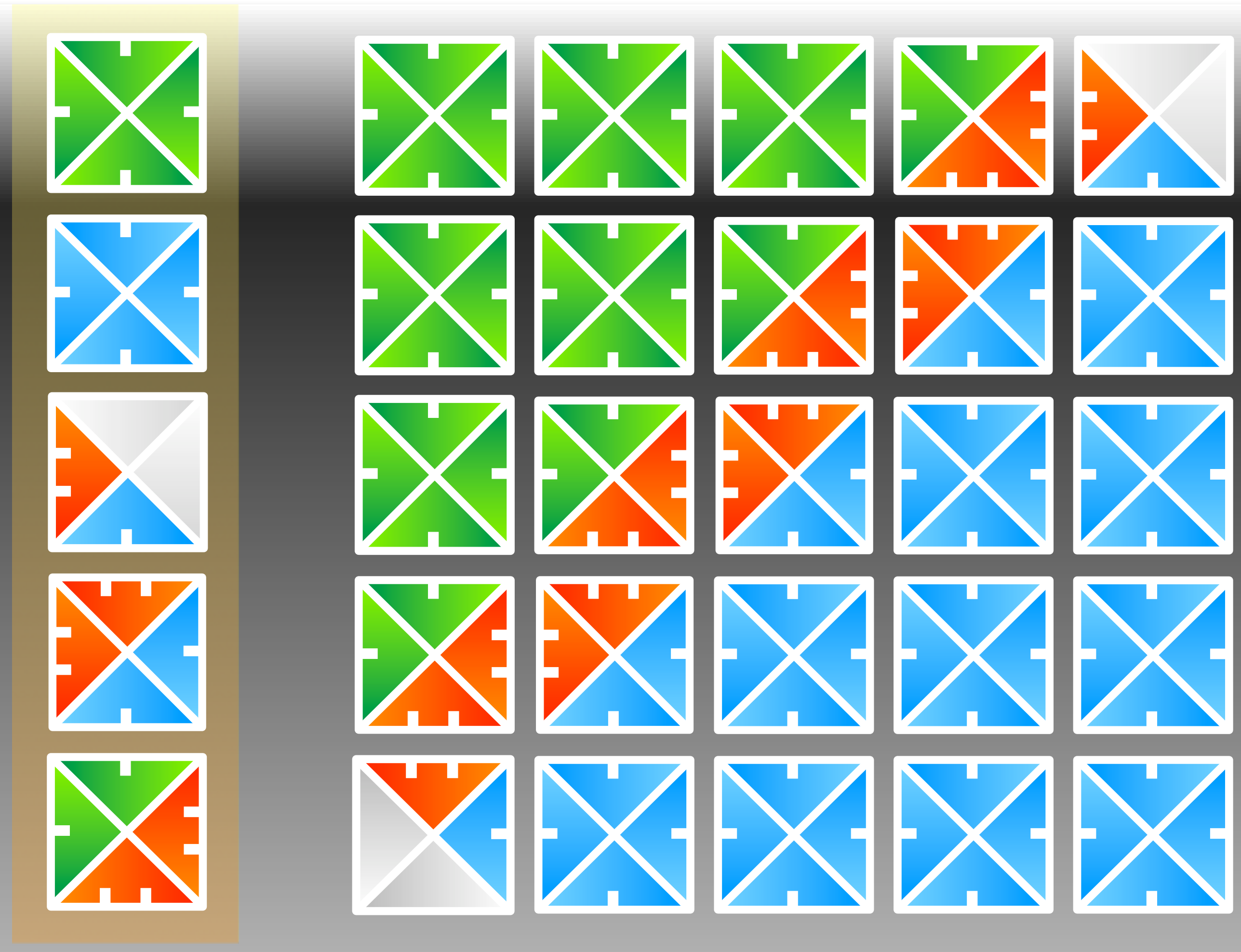
Constantine Evans, PhD Thesis, Caltech 2014

Algorithmic questions:

- Minimize the number of tiles?
- Minimize assembly time?
- Is there a universal set of tiles? (i.e. a programming language)

Minimize the number of tiles

- **Undecidable** problem in general
- For the square, **5 tiles are enough and required:**

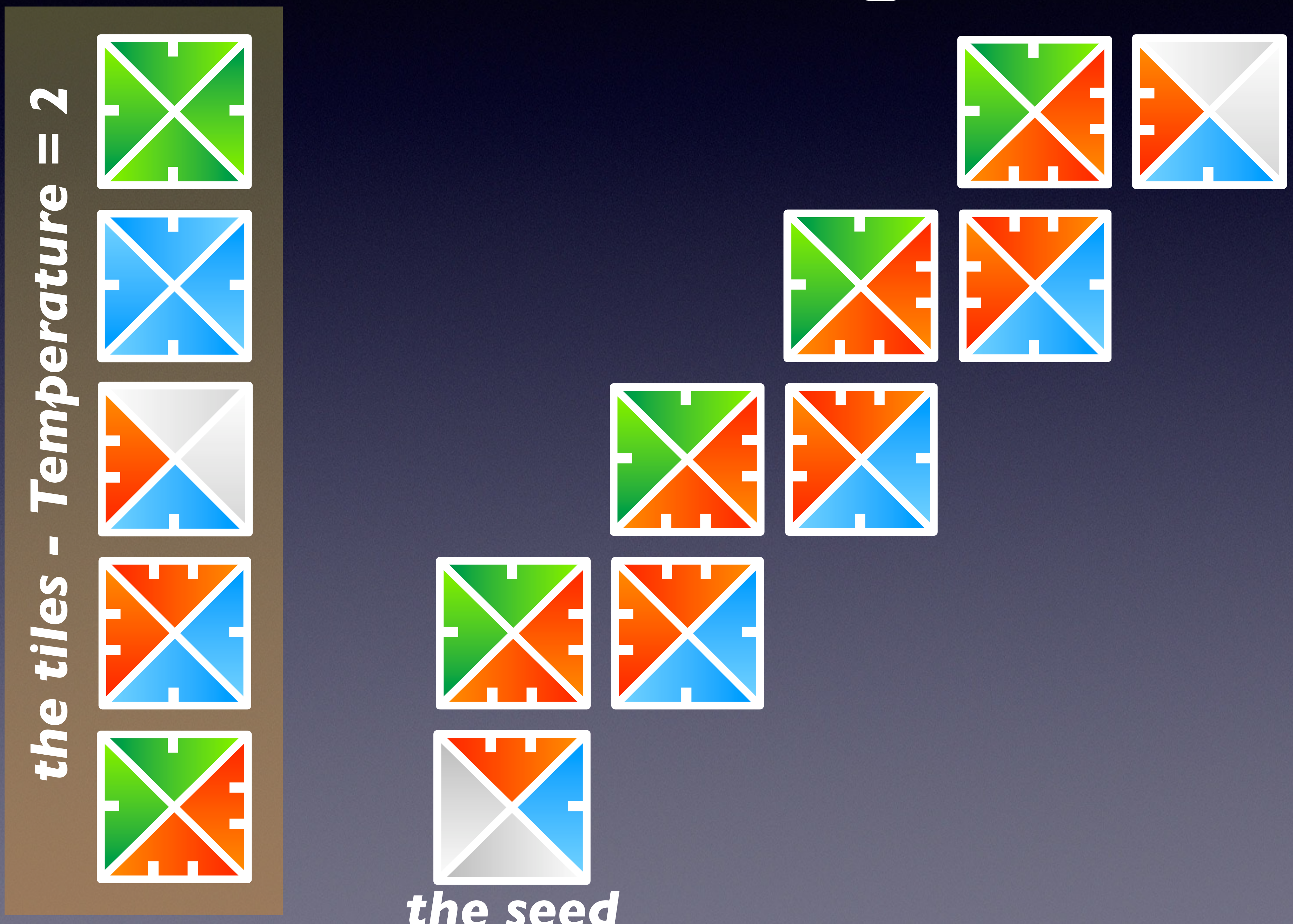


Becker, Rapaport, Rémila, 2006

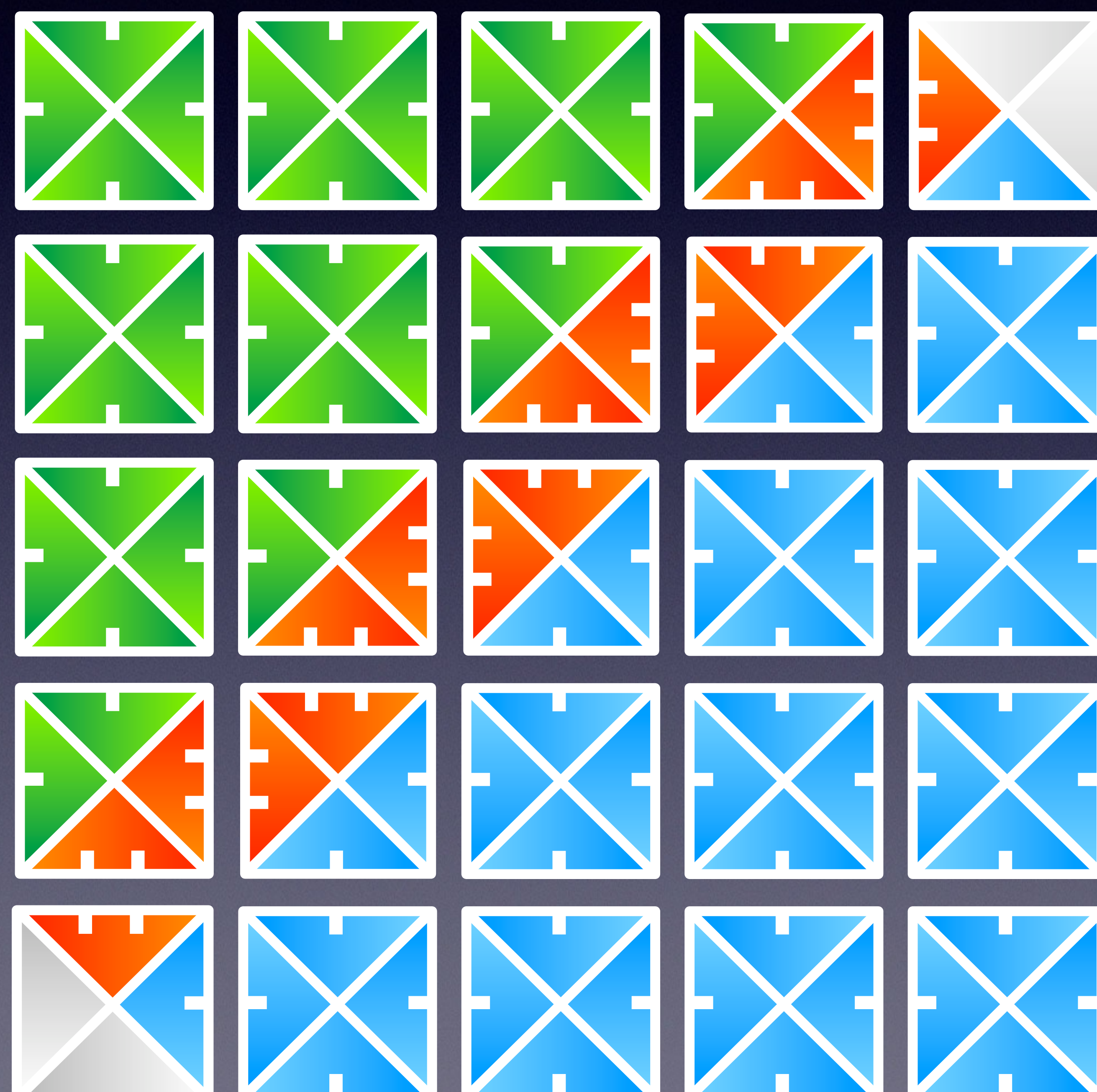
Minimizing Assembly time

- Undecidable problem in general
- Squares can be assembled in optimal time: $2n - 2$

An example:
Assembling a square



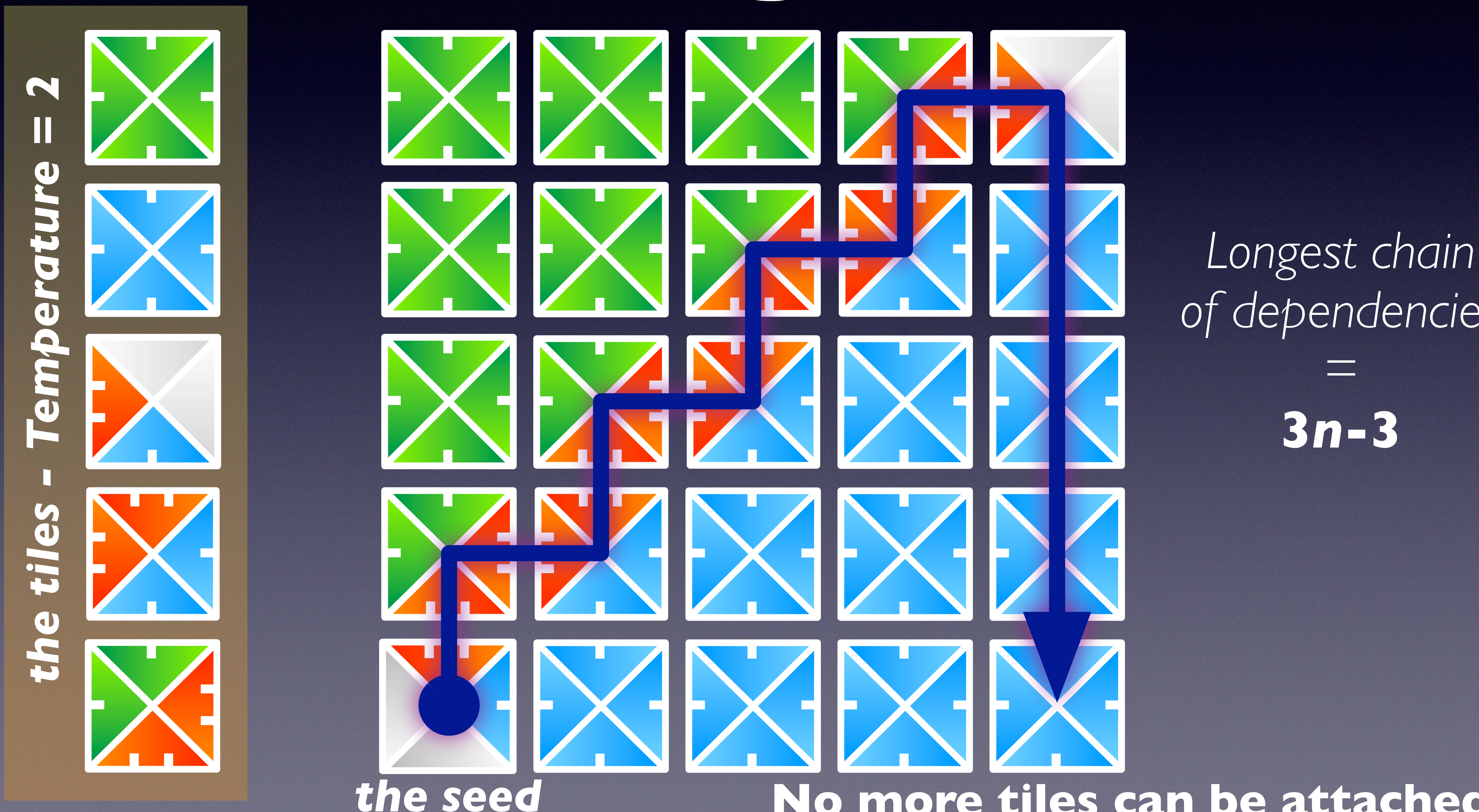
An example:
Assembling a square



the seed

No more tiles can be attached

An example:
Assembling a square



Longest chain of dependencies = **3*n*-3**

Assembling vs Tiling & Cellular Automata

Facts

Irrevocability.
As opposed to CA, the "state/tile" of a cell cannot change

Everything that can bind, may bind so be careful with signals self-ignition.

Guaranteeing an order.
Being sure of the predecessors of each cell to guarantee the global behavior

Only one "main signal" per coordinate.
Otherwise it is not possible to guarantee the predecessors

Some consequences

Filling tiles carry information and are not interchangeable.
As opposed to quiescent states in CA or "blank tiles" in tilings

There exists flows of information within the shape.
Signals cannot go against the flows but still have to intersect predictably

Ordered Tilesystem

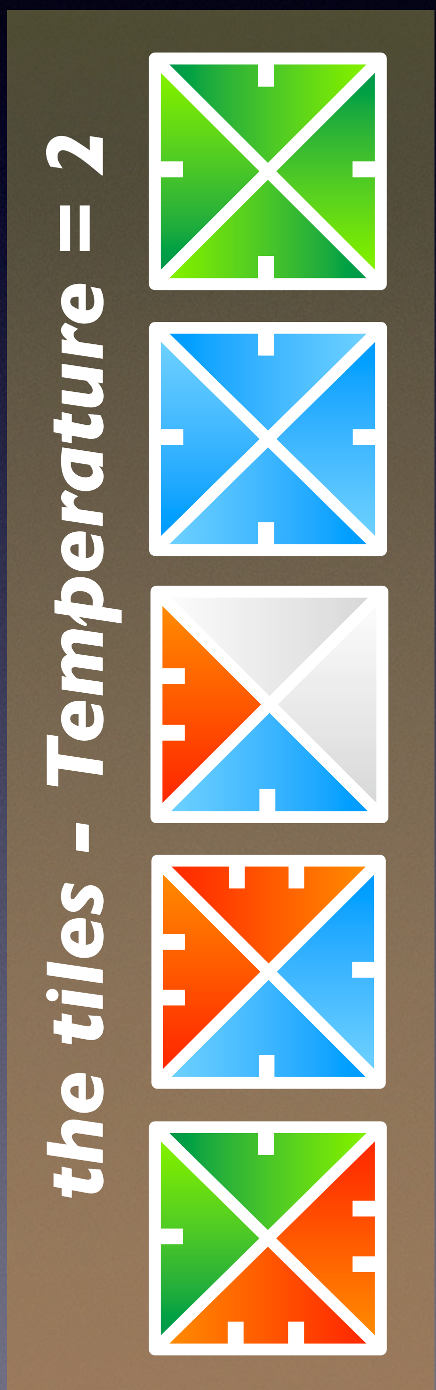
A tilesystem is **ordered** *if for each production, the predecesors cells of each cell are* **independent** *of the construction path.*

Consequences

- *No one has more than* ***T° predecessors***.
- *The only* ***non-determinism*** *relies in the choice of the tile to attach, which determines which shape is assembled.*

Example of an ordered tile system

Example of an ordered tile system



Rank

Rank.
The **rank** of a site *(i,j)* in a given shape is the length of its longest chain of dependancies from the seed.

Time model

Poisson Markov Chain Model.
Each tile appears at each unoccupied site according to some Poisson process at a **rate** proportional to its **concentration**.

Only **matching** tile with **enough bonds** remains attached to the current agregate.

Time & order

Theorem. *[Adleman et al, 2001]*
The expected time to build a shape ***P*** is:

$$O(c \cdot rank(P))$$

where ***c*** only depends on the concentrations and ***rank(P)*** is a highest rank in the shape ***P***.

⇒ we focus on **minimizing the highest rank**

Real time

Lower bounding the construction time.
Given that tiles are placed one next to the others, $||P||_1$ is a lower bound on the highest rank of a site of a shape P.

Real time construction.
A shape P is built in **real time** if

$$\text{the highest rank of a site} = ||P||_1$$

For the $n \times n$ square S_n : $||S_n||_1 = 2n - 2$

Skeleton

understanding the flow of information

Skeleton. *The* ***skeleton*** *of a shape in an ordered tile system is the set of the sites with* ***at most one predecesor****.*

the *y-skeleton* in orange
opens the rows

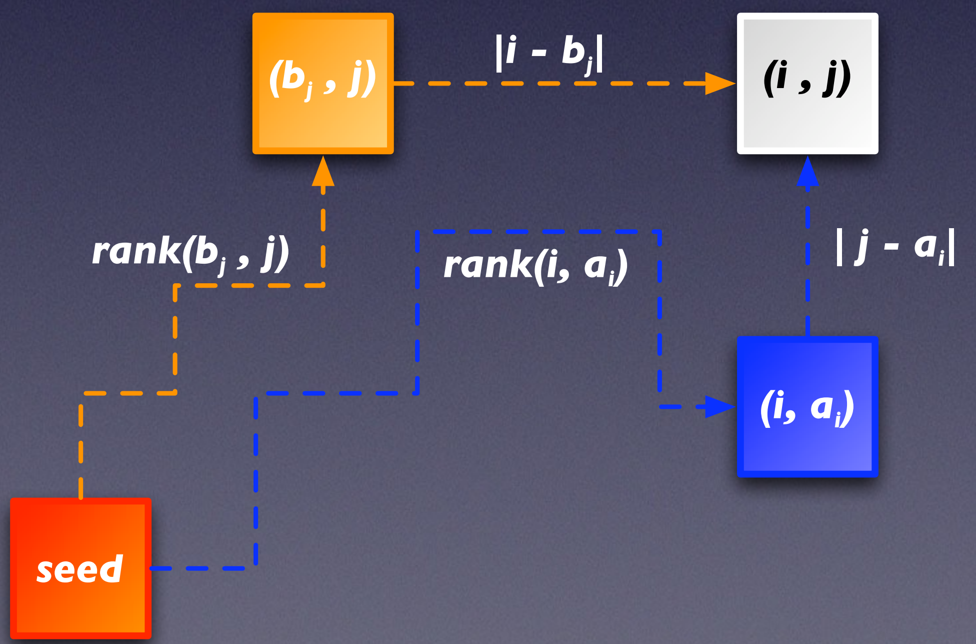
the *x-skeleton* in blue
opens the columns

Assembling a Square in Real Time

Lower bounding the rank

Let $(i, a_i)_{i \geq 0}$ and $(b_j, j)_{j \geq 0}$ be the *x*- and *y*-skeletons

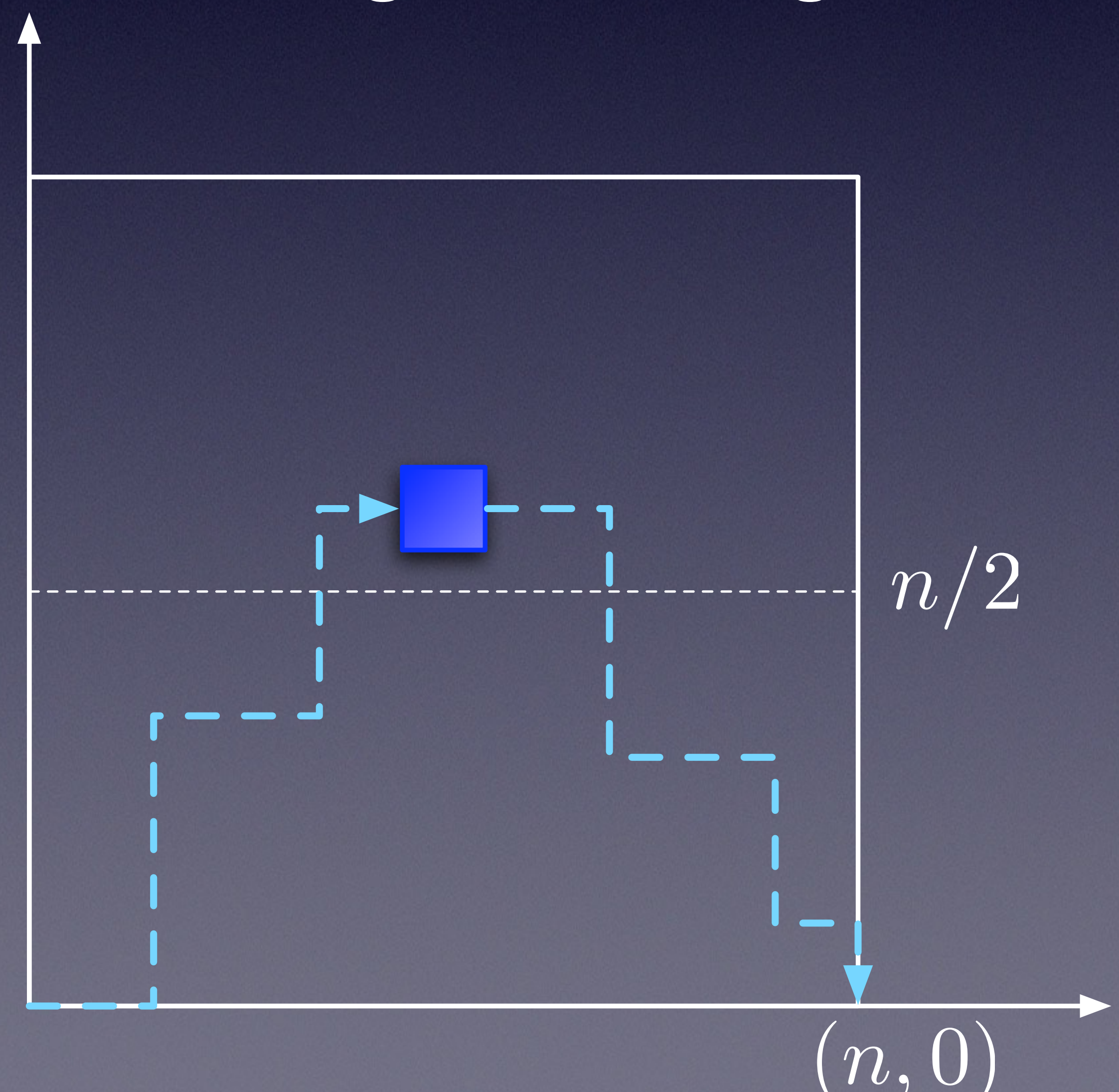
Since the *x*- and *y*-skeletons sites are the **first** tiled on each column and each row respectively, then for each site (i,j):



$$\mathrm{rank}(i,j) \geqslant \max\{\mathrm{rank}(i,a_i) + |j - a_i|, \mathrm{rank}(b_j,j) + |i - b_j|\}$$

Where should be the skeleton?

the *x*-skeleton **cannot** go above $n/2$
the *y*-skeleton **cannot** go to the right of $n/2$

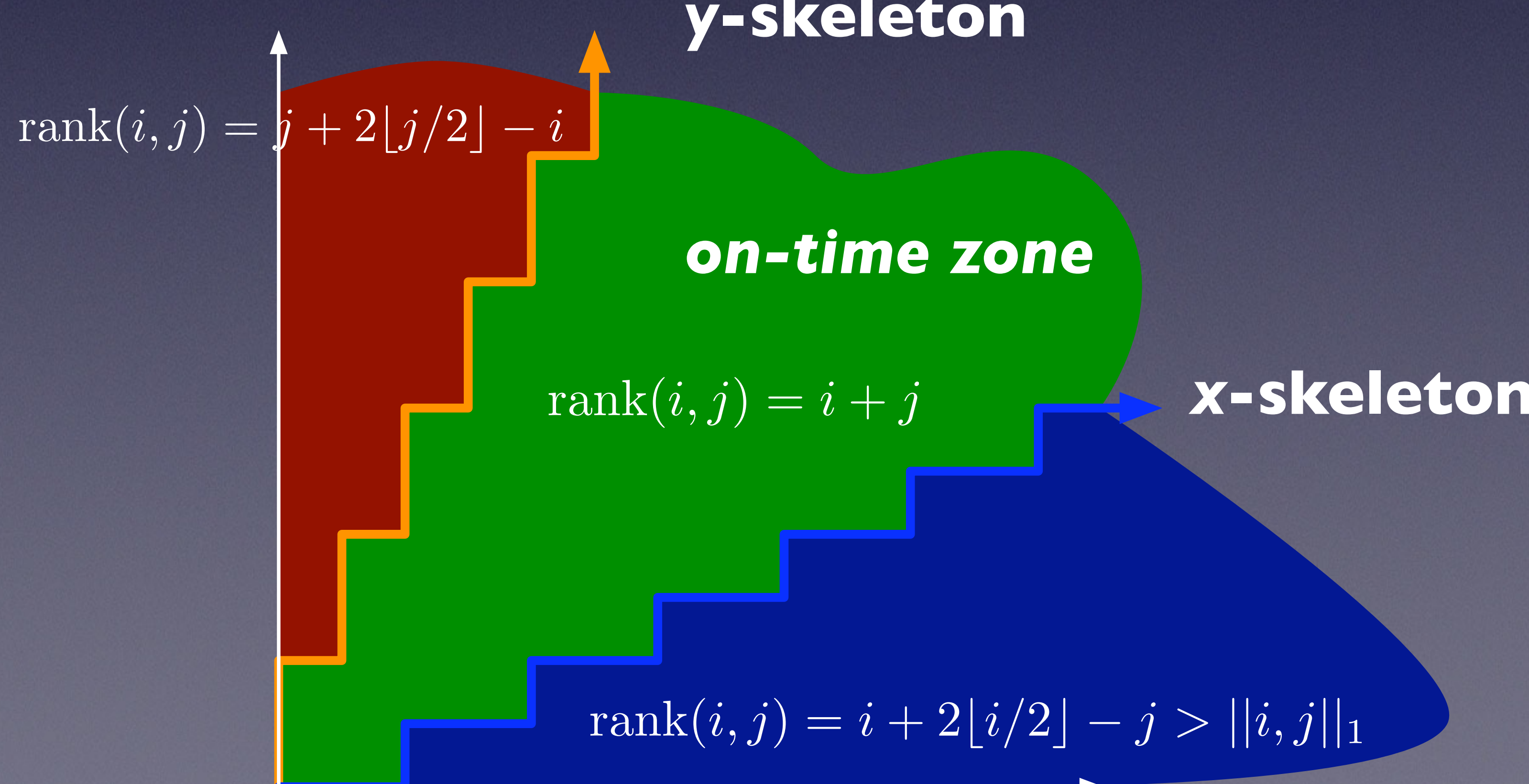


Rank function induced by the skeleton

The skeleton: $a_i = (i, \lfloor i/2 \rfloor)$ and $b_j = (\lfloor j/2 \rfloor, j)$

The rank induced:

$$rank(u) = \max\{||a_i||_1 + ||u - a_i||_1, |b_j||_1 + ||u - b_j||_1)$$



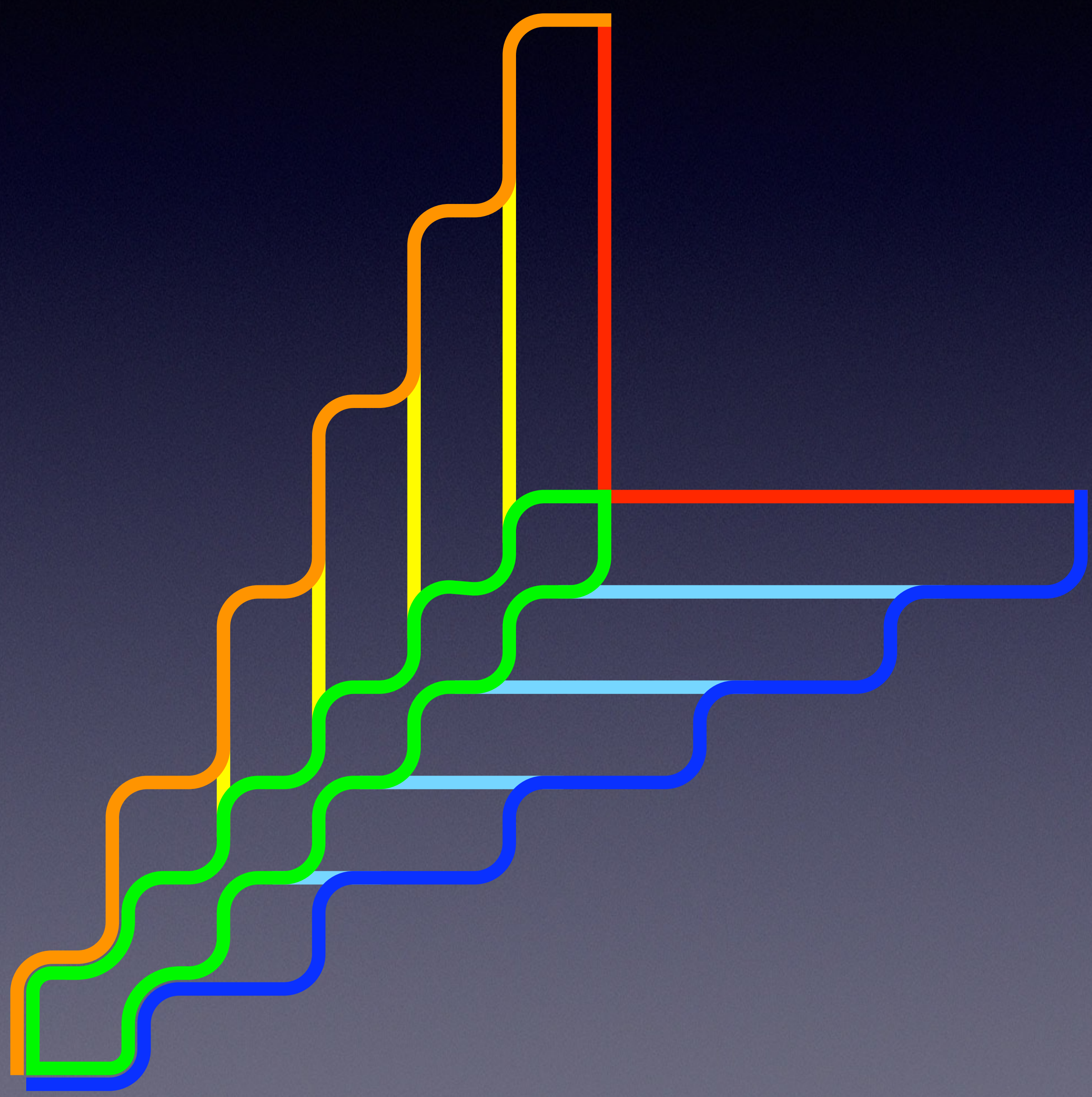
Order induced by the skeleton

Key to construct the tileset:

1) being able to **guess** the types of its **successors** from its own **predecesors**

2) **synchronizing** the two parts of the skeleton

The resulting tileset



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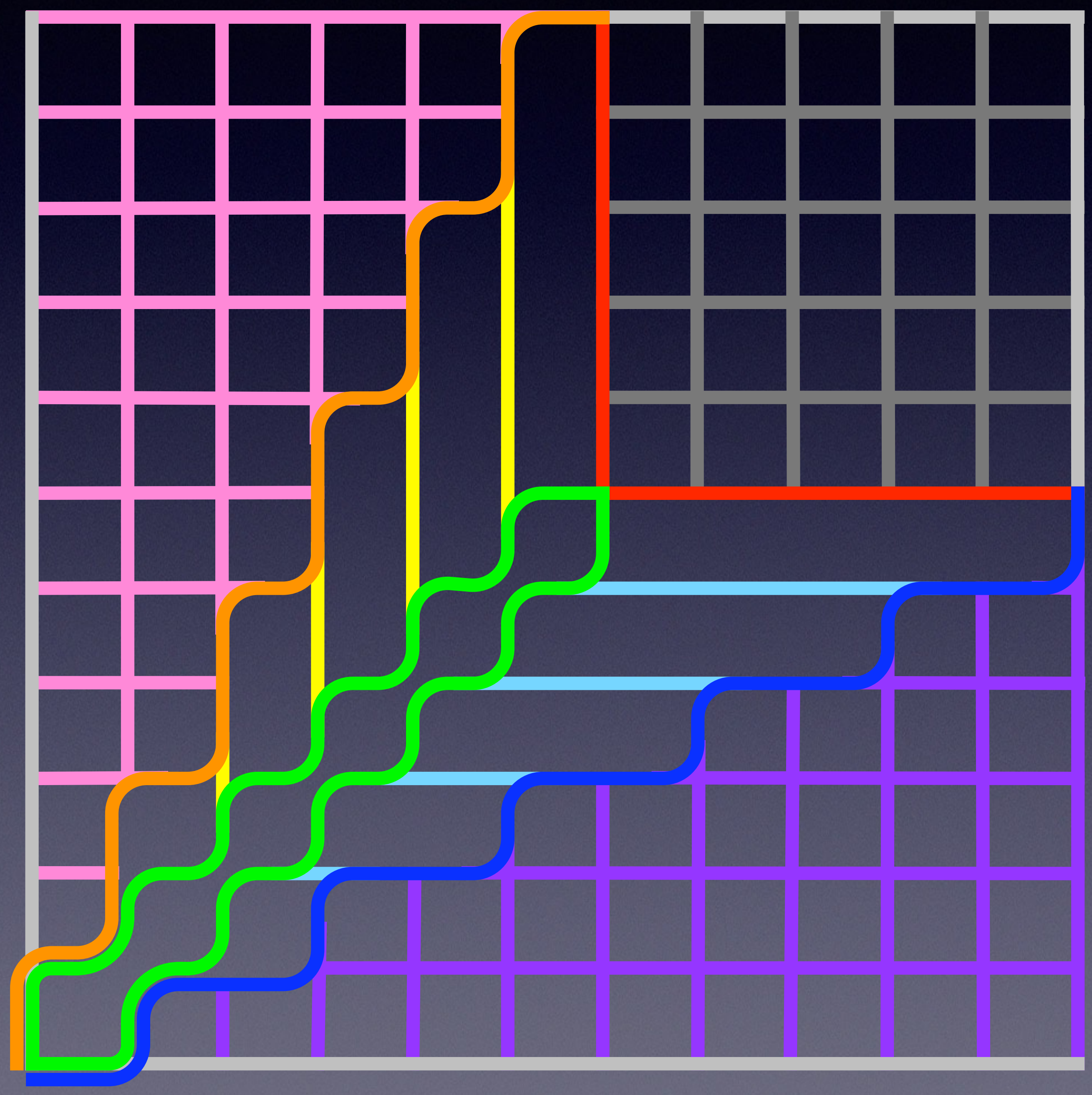

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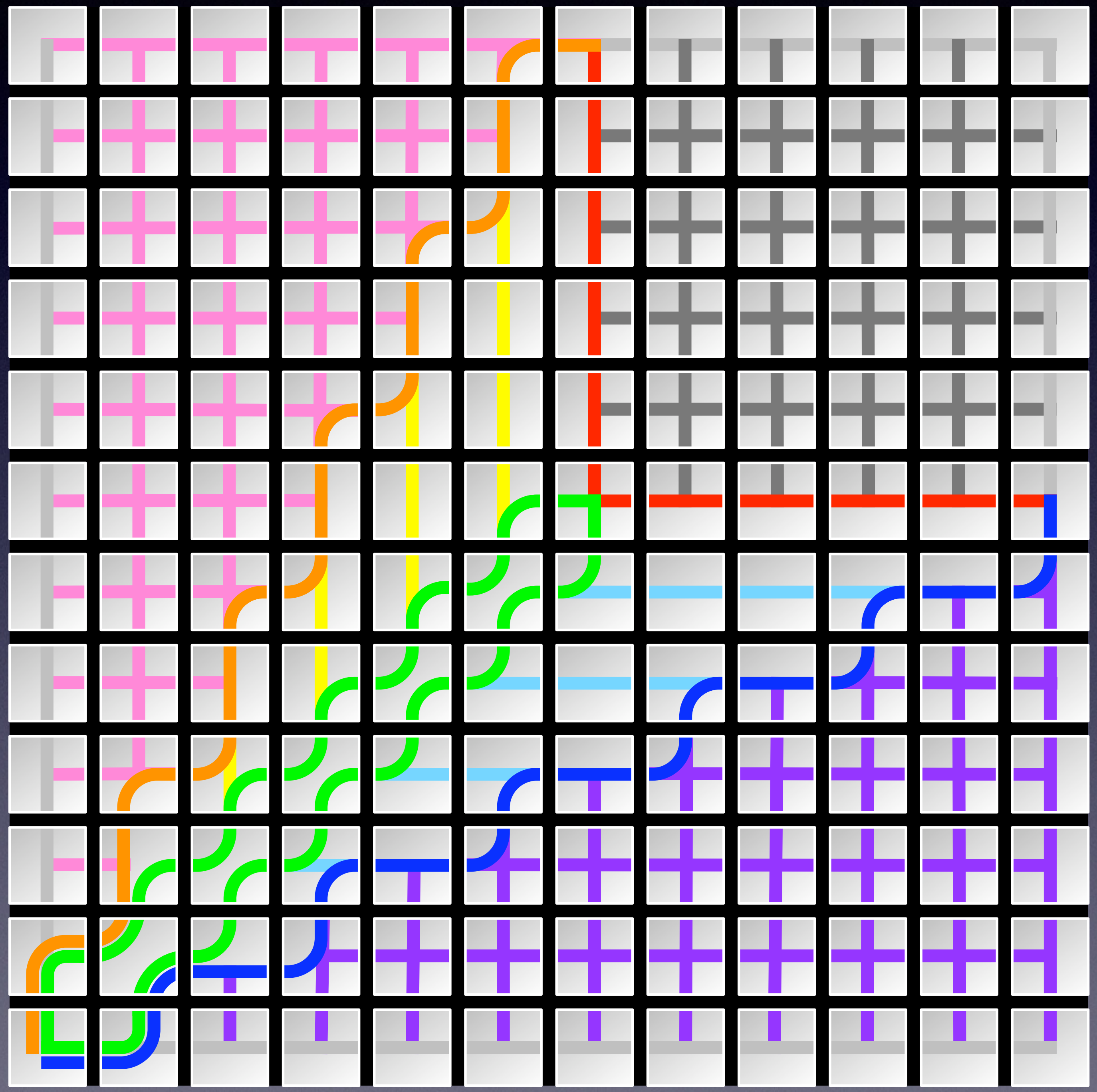

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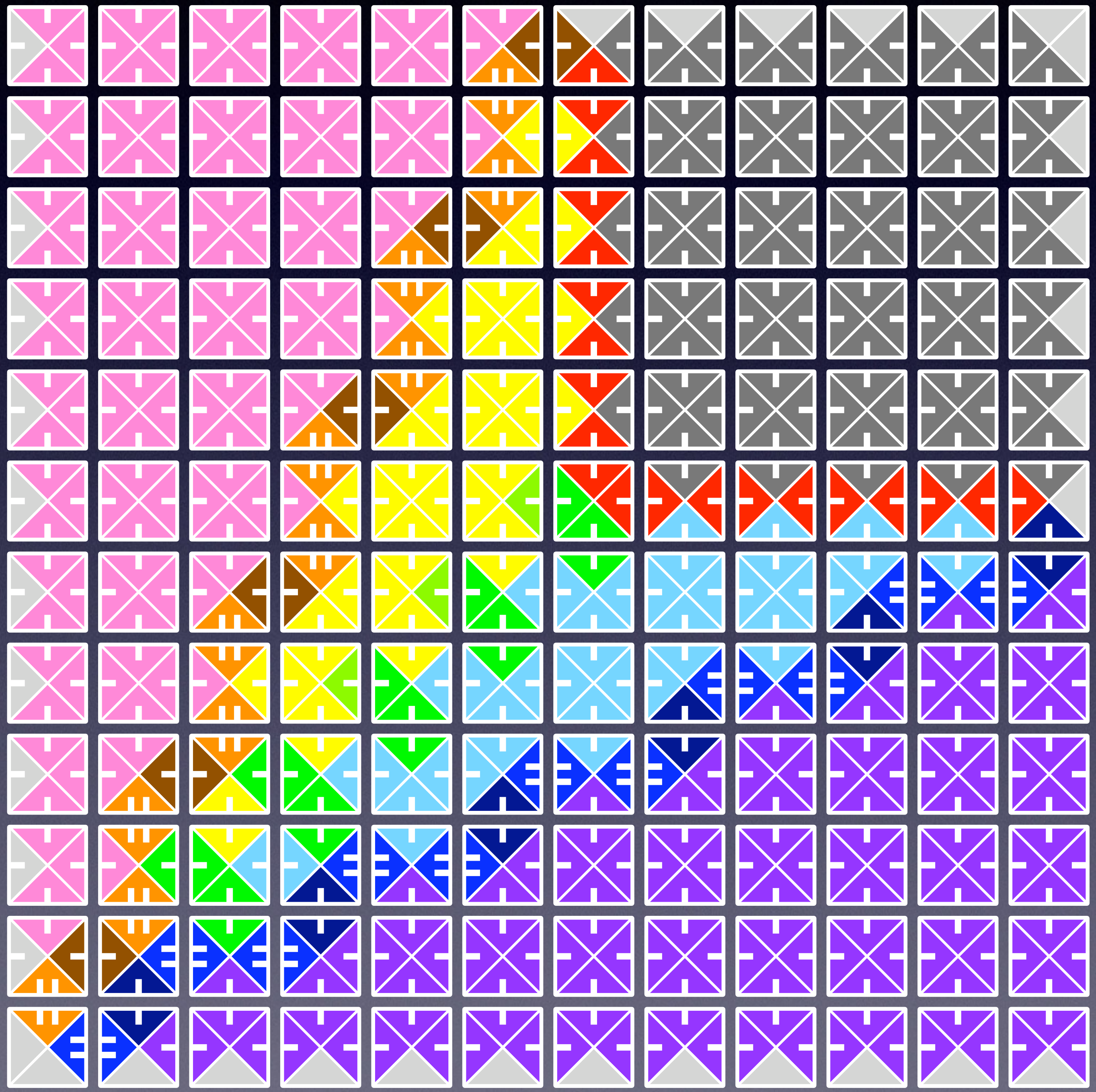
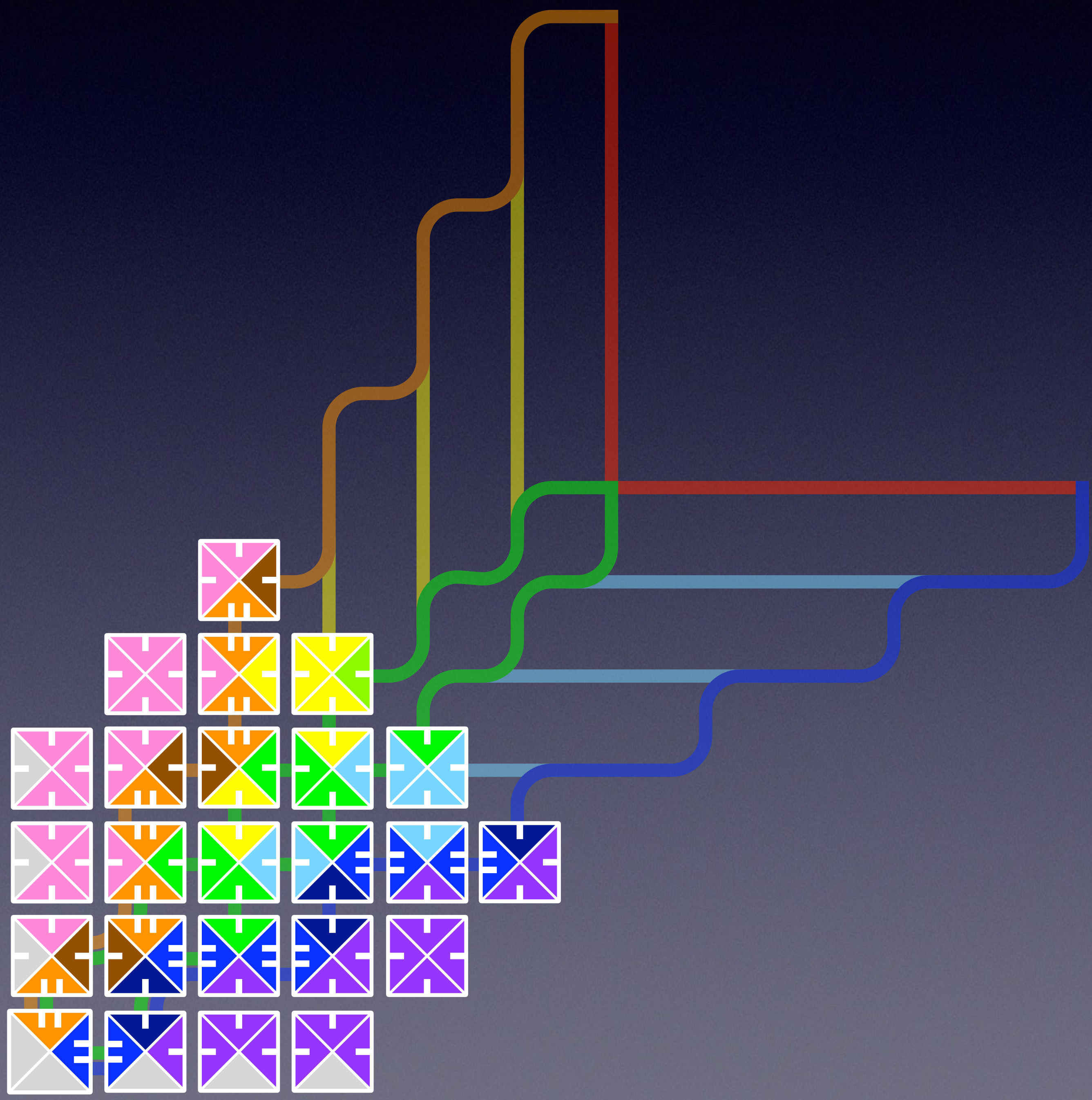


Running the tileset



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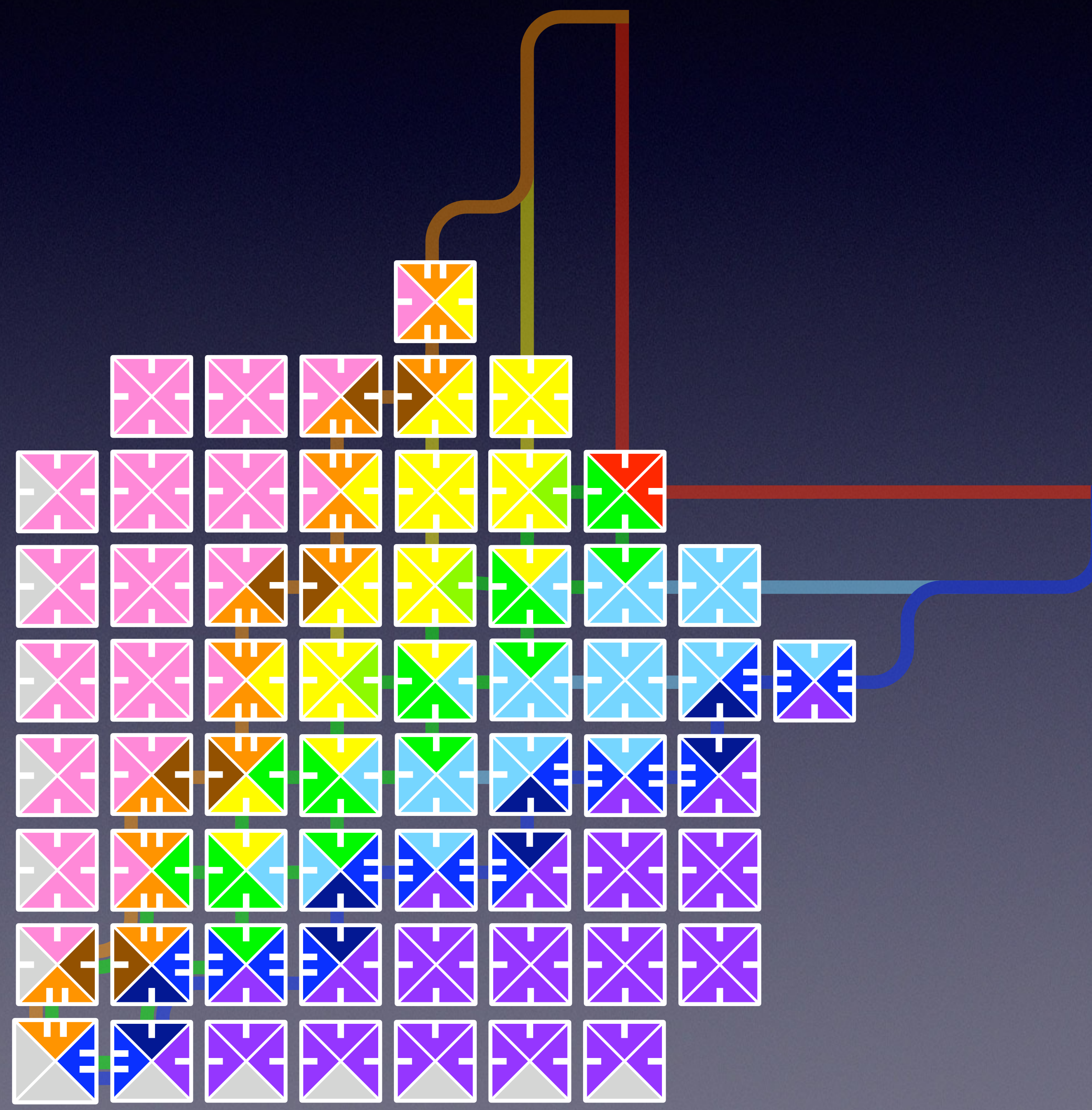

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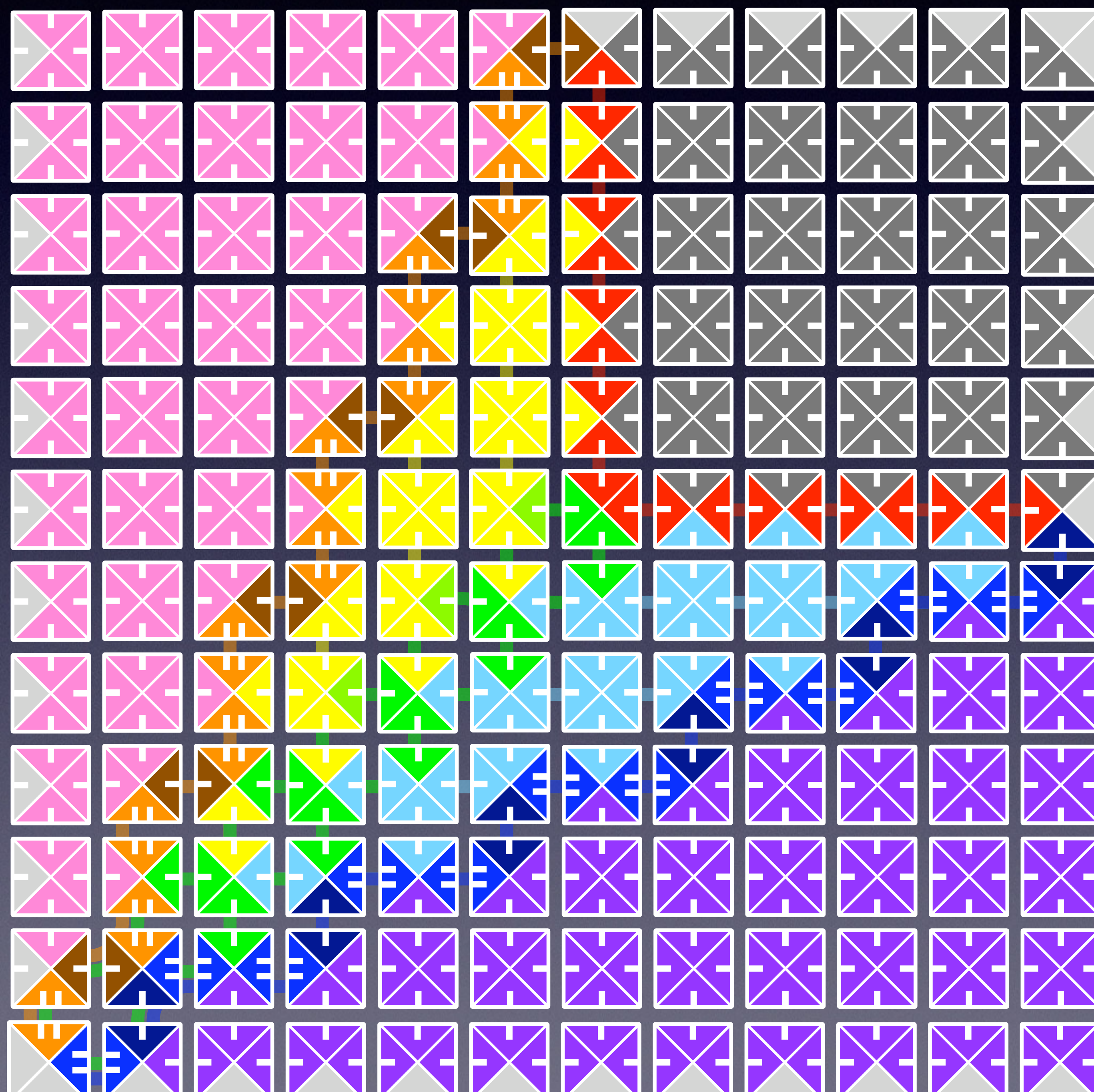
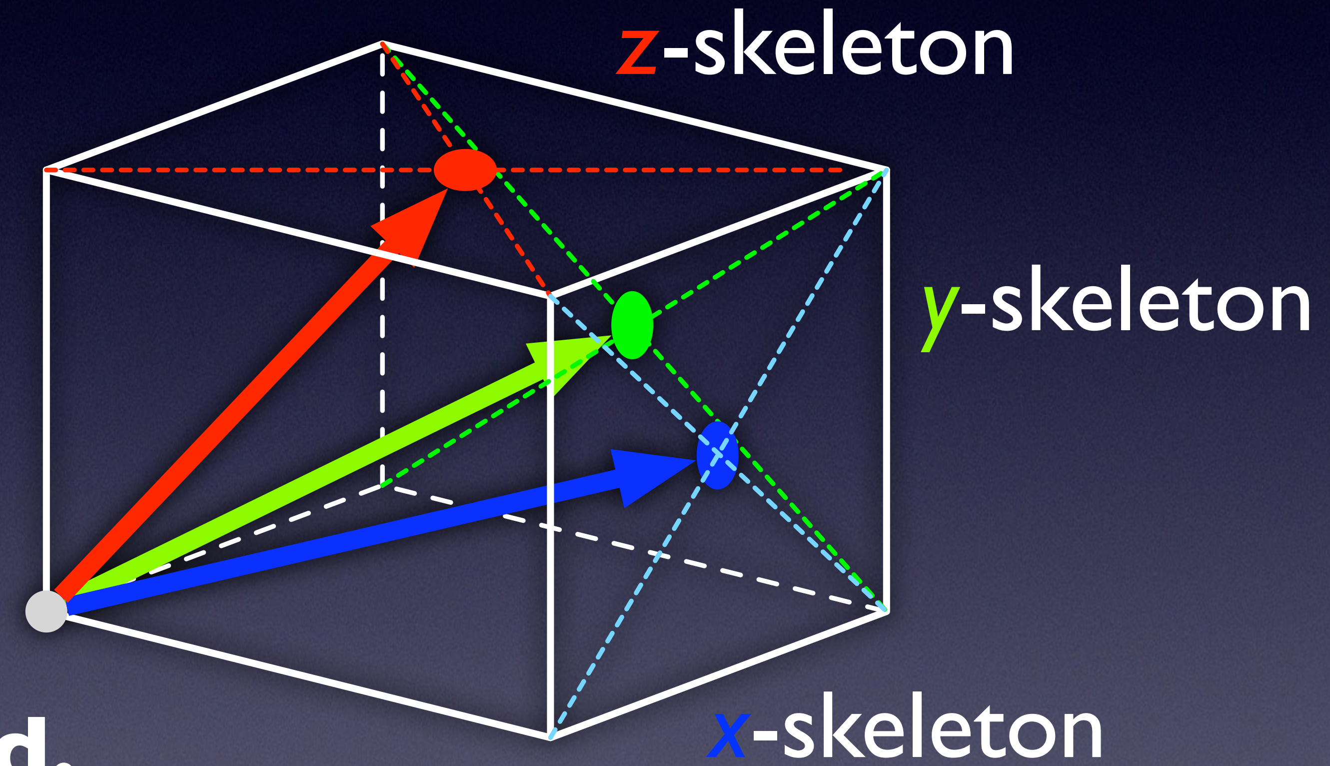


Assembling cubes in real time

The skeleton & its rank function

The skeleton.

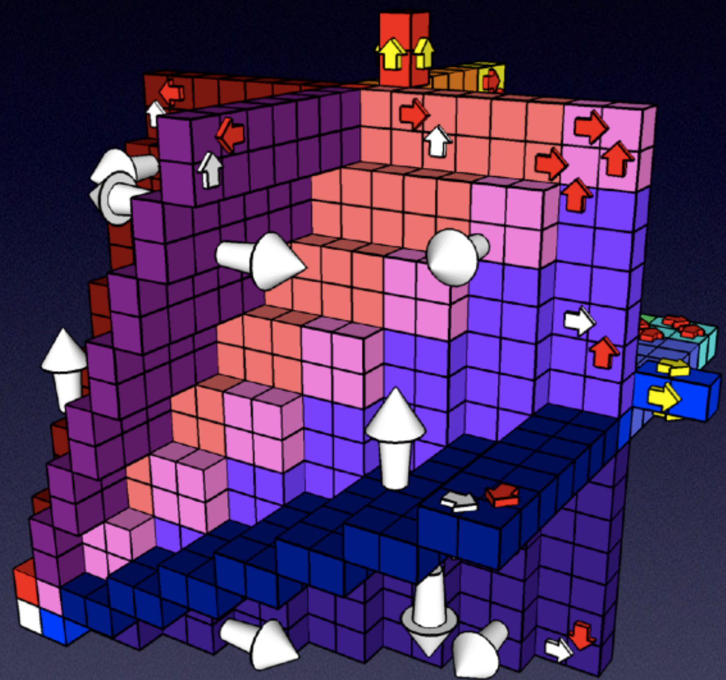
$$\begin{cases} a_i = (i, \lfloor i/2 \rfloor, \lfloor i/2 \rfloor) \\ b_j = (\lfloor j/2 \rfloor, j, \lfloor j/2 \rfloor) \\ c_k = (\lfloor k/2 \rfloor, \lfloor k/2 \rfloor, k) \end{cases}$$

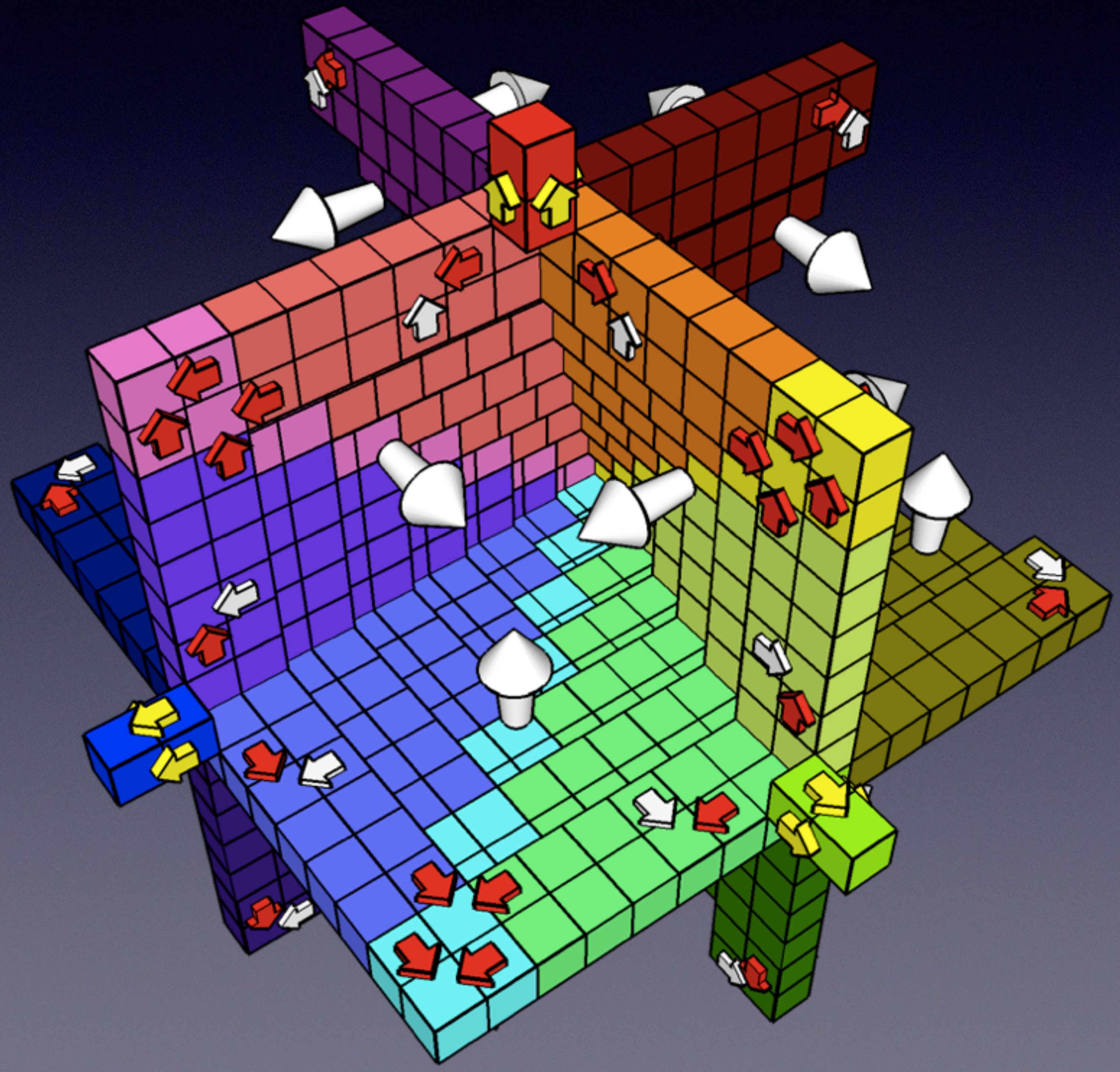


The rank function induced.

$$\operatorname{rank}(u) = \max \begin{cases} ||a_i||_1 + ||u - a_i||_1 \\ ||b_j||_1 + ||u - b_j||_1 \\ ||c_k||_1 + ||u - c_k||_1 \end{cases}$$

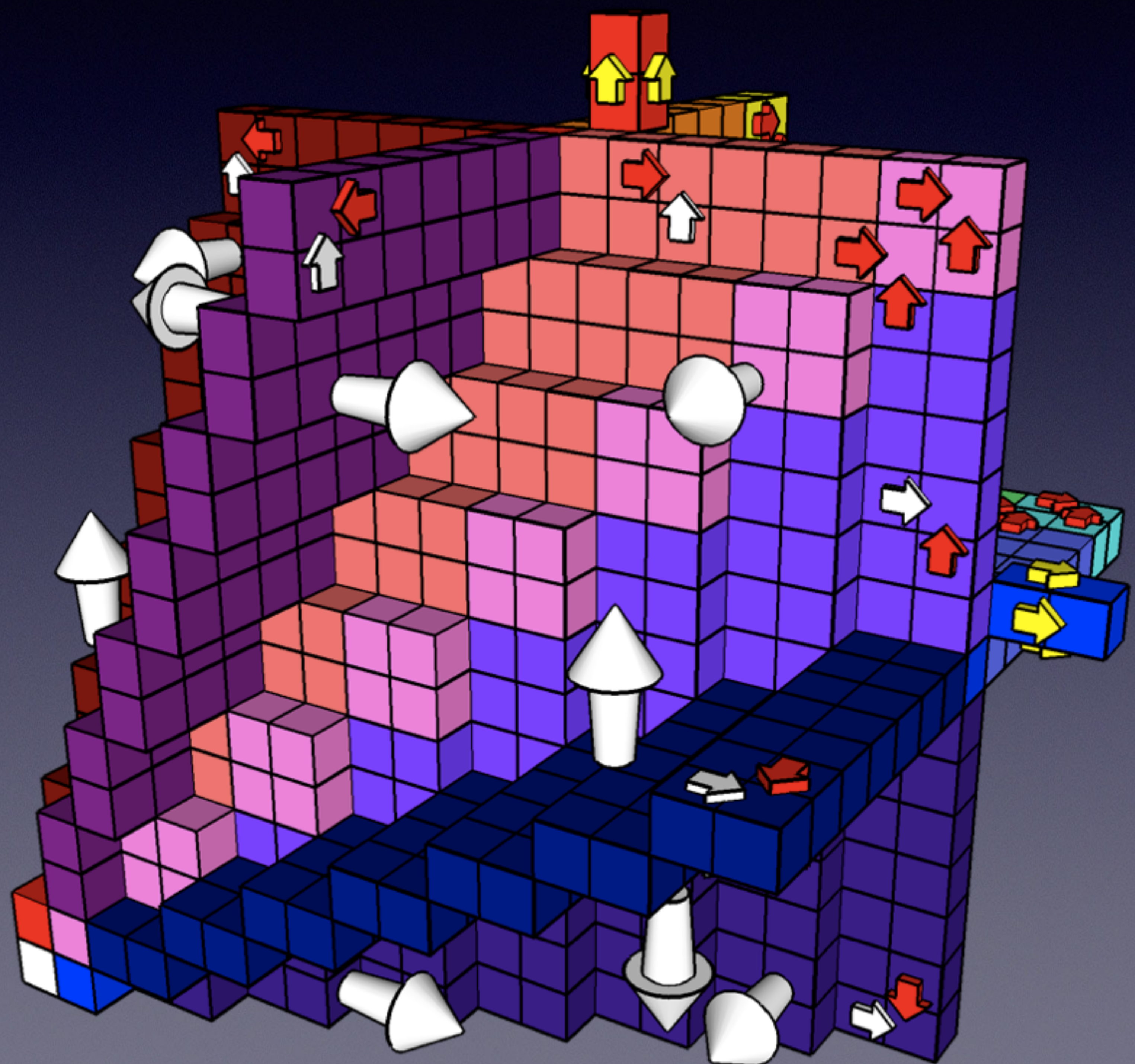
Variations of the rank function

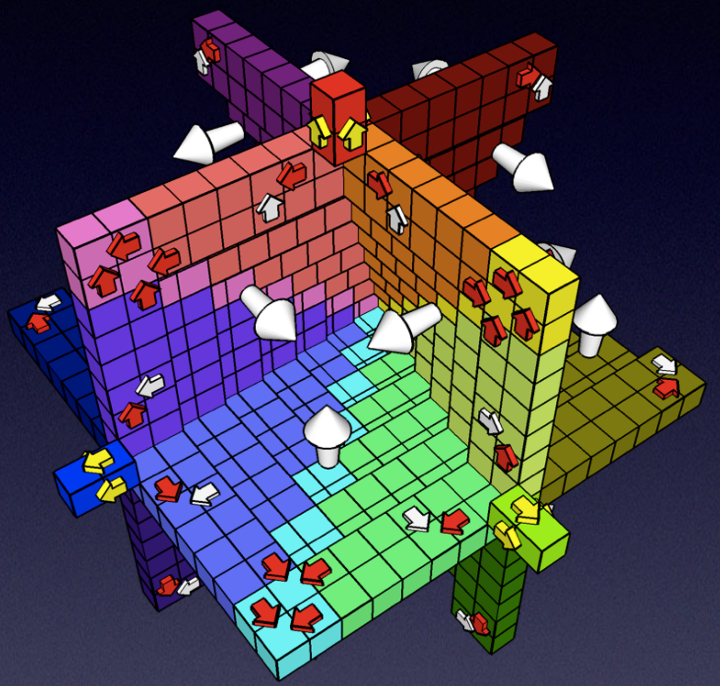




Key step:
determining the successors from the predecessors

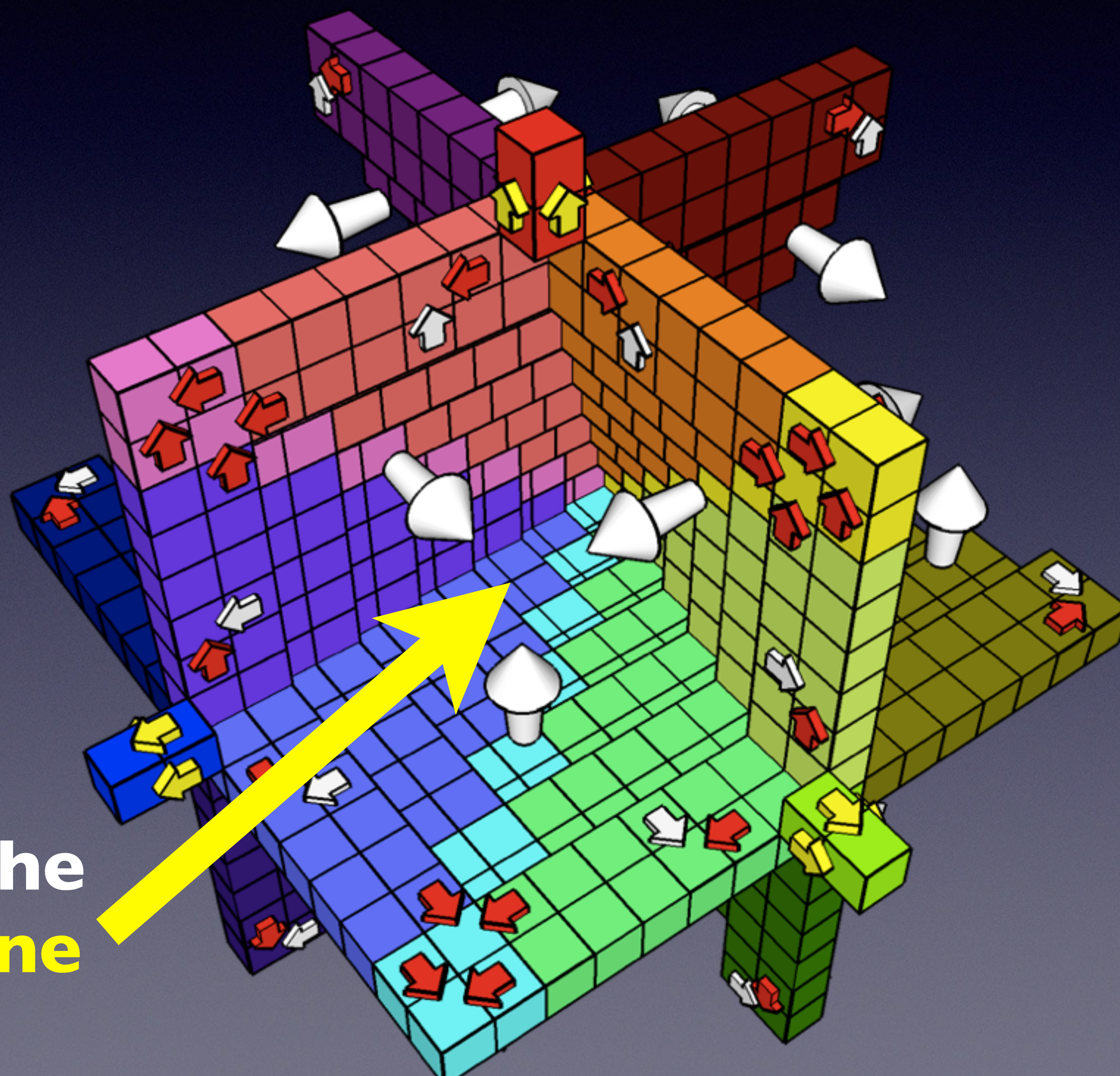
Variations of the rank function





Key step:
determining the successors from the predecessors

Synchronizing the 3 skeleton branches



Use again the **on-time zone**

Time optimal cube assembly