DNA24 — 2018

Molecular Shape folding with Oritatami

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Joint work with

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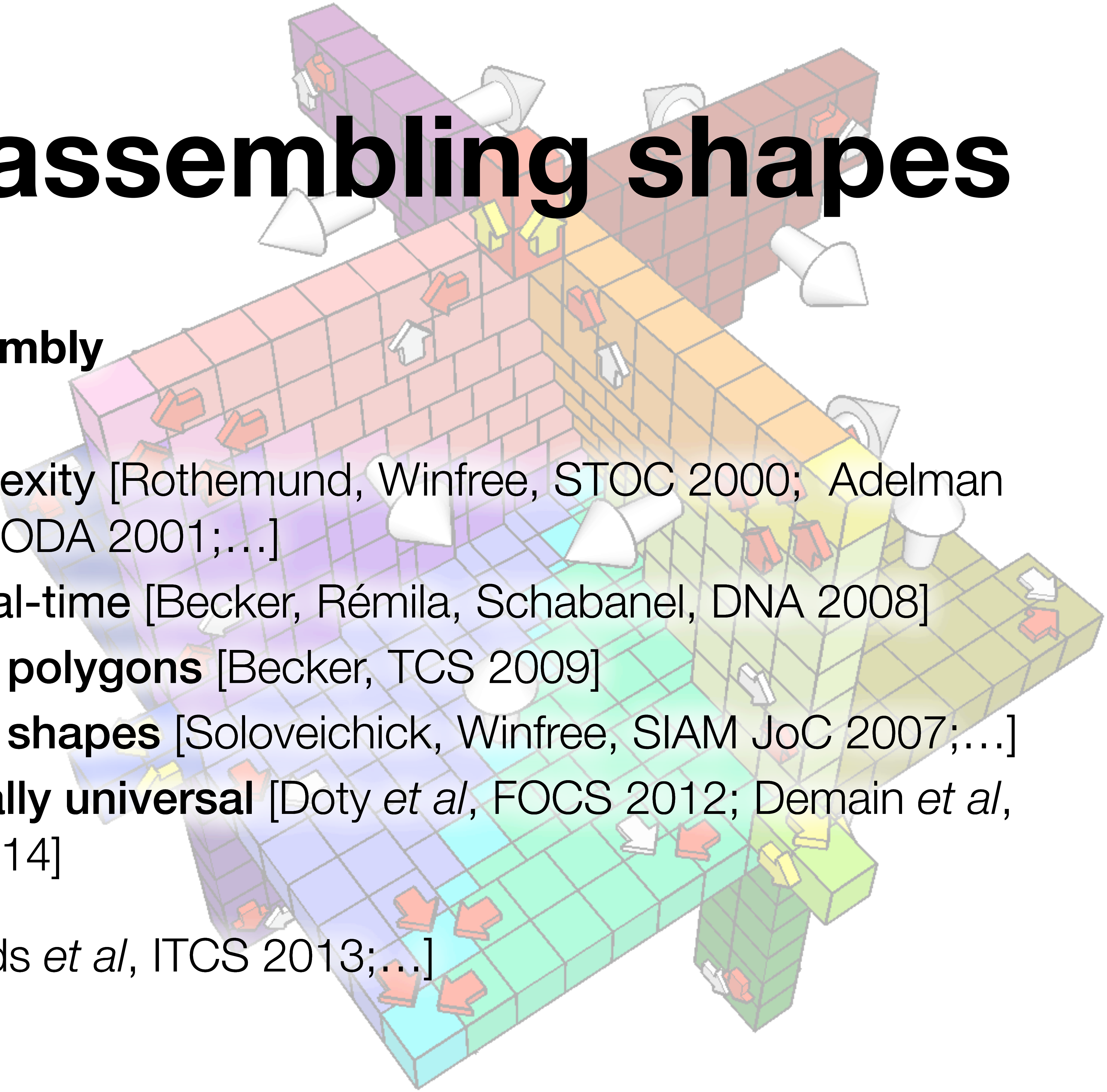
Self-assembling shapes

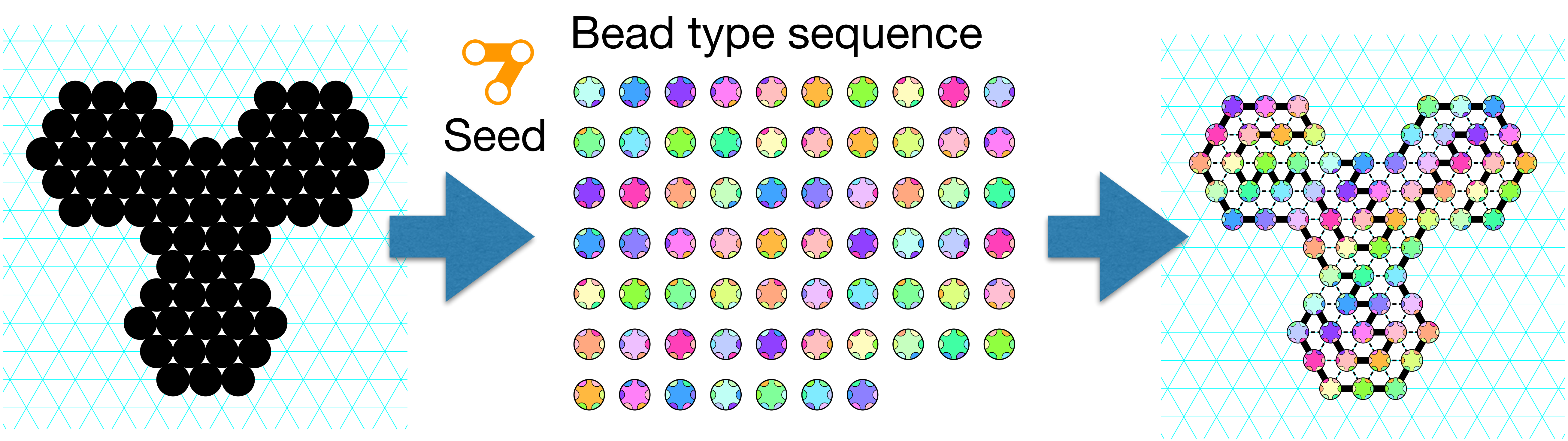
Tile self-assembly

- **Squares:**
  - **Complexity** [Rothemund, Winfree, STOC 2000; Adelman *et al*, SODA 2001;…]
  - **Optimal-time** [Becker, Rémila, Schabanel, DNA 2008]
- **Arbitrary polygons** [Becker, TCS 2009]
- **Arbitrary shapes** [Soloveichick, Winfree, SIAM JoC 2007;…]
- **Intrinsically universal** [Doty *et al*, FOCS 2012; Demain *et al*, ICALP 2014]

Nubots [Woods *et al*, ITCS 2013;…]

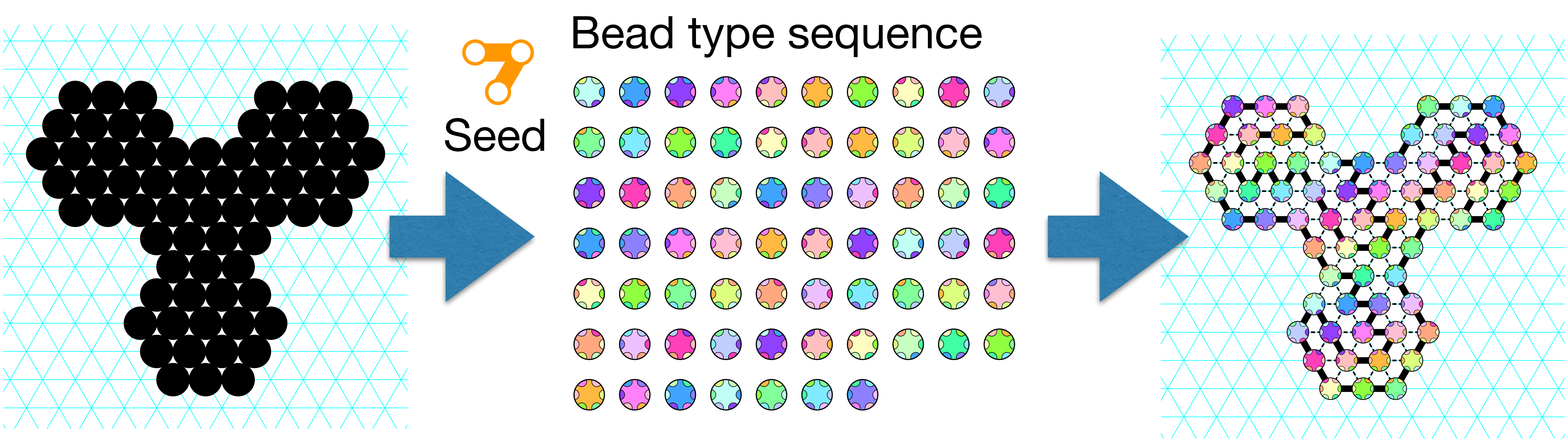


Goal: Given a shape S, Find an oritatami system, i.e. a *sequence of bead types*, that folds into S



An Oritatami system folds a shape if:

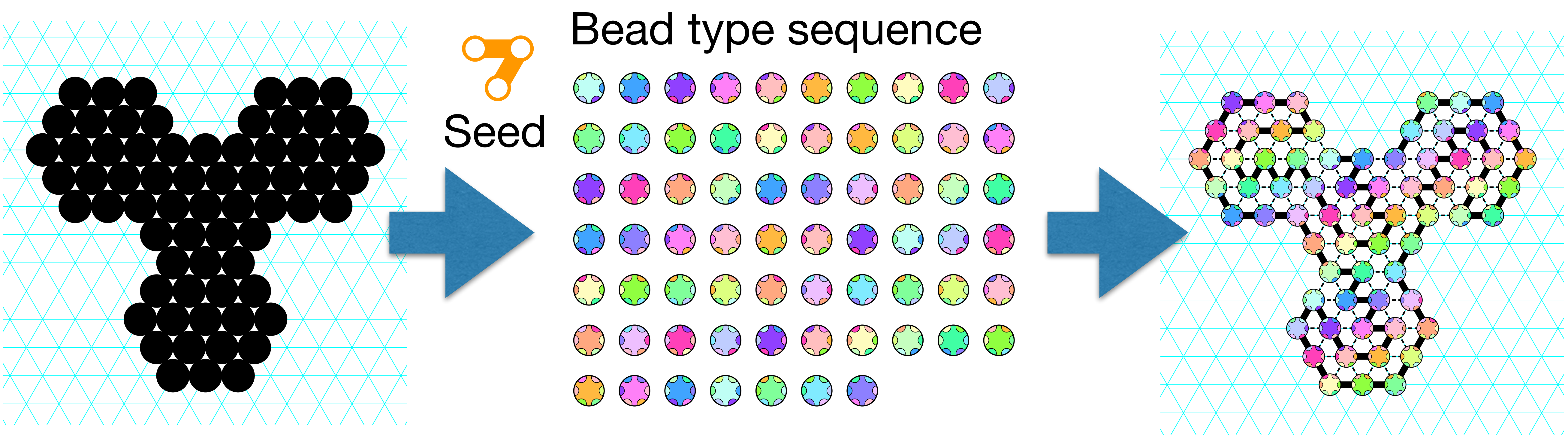
Starting from the seed configuration,
it folds deterministically to occupy all the positions of the shape and only them



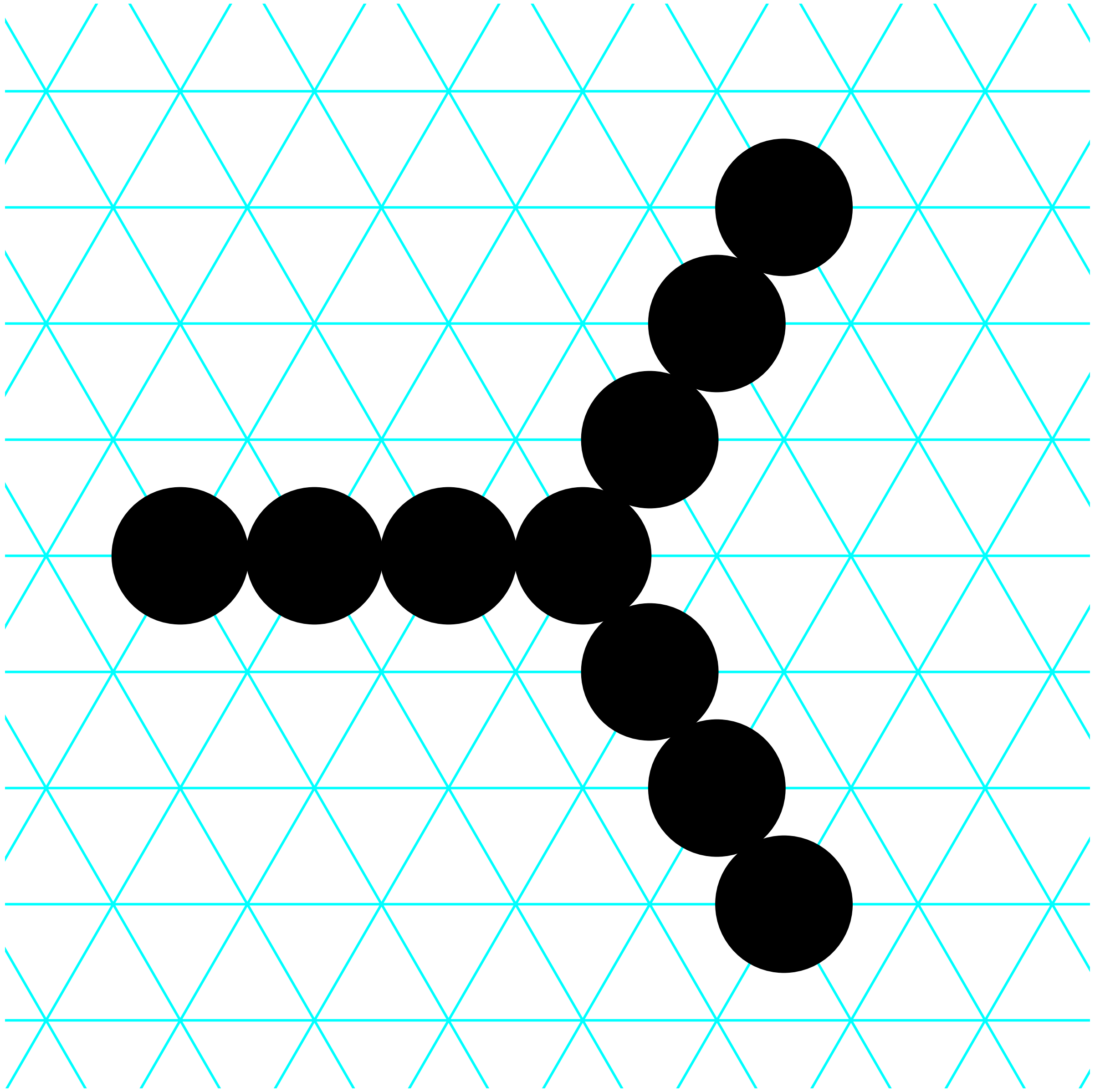
Seek an Universal construction

- **Fixed** finite size seed
- **Fixed** finite set of bead types

(independent of the shape)



Trivial fact:
Foldable shapes are Hamiltonian



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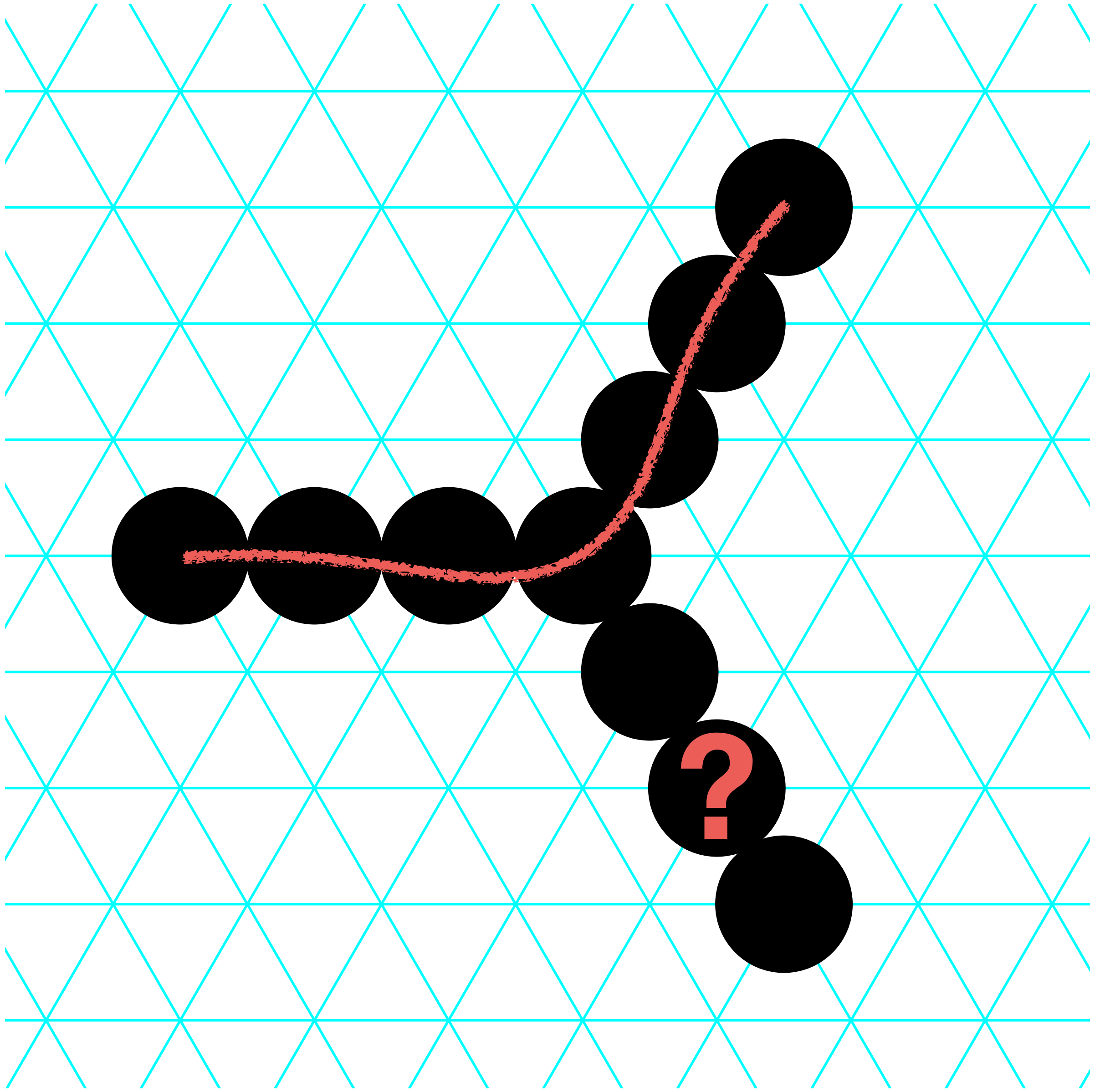
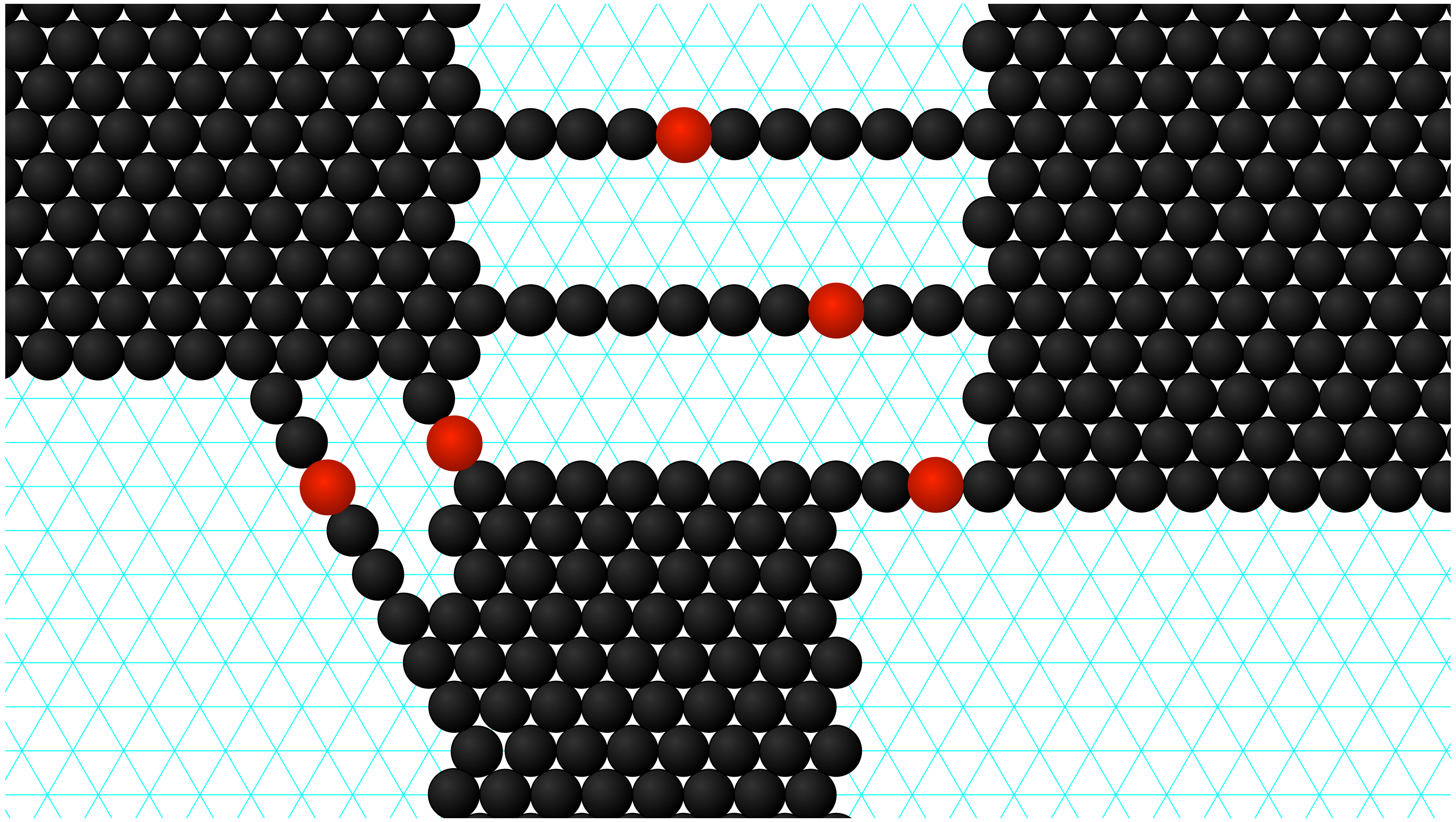
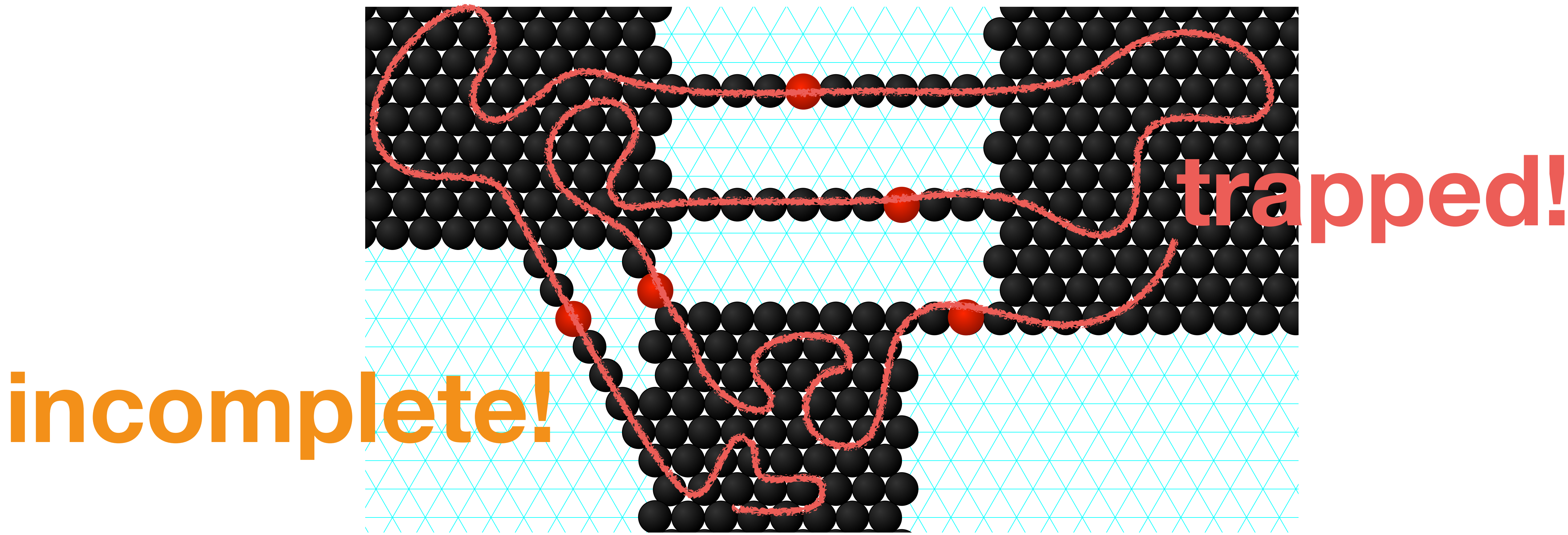


Fact: Finitely cutable *infinite* shapes cannot be folded



A **finite set of points** cutting the shape into several infinite pieces

Fact: Finitely cutable *infinite* shapes cannot be folded

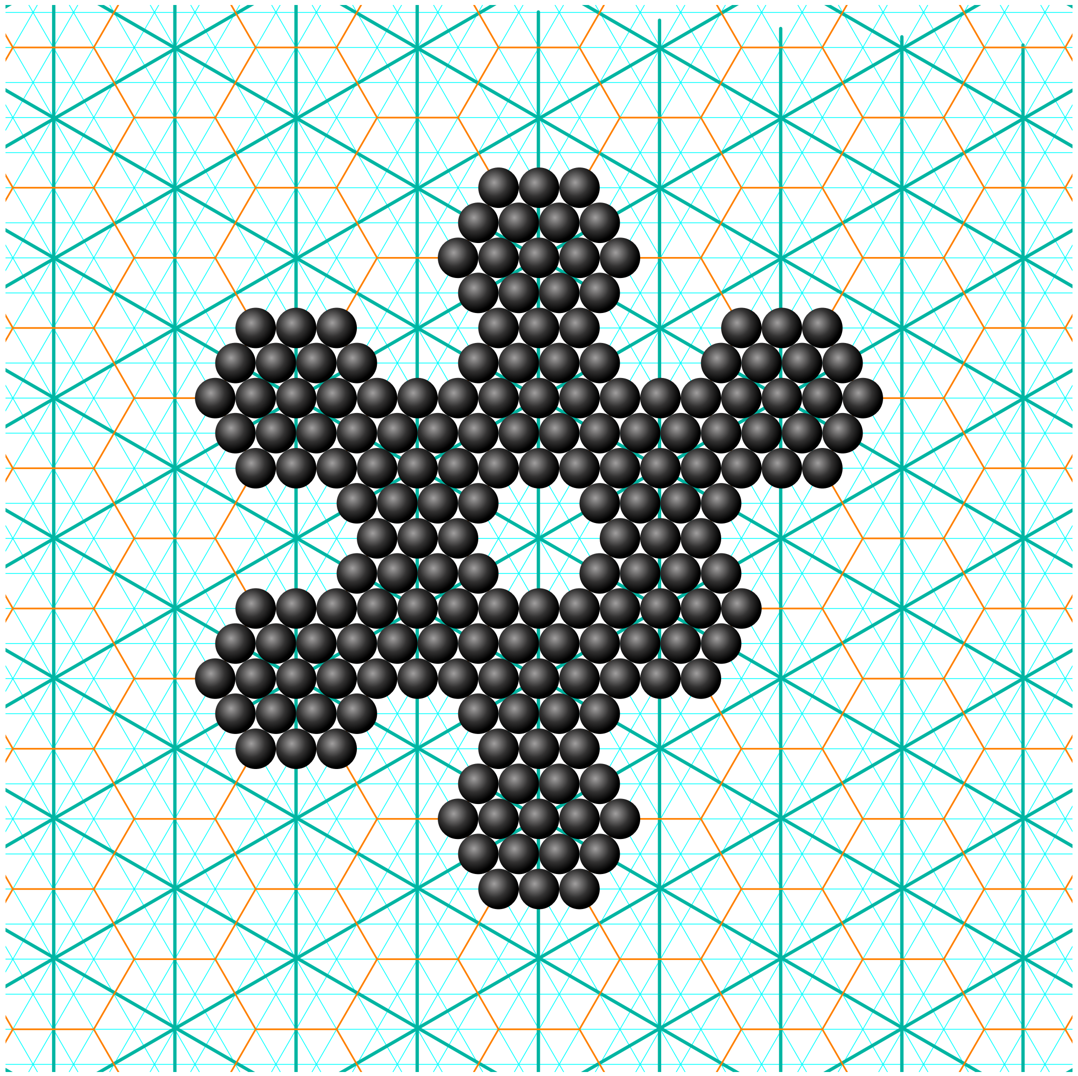


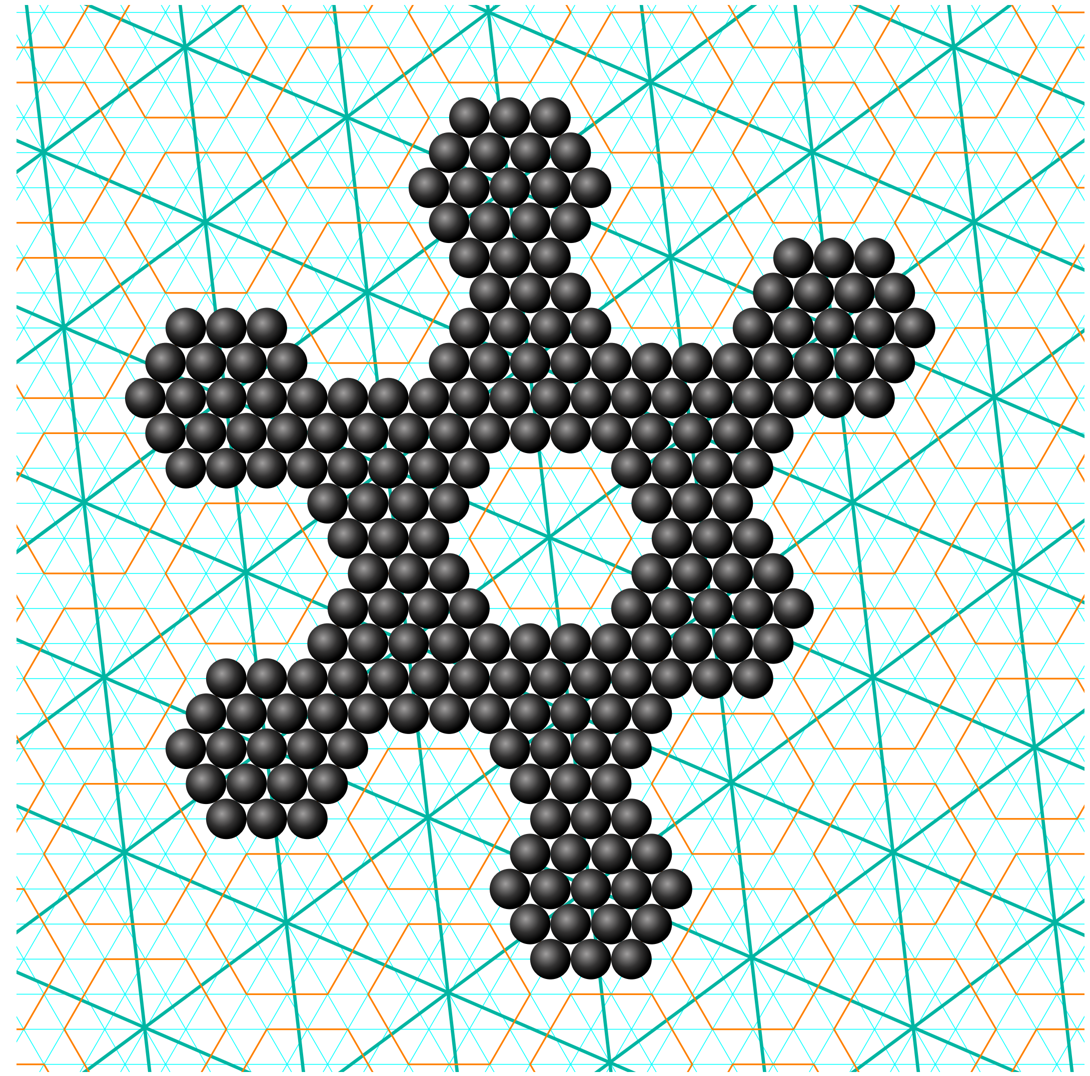
A **finite set of points** cutting the shape
into several infinite pieces

Oritatami systems are thus essentially different from tile assembly systems (aTam)

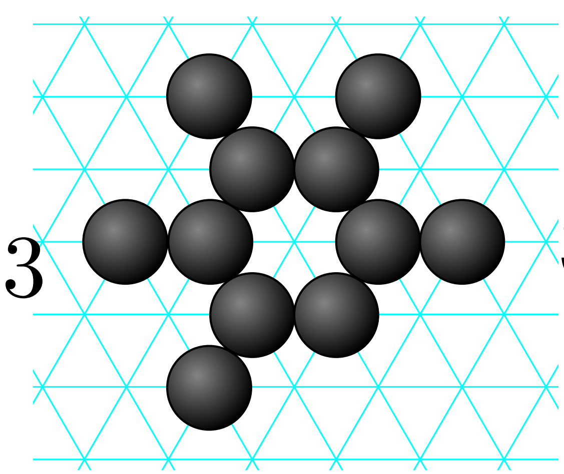
Consider upscaling schemes

Upscaling schemes





scale $\mathscr{A}_{n},\ n=3$



scale $\mathscr{B}_{n},\ n=3$

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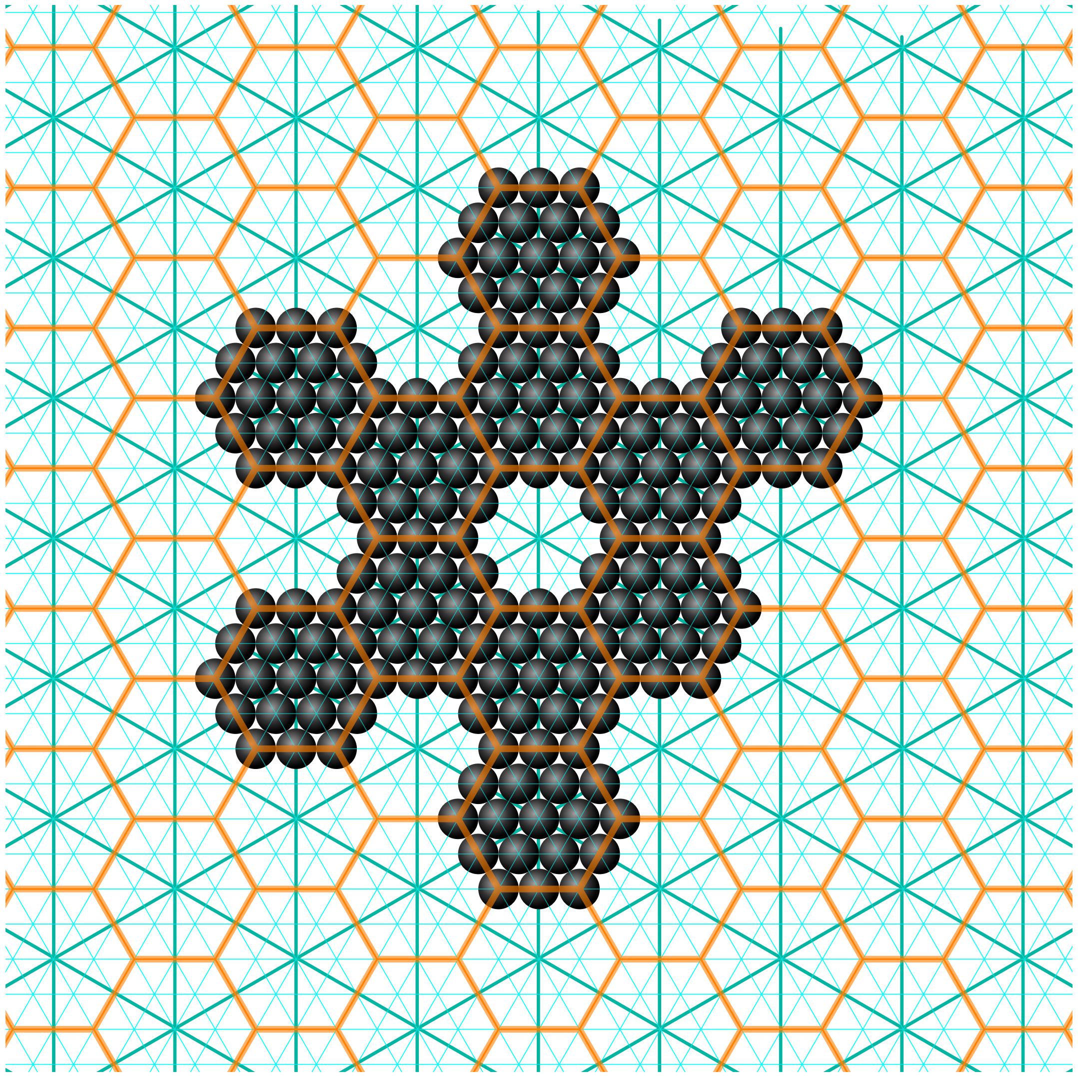

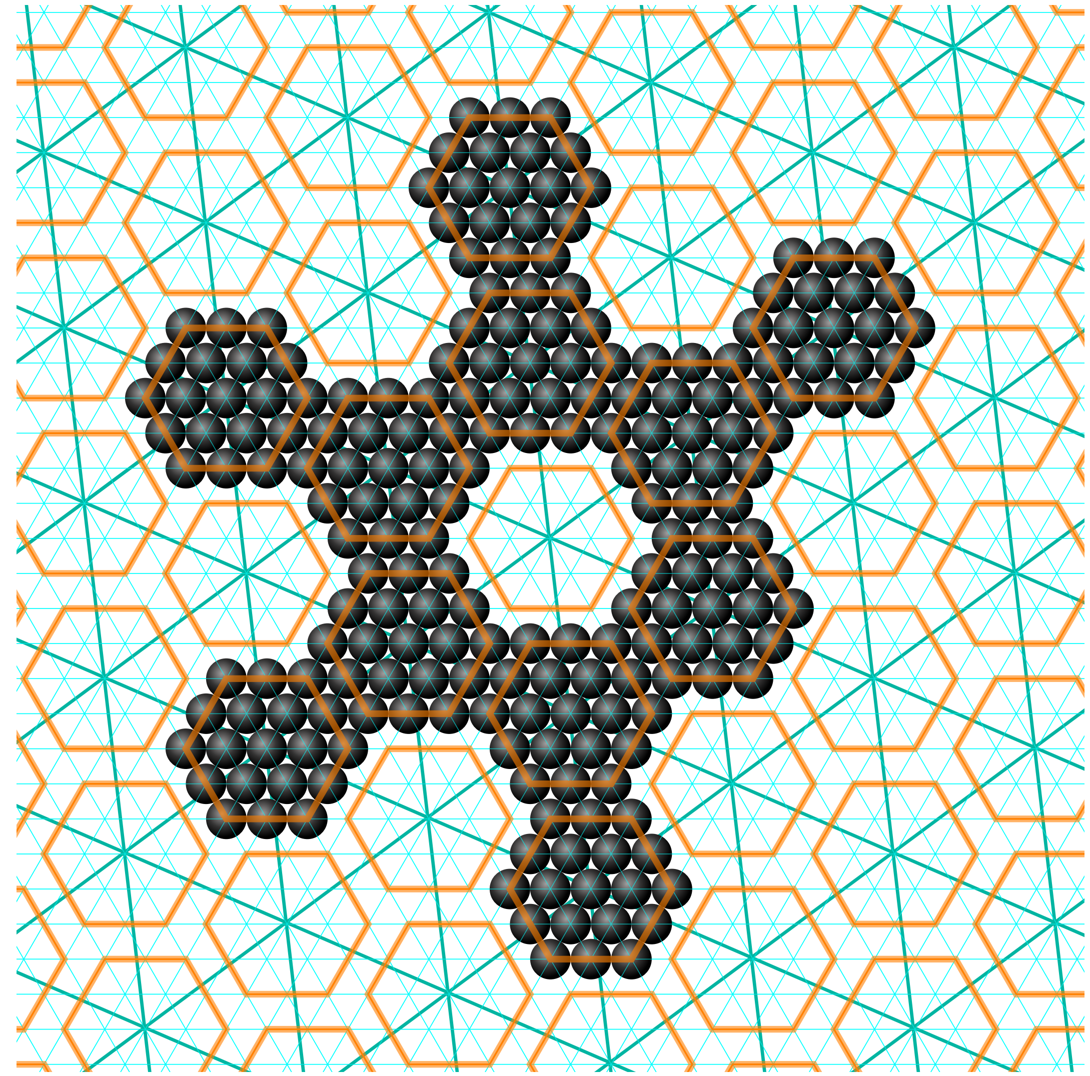

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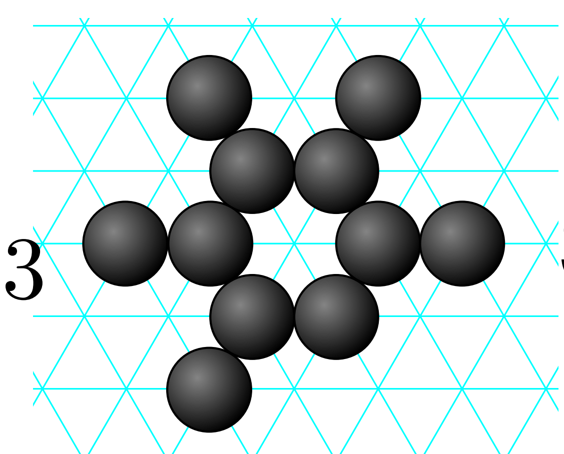
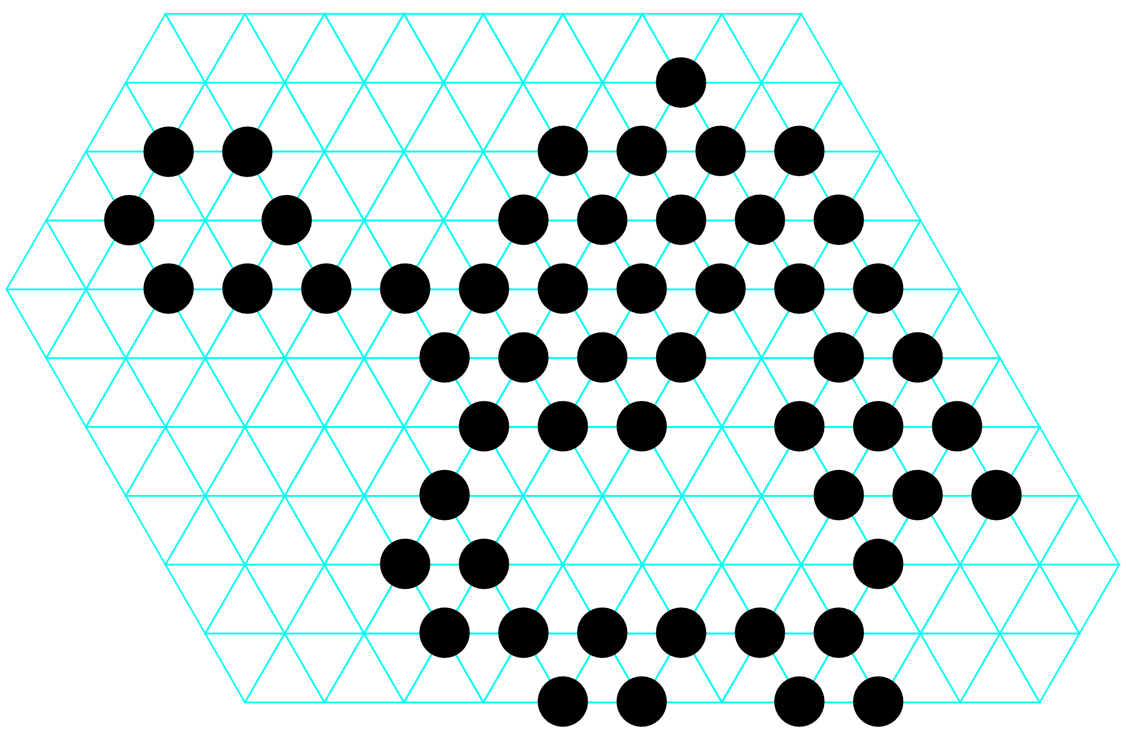
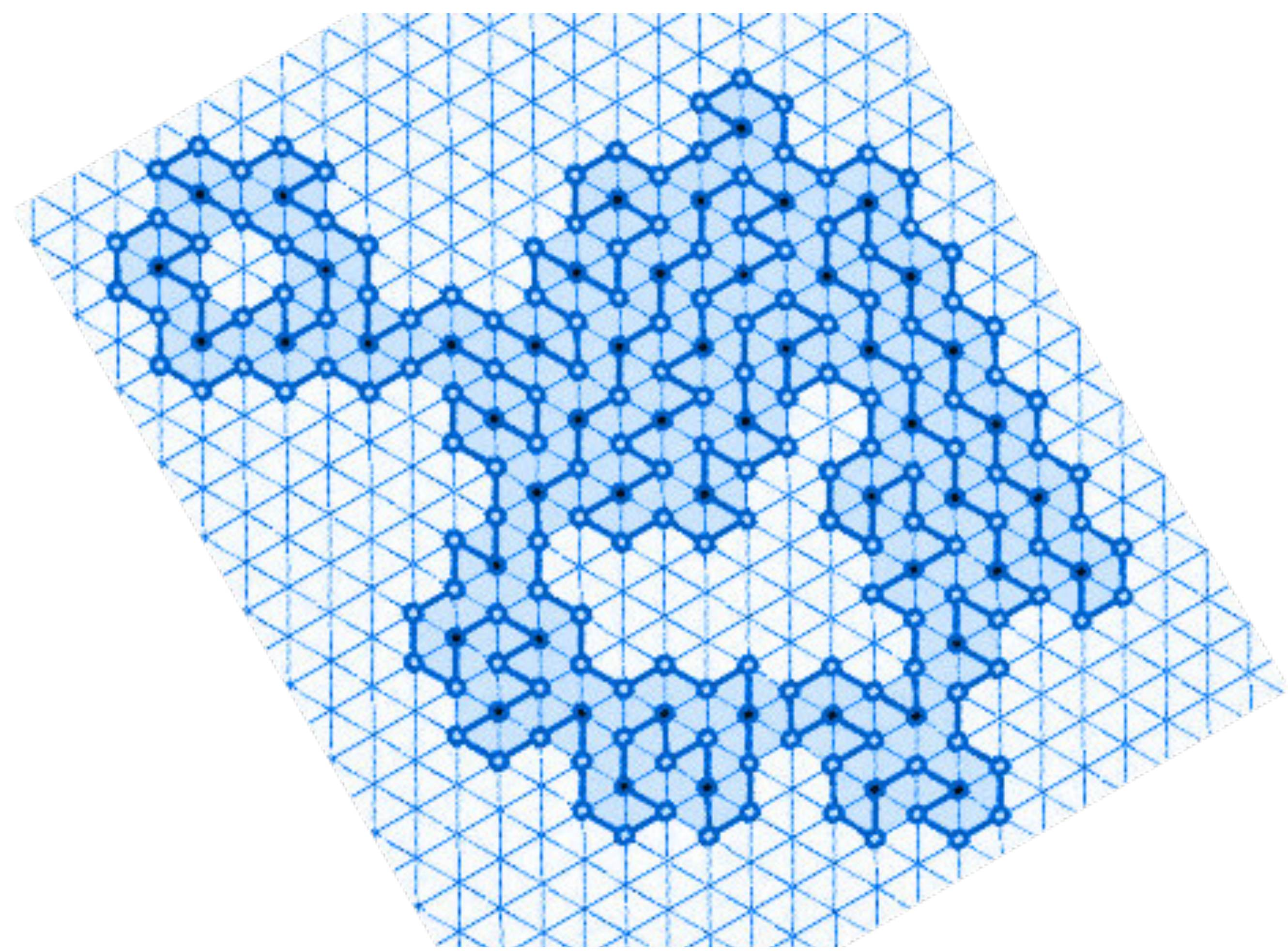


scale $\mathcal{B}_{n},\ n = 3$

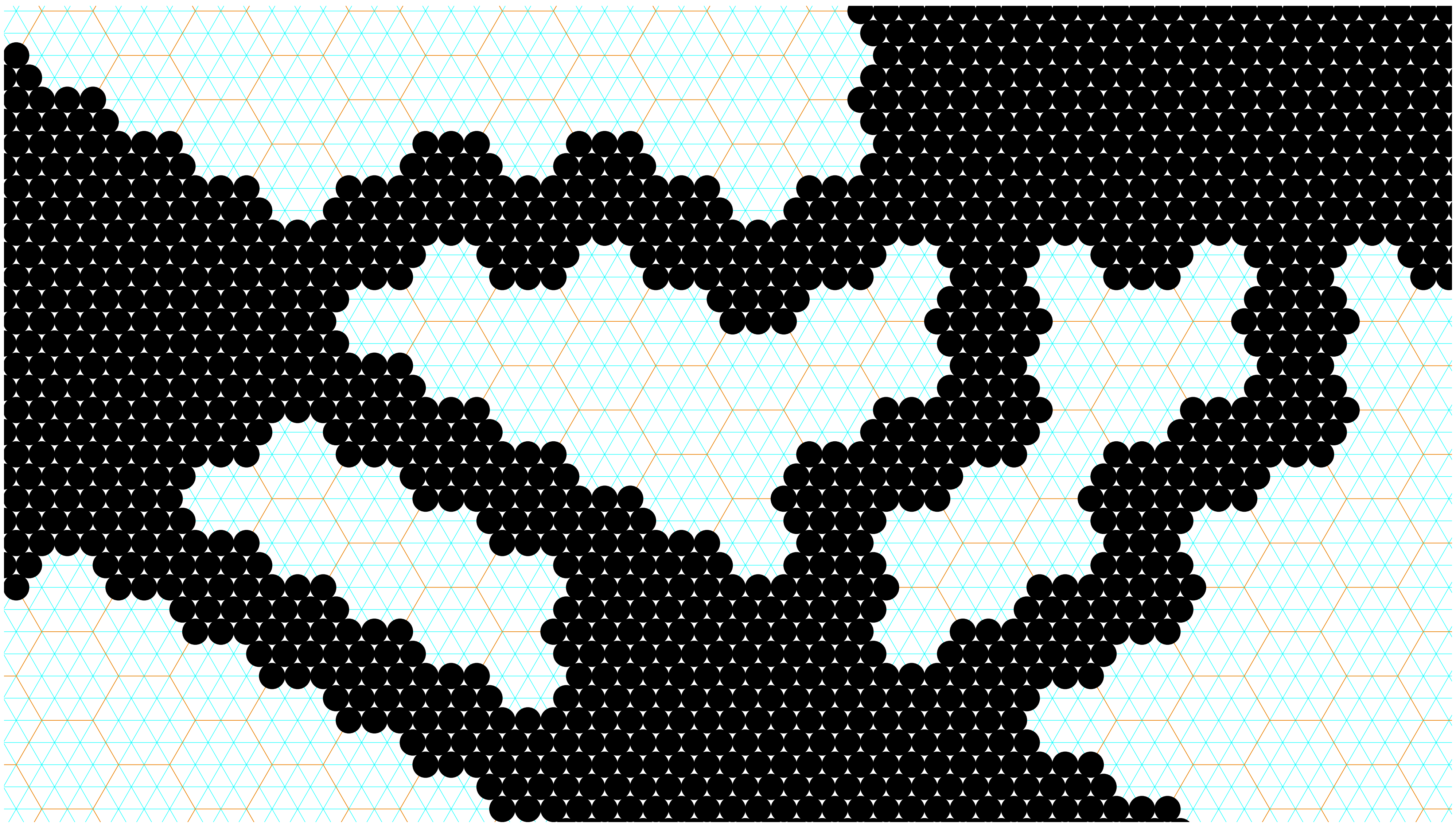
Finite shapes are Hamiltonian at scale $\mathcal{A}_2$

Theorem. There is a quadratic algorithm that computes an Hamiltonian path for any finite shape at scale $\mathcal{A}_2$





Upscaling does not help with finitely cutable infinite shapes



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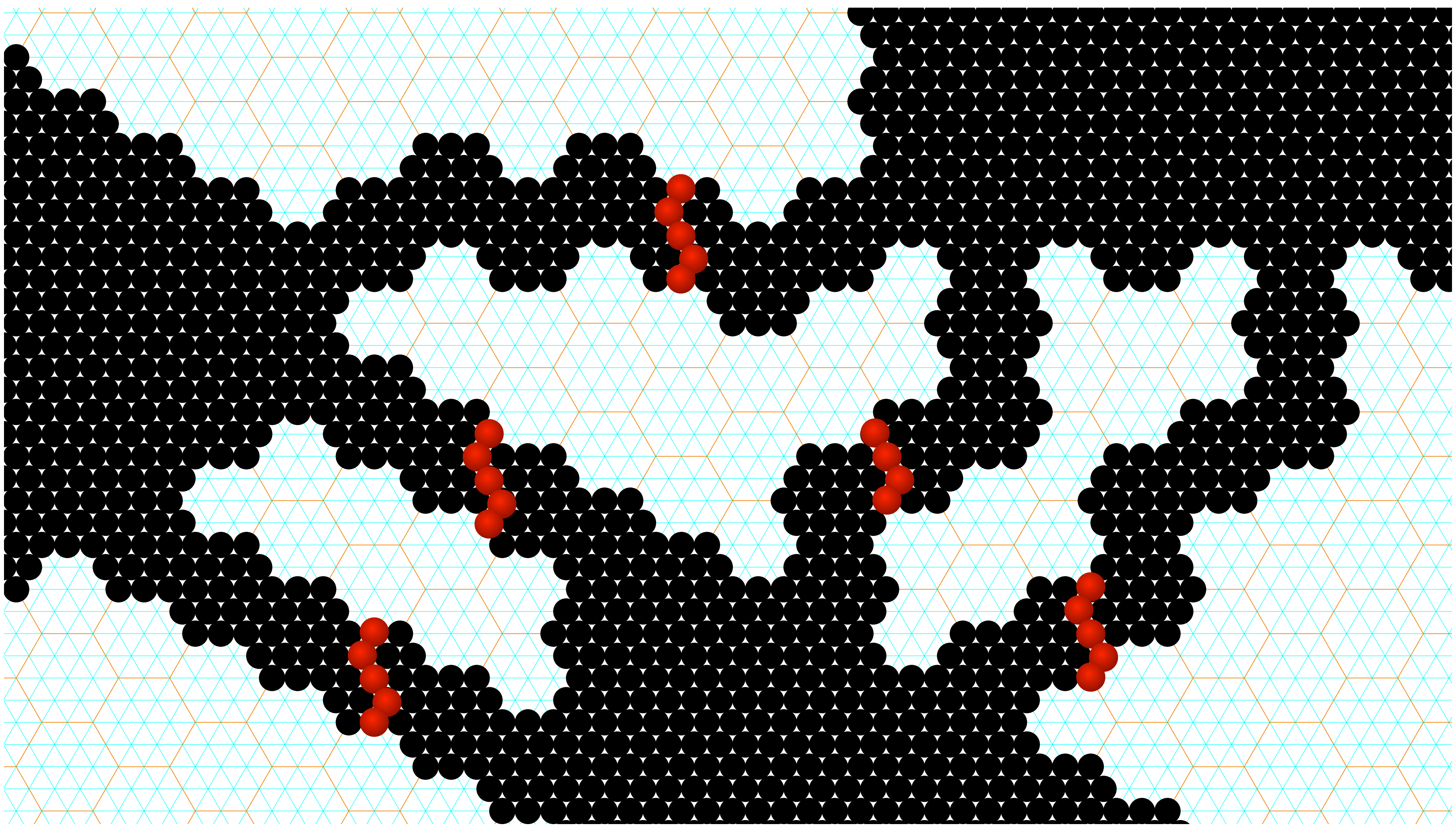

Thus, we focus on **finite shapes**

Scale $\mathscr{B}_n$

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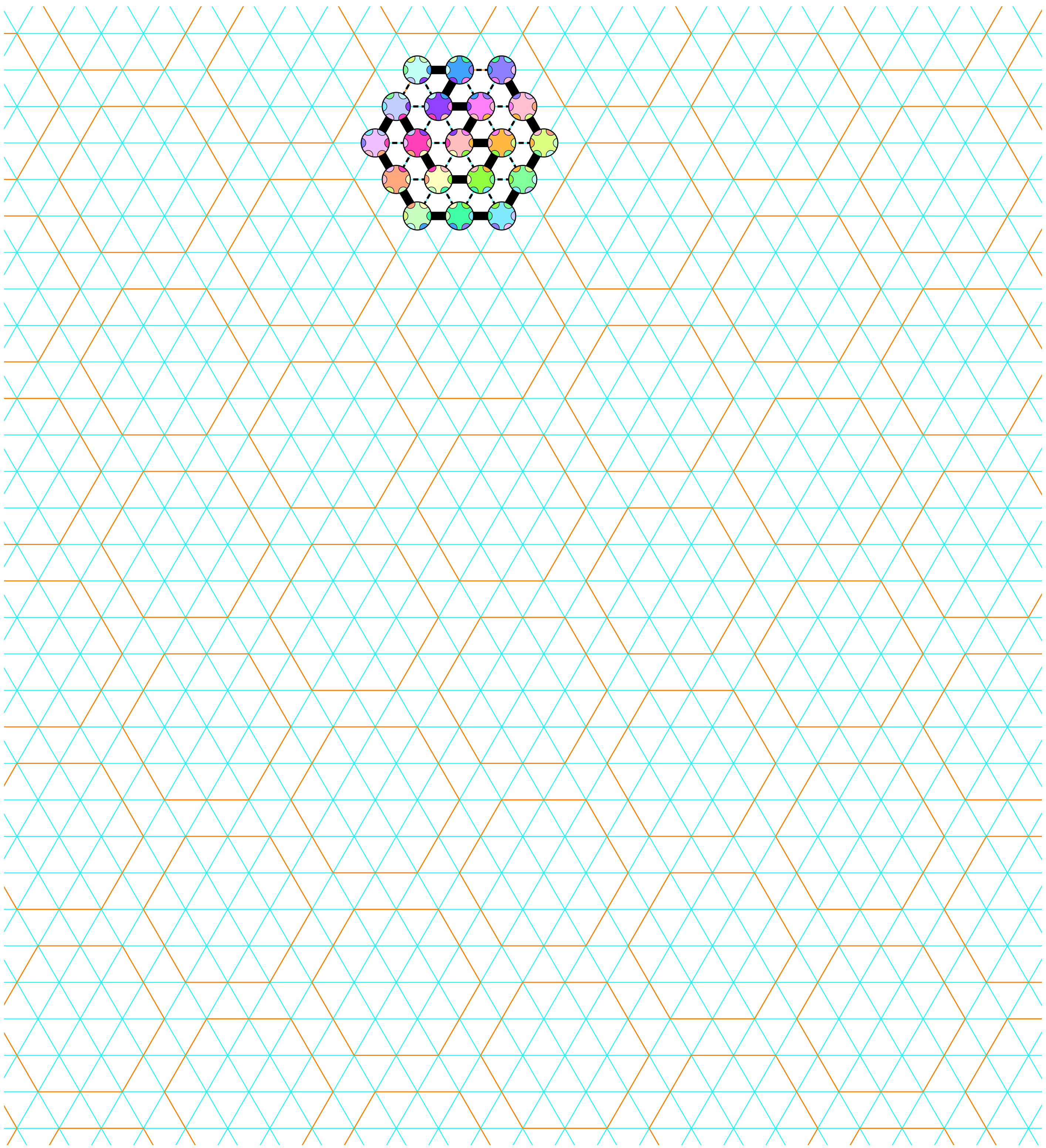
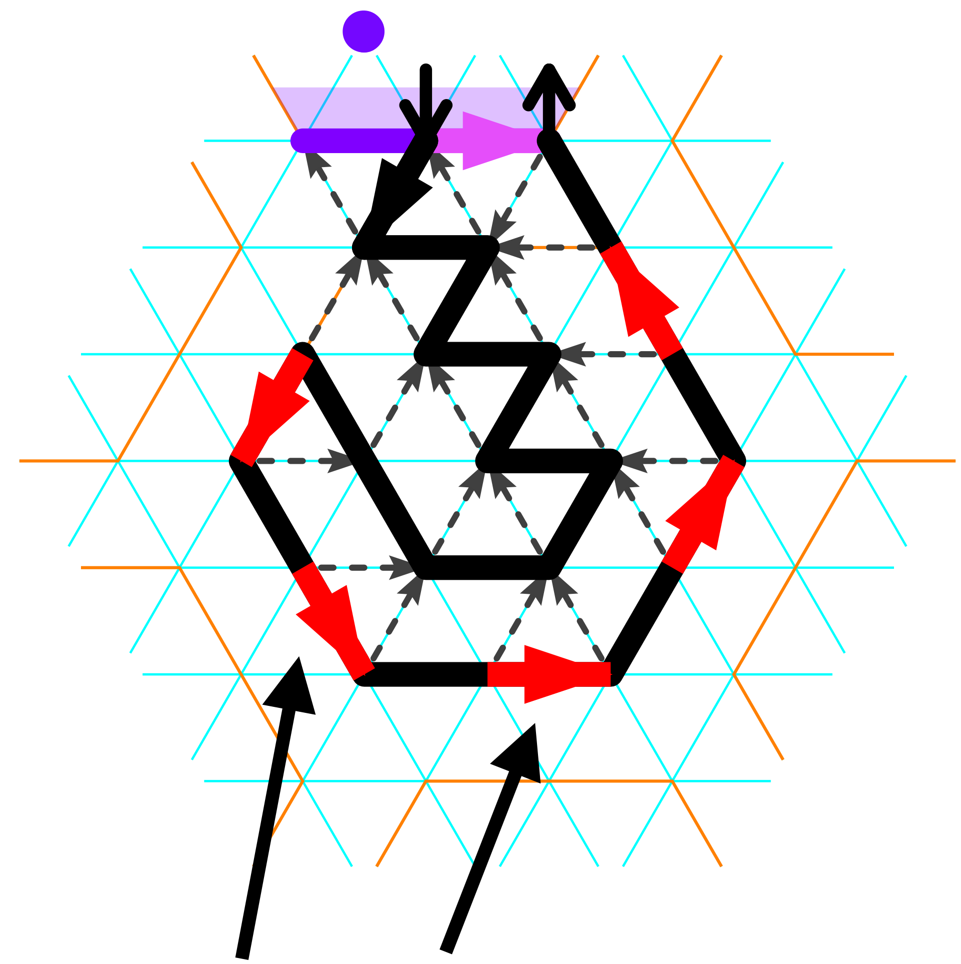


Use a unique pattern



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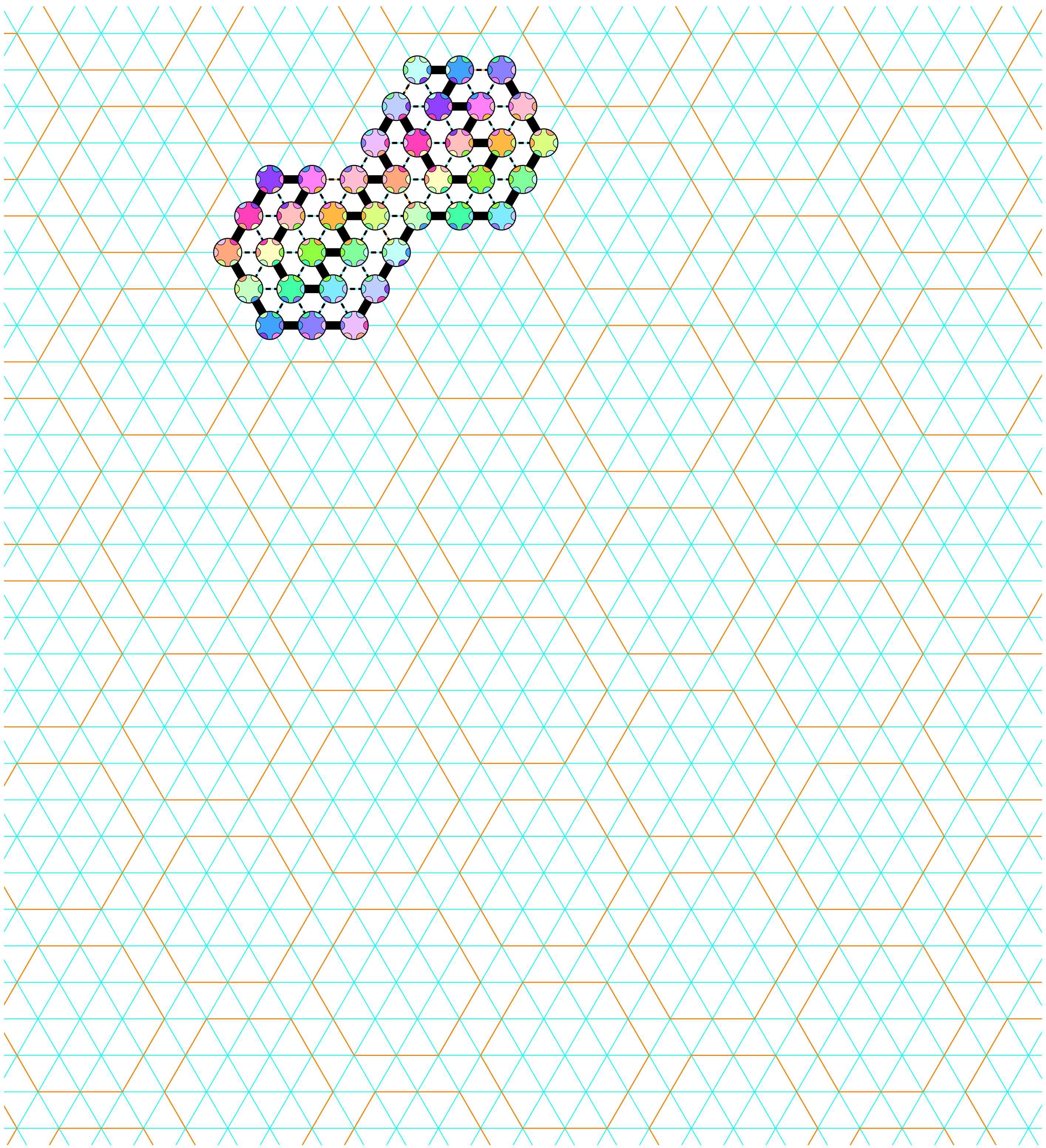

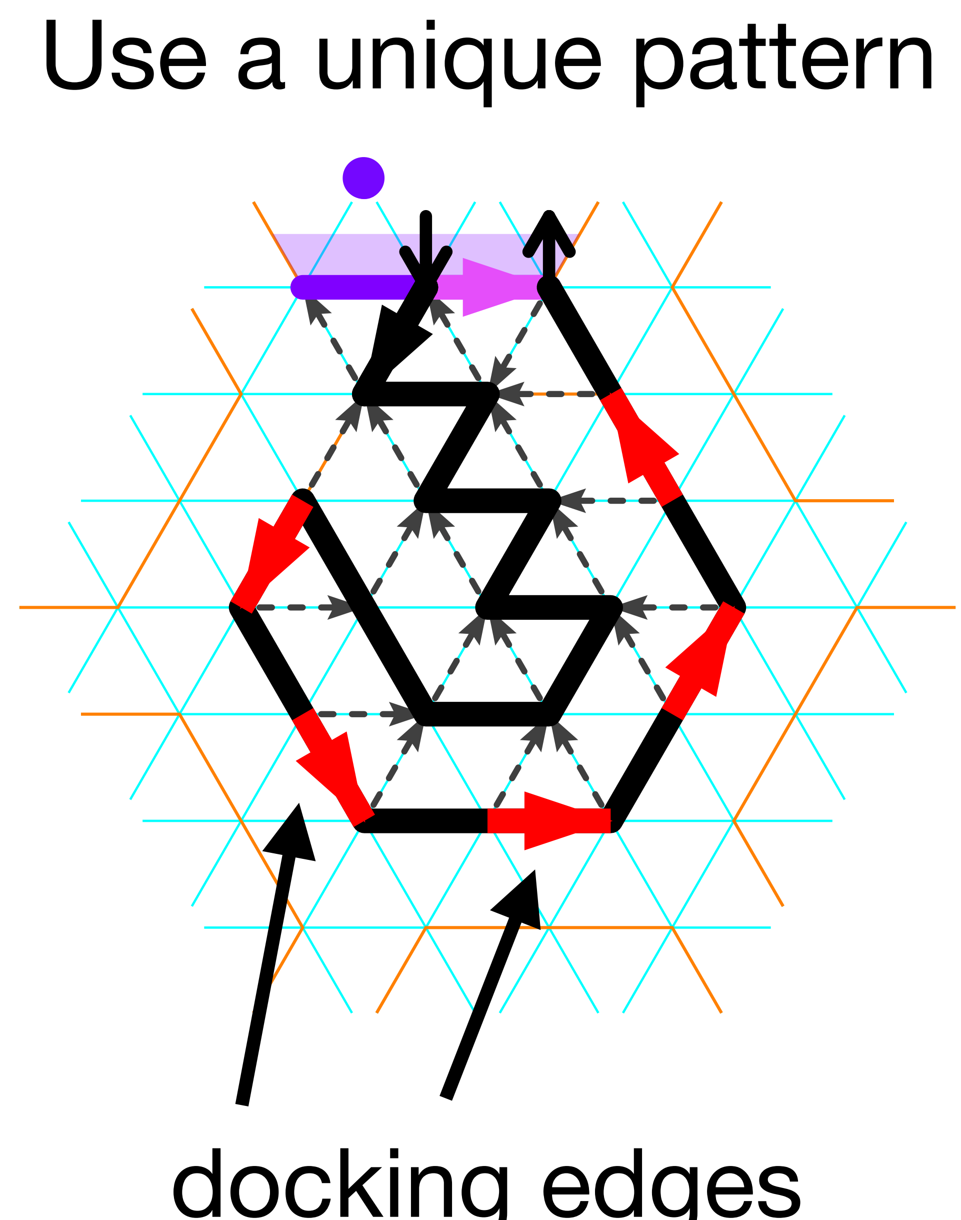

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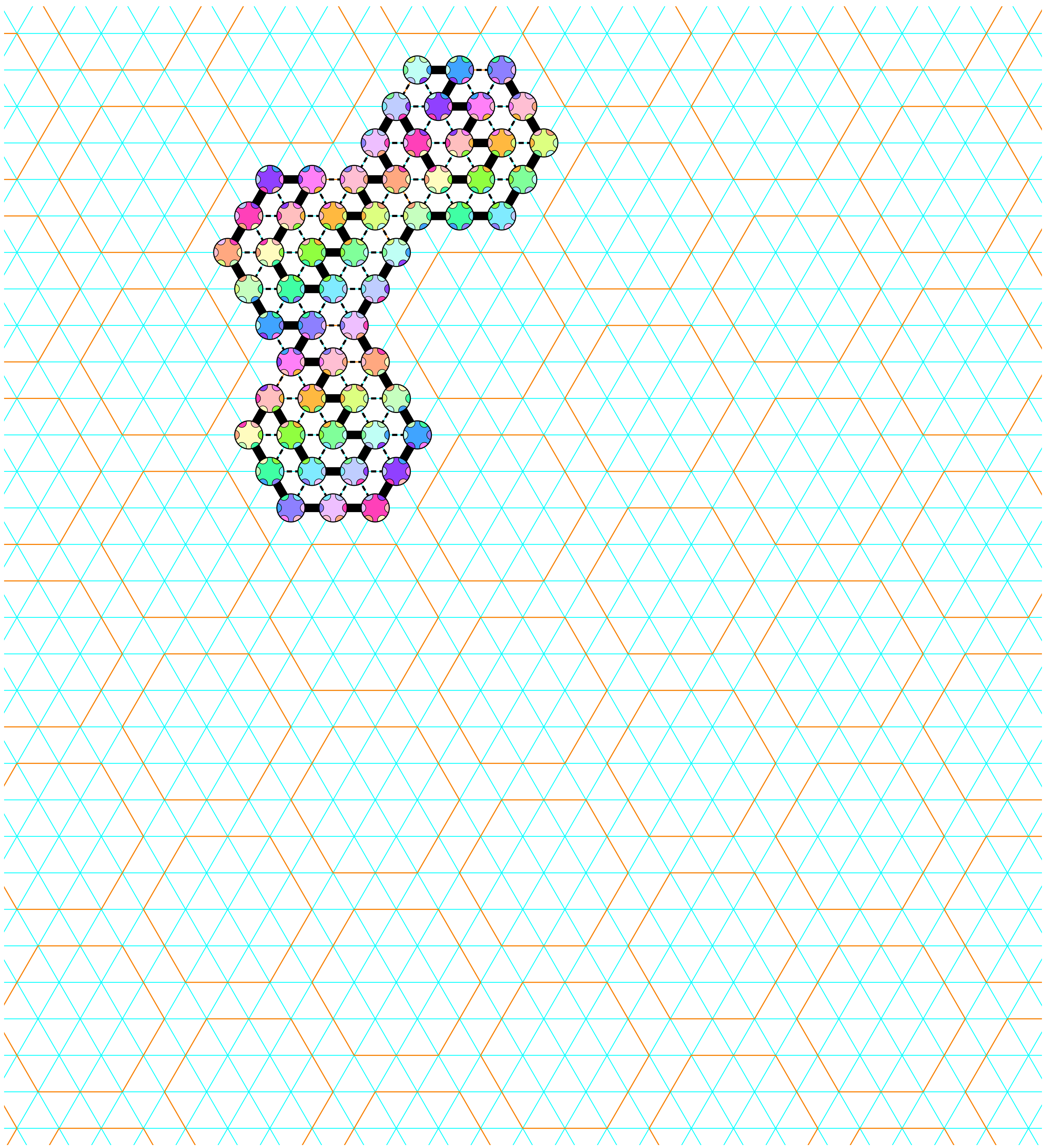

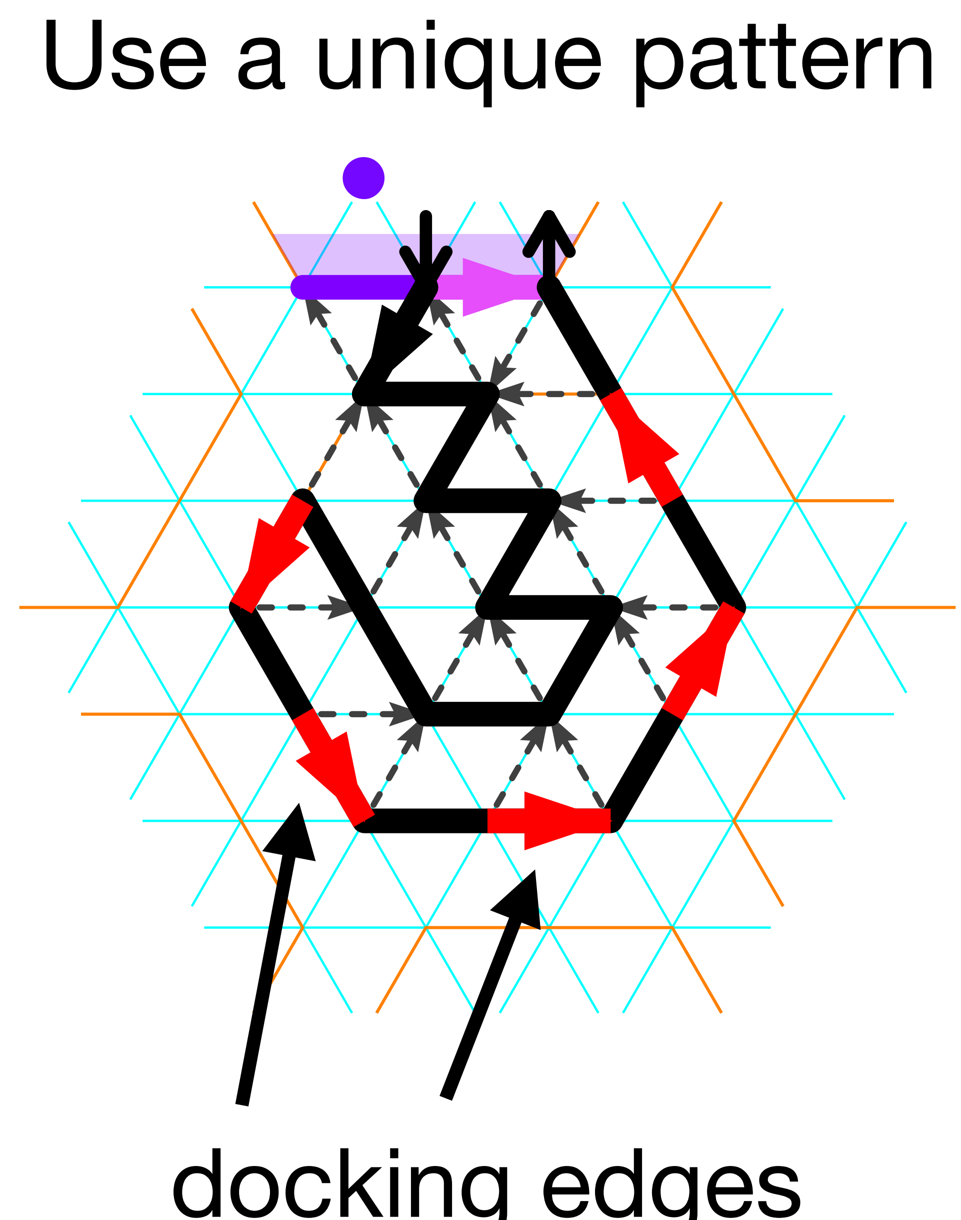

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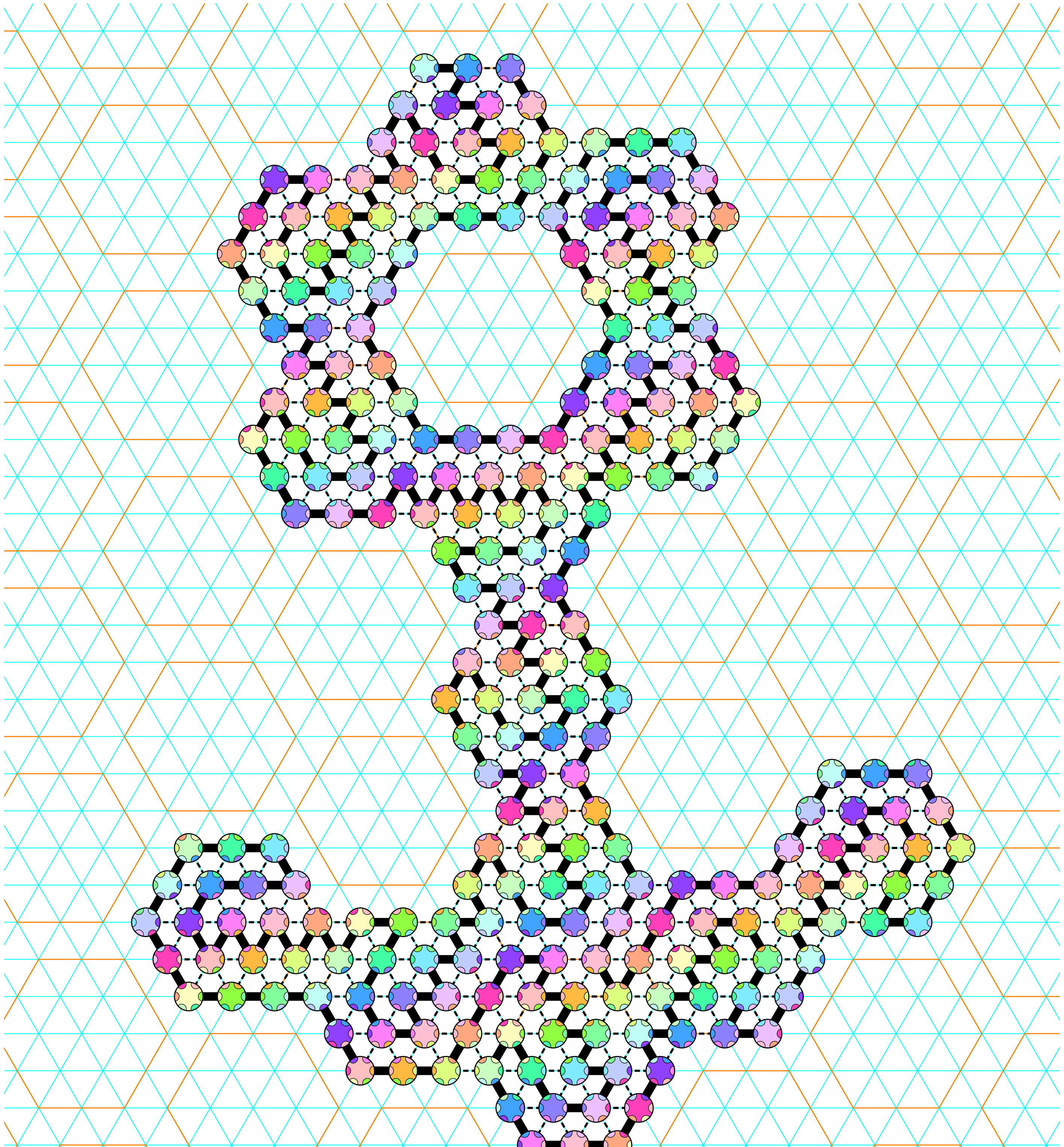

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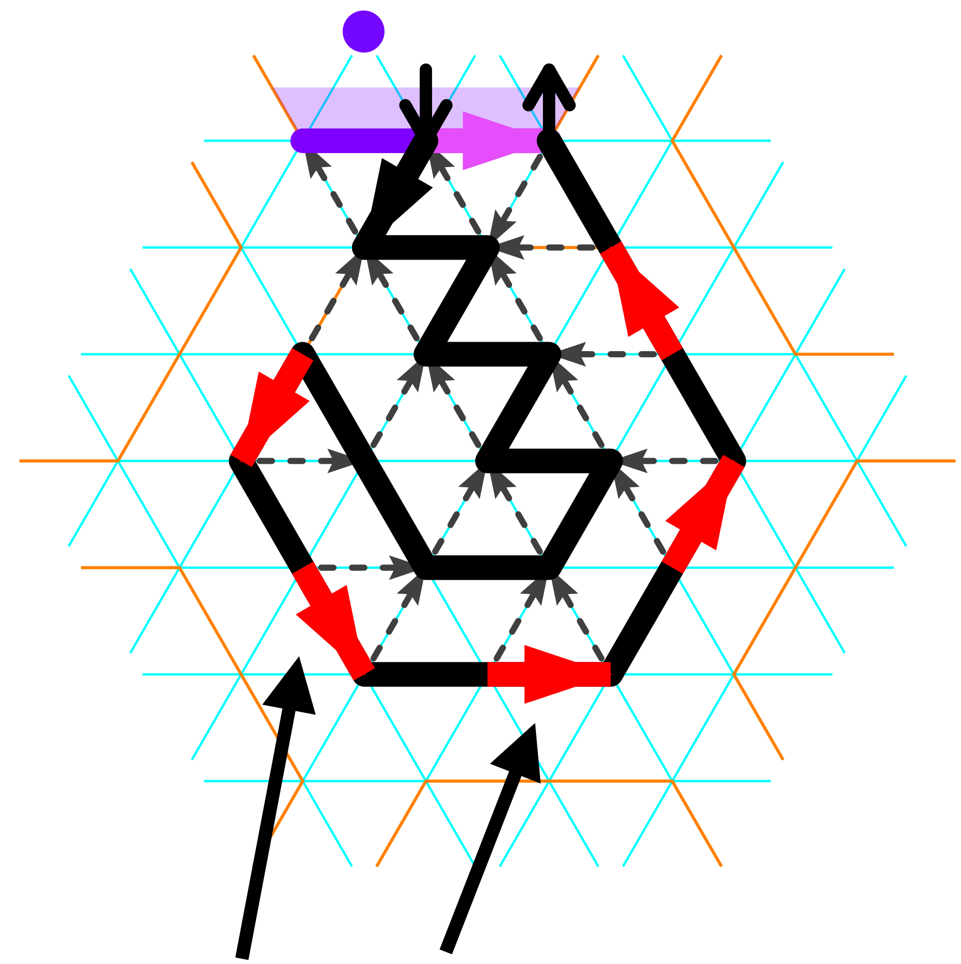
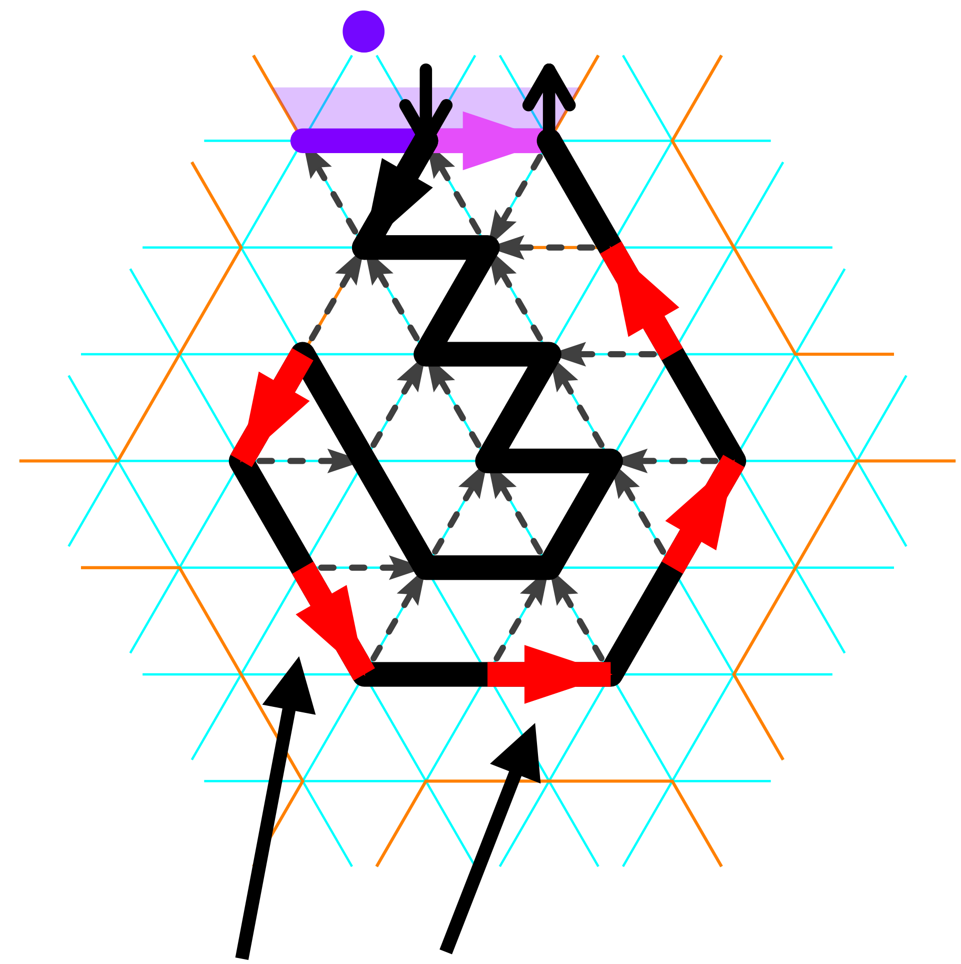


docking edges

scale $\mathscr{B}_n$

Use a unique pattern



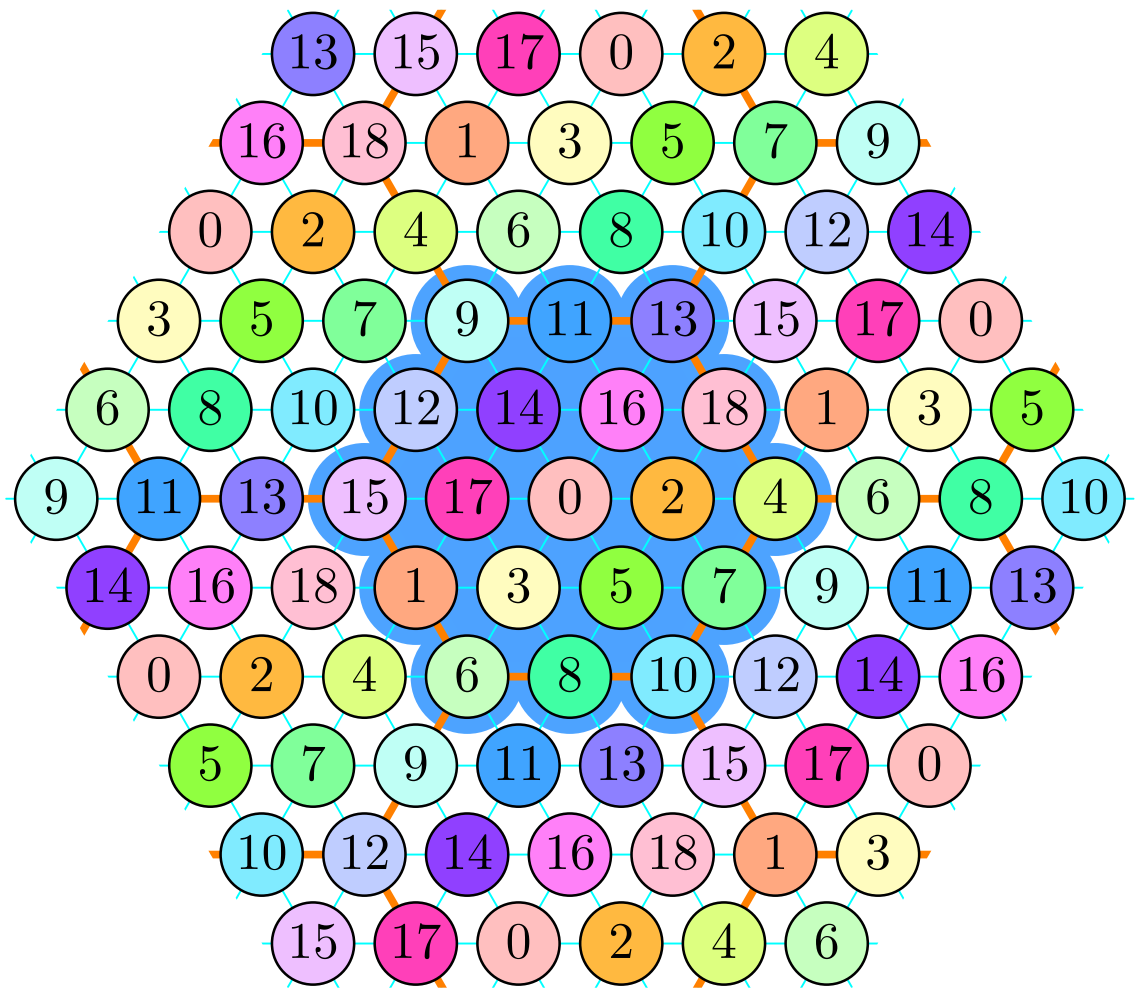
Theorem. All finite shapes can be folded at scale $\mathscr{B}_n$ *for* $n \geq 3$

Proof. By induction:

For **all red edges**, the corresponding **three purple positions** are filled before.

How many bead types are needed ?

Affine coloring of hexagons



Theorem. Let H_n be the hexagon of radius n,

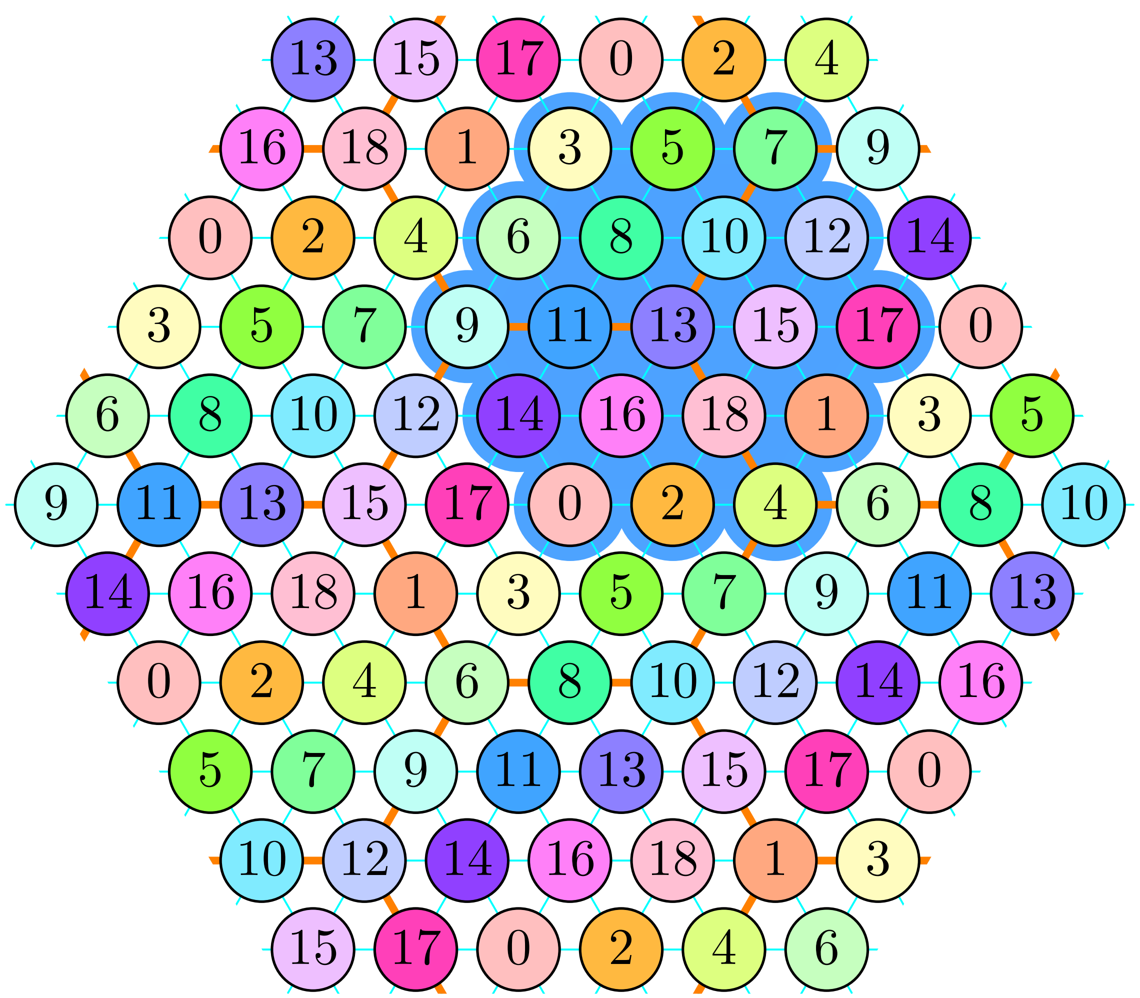
$$c(i,j) = ni + (n+1)j \bmod |H_n|$$

is a proper coloring of H_n

Corolary 1. As it is affine, it is a proper coloring of *any* translation of H_n

Corolary 2. Furthermore, the colors of the neighbors of a given node are fixed translations modulo $|H_n|$ of its own color

Affine coloring of hexagons



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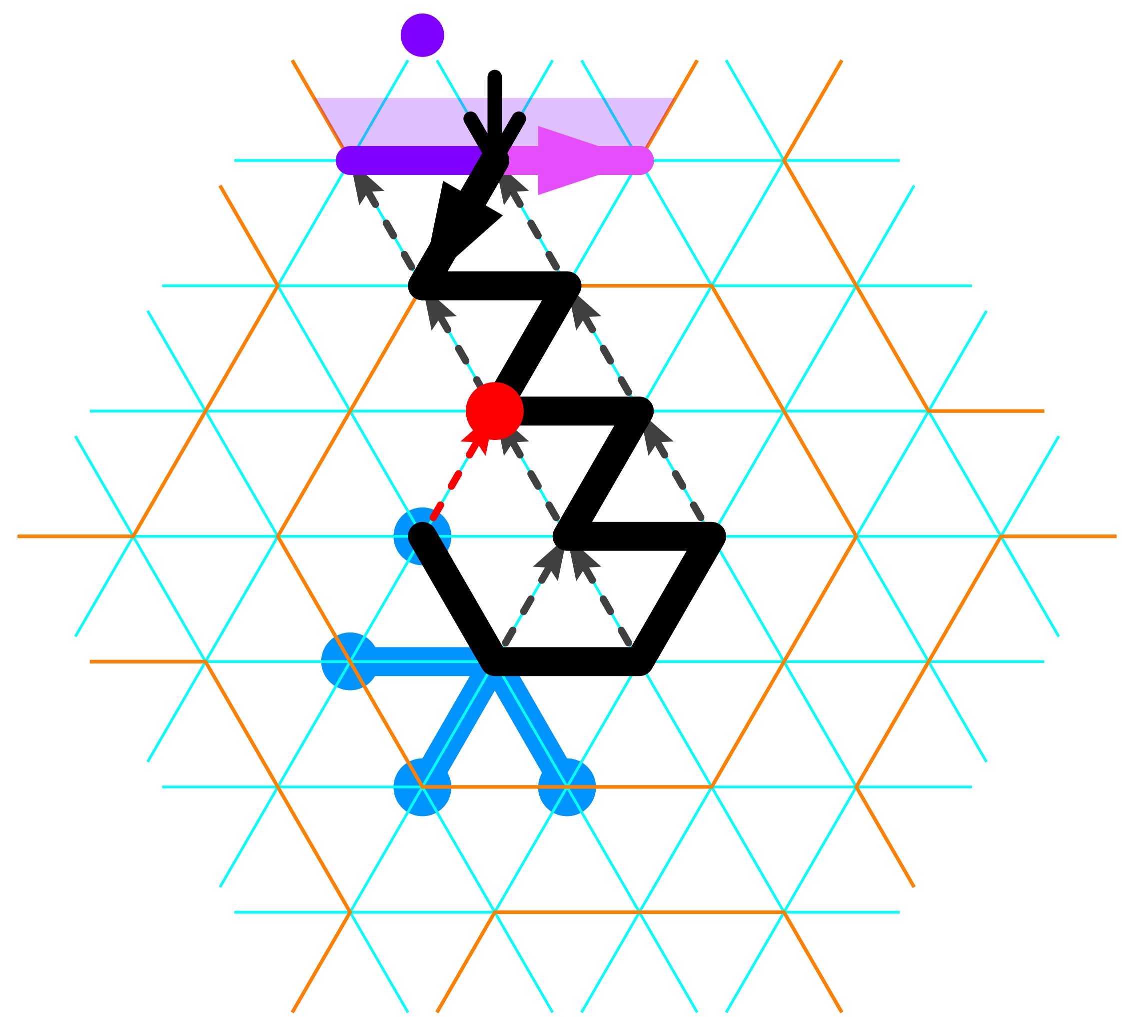
Tight oritatami Systems

An oritatami system is *tight* if:

- delay **δ = 1**
- **every bead destination** has a **tight neighbor,** i.e. such that there is only **one available position** next to it



For tight oritatami system, each bead's position is uniquely determined by whom it is attracted to

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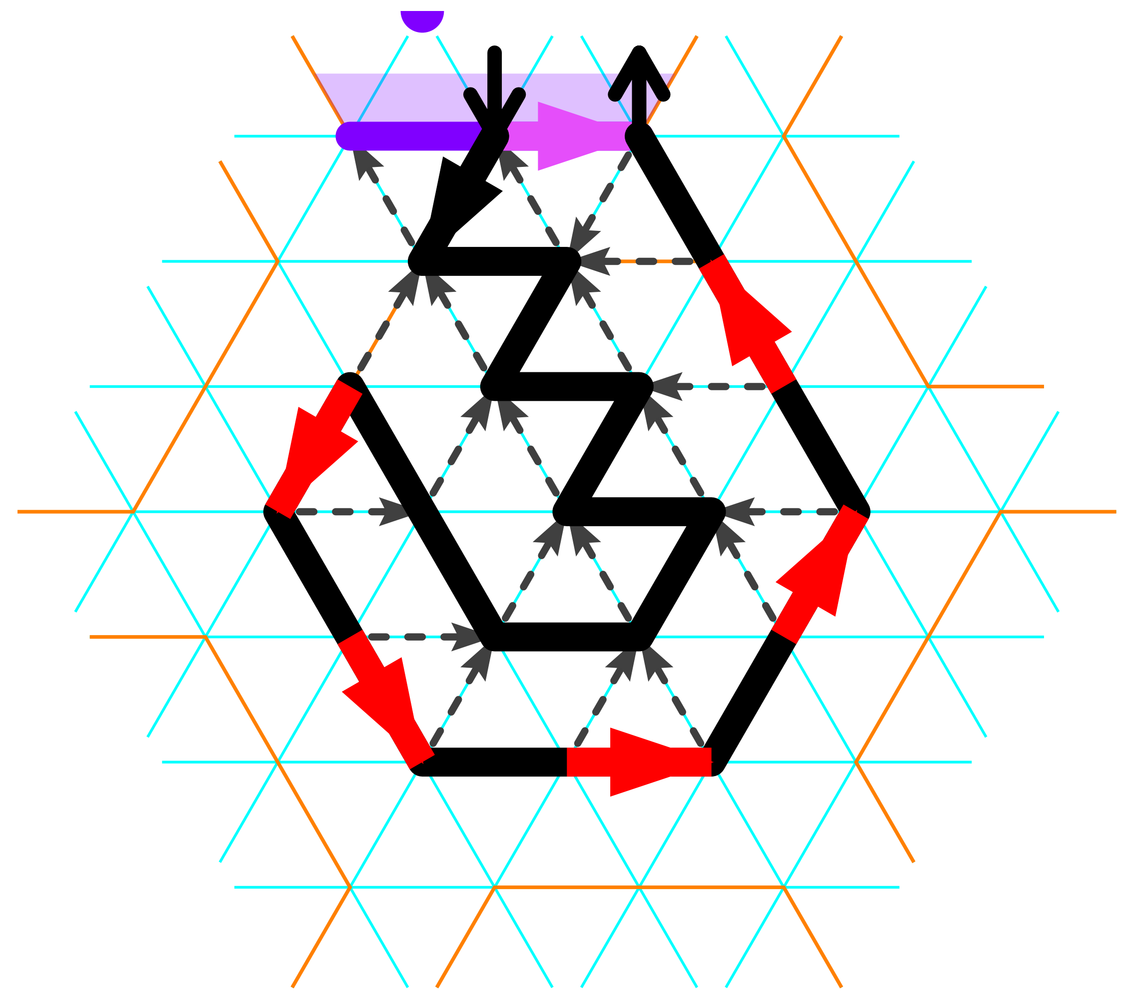
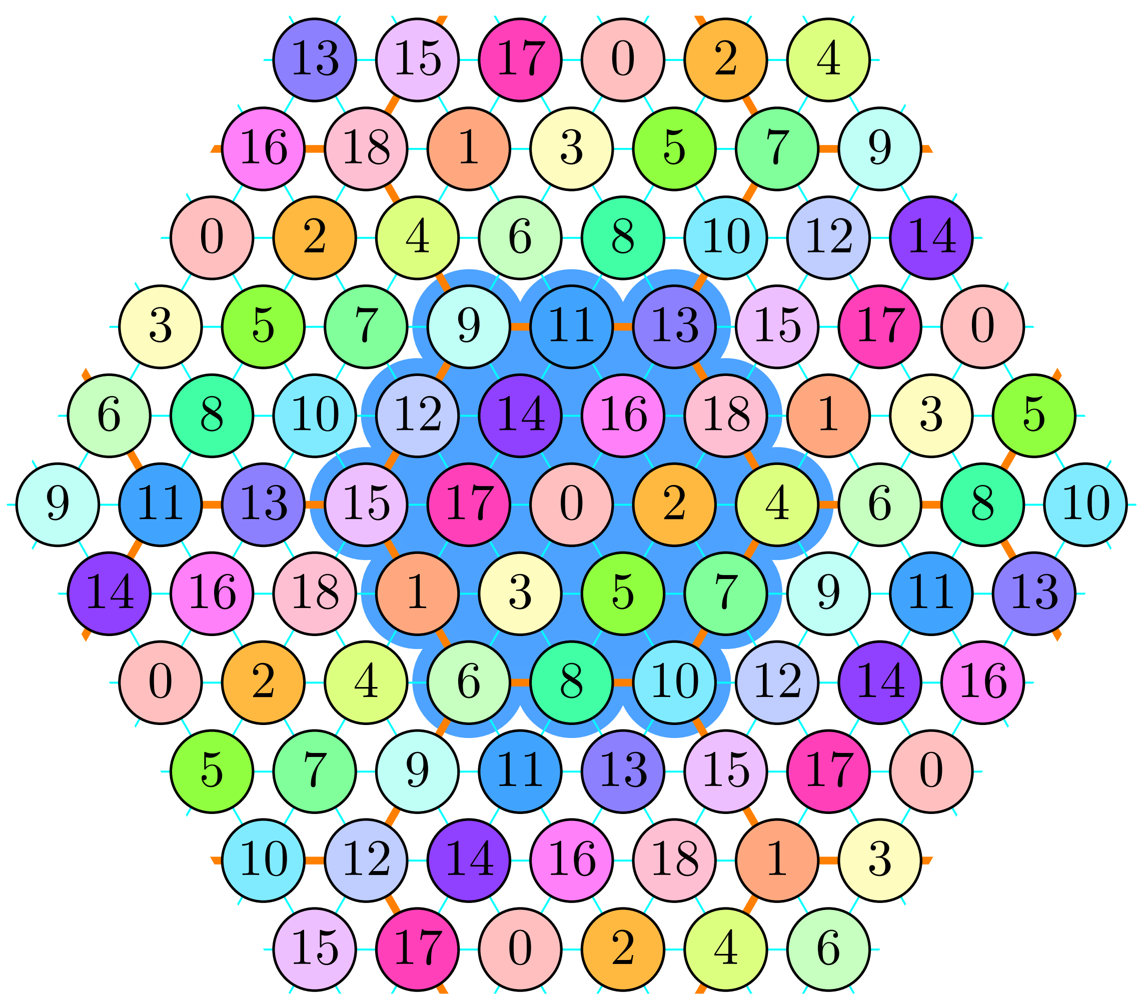


For tight oritatami system, each bead's position is uniquely determined by whom it is attracted to

19 bead types are enough for tight oritatami systems



Each bead located at (i,j) receives bead type:

$$\boldsymbol{c(i,j)}$$

and $\boldsymbol{c}$❤️$\boldsymbol{c'}$ iff

$$\boldsymbol{c' = c + \Delta c(d) \bmod 19}$$

For tight oritatami system, each bead's position is fully determined by whom it is attracted to

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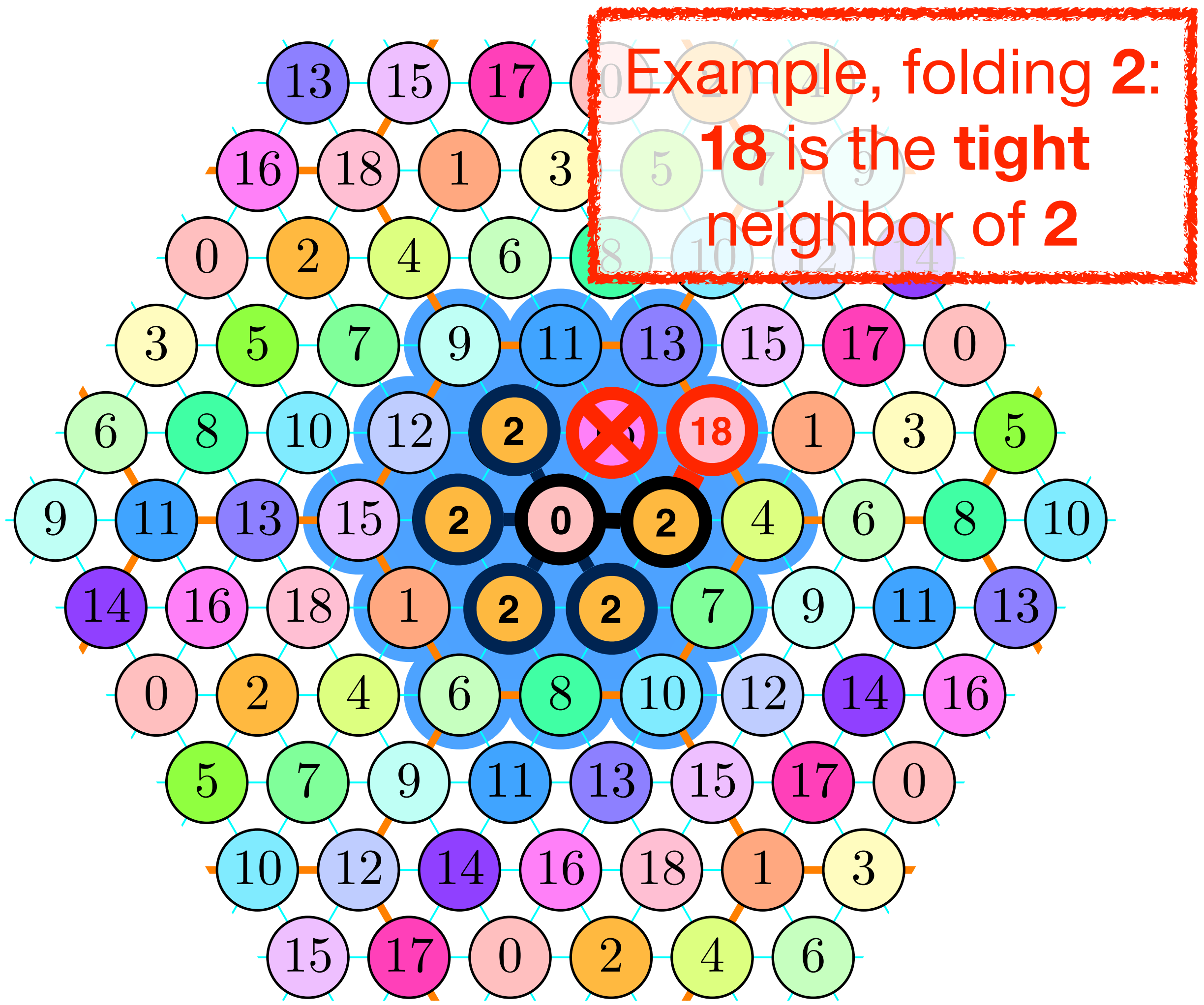

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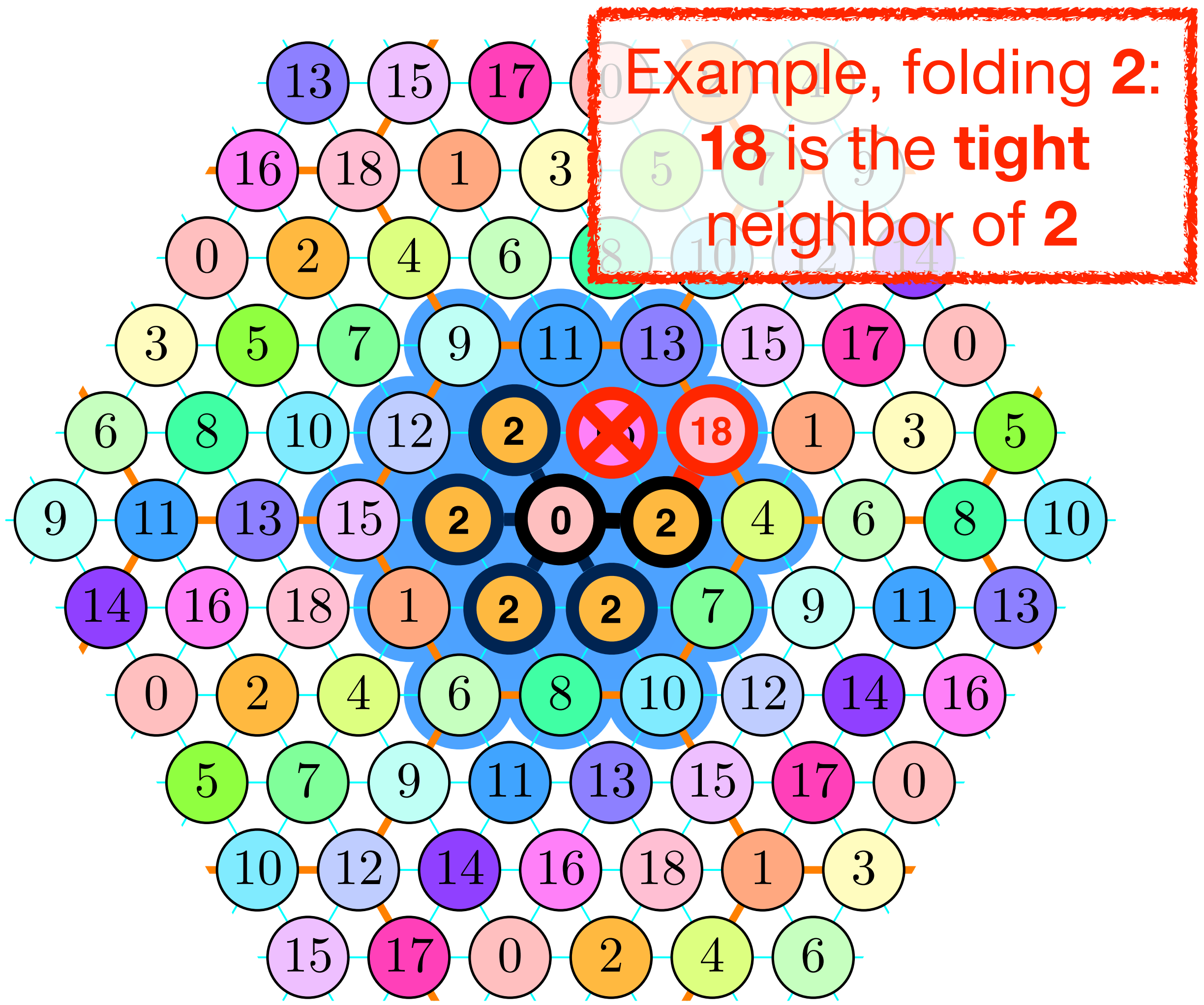

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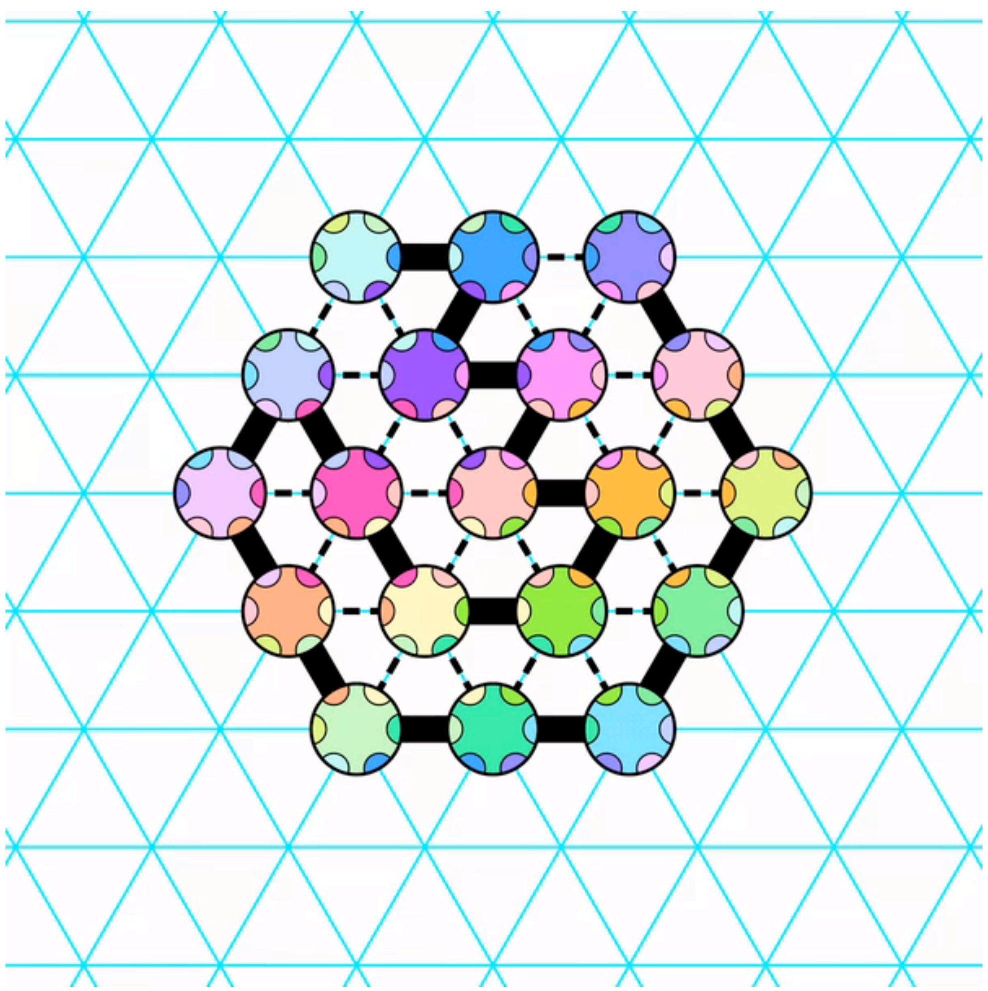

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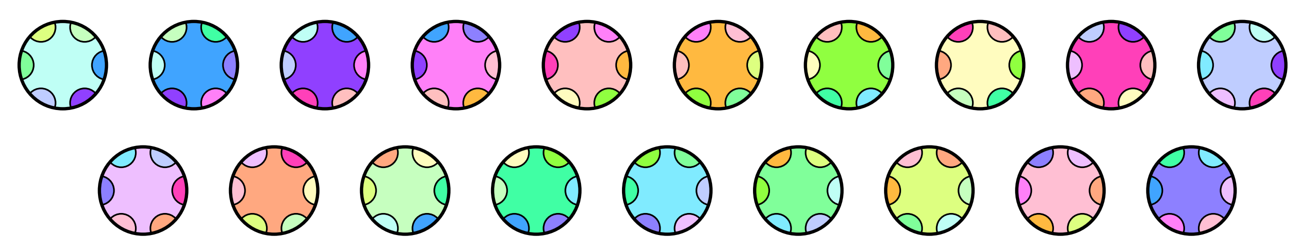

Theorem. 19 beads types are enough

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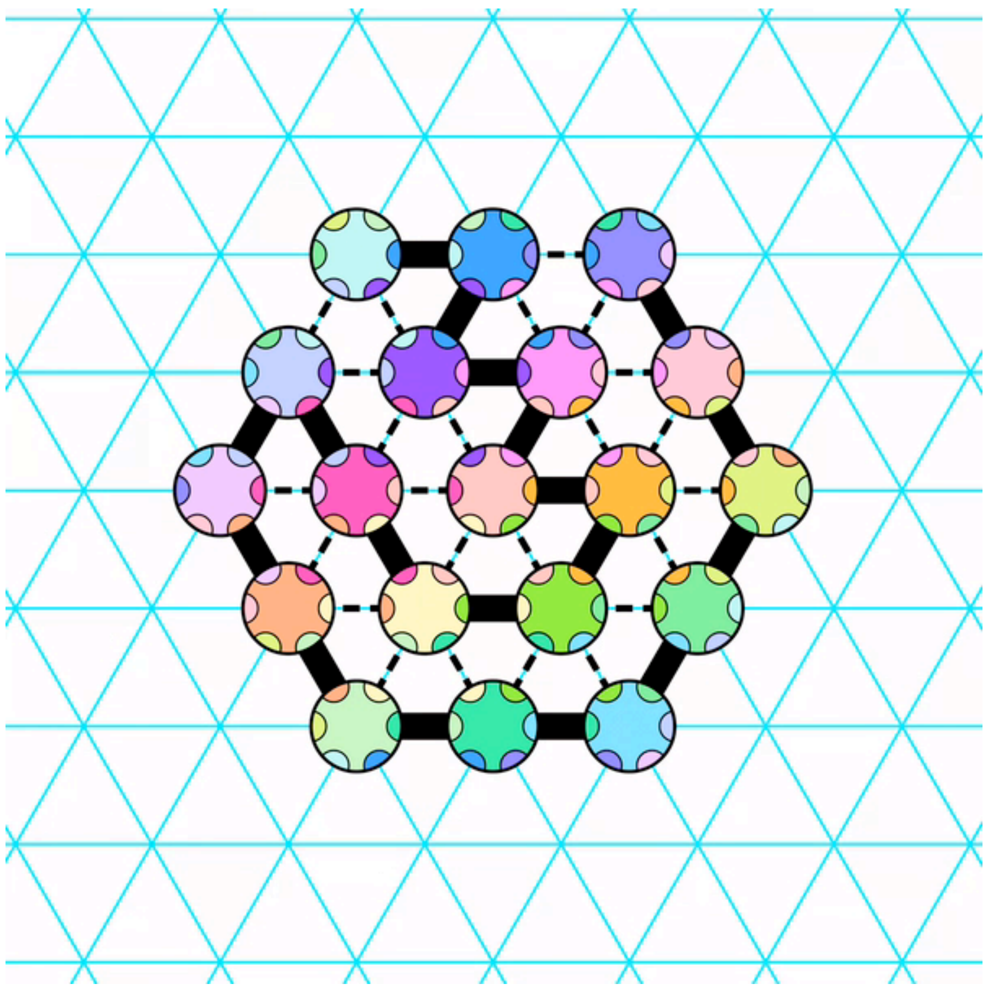

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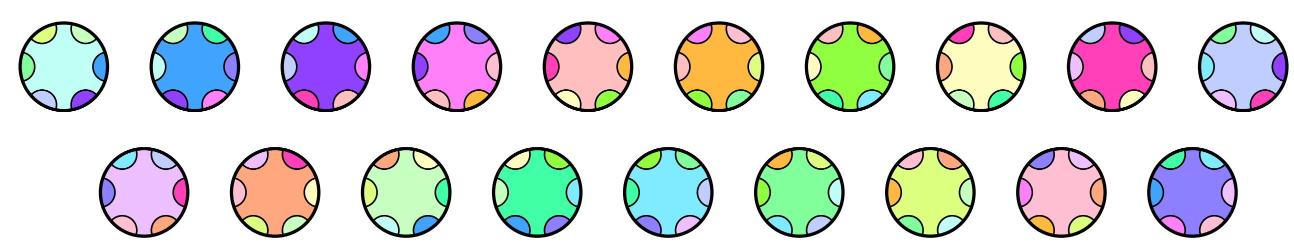
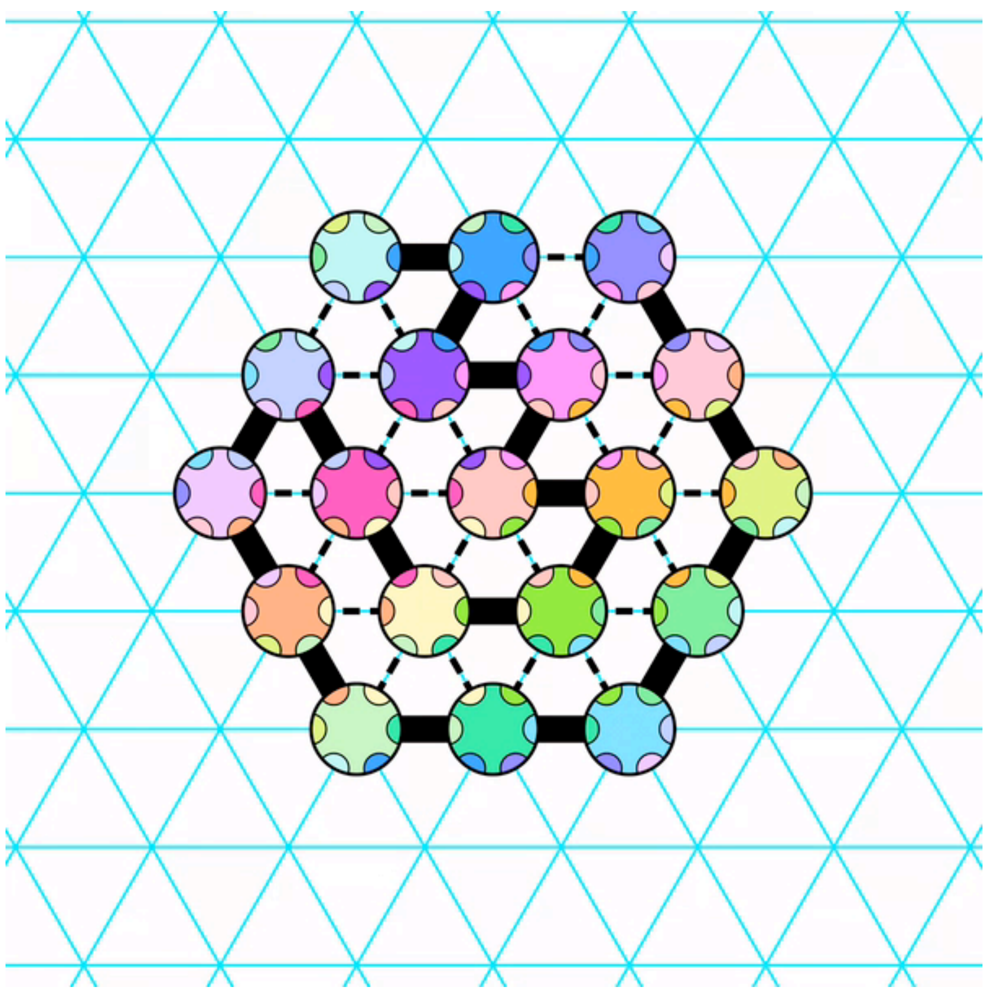


Theorem. There is a **constant-time incremental** algorithm that outputs a tight oritatami system using **19 bead types** that folds any finite shape at scale $\mathscr{B}_{n\,\geq\,3}$ from a **seed of size 3**

19 bead types are enough for tight oritatami systems



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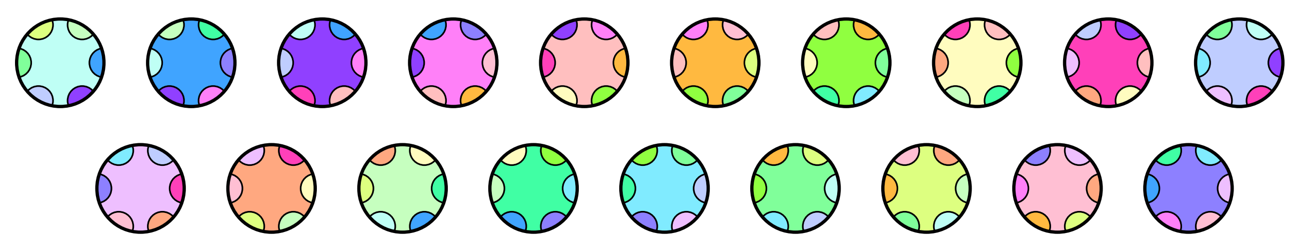


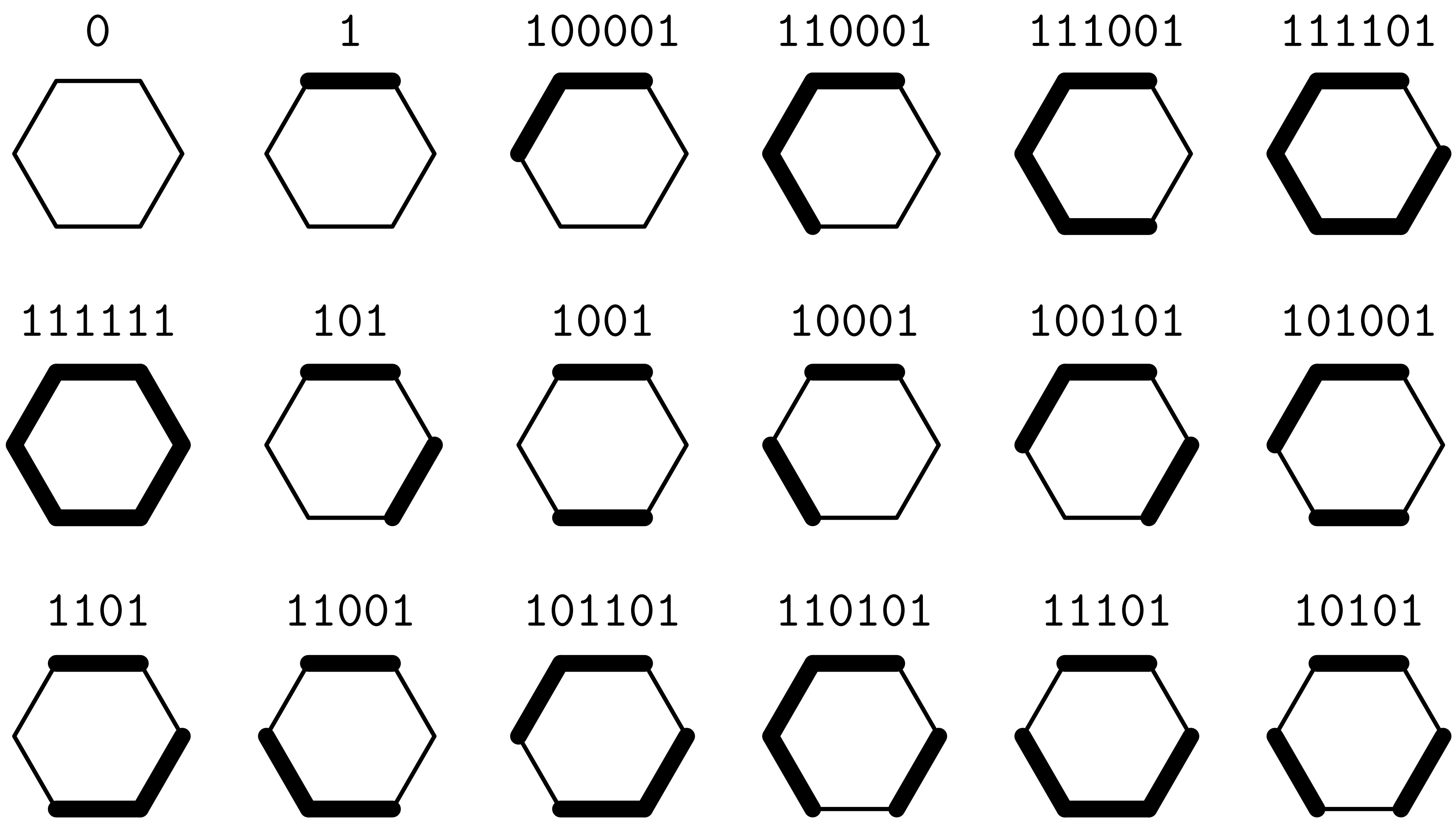
Theorem. There is a **constant-time incremental** algorithm that outputs a tight oritatami system using **19 bead types** that folds any finite shape at scale $\mathcal{B}_{n \geq 3}$ from a **seed of size 3**

Scale $\mathcal{A}_n$

scale $\mathcal{A}_n$

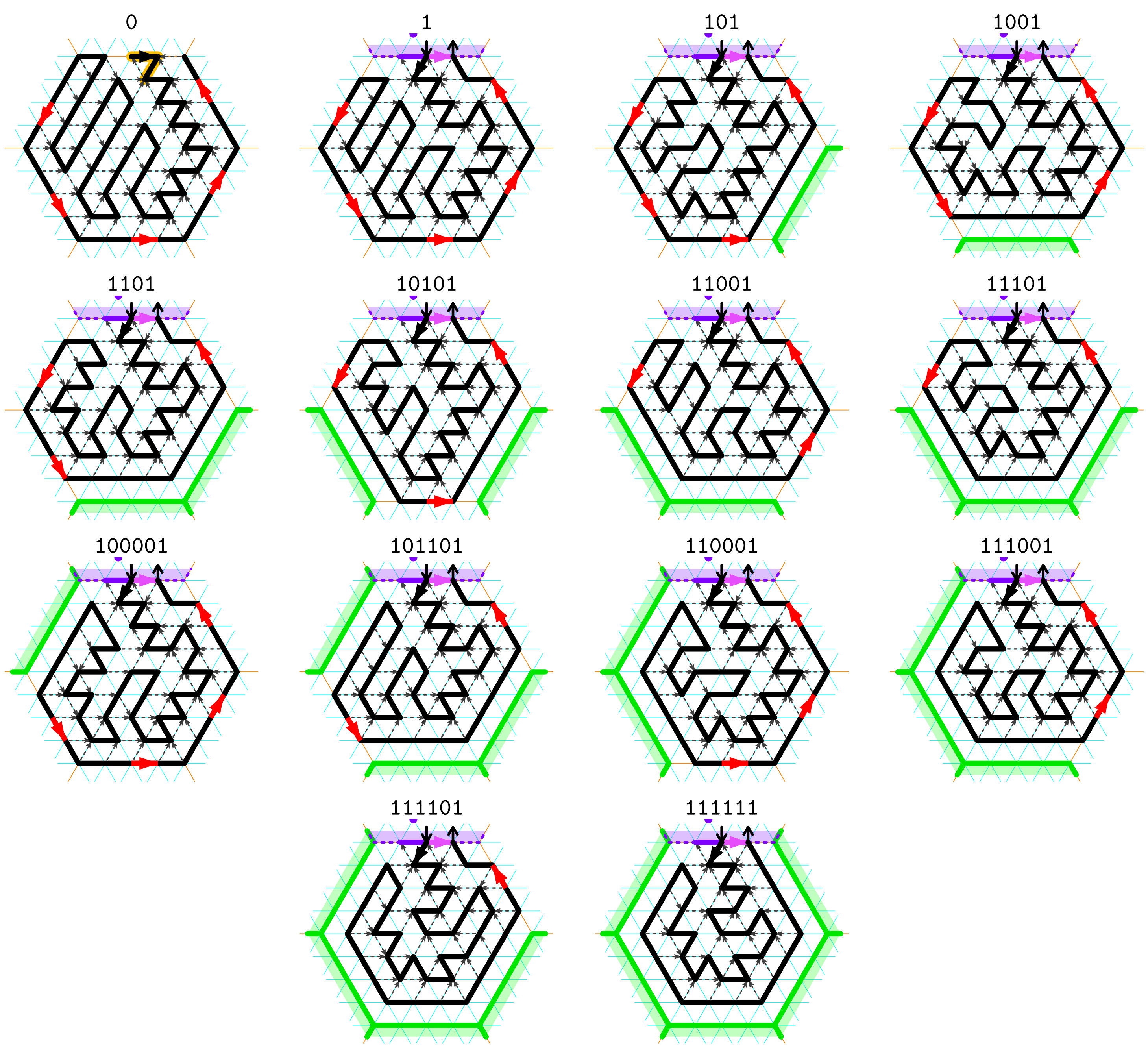
At scale $\mathcal{A}_n$, cells share sides

Plug on the **clockwise-most occupied side** of the cell



The 18 possible configurations

scale $\mathcal{A}_{n\geq 5}$



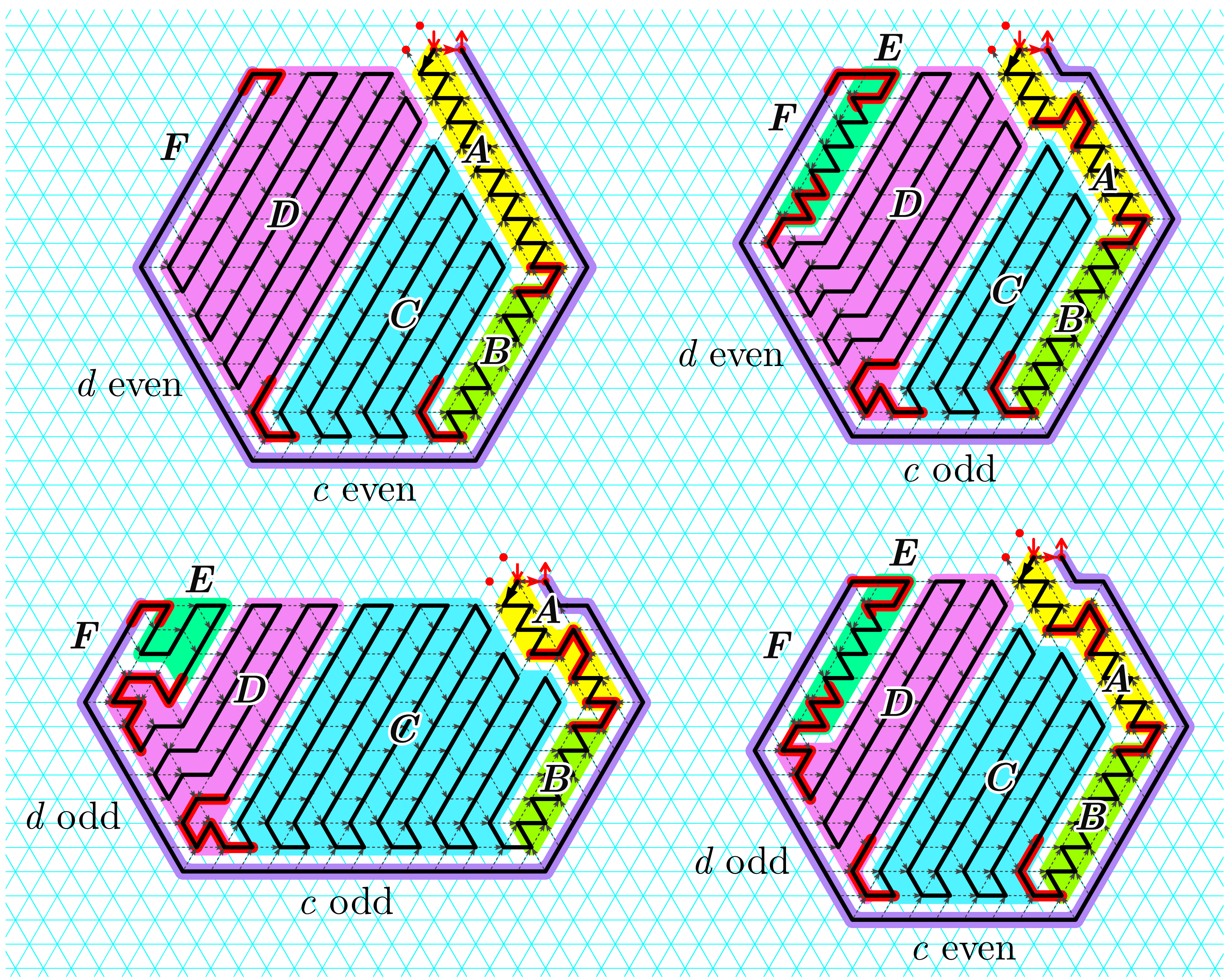
This design ensure that:

- the **purple sites** are always occupied before folding the path
- the path is **tight** and **self-supported**

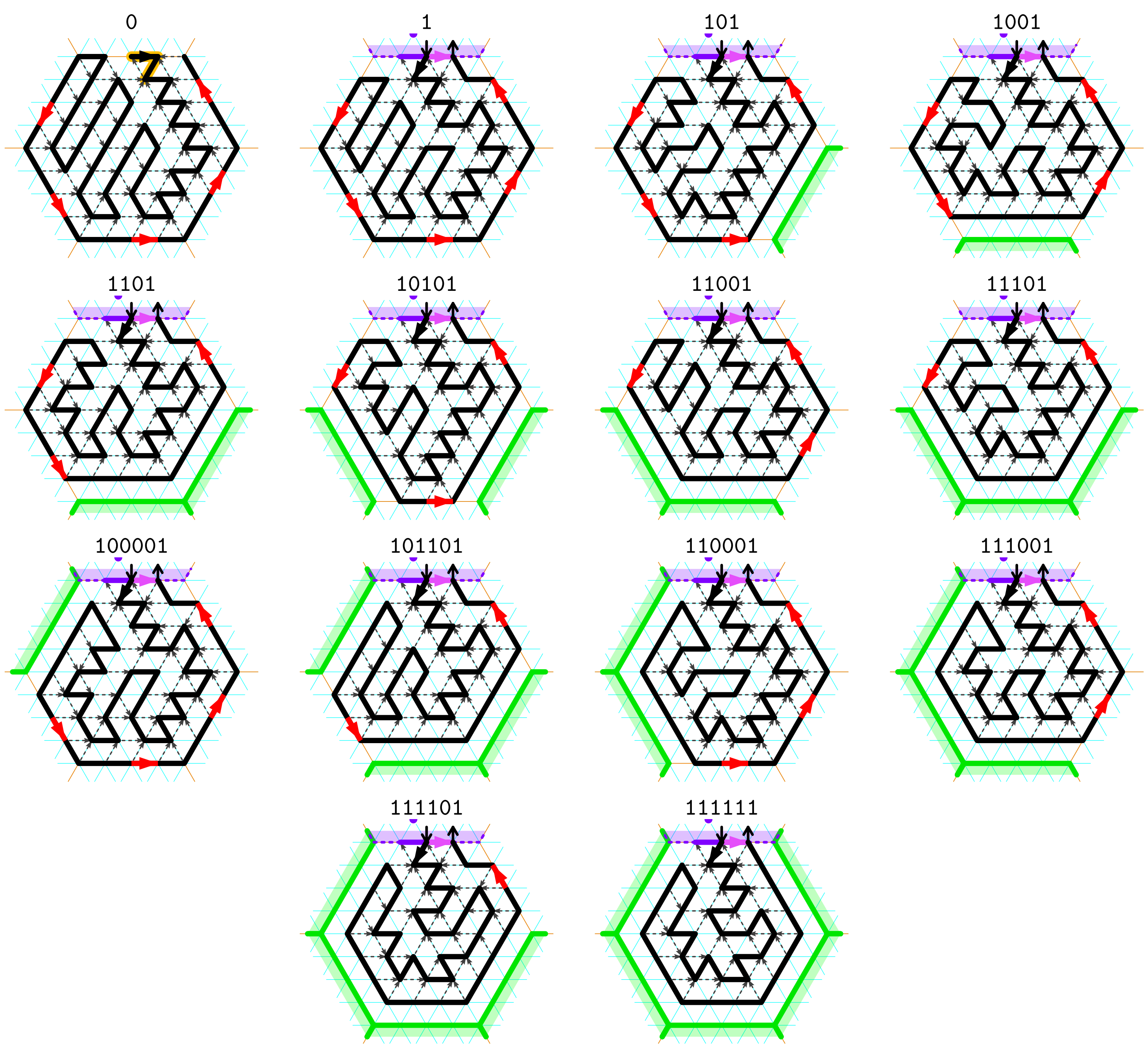
➡ One can **plug on *any* occupied side** to extend the path

Tight paths for pseudo-hexagons

Theorem. There is an algorithm that outputs a tight self-supported path for filling any configuration of an hexagon of radius ≥ 5



scale $\mathcal{A}_{n\geq5}$



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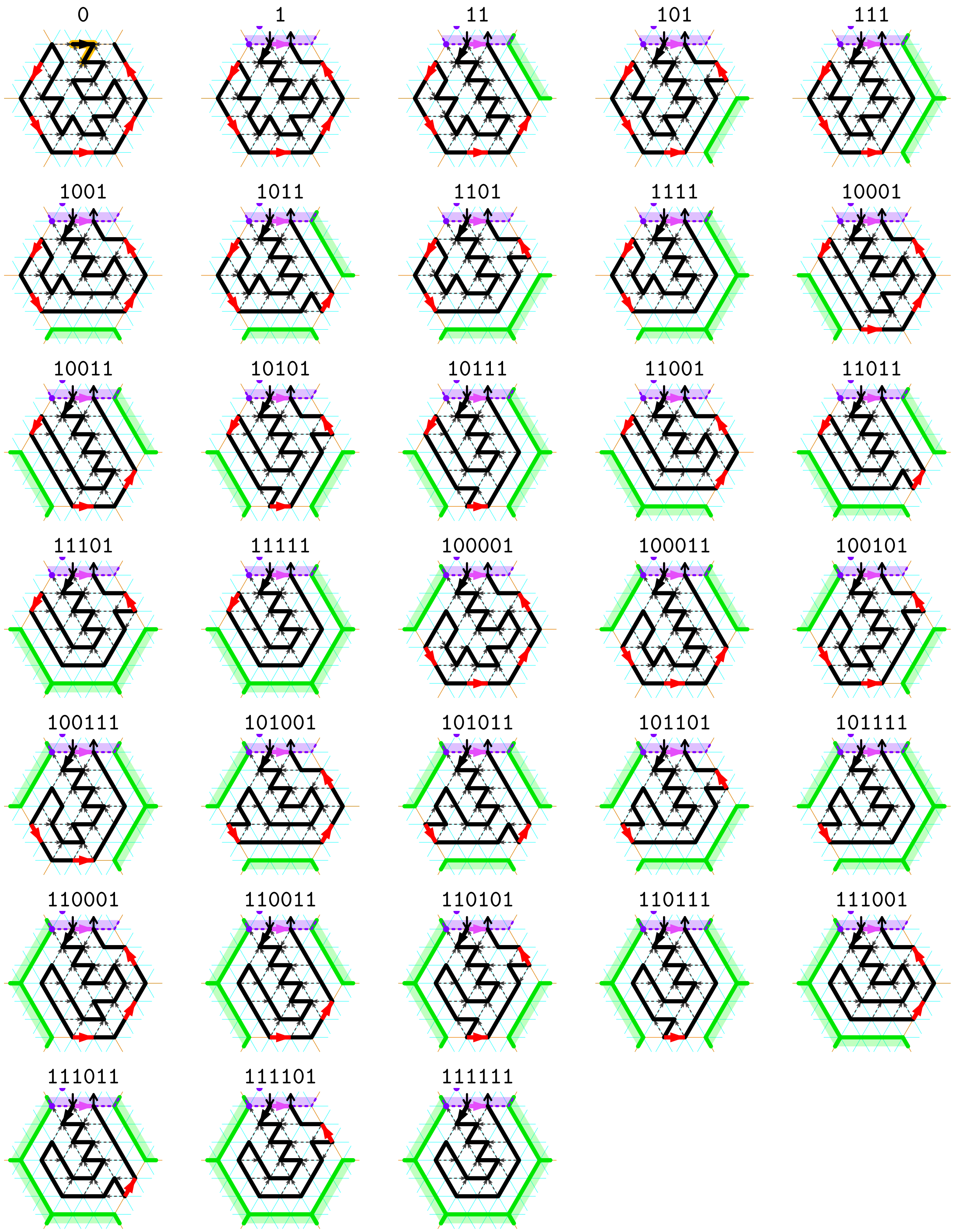
Scale $\mathcal{A}_4$



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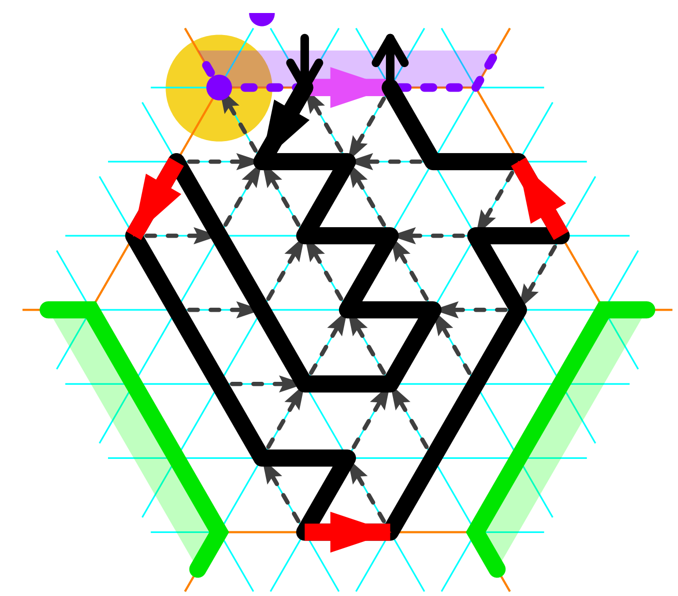
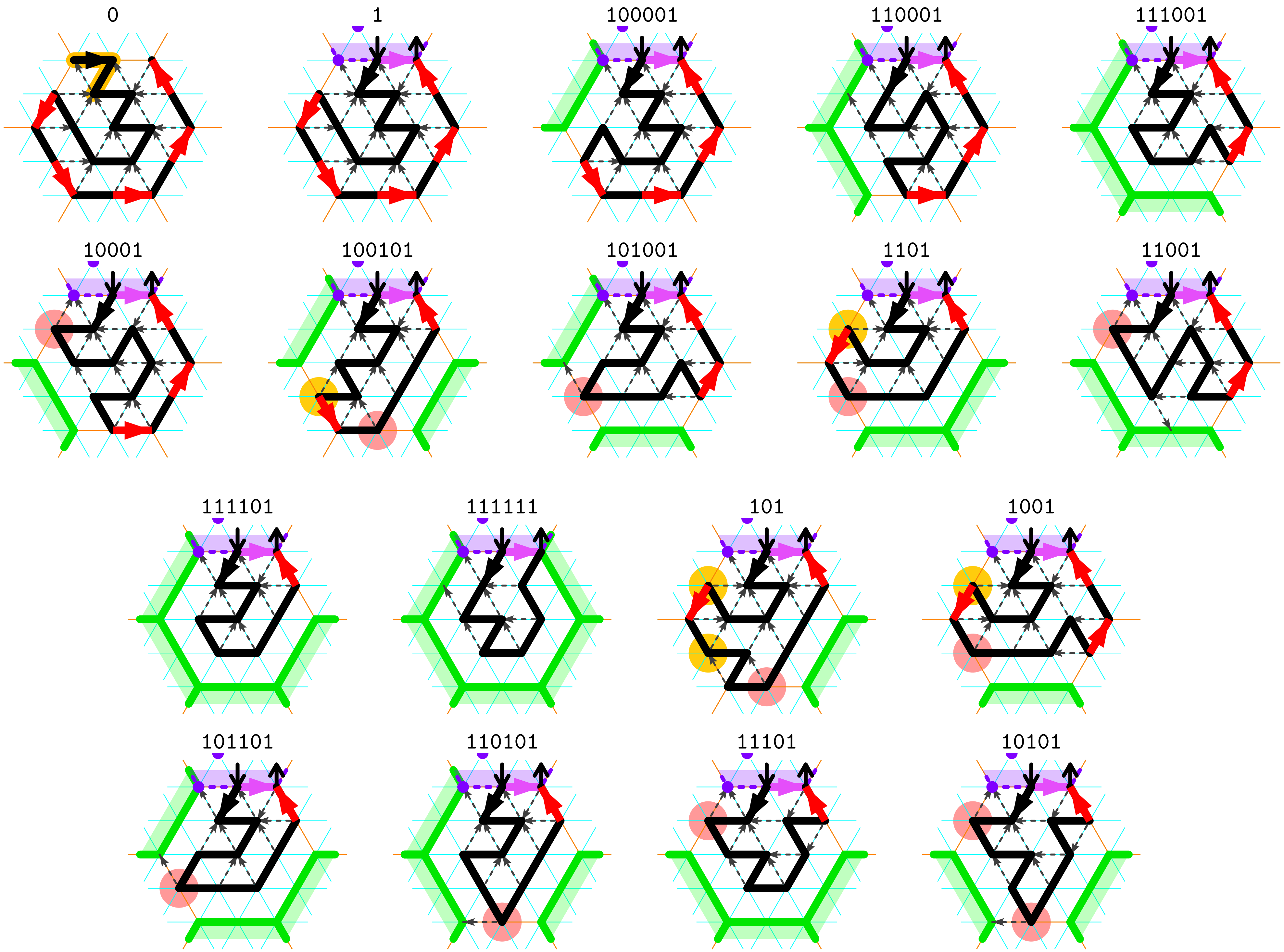


We cannot guarantee the presence of the left purple bead **unless we plug on the latest occupied side** on the current path

$\Longrightarrow$ 32 cases

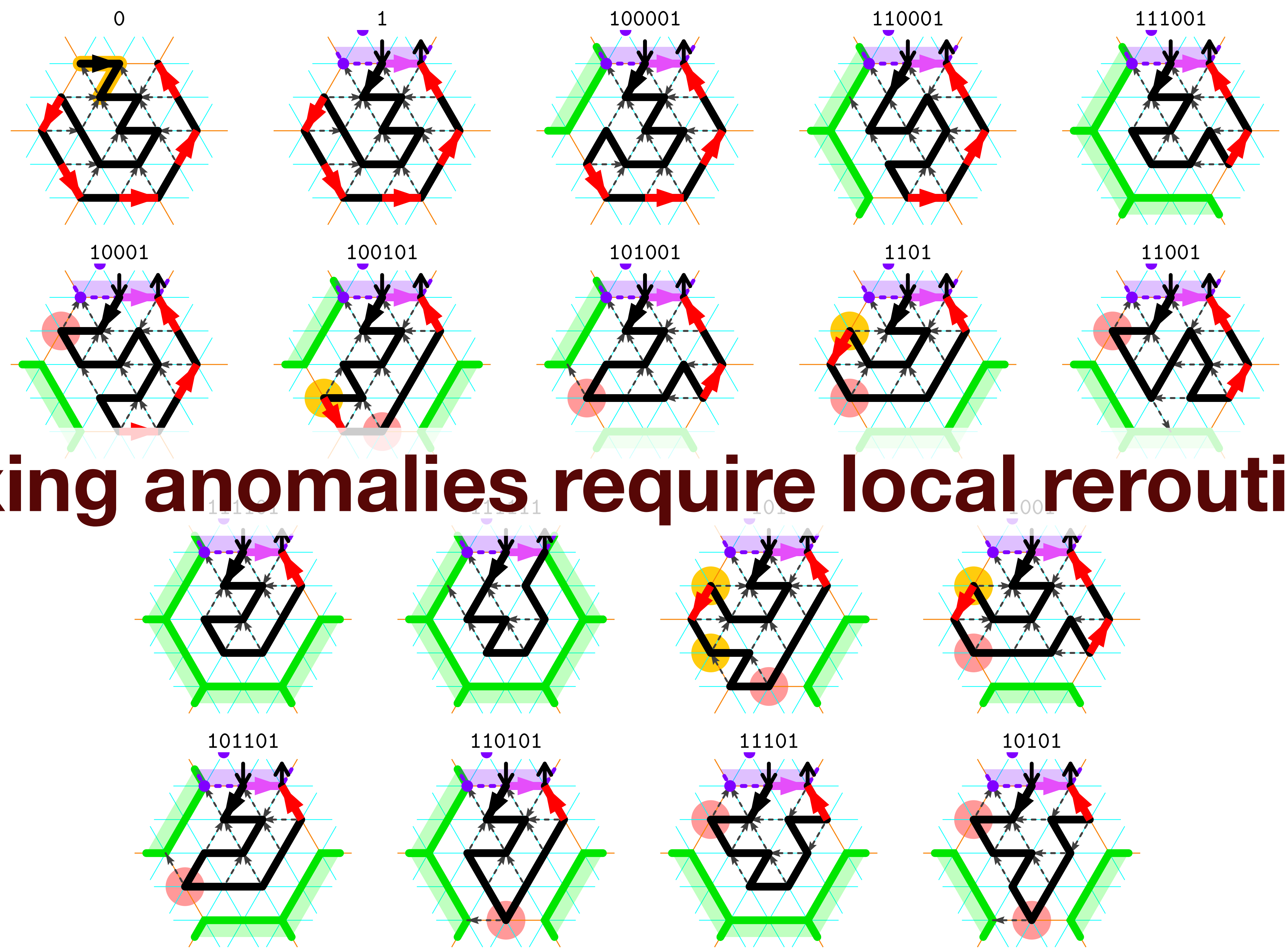
Scale $\mathcal{A}_3$

Scale $\mathcal{A}_3$: Basic cases



Time anomaly: No docking edge **Path anomaly:** Blocking docking edge

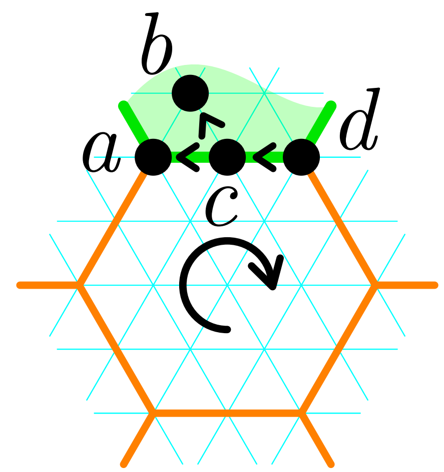
Scale $\mathcal{A}_3$: Basic cases



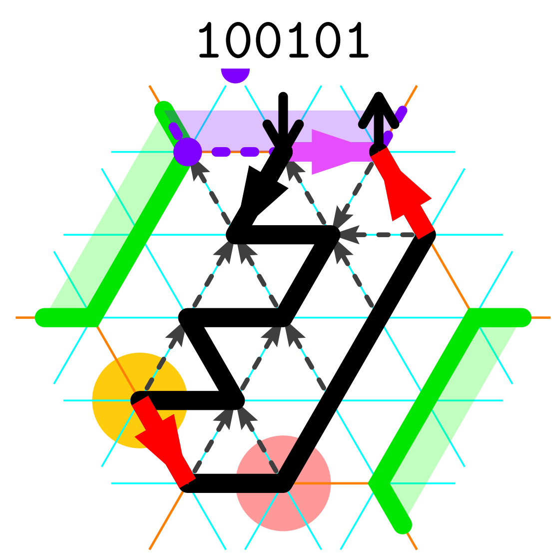
Fixing anomalies require local rerouting

Time anomaly: No docking edge **Path anomaly:** Blocking docking edge

Scale $\mathcal{A}_3$: Invariants



For every occupied side of an empty cell:
time(a), time(b) < time(c) < time(d)

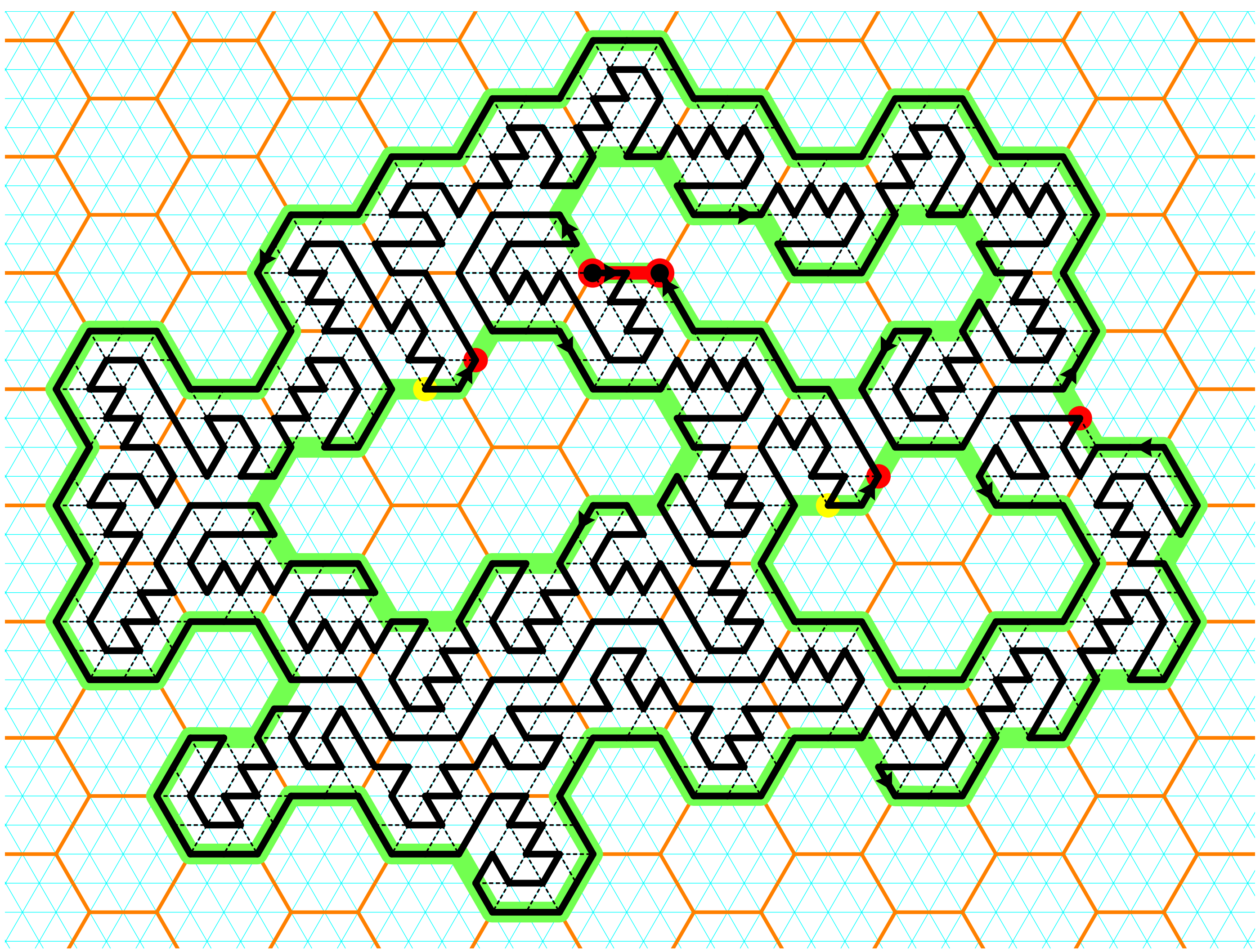


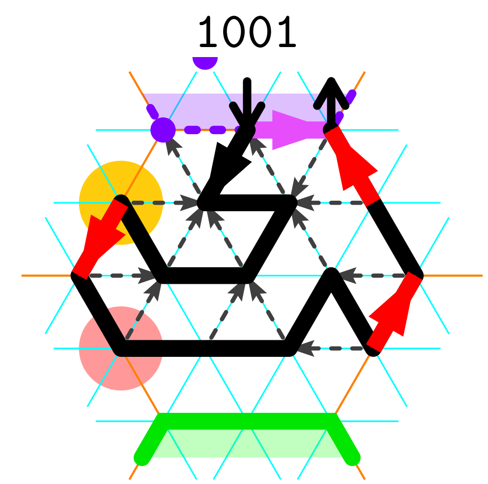
the clockwise-most side of a segment in an empty cell is always the latest on the path if it is not a time-anomaly

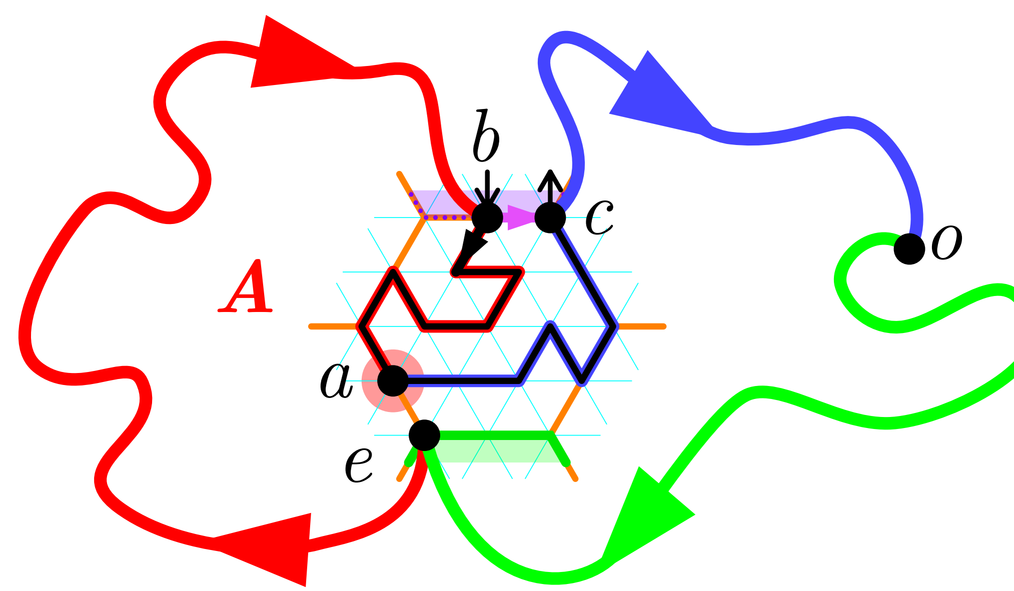
Scale $\mathcal{A}_3$: time-anomalies

Lemma. There is **exactly one single time-anomaly** on the boundary of every empty zone A

Proof by Jordan's theorem







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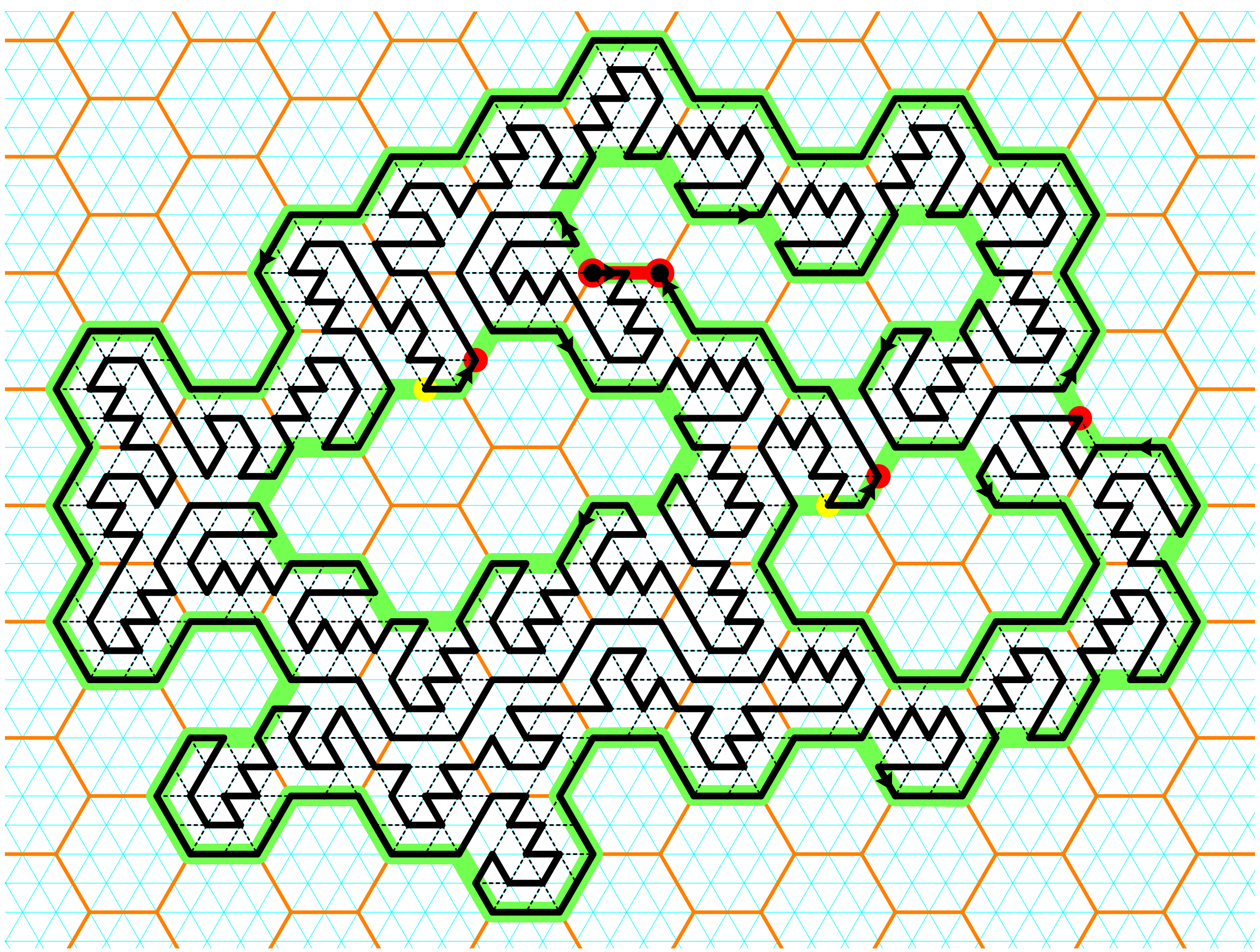
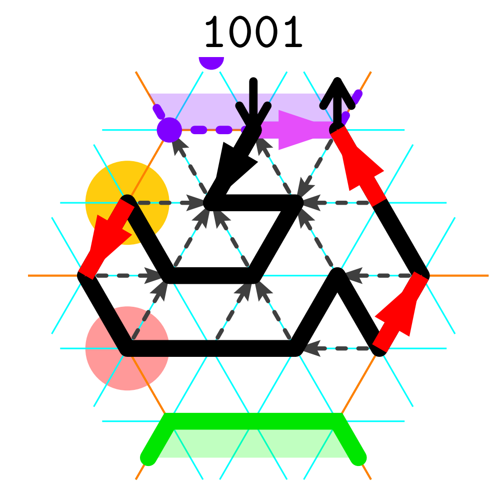
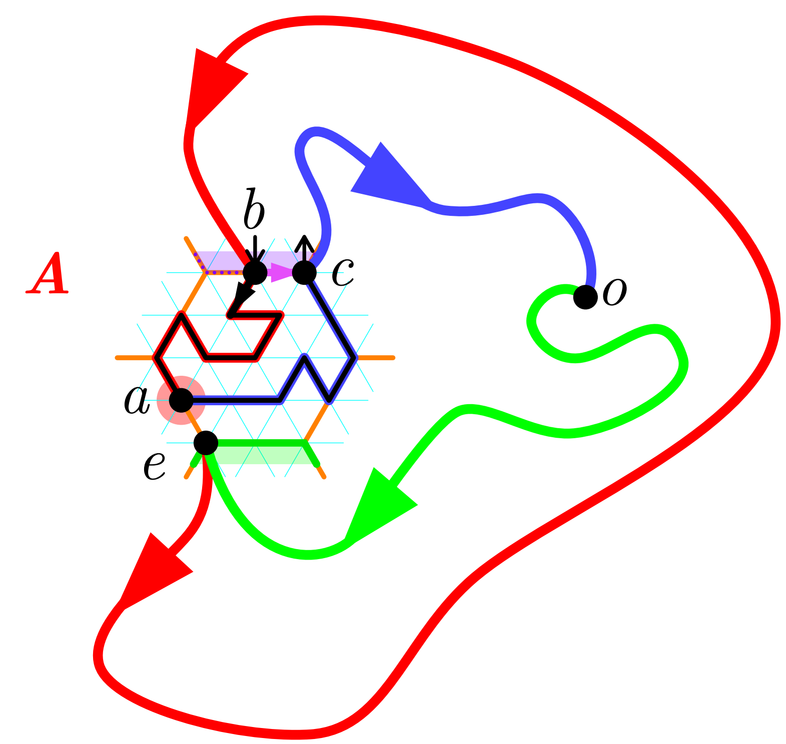
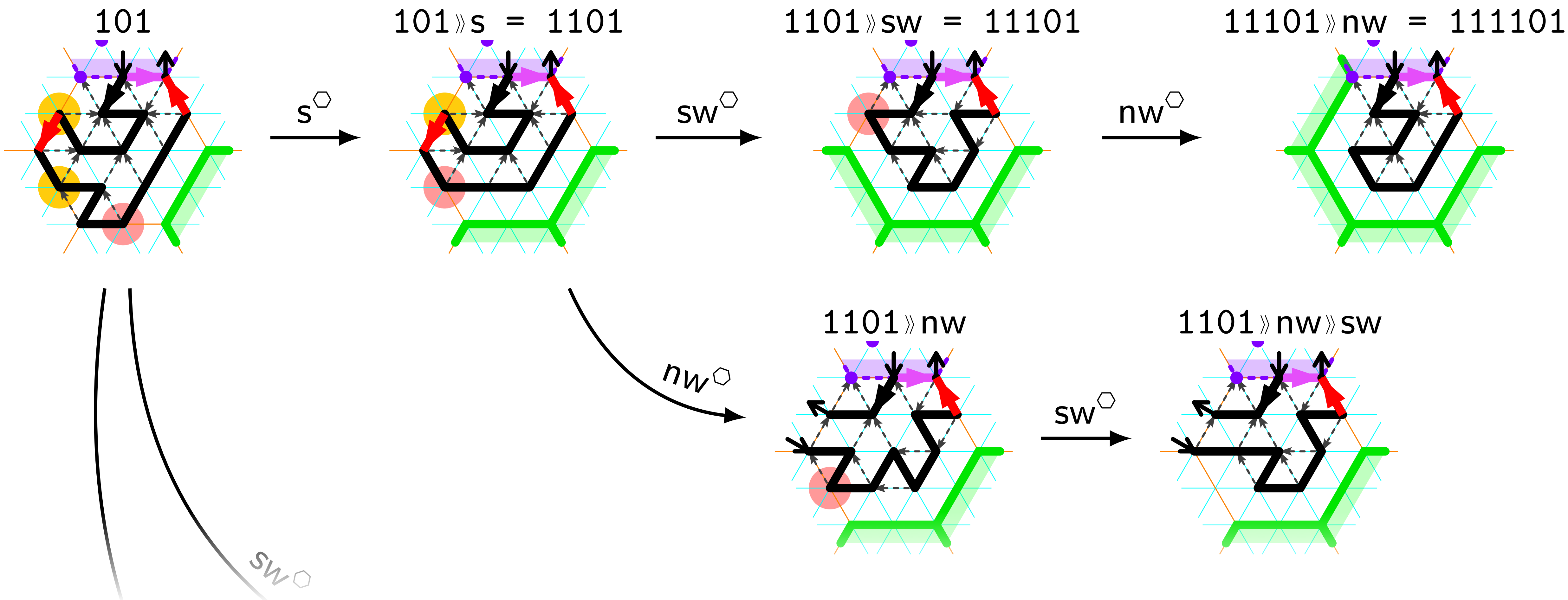


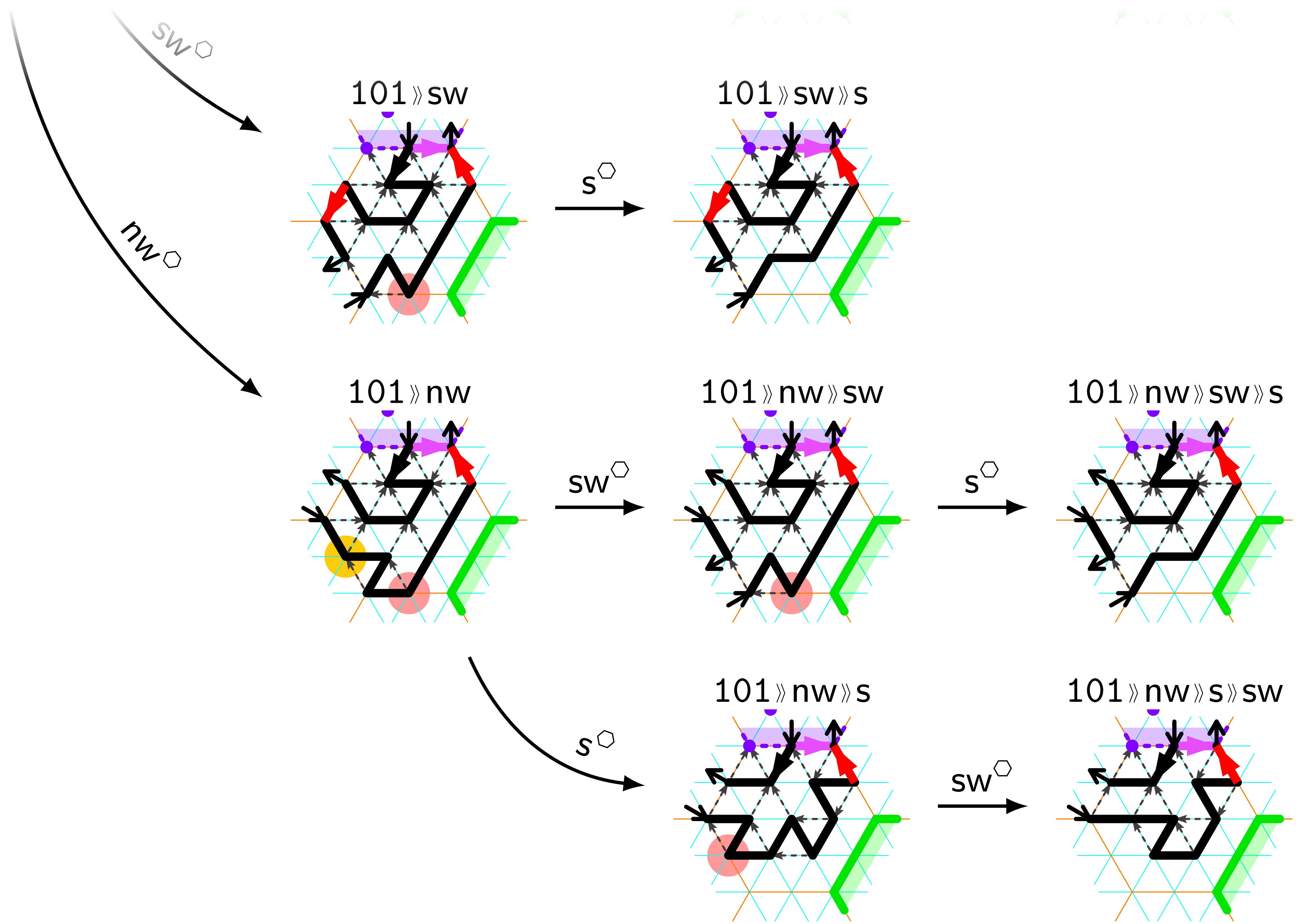




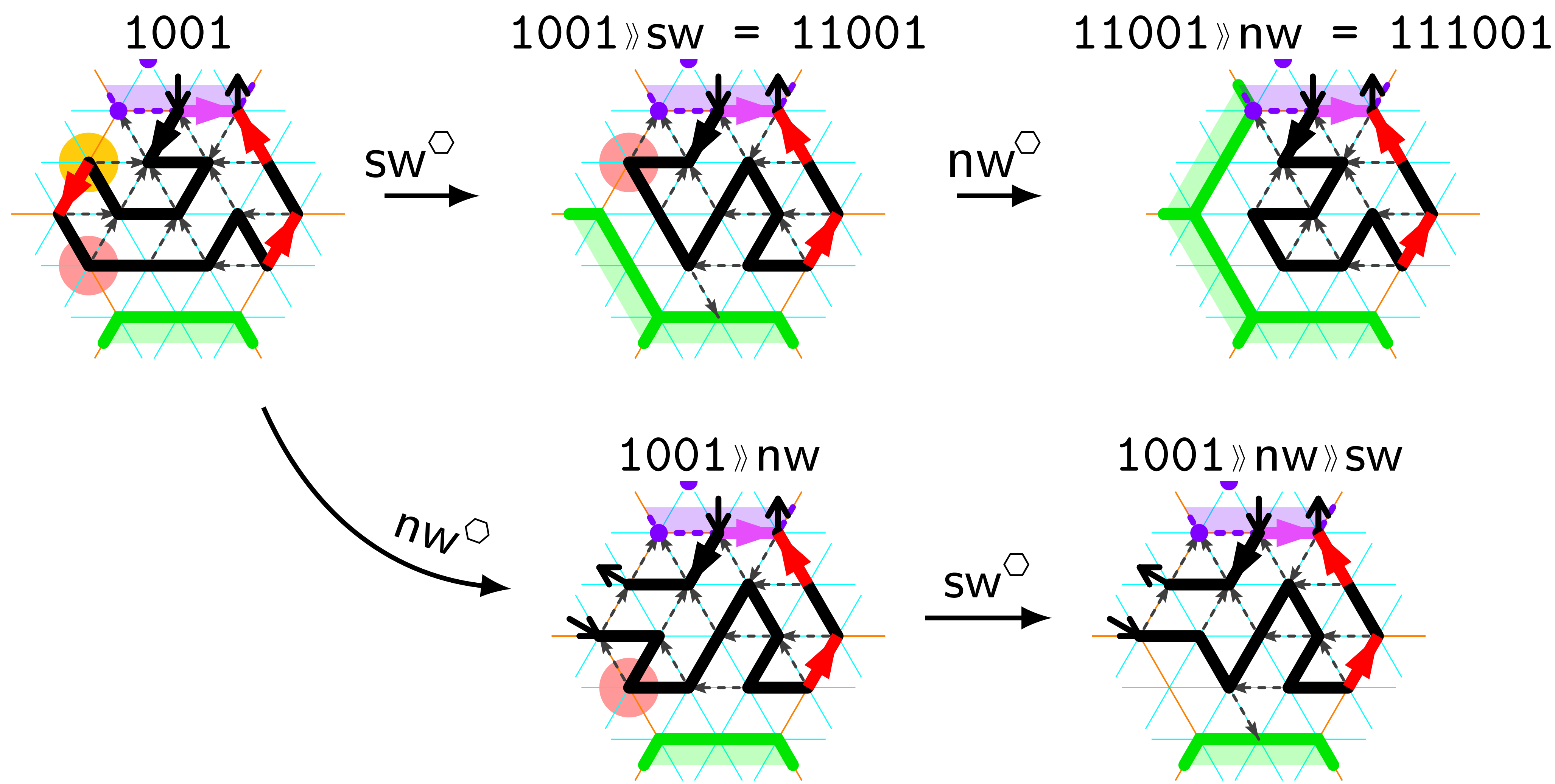
Scale $\mathcal{A}_3$: Fix anomalies



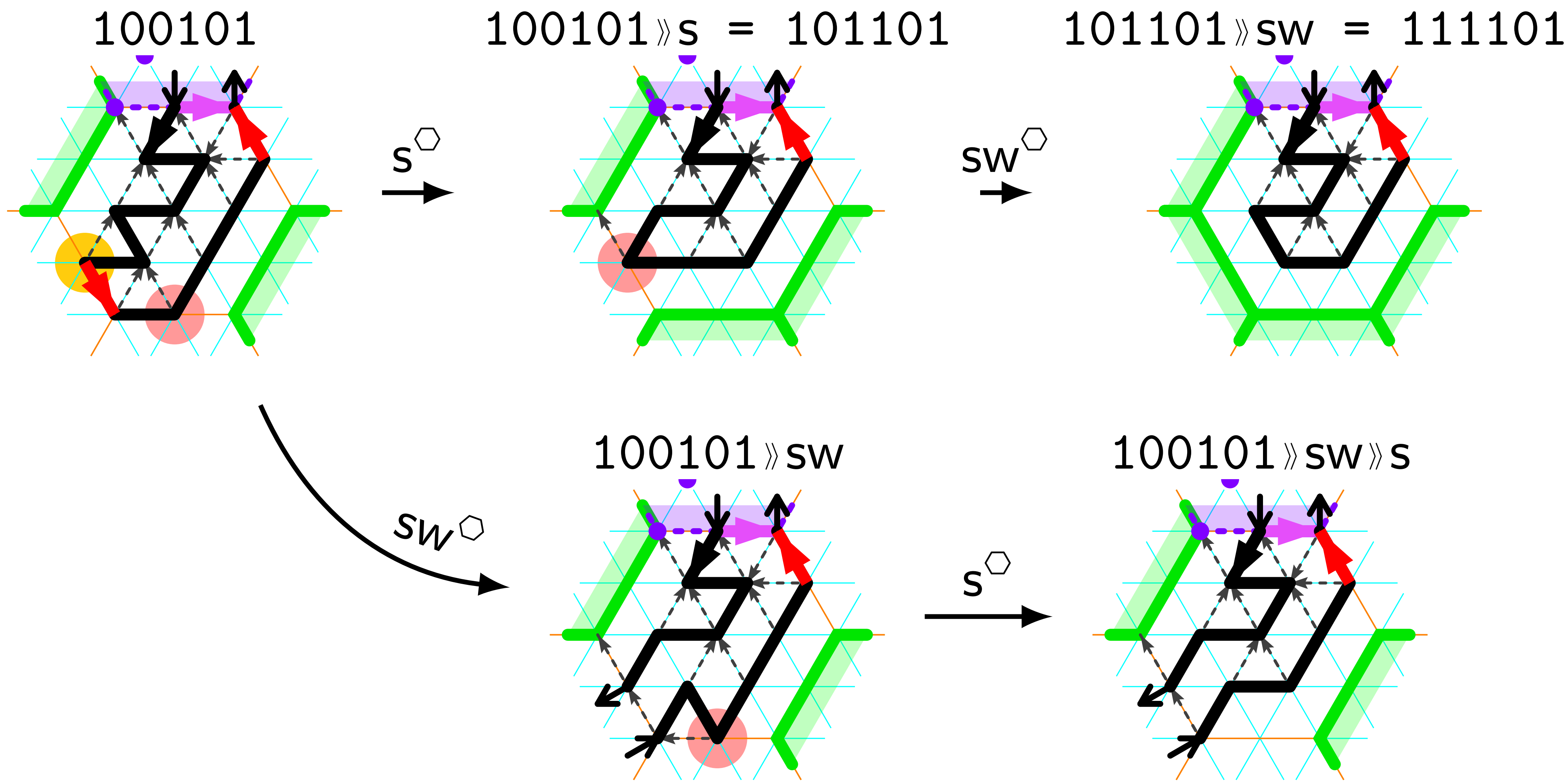
Scale $\mathcal{A}_3$: Fix anomalies



Scale $\mathcal{A}_3$: Fix anomalies

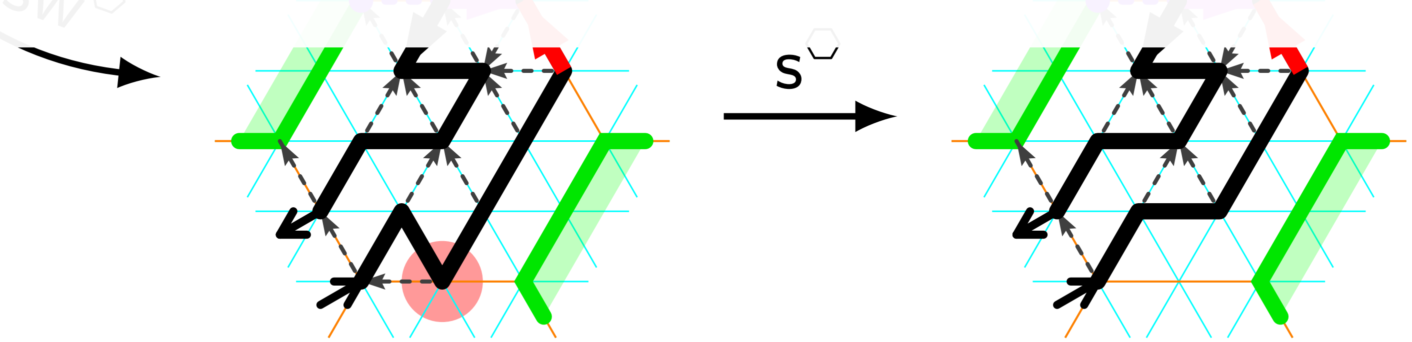


Scale $\mathcal{A}_3$: Fix anomalies

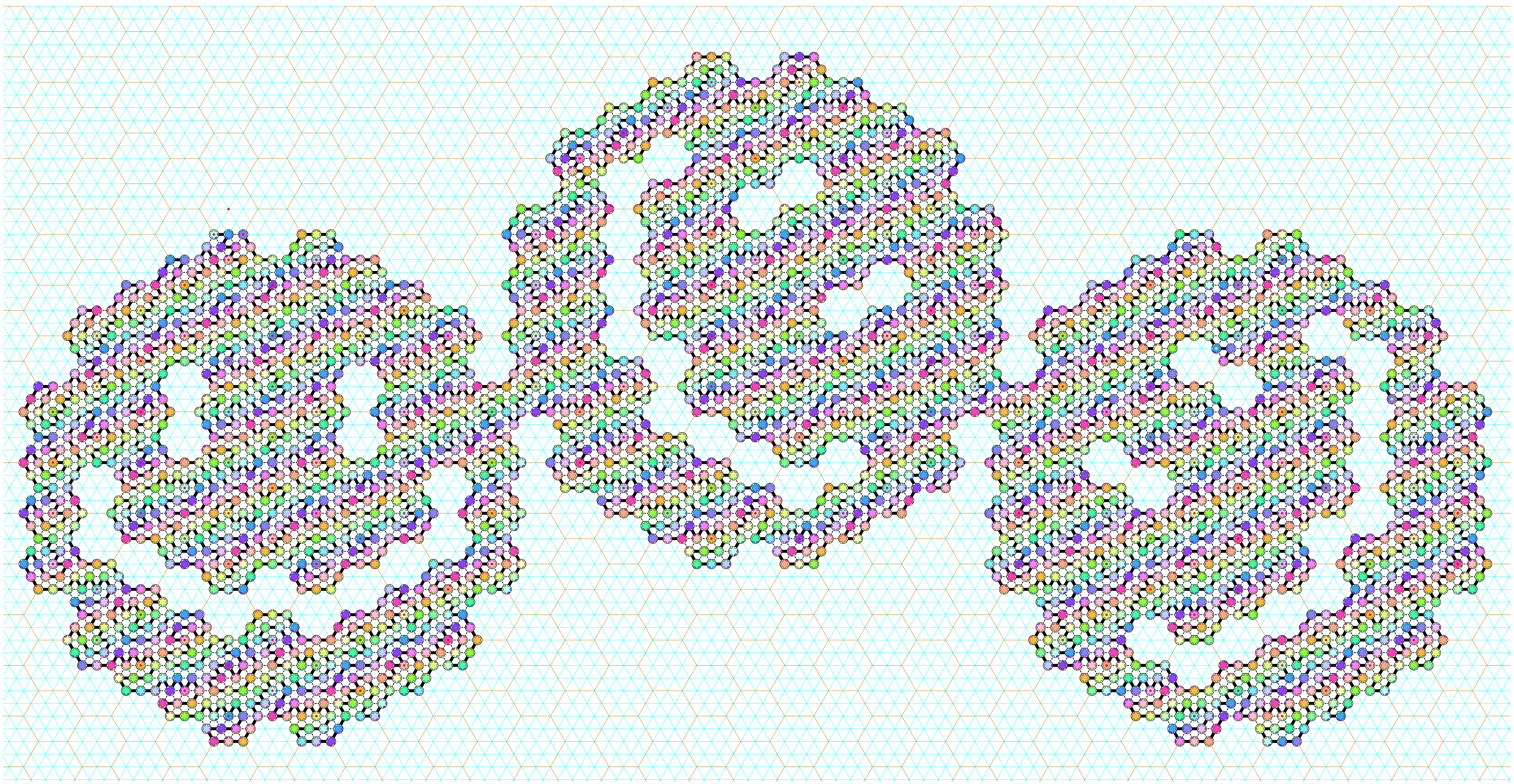


Scale $\mathscr{A}_3$: Fix anomalies

Theorem.
There is an **log-time incremental** algorithm that outputs a tight oritatami system using **19 bead types** that folds any finite shape at scale $\mathscr{A}_3$ from a **seed of size 3**

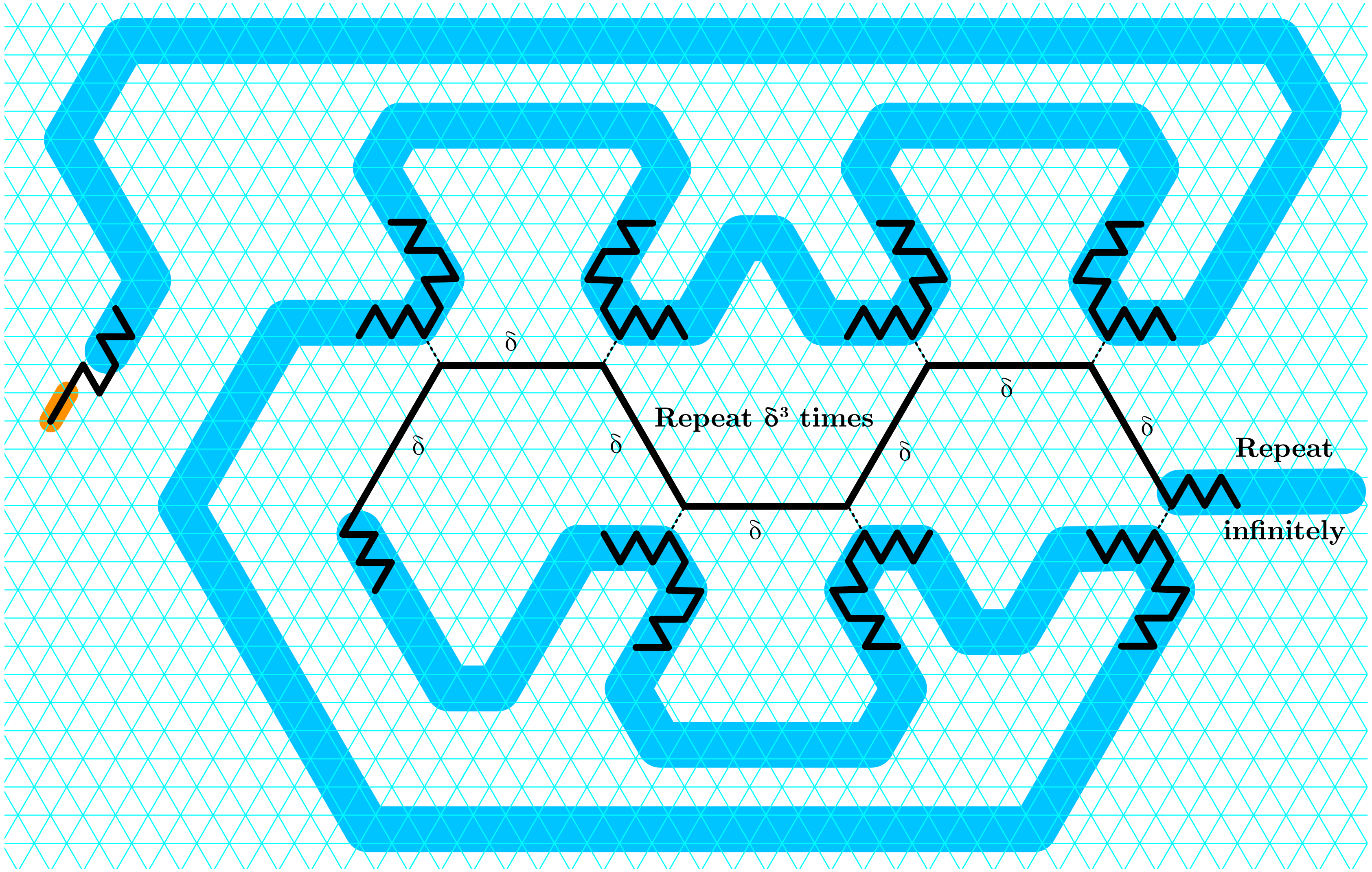


An example



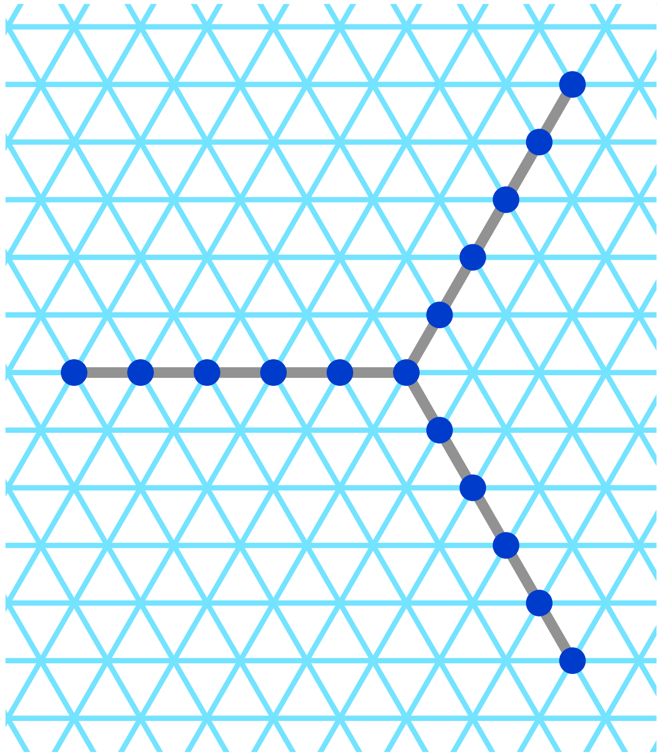
Would increasing the delay instead of upscaling help?

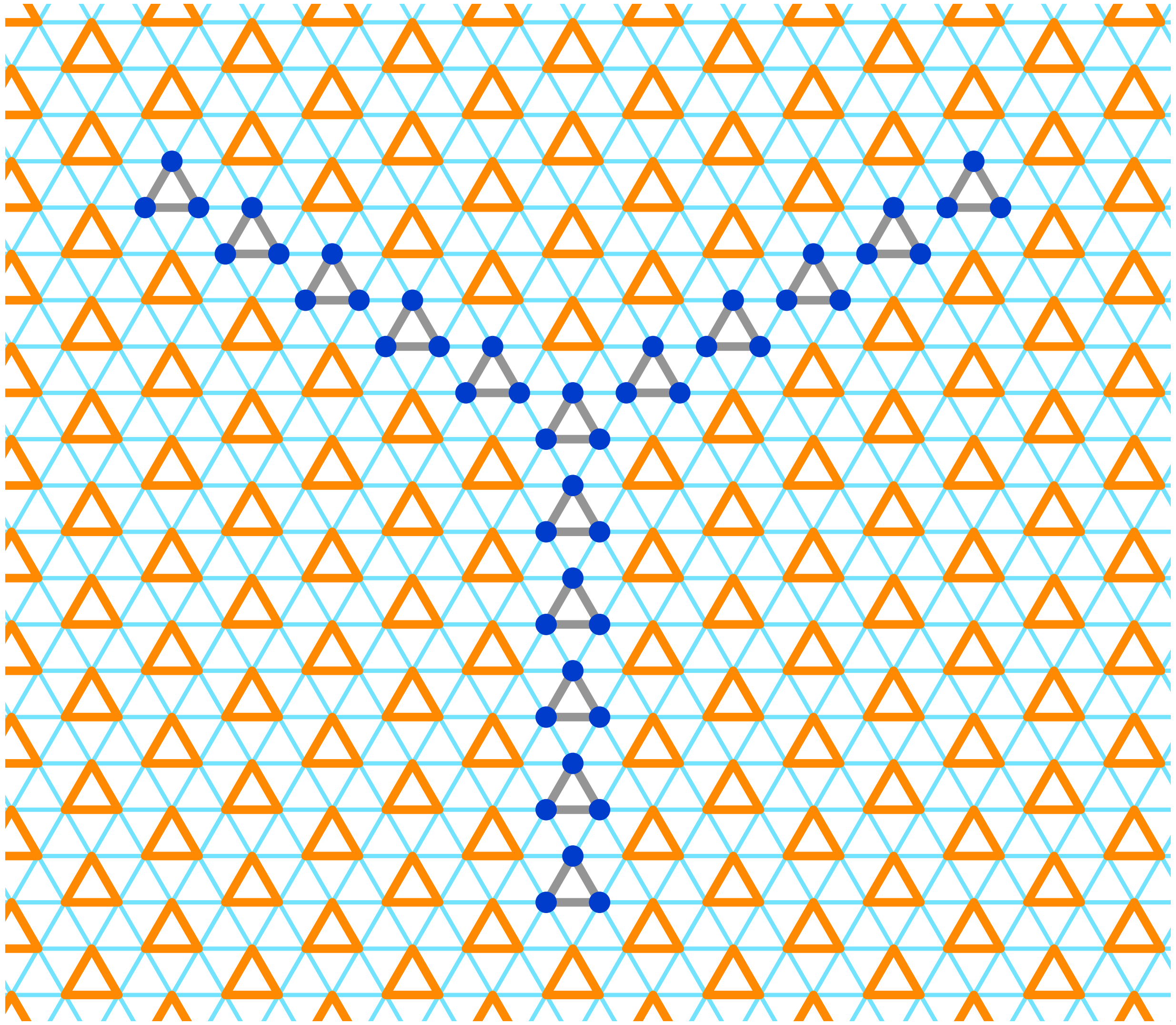
Theorem. For any delay δ, there is an infinite shape that cannot be folded by no oritatami system with delay δ



A shape impossible to build at scale < 3?

The three arms star

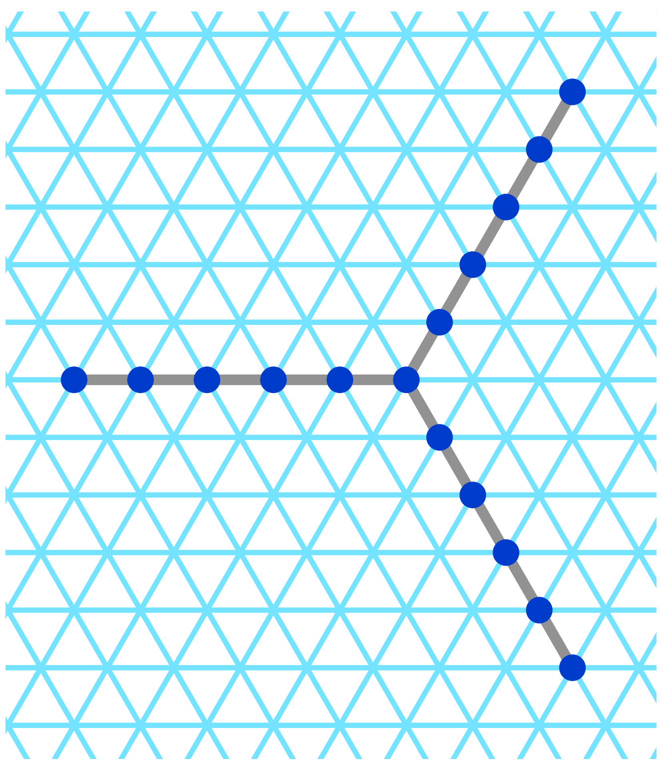


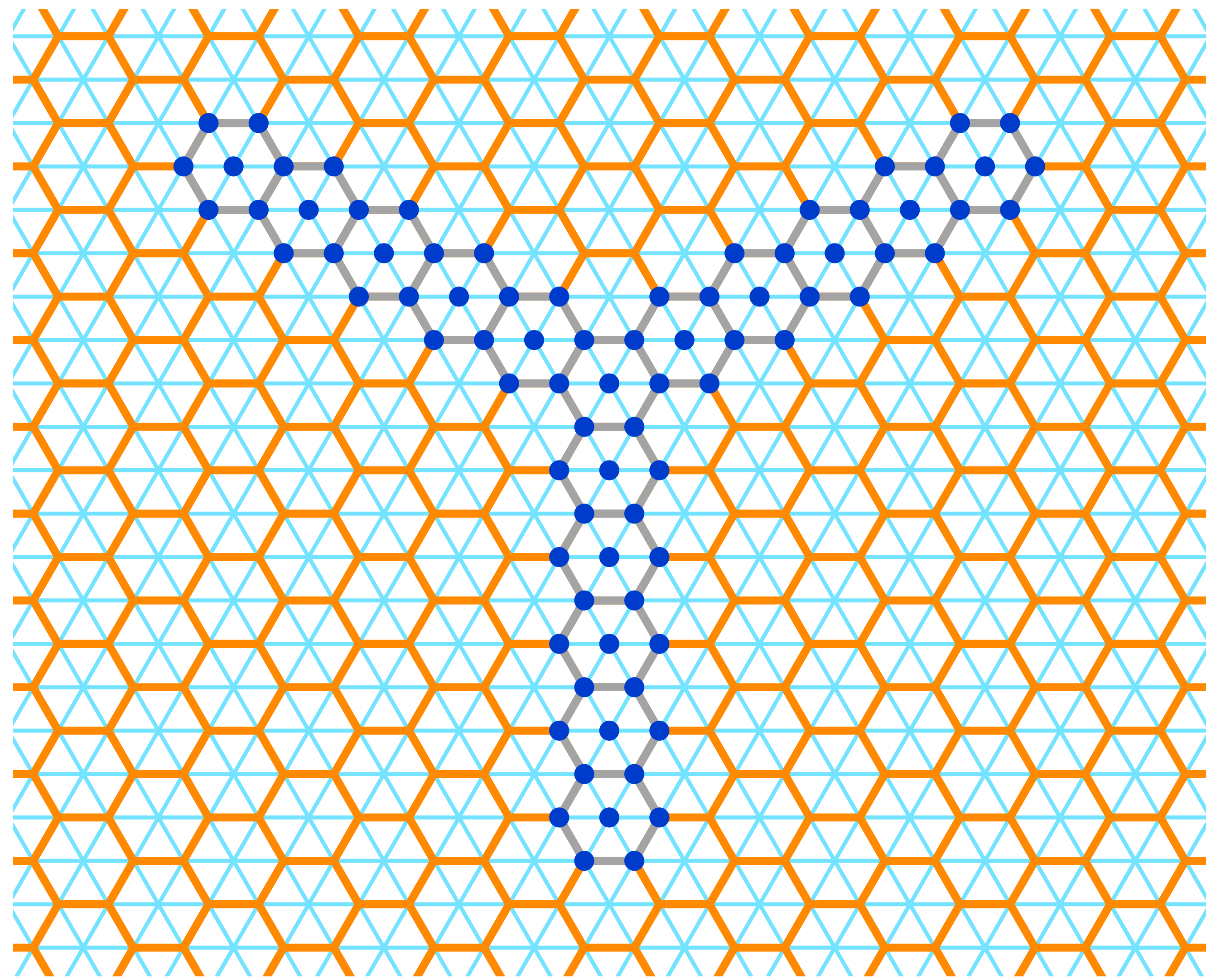


Impossible at this scale: not Hamiltonian

A shape impossible to build at scale < 3?

The three arms star

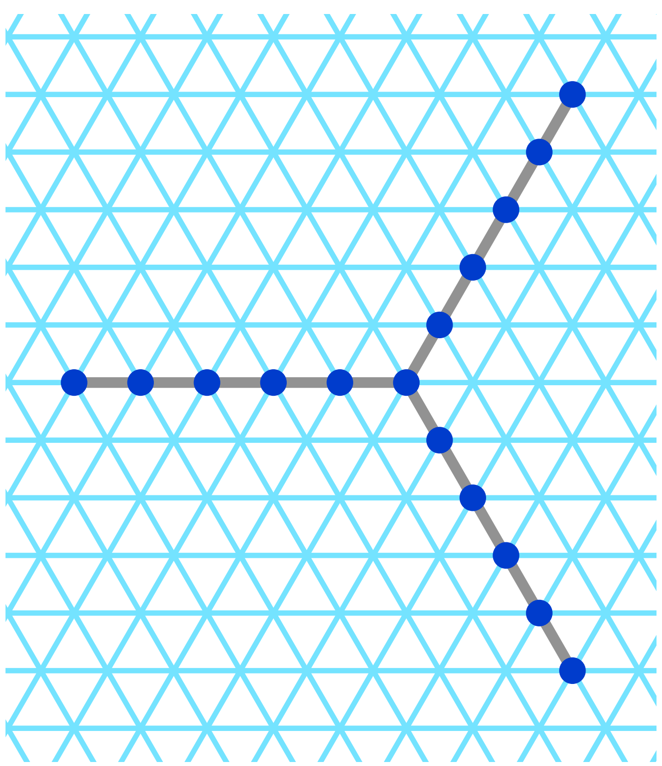


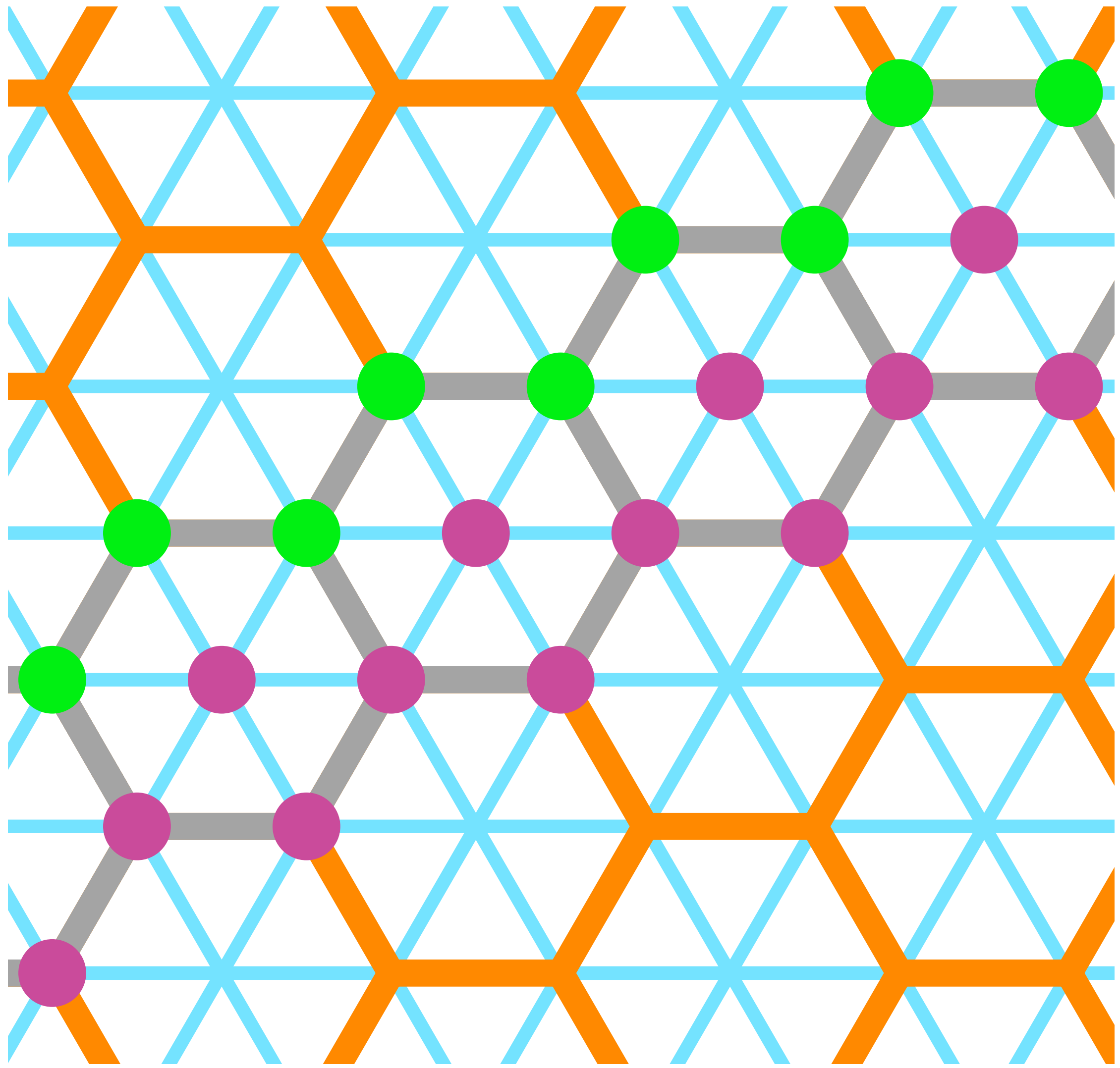


At least one arm must be folded from the center back and forth

A shape impossible to build at scale < 3?

The three arms star

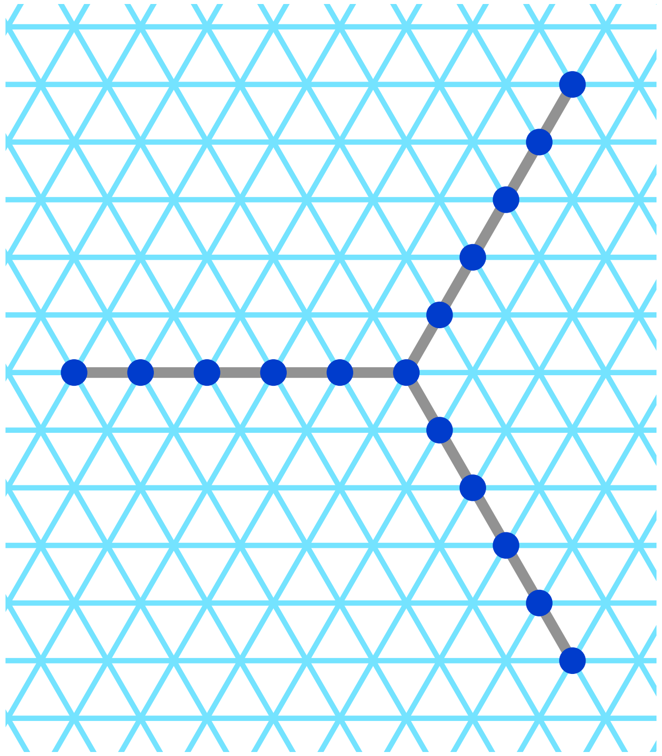


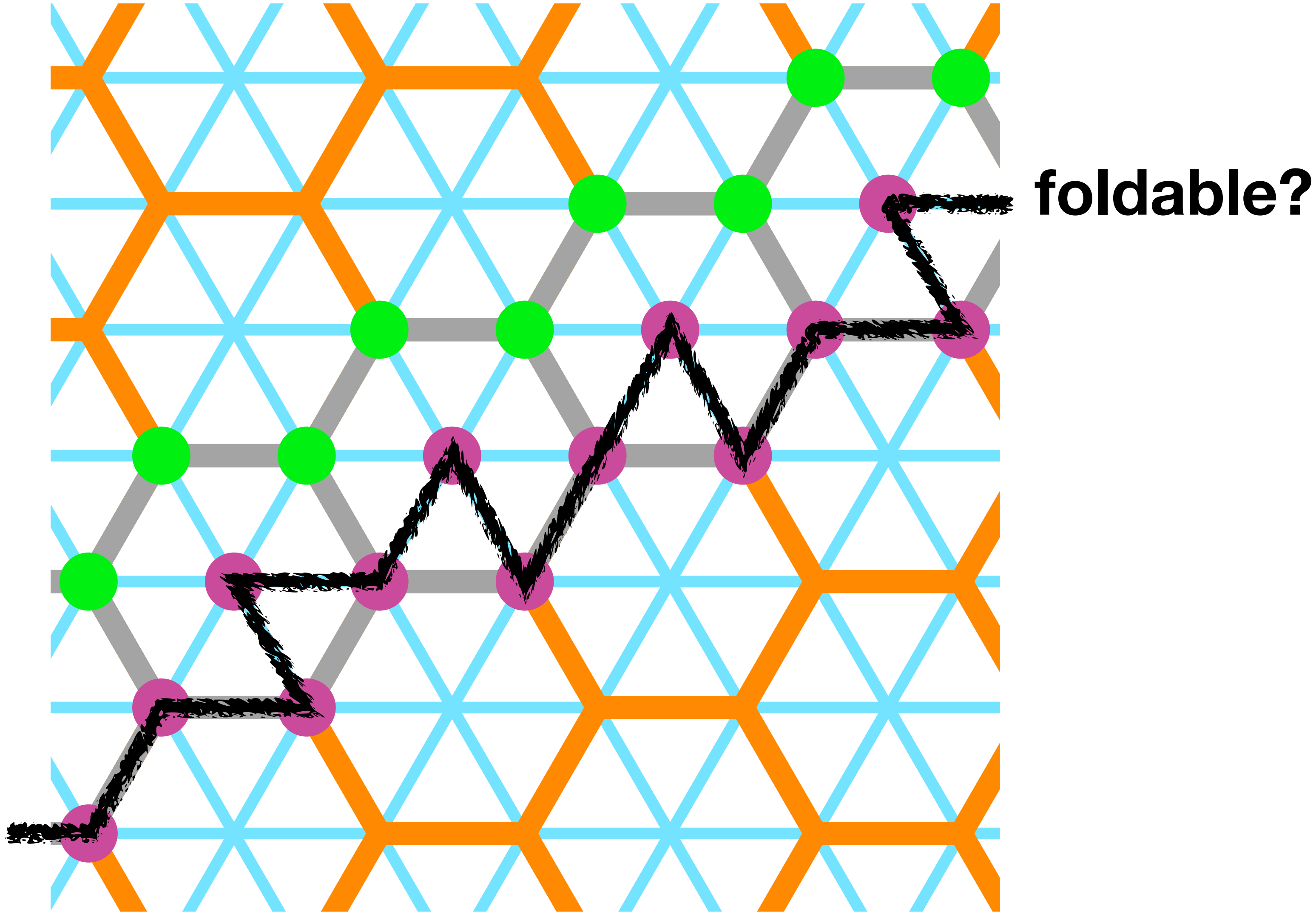


In this arm, **pink** must be filled before **green**… Is it possible?

A shape impossible to build at scale < 3?

The three arms star





In this arm, **pink** must be filled before **green**… Is it possible?

Conclusion

- A **nearly-constant time incremental algorithm** that outputs a **19-bead types** tight oritatami system that folds ***any* finite shape** at all **scale A_n** and **B_n with $n \geq 3$,** from a **seed of size 3**
- As opposed to the number of tile types in aTAM, the **number of bead types** does **not depend on the Kolmogorov complexity** of the shape
- **Universal set of bead types** for tight oritatami systems (with arbitrary delay δ as well)
- **Conjecture:** The three arms star cannot be folded at scale A2 and B2 for all delay

Scary Pacman