

# Algorithmic self-assembly with DNA tiles

## Tutorial

David Doty (UC-Davis)

23<sup>rd</sup> International Meeting on DNA Computing and Molecular Programming

University of Texas–Austin

September 2017

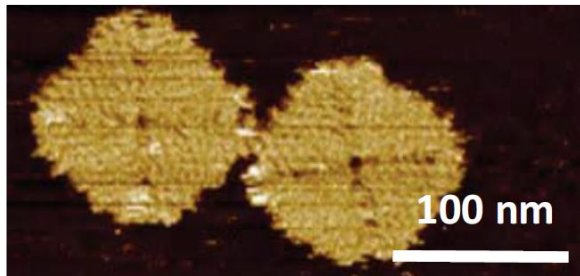
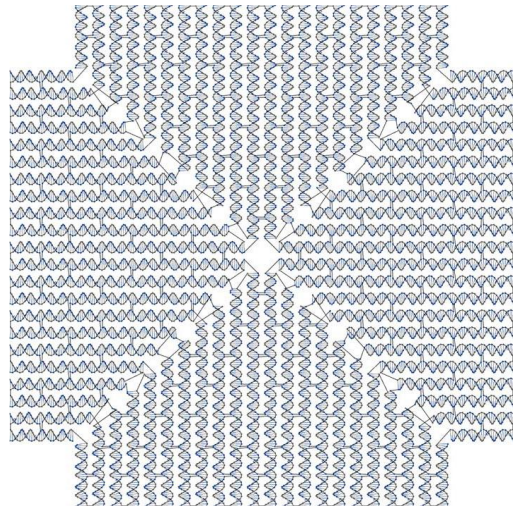


# DNA tile self-assembly

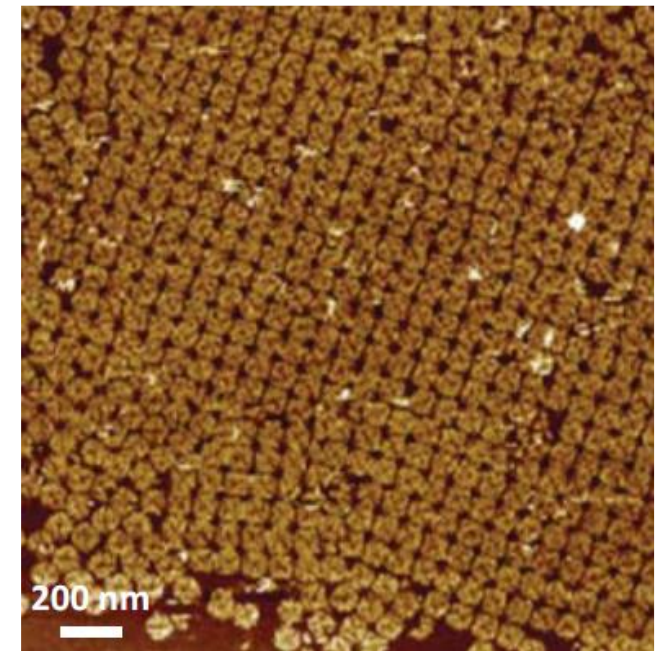
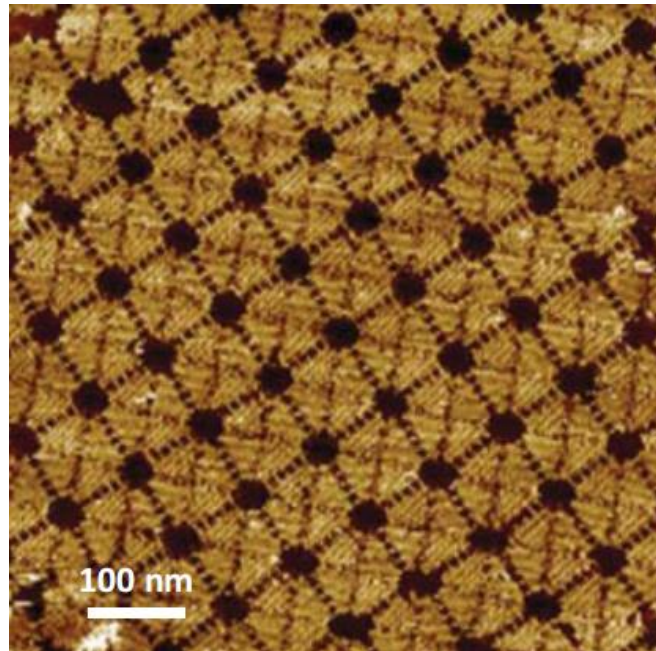
# DNA tile self-assembly

monomers (“tiles” made from DNA) bind into a crystal lattice

tile

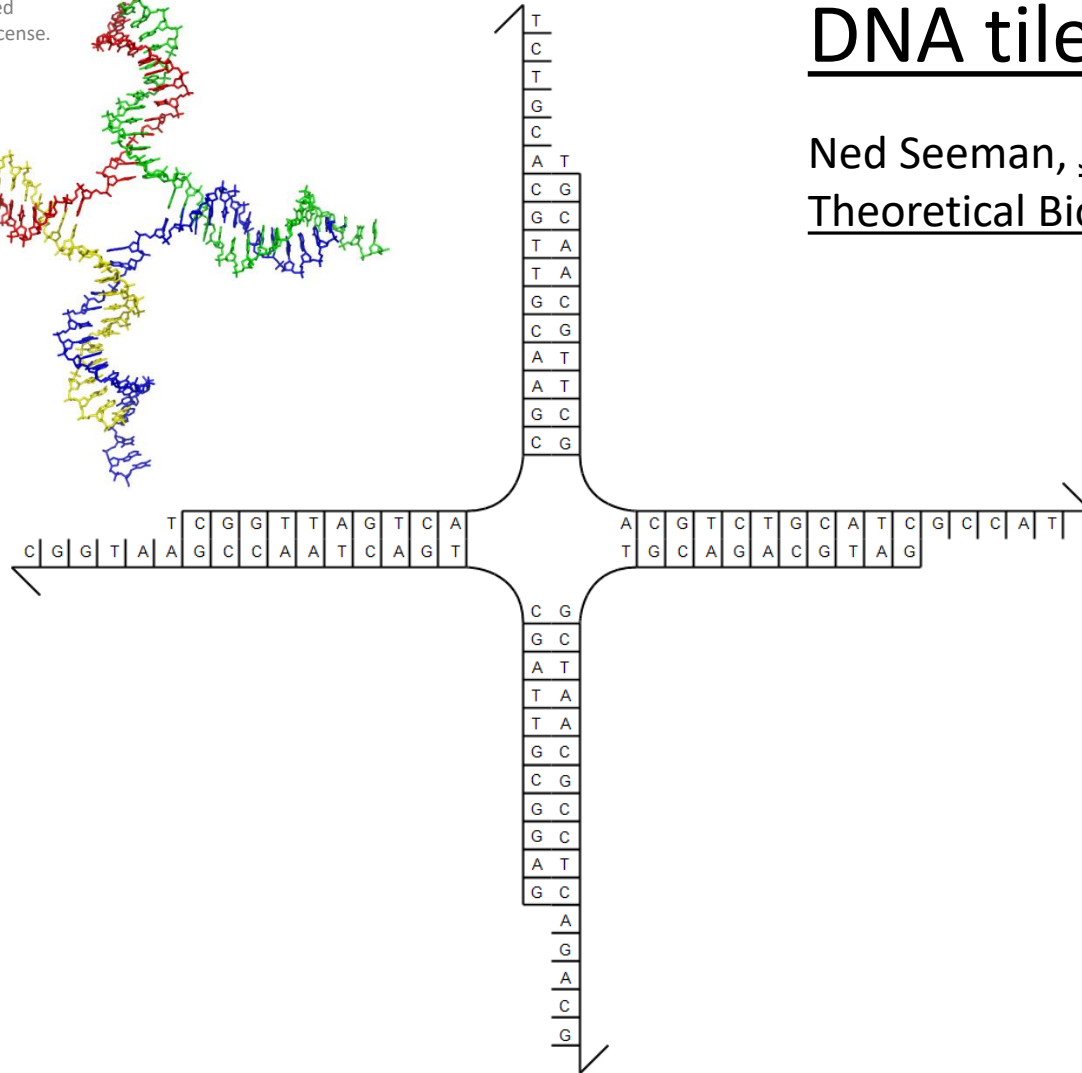
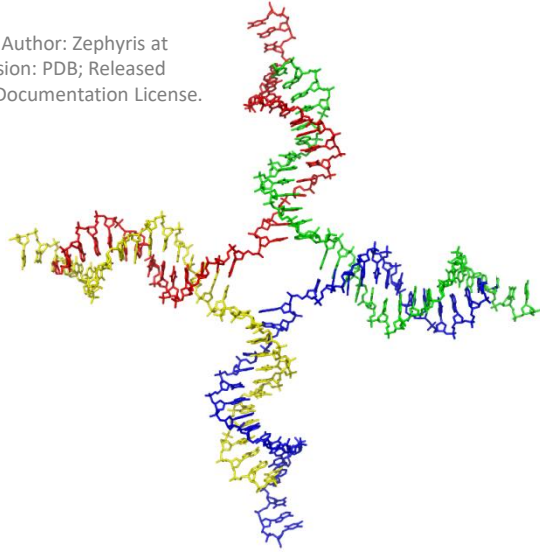


lattice



# Practice of DNA tile self-assembly

Source:en.wikipedia; Author: Zephyris at en.wikipedia; Permission: PDB; Released under the GNU Free Documentation License.



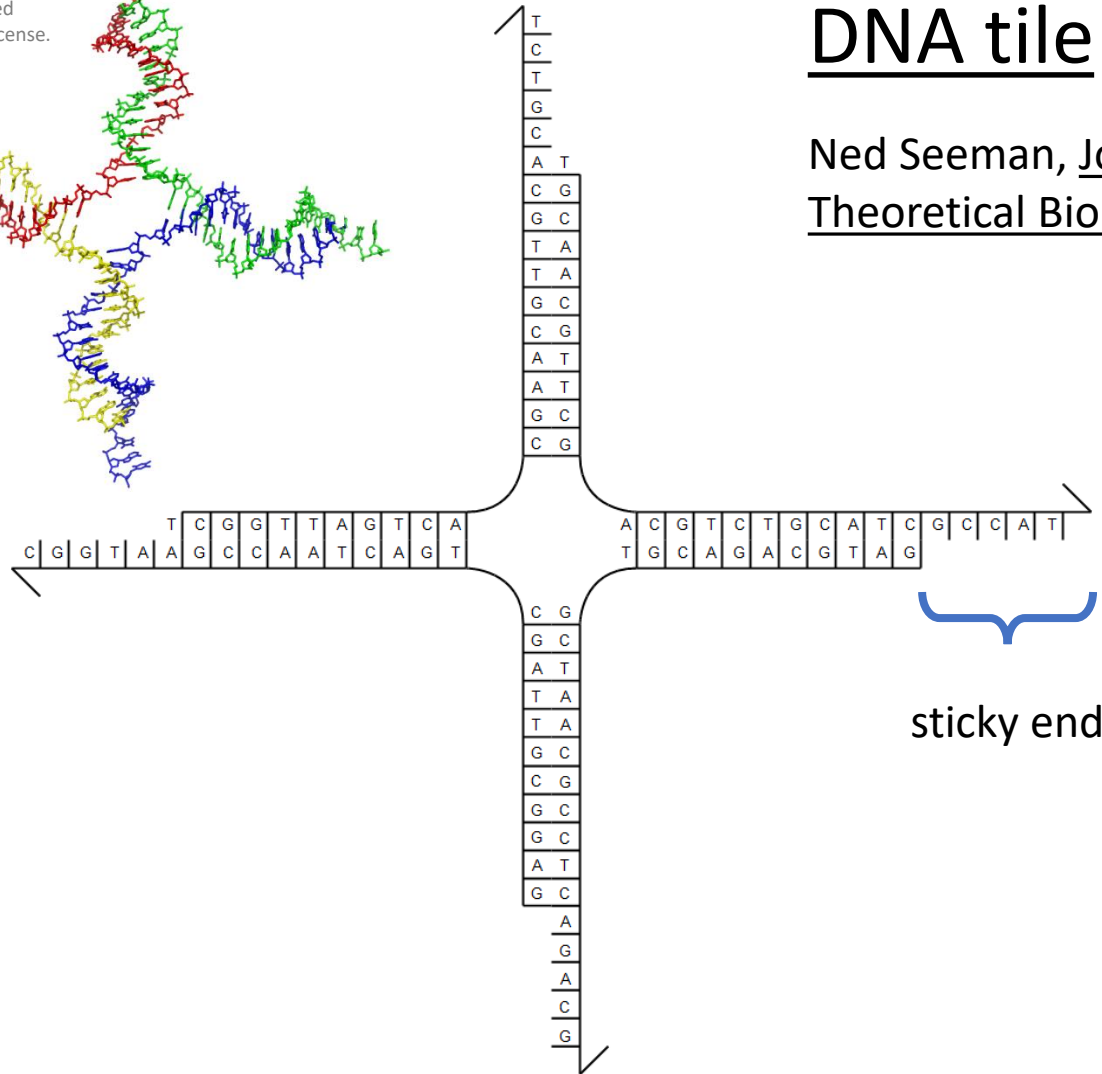
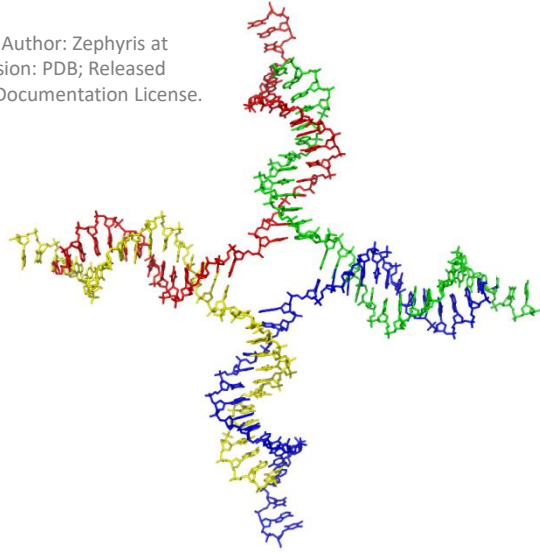
## DNA tile

Ned Seeman, Journal of Theoretical Biology 1982



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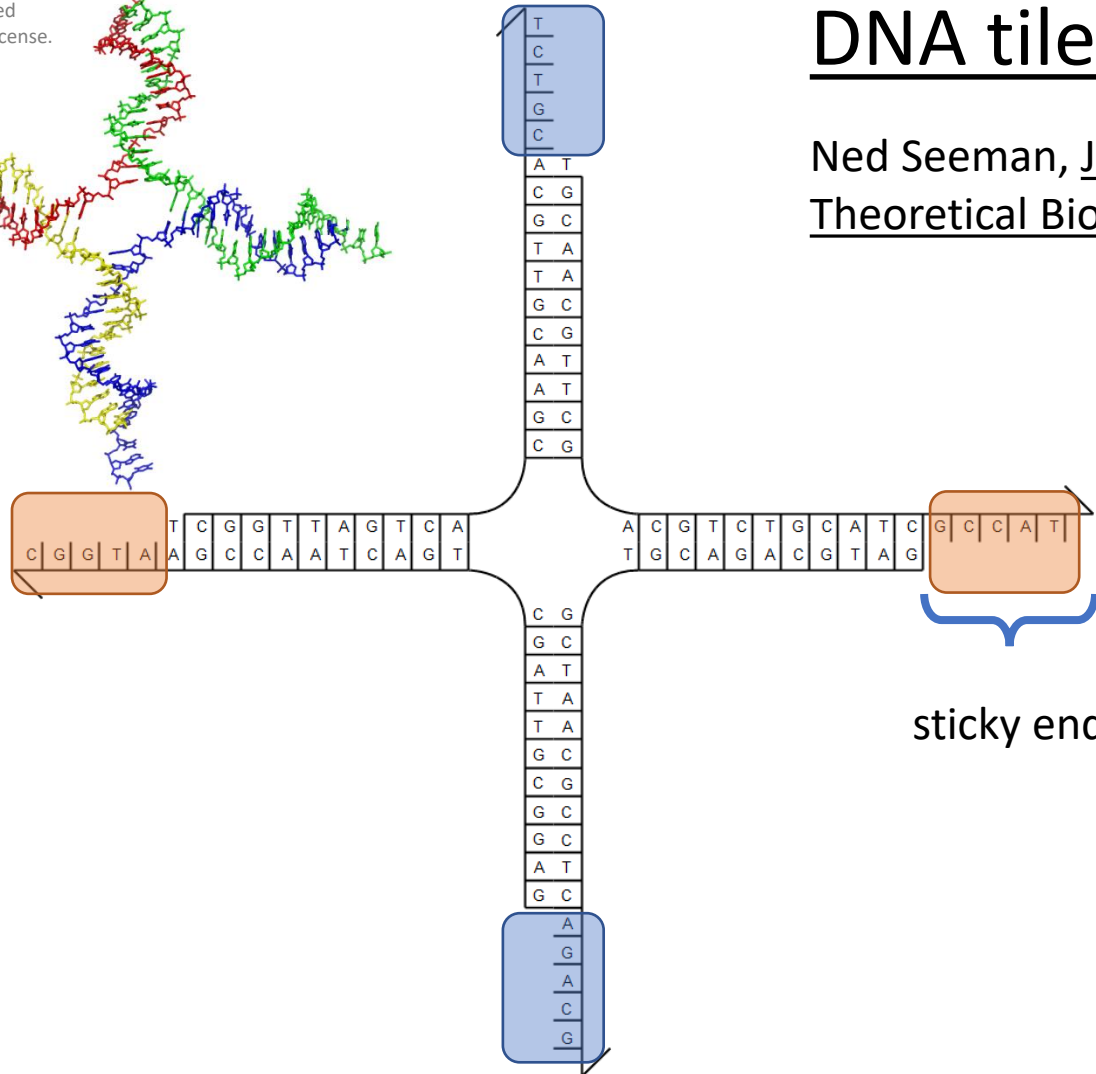
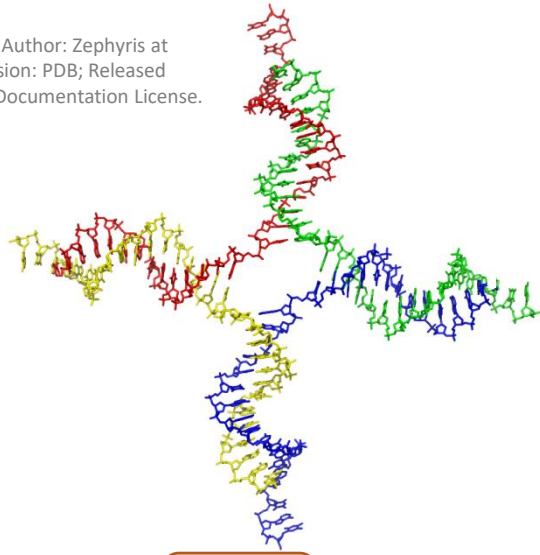
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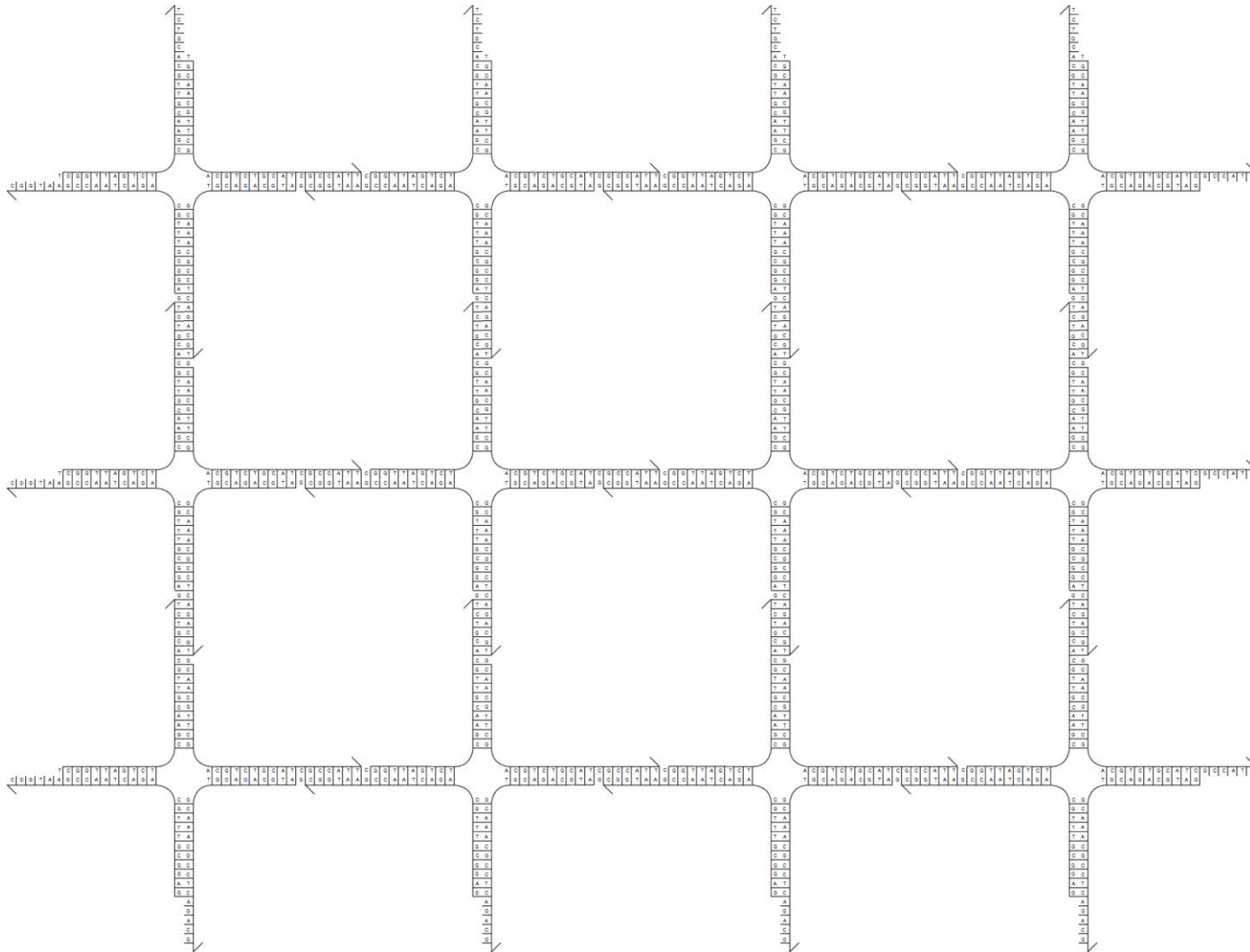
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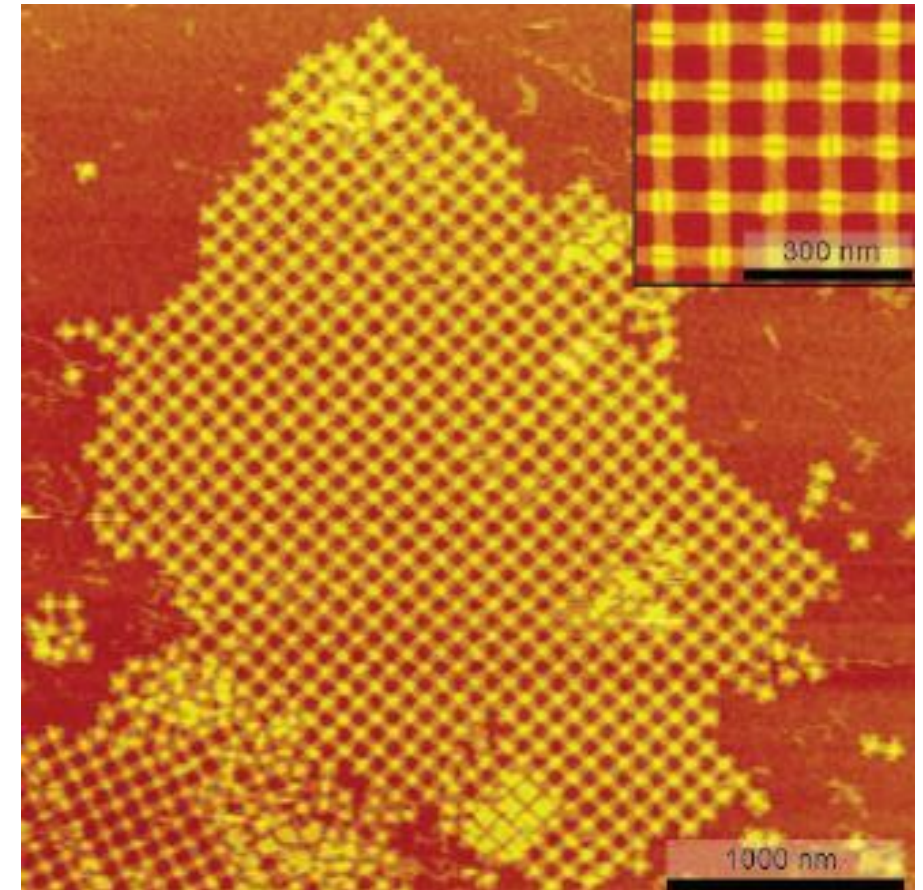


# Practice of DNA tile self-assembly

Place many copies of DNA tile in solution...



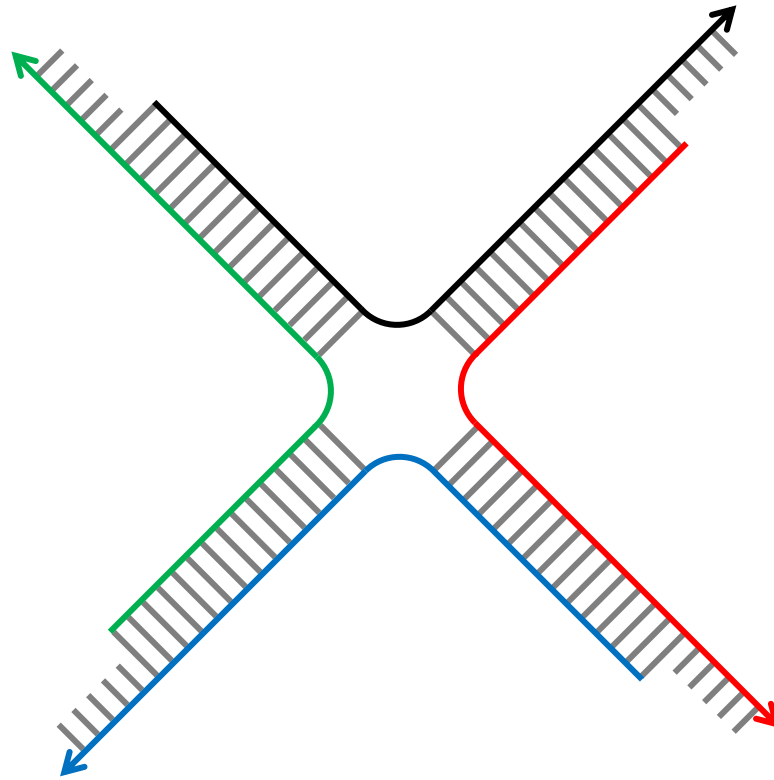
(not the same tile motif in this image)



Liu, Zhong, Wang, Seeman, *Angewandte Chemie* 2011

# Practice of DNA tile self-assembly

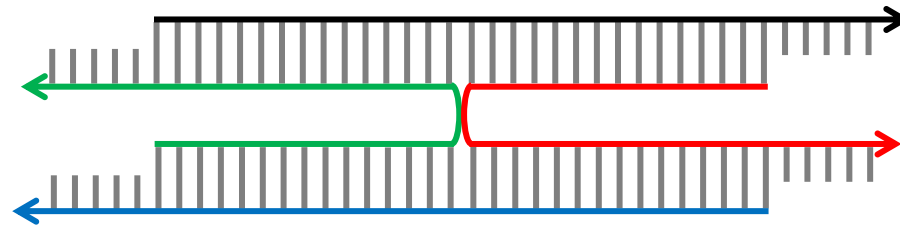
What really happens in practice to Holliday junction (“base stacking”)





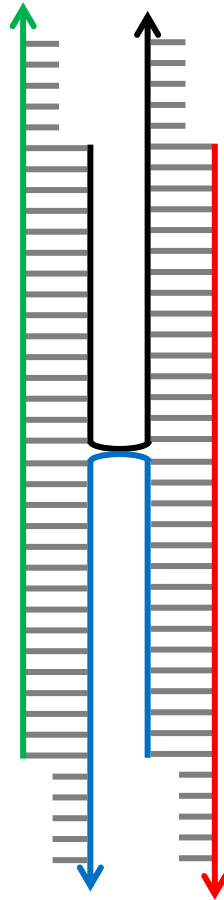
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What really happens in practice to Holliday junction (“base stacking”)



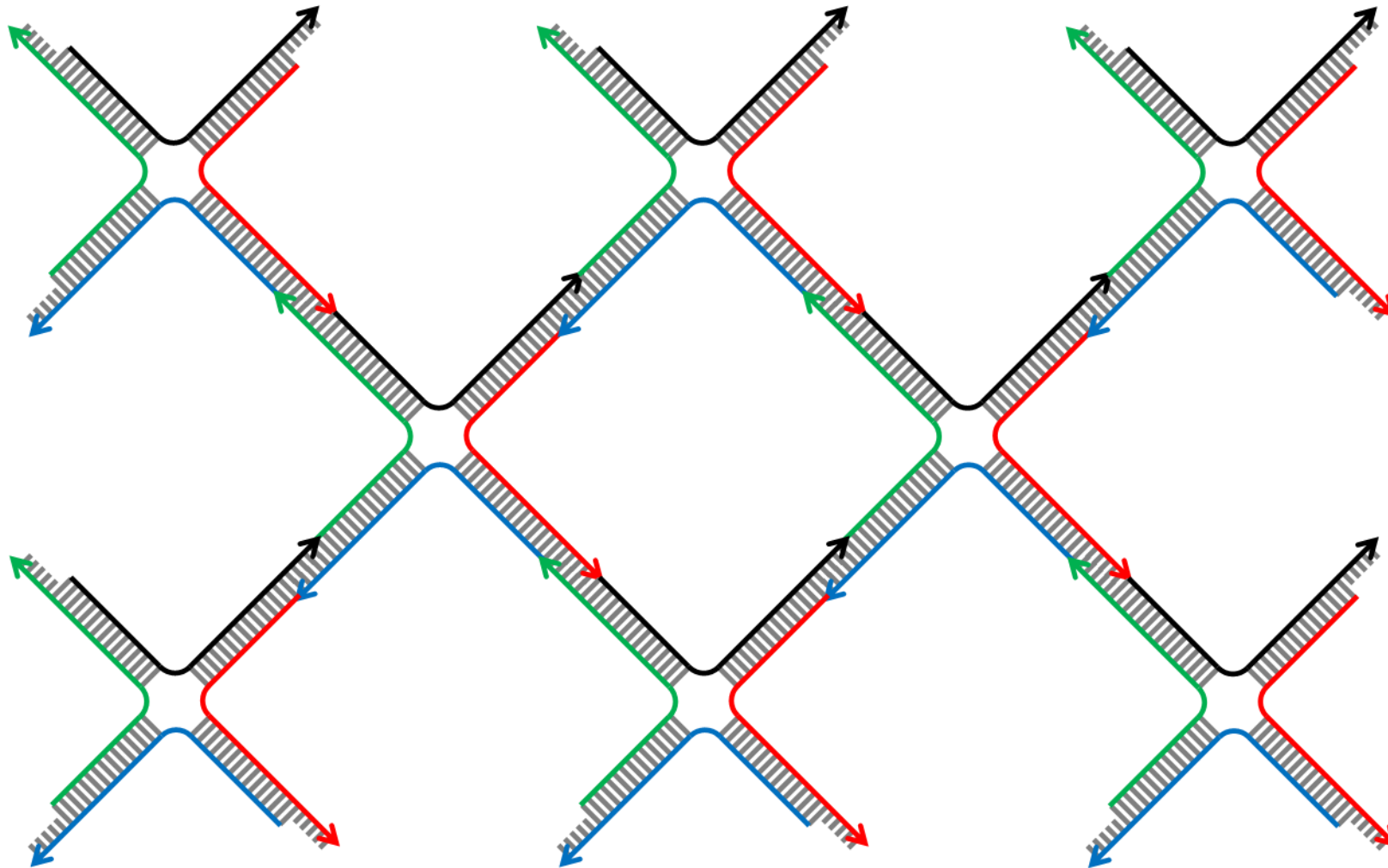
# Practice of DNA tile self-assembly

What really happens in practice to Holliday junction (“base stacking”)



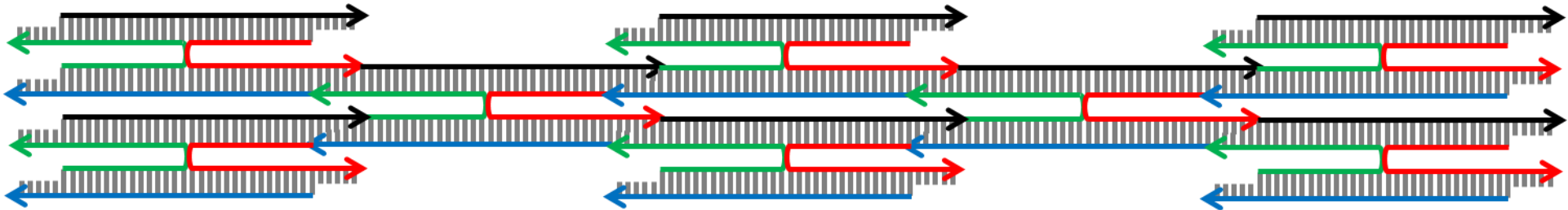
# Practice of DNA tile self-assembly

What really happens in practice to Holliday junction (“base stacking”)

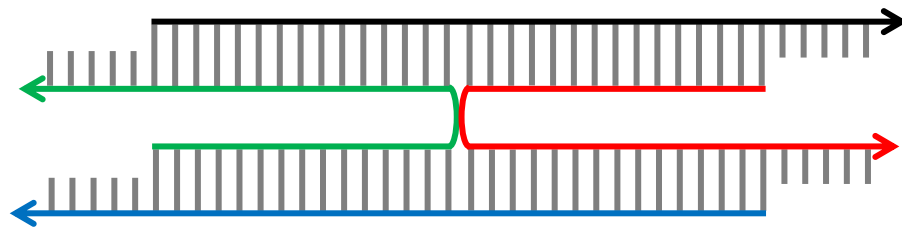


# Practice of DNA tile self-assembly

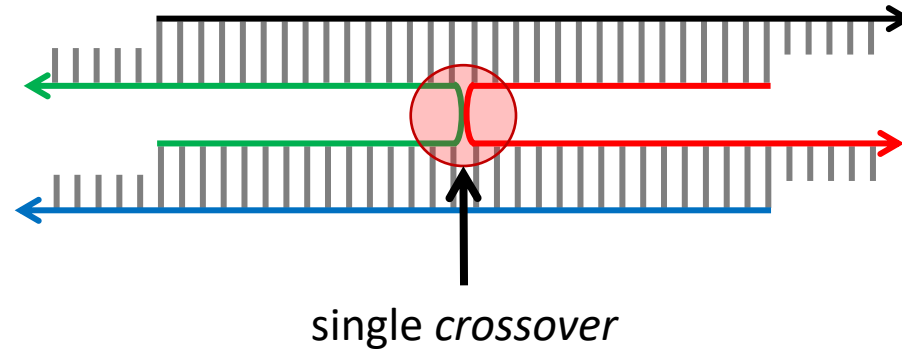
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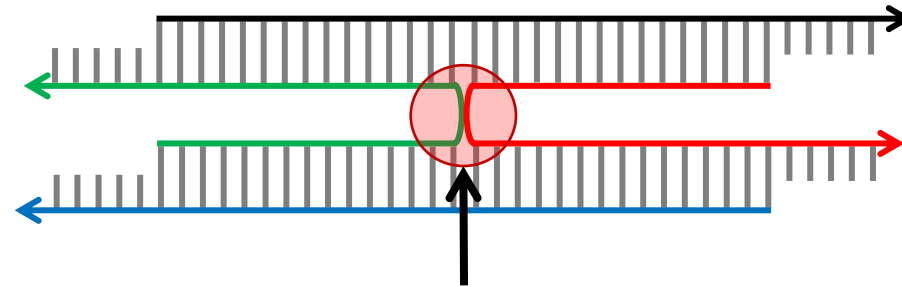
# Practice of DNA tile self-assembly



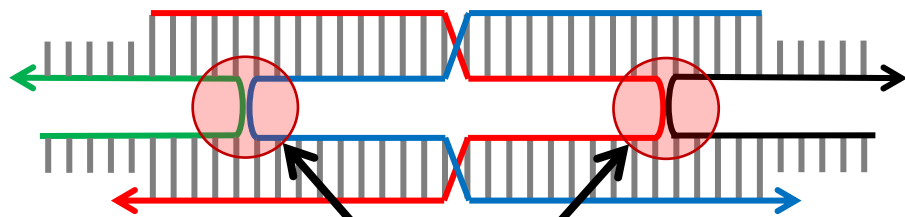
# Practice of DNA tile self-assembly



# Practice of DNA tile self-assembly



single crossover



double crossover

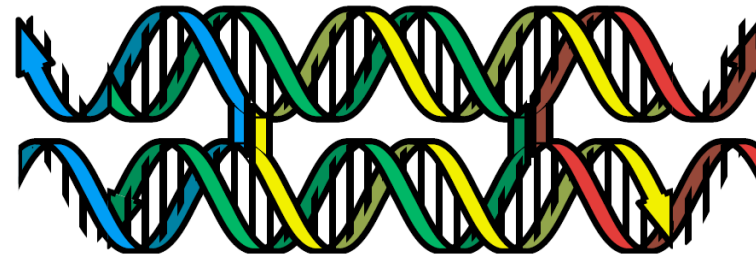
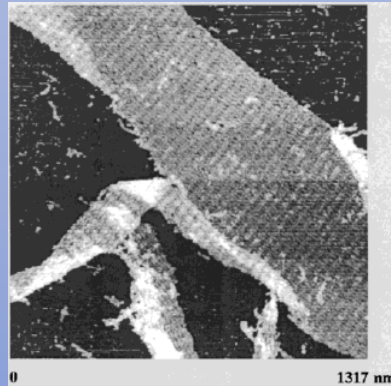
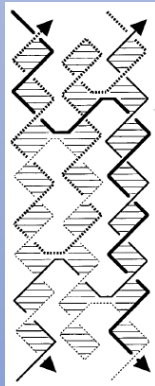


Figure from Schulman, Winfree, *PNAS* 2009

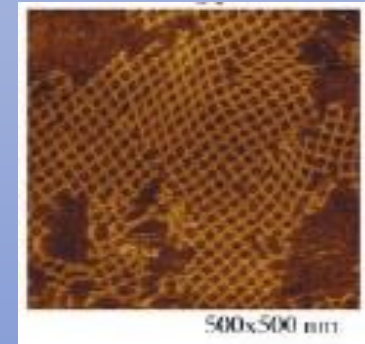
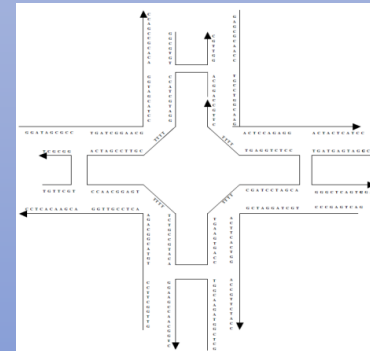
# Practice of DNA tile self-assembly

## other tile motifs

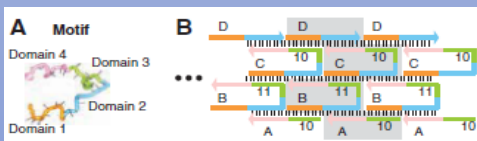
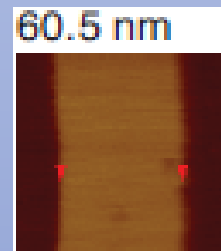
**triple-crossover tile** (LaBean, Yan, Kopatsch, Liu, Winfree, Reif, Seeman, *JACS* 2000)



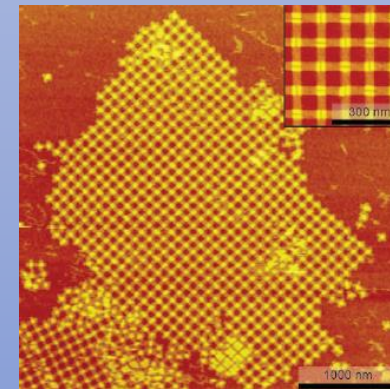
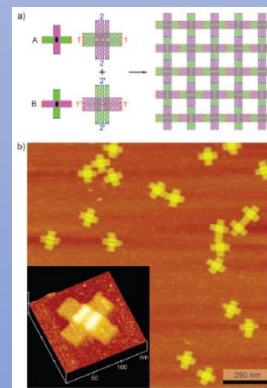
**4x4 tile** (Yan, Park, Finkelstein, Reif, LaBean, *Science* 2003)



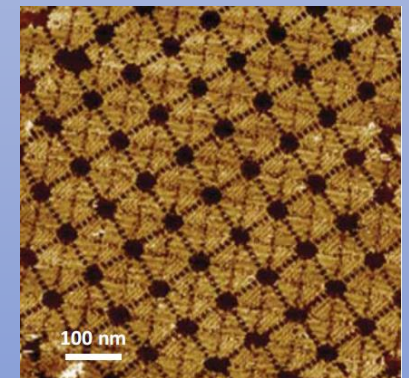
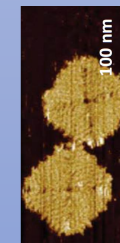
**single-stranded tile** (Yin, Hariadi, Sahu, Choi, Park, LaBean, Reif, *Science* 2008)



**DNA origami tile** (Liu, Zhong, Wang, Seeman, *Angewandte Chemie* 2011)



Tikhomirov, Petersen, Qian, *Nature Nanotechnology* 2017





# Theory of *algorithmic* self-assembly

What if...

... there is more than one tile type?

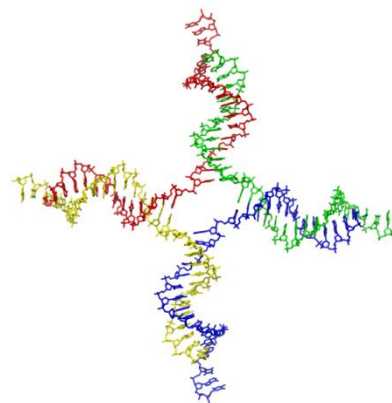
... some sticky ends are “weak”?



Erik Winfree

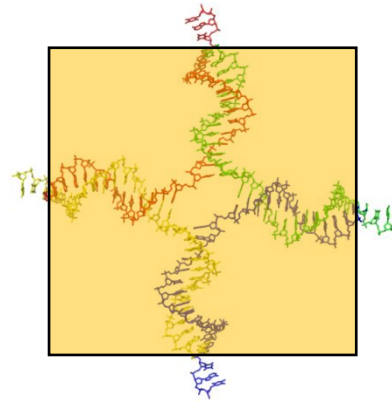
# Abstract Tile Assembly Model

Erik Winfree,  
Ph.D. thesis,  
Caltech 1998



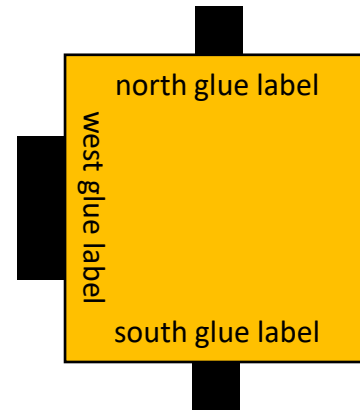
# Abstract Tile Assembly Model

- **tile type** = unit square



# Abstract Tile Assembly Model

- **tile type** = unit square
- each side has a **glue** with a **label** and **strength** (0, 1, or 2)



strength 0



strength 1 (weak)

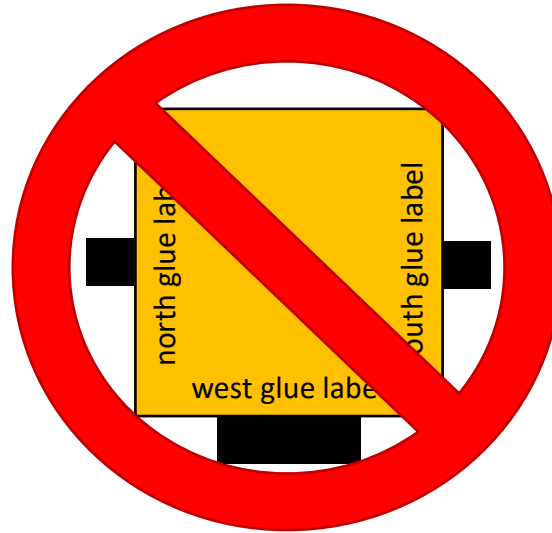


strength 2 (strong)



# Abstract Tile Assembly Model

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- tiles cannot rotate



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strength 1 (weak)

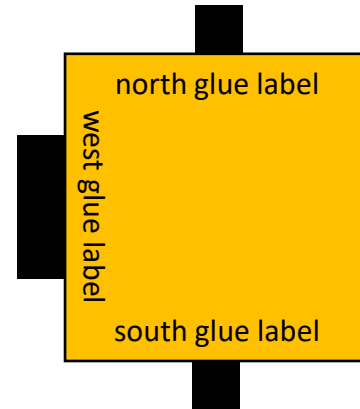


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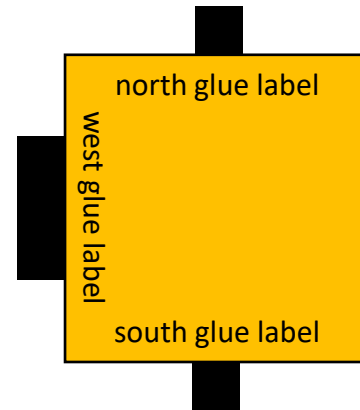
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- finitely many tile **types**
- infinitely many **tiles**: copies of each type

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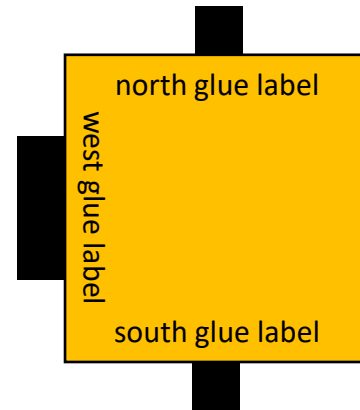
strength 2 (strong)



- finitely many tile **types**
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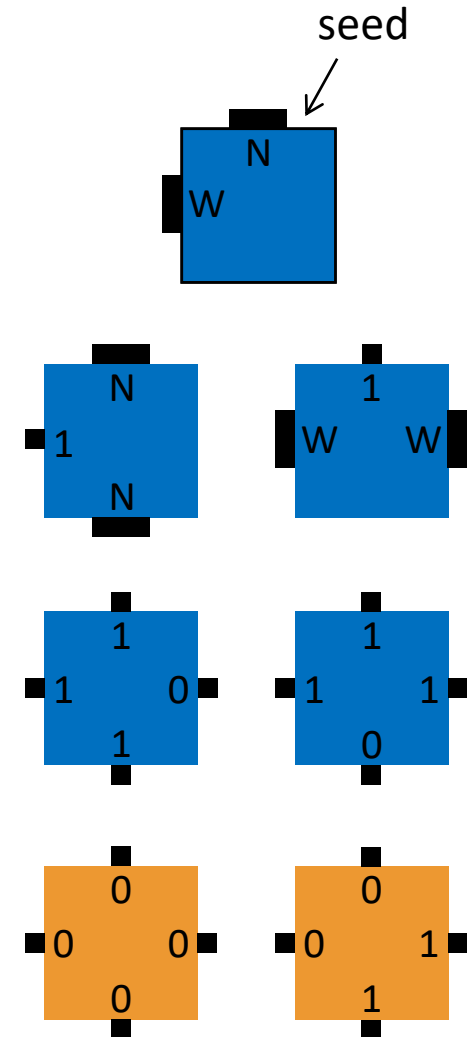
strength 2 (strong)



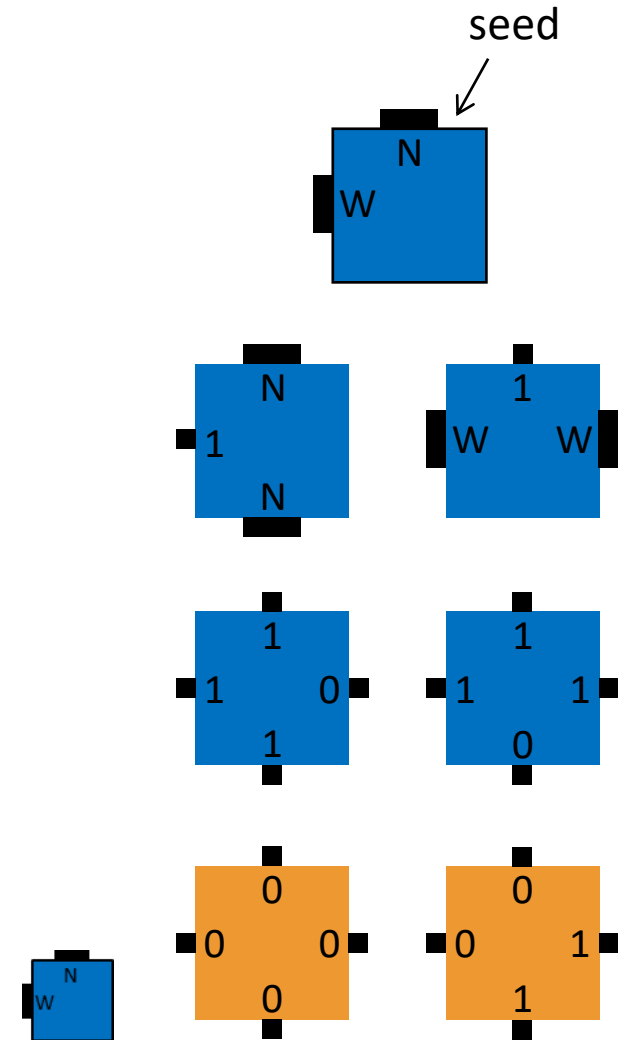
- finitely many tile **types**
- infinitely many **tiles**: copies of each type
- assembly starts as a single copy of a special **seed** tile
- tile can bind to the assembly if total binding strength  $\geq 2$  (**two weak glues** or **one strong glue**)



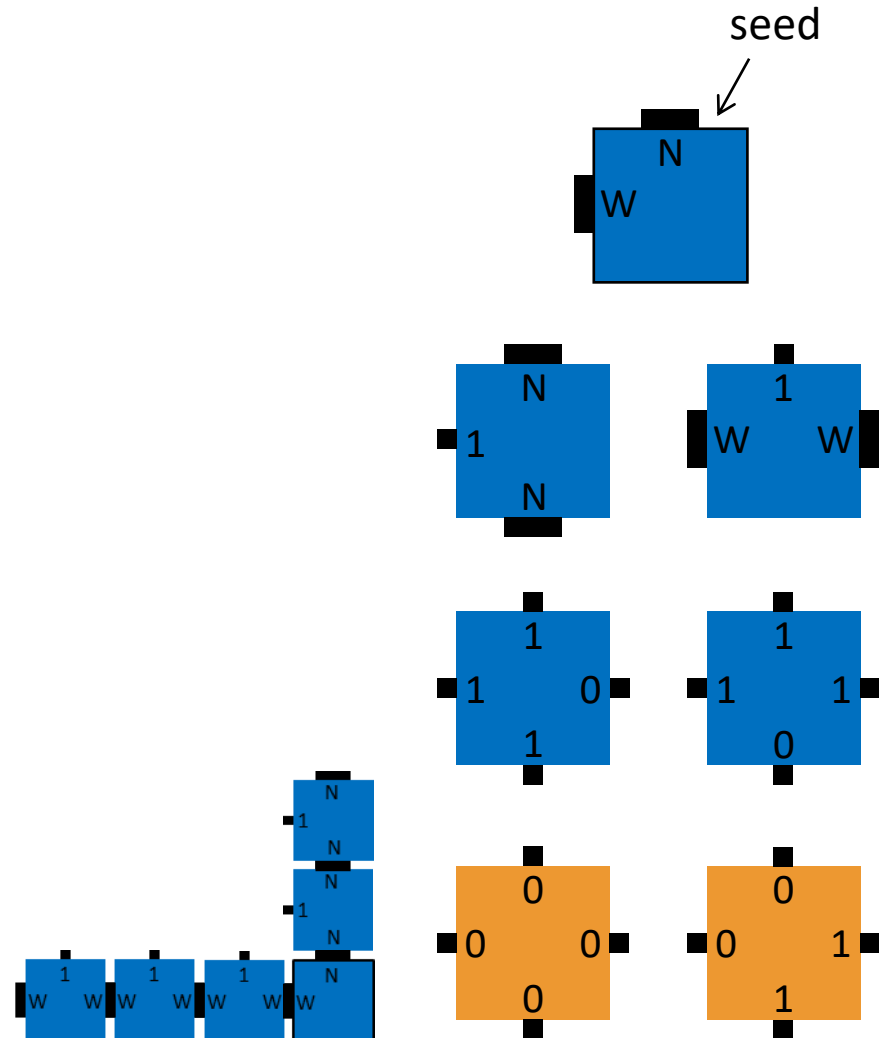
# Example tile set



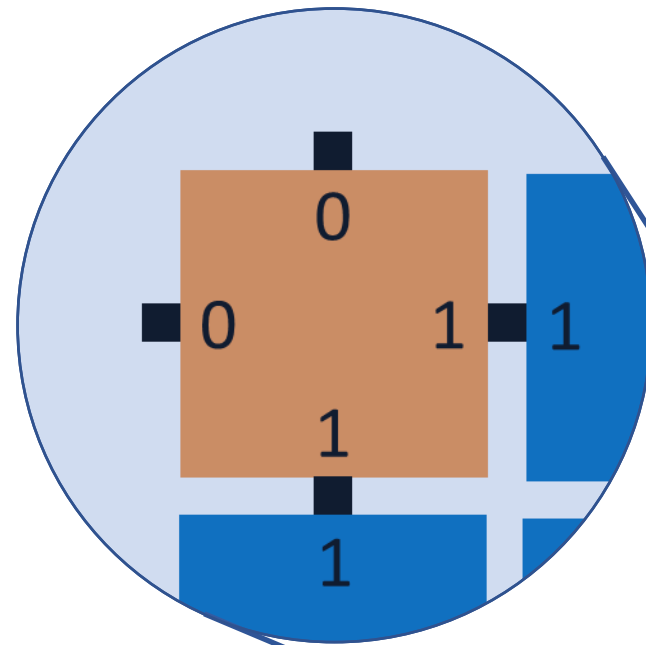
# Example tile set



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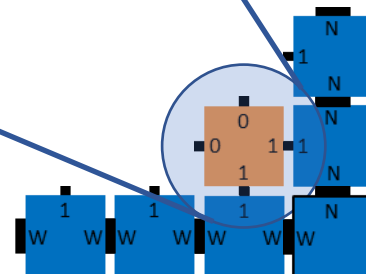
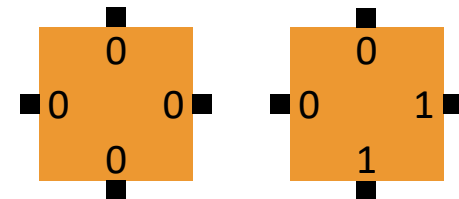
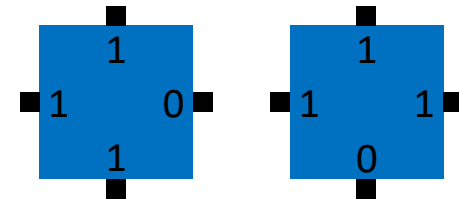
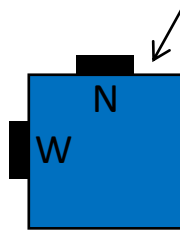


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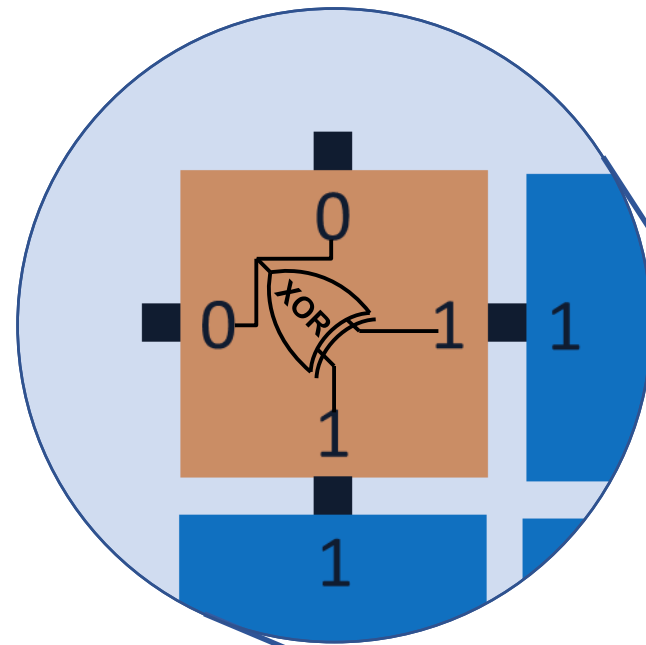


“cooperative binding”

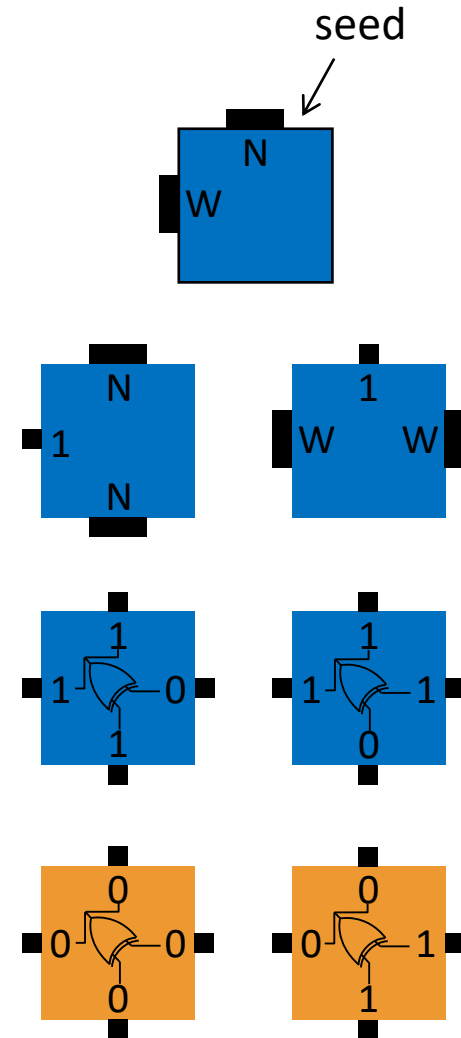
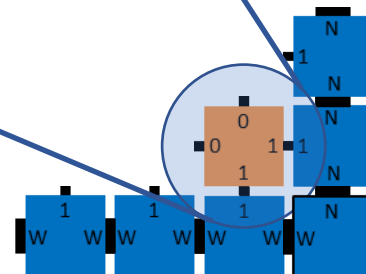
seed



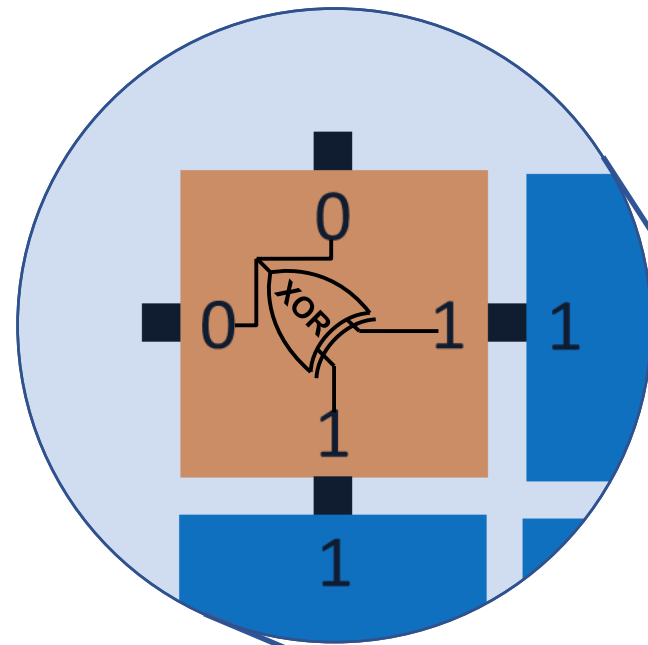
# Example tile set



“cooperative binding”

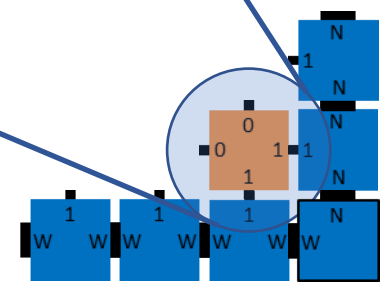
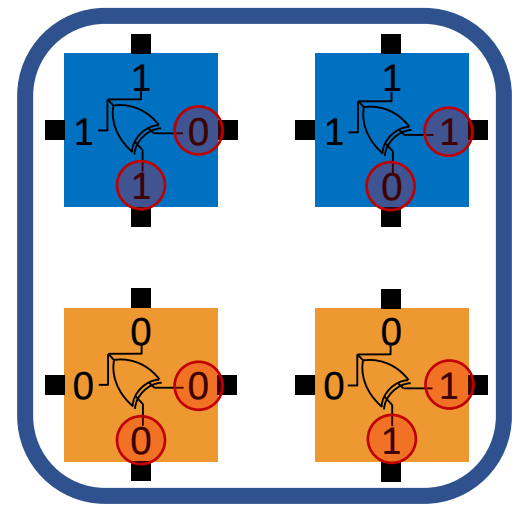
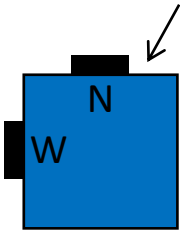


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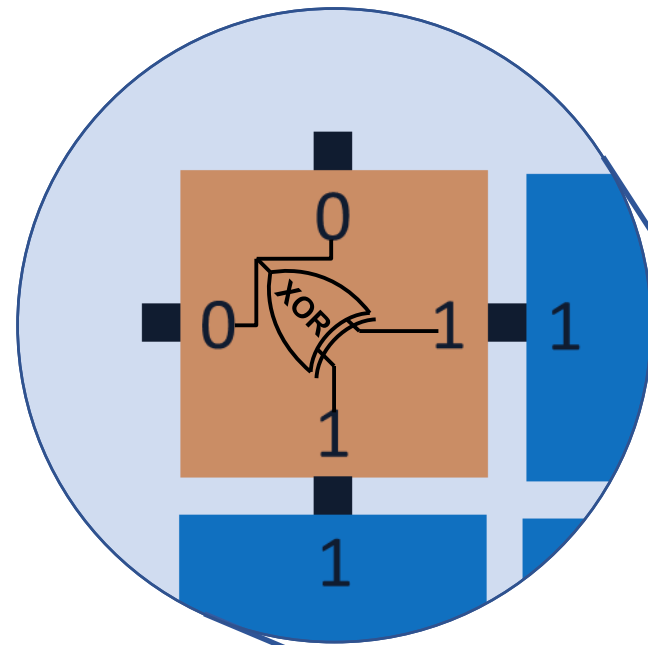


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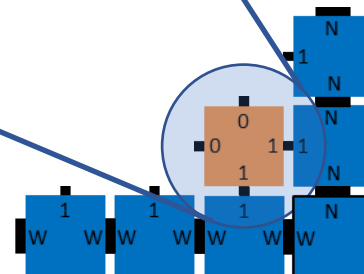
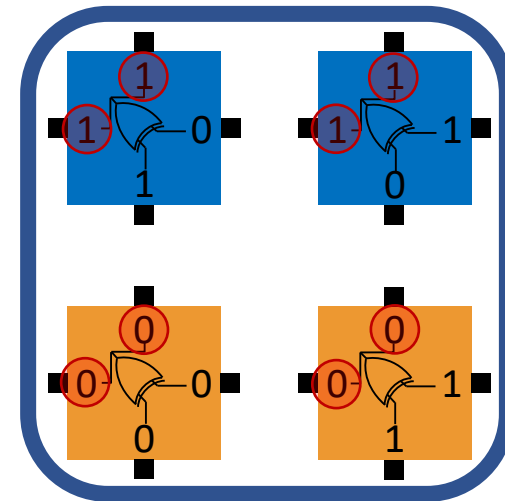
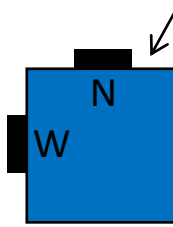


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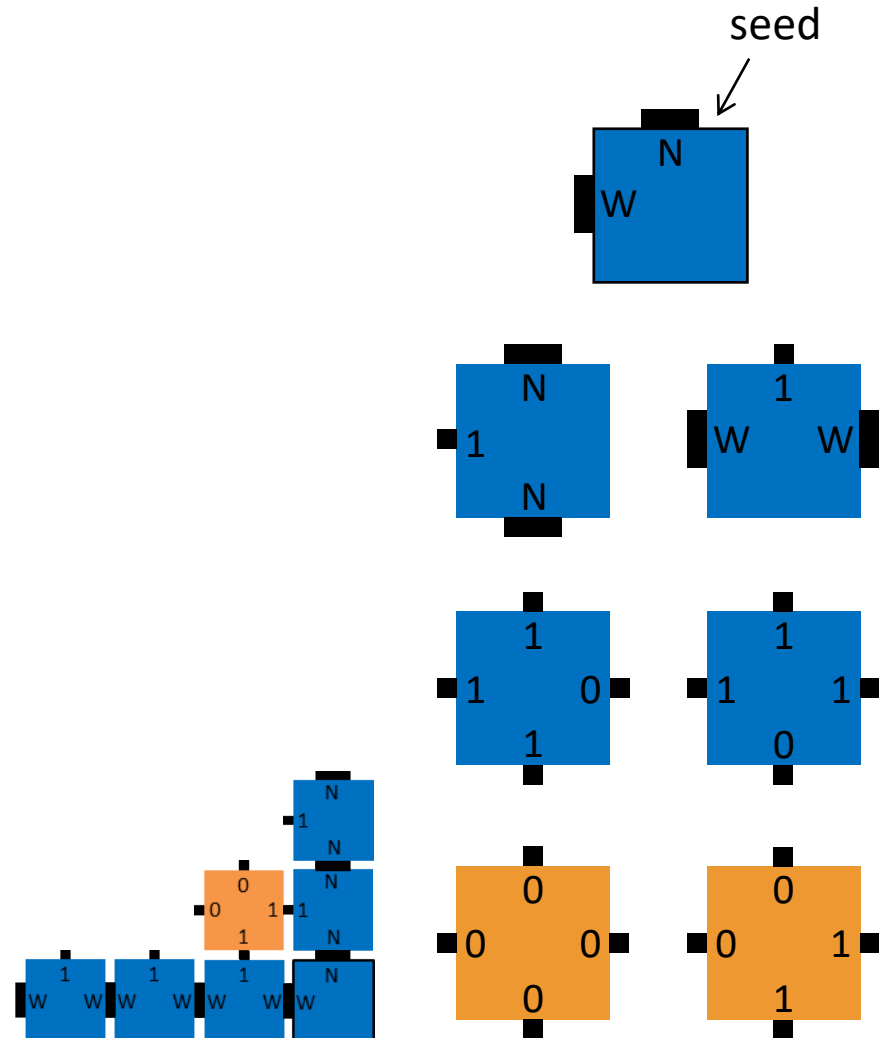


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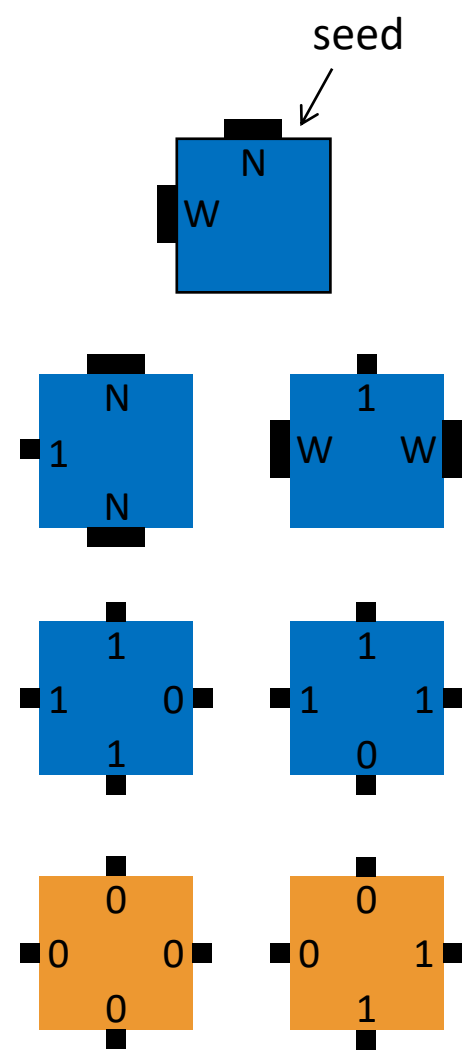
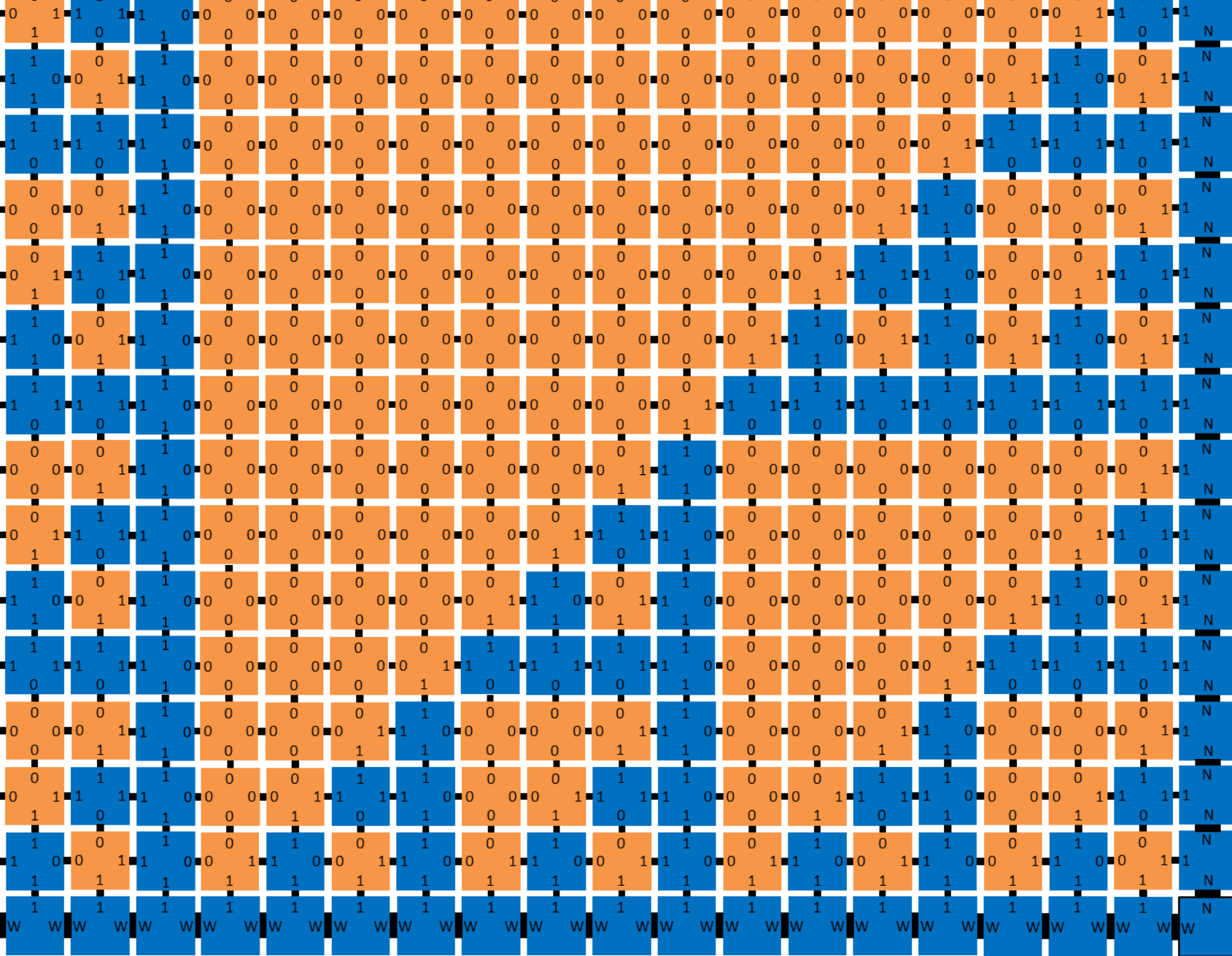
seed

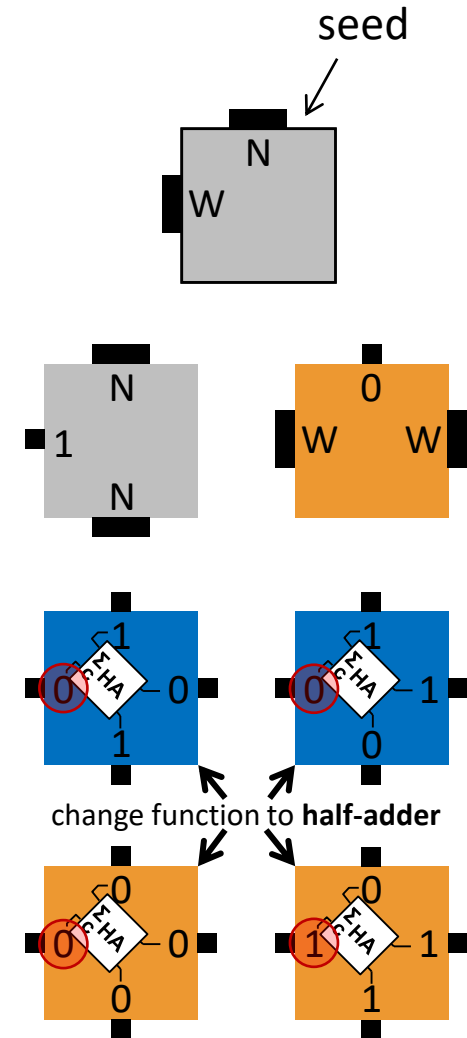
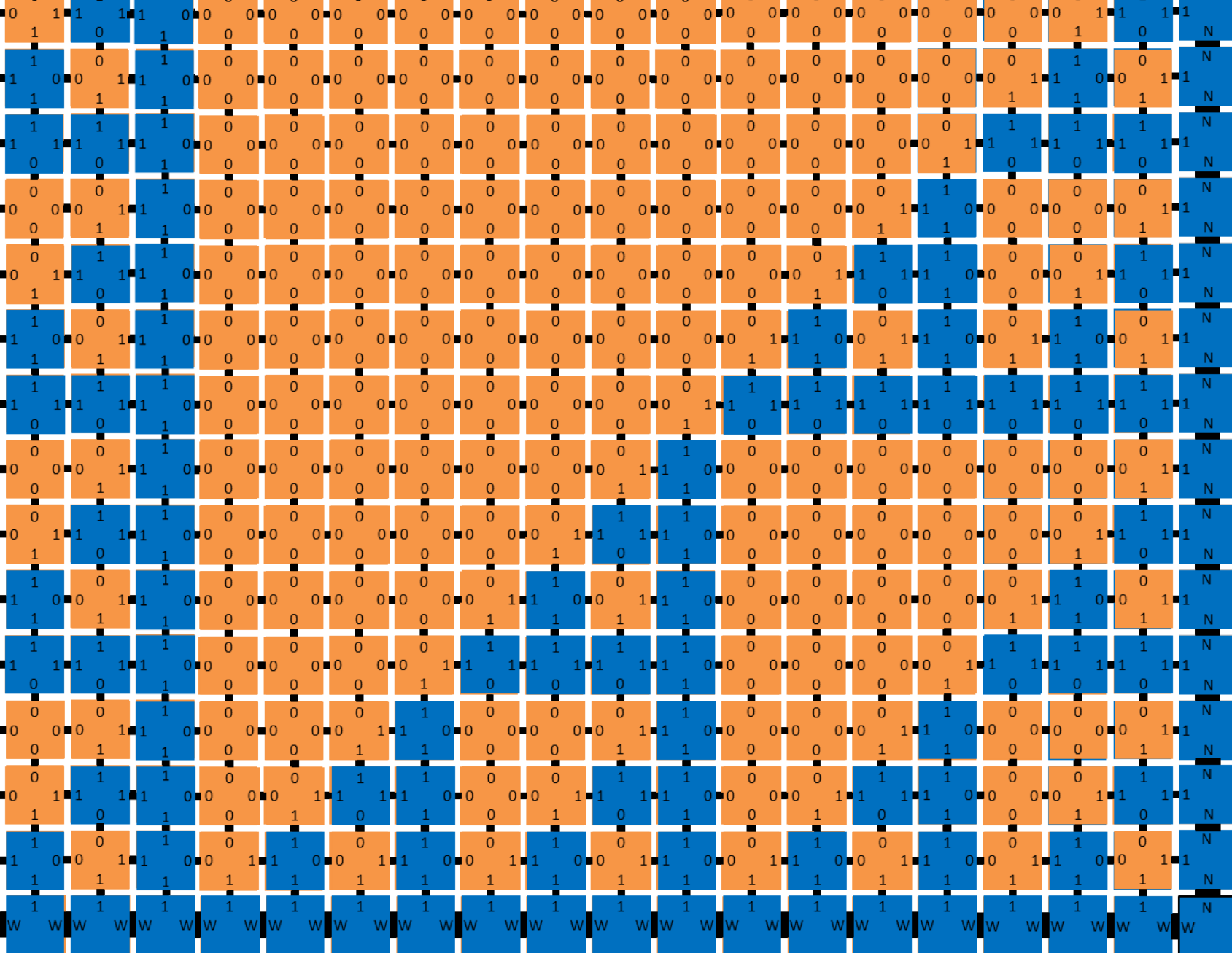


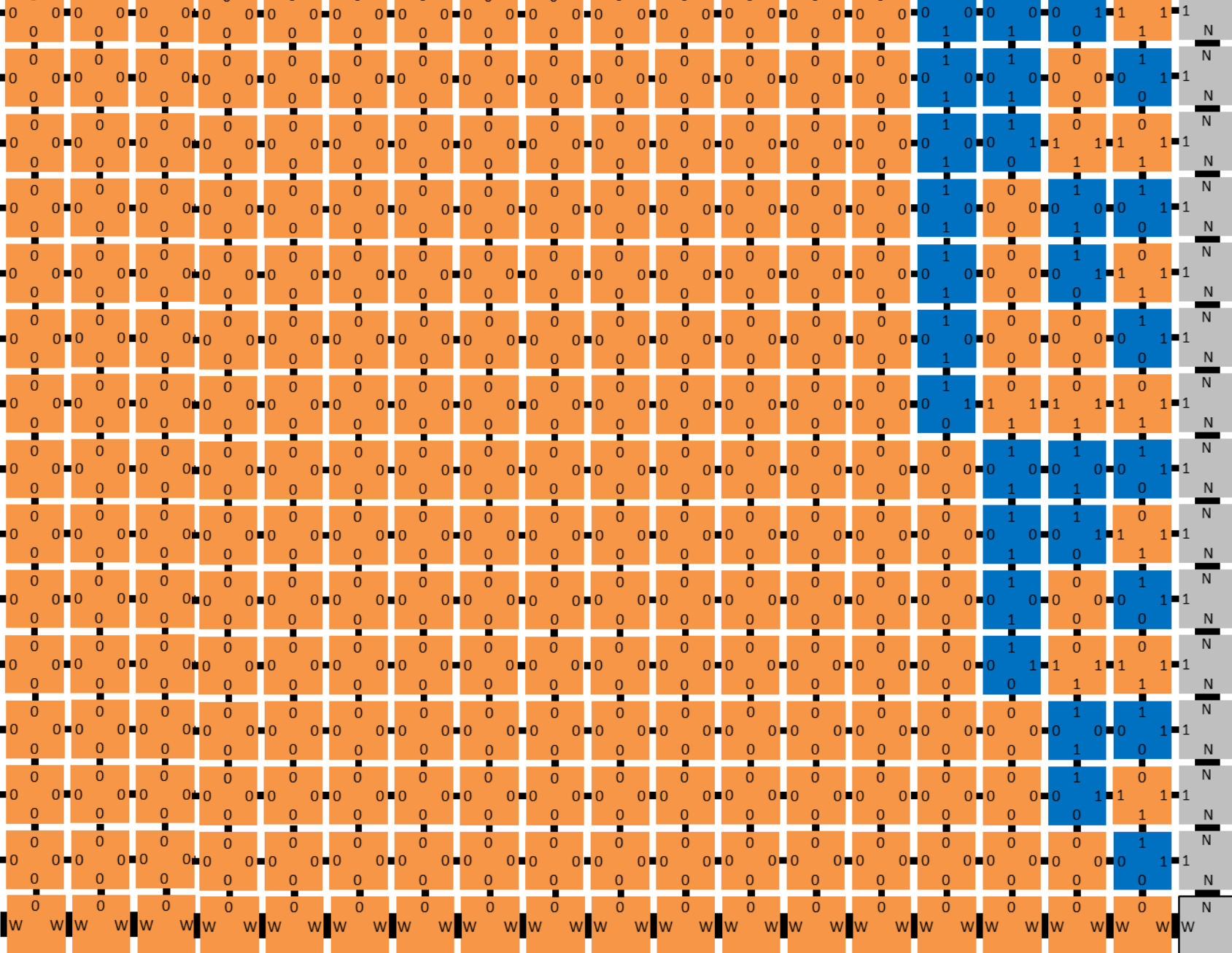
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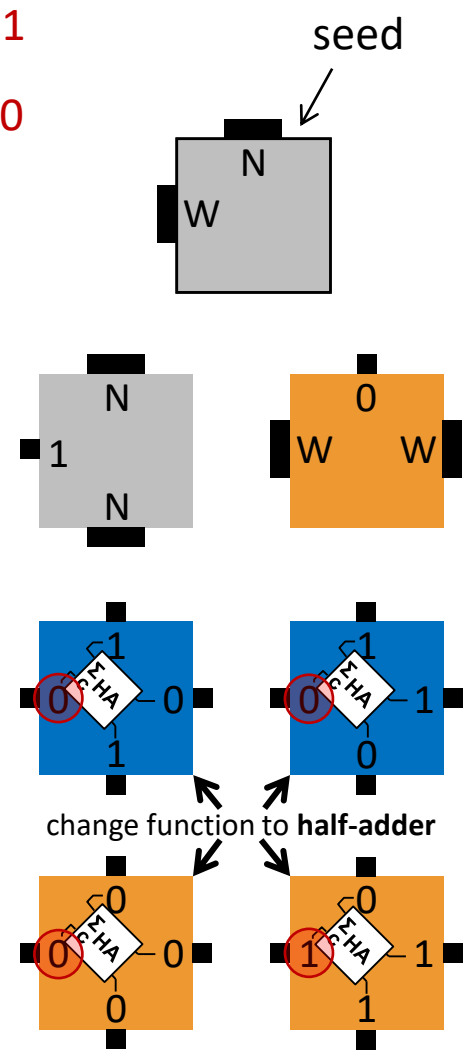




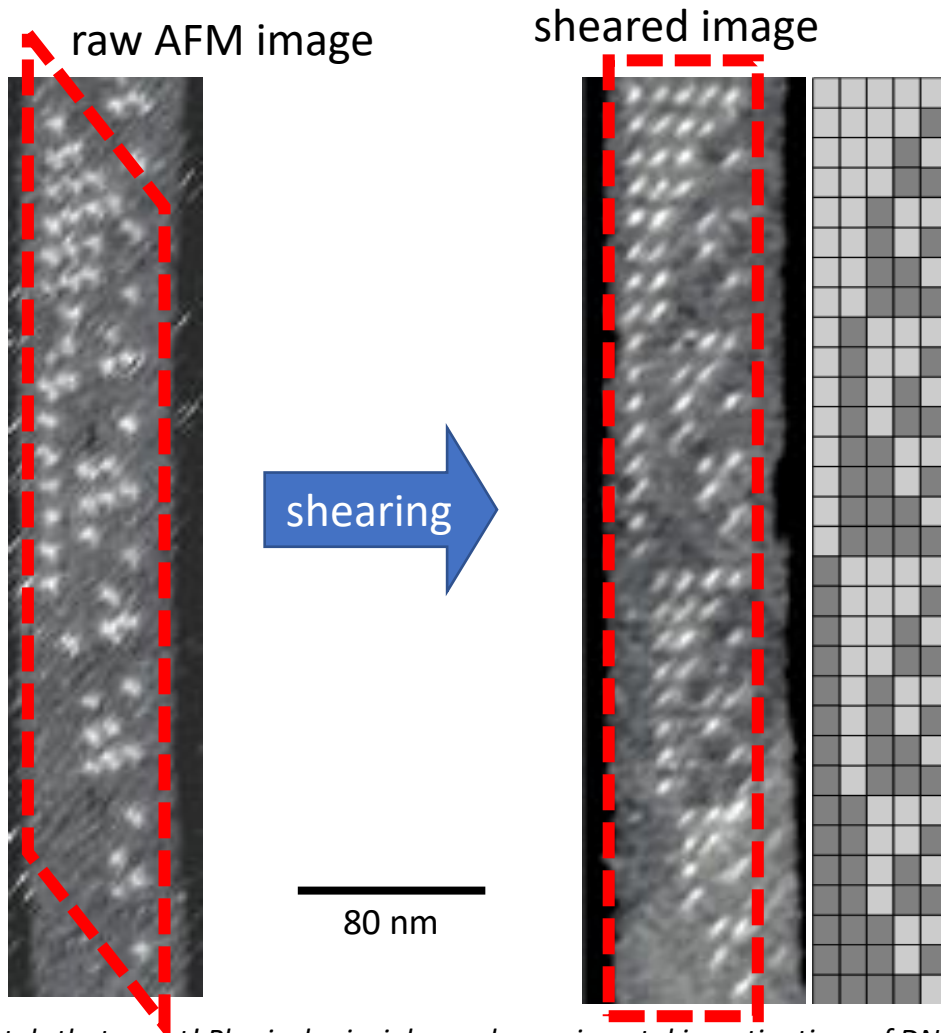




14  
13  
12  
11  
10  
9  
8  
7  
6  
5  
4  
3  
2  
1  
0

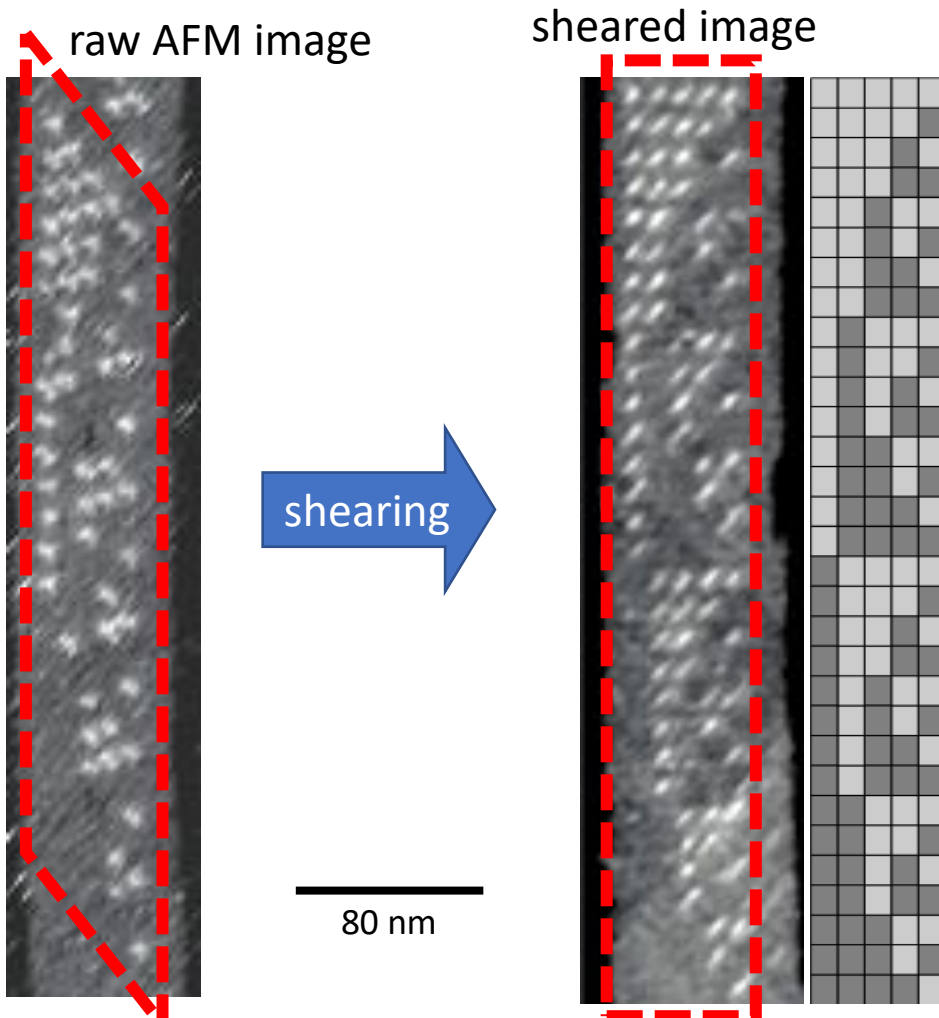


# Algorithmic self-assembly in action



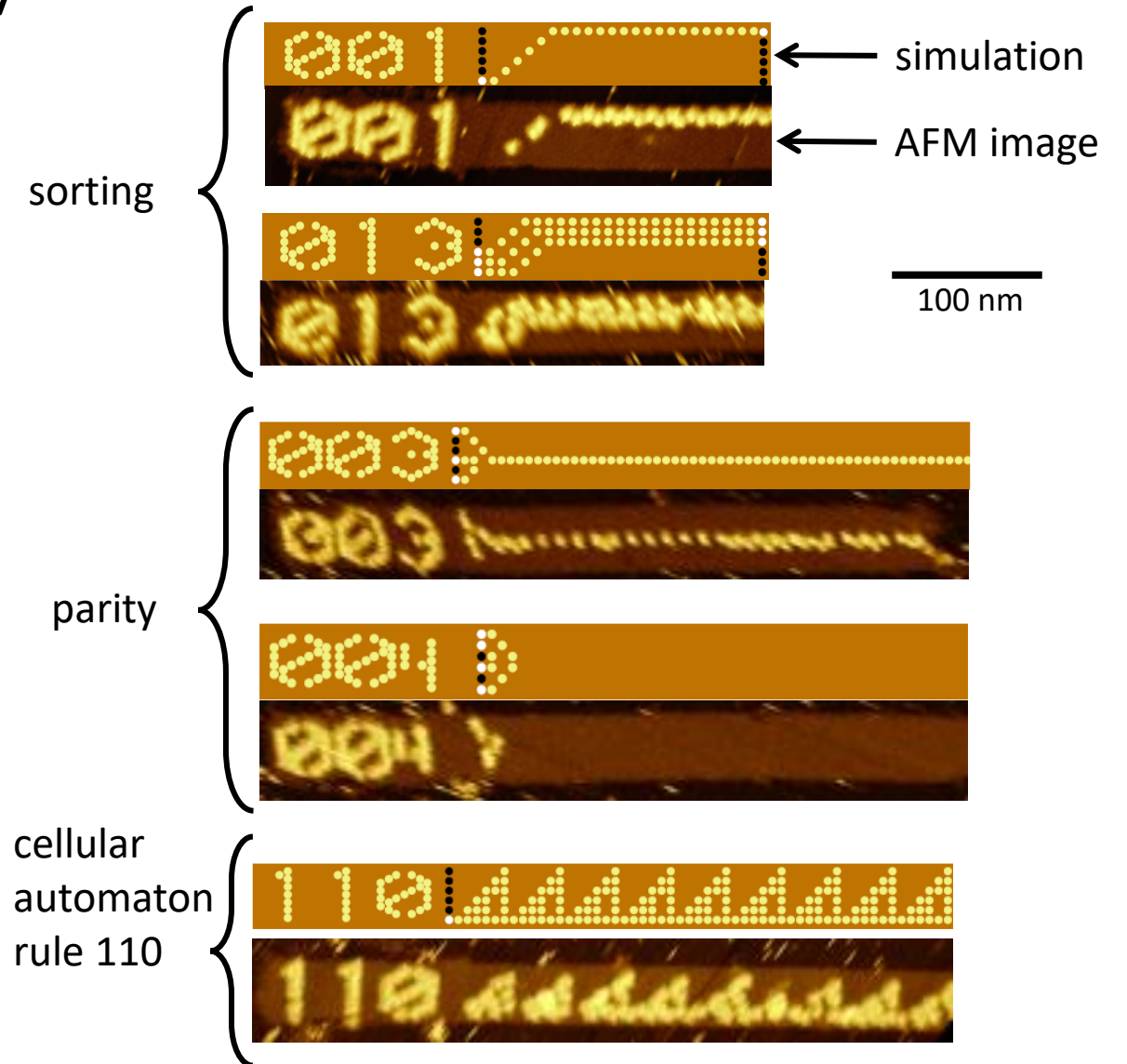
[Crystals that count! Physical principles and experimental investigations of DNA tile self-assembly, Constantine Evans, Ph.D. thesis, Caltech, 2014]

# Algorithmic self-assembly in action



[Crystals that count! Physical principles and experimental investigations of DNA tile self-assembly, Constantine Evans, Ph.D. thesis, Caltech, 2014]

Track B talk by Damien Woods at 11:30am tomorrow!

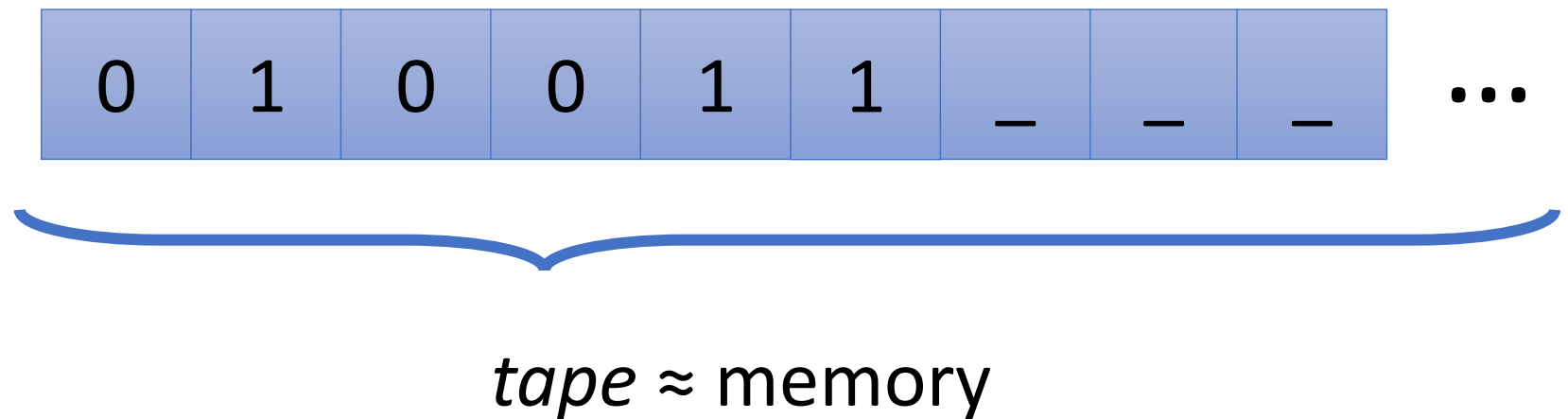


[Iterated Boolean circuit computation via a programmable DNA tile array. Woods, Doty, Myhrvold, Hui, Wu, Yin, Winfree, [in preparation](#)] 13

How computationally powerful  
are self-assembling tiles?

# Turing machines

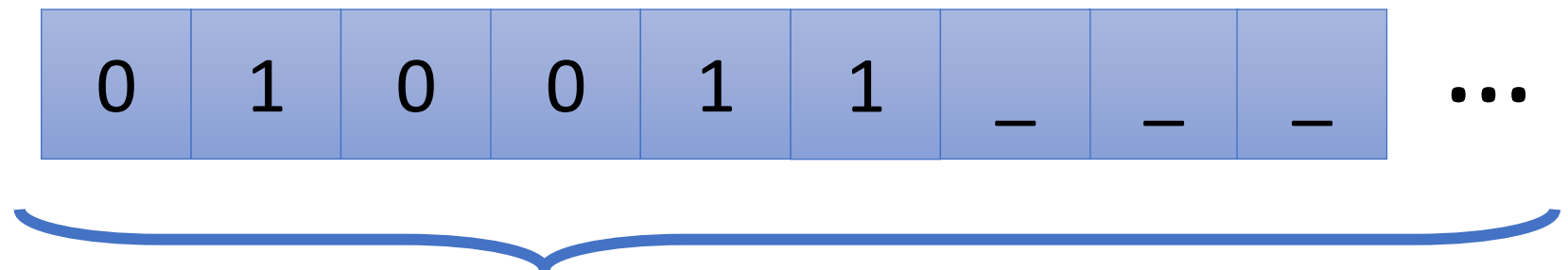
# Turing machines





# Turing machines

*state*  $\approx$  line of code

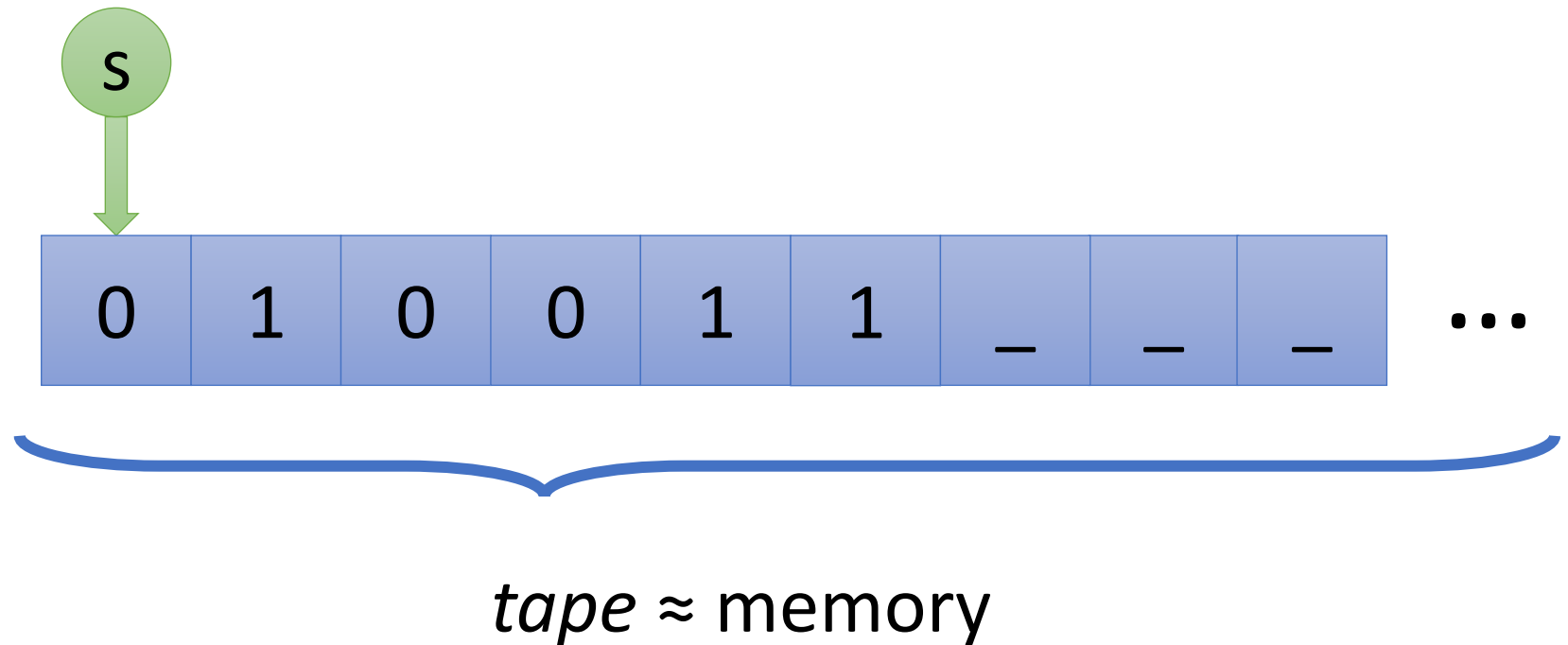


*tape*  $\approx$  memory

# Turing machines

*state*  $\approx$  line of code

initial state = s

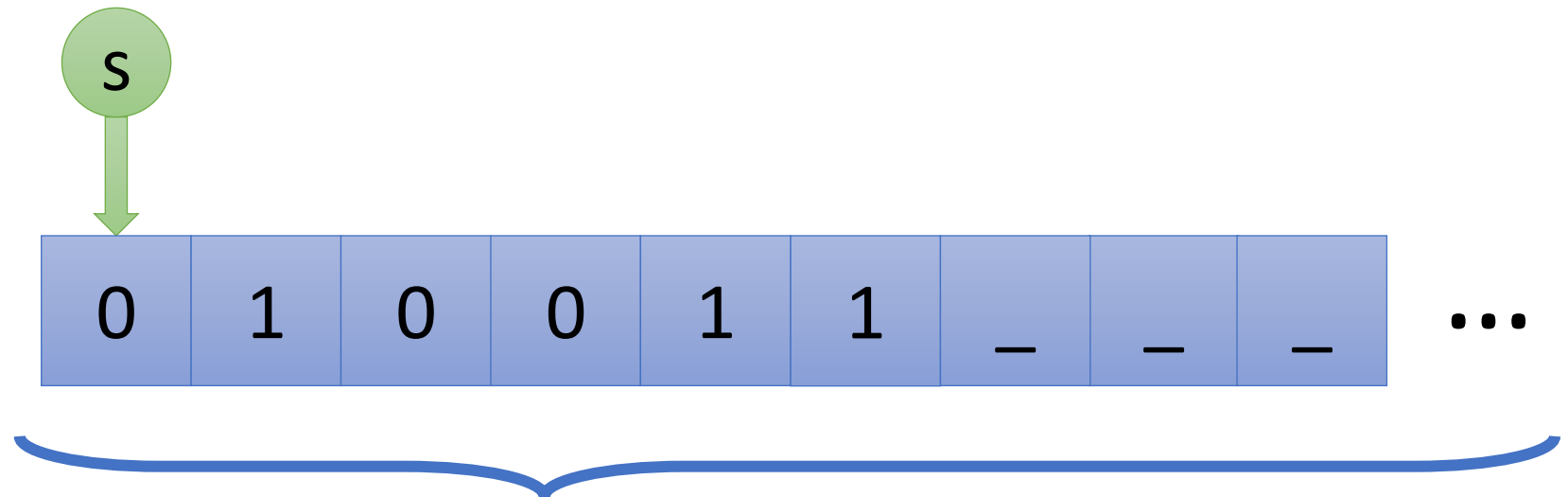


# Turing machines

*state*  $\approx$  line of code

initial state = *s*

*s*,0: *q*,0, $\rightarrow$



*transitions*  
(instructions)

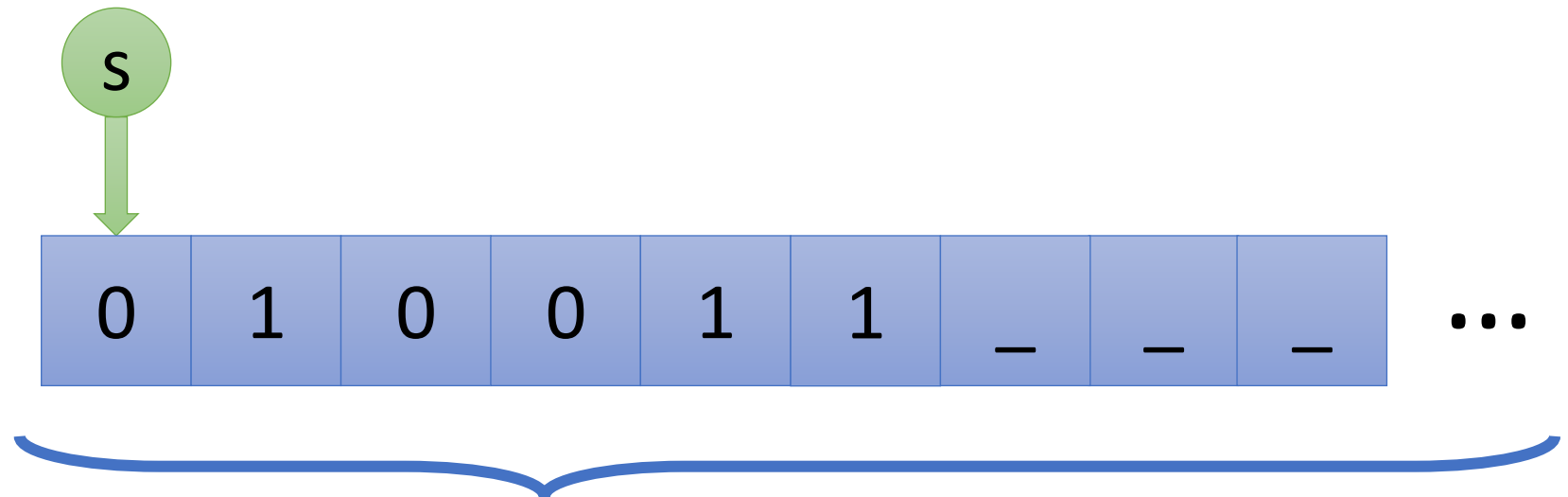
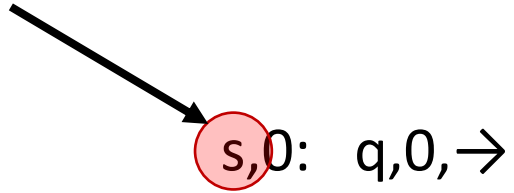
*tape*  $\approx$  memory

# Turing machines

*state*  $\approx$  line of code

initial state = *s*

current state



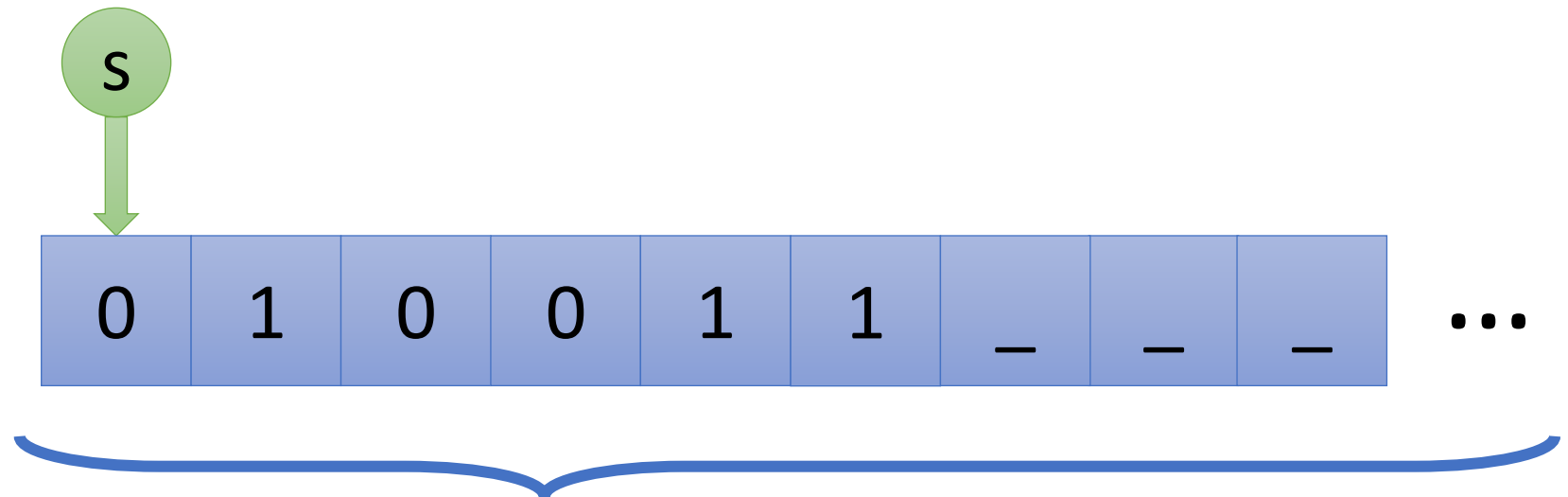
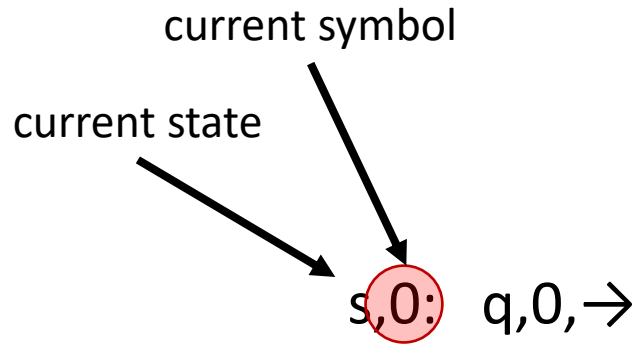
*transitions*  
(instructions)

*tape*  $\approx$  memory

# Turing machines

*state*  $\approx$  line of code

initial state =  $s$



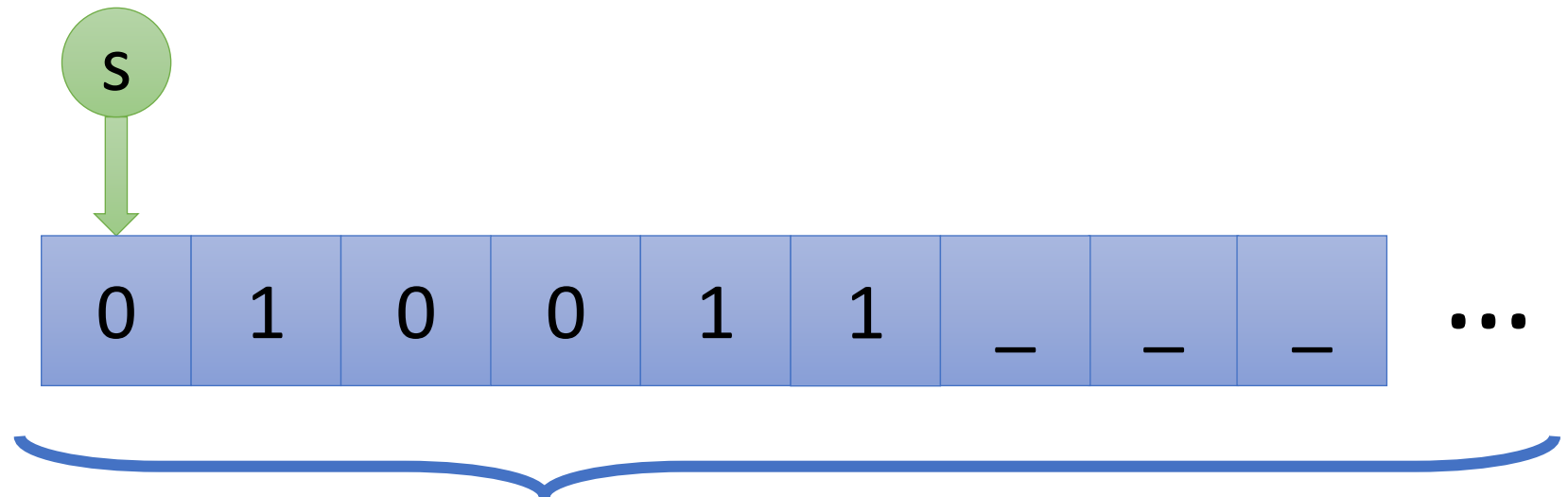
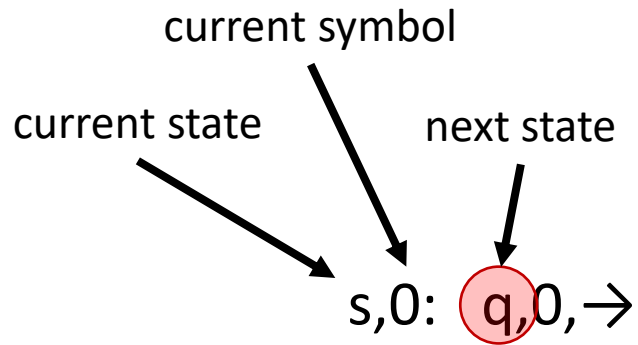
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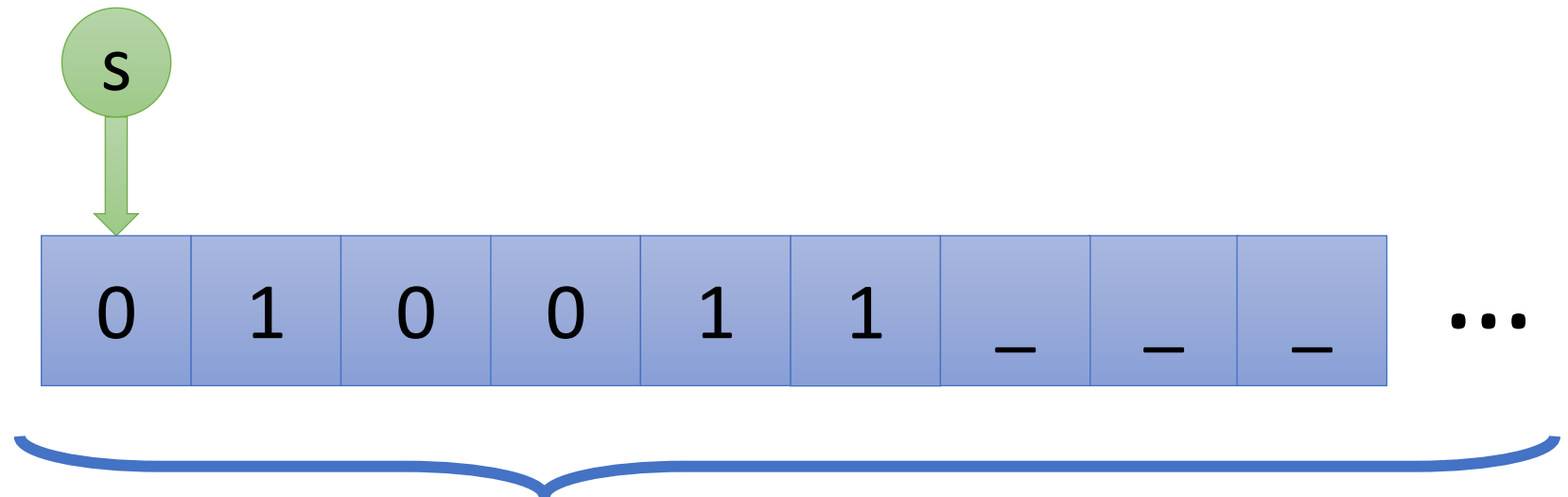
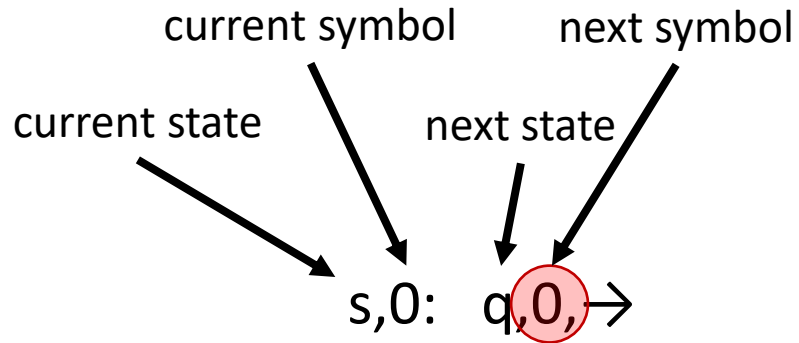
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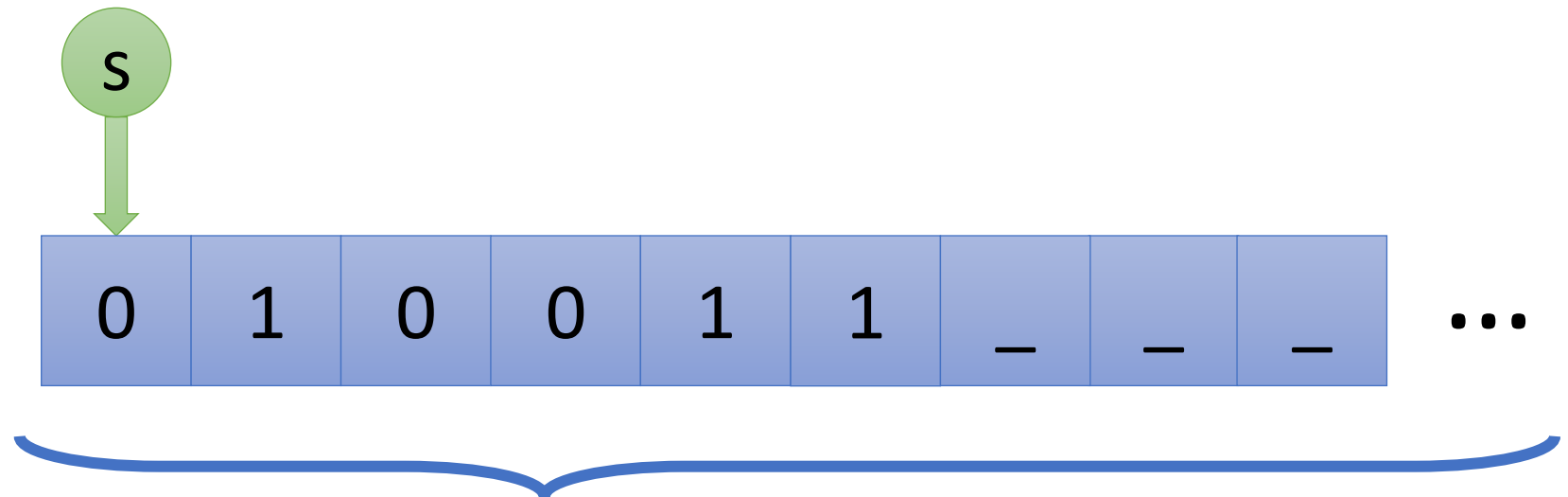
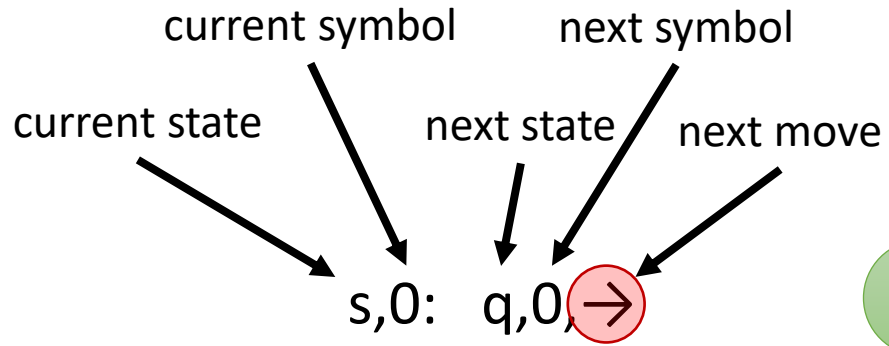
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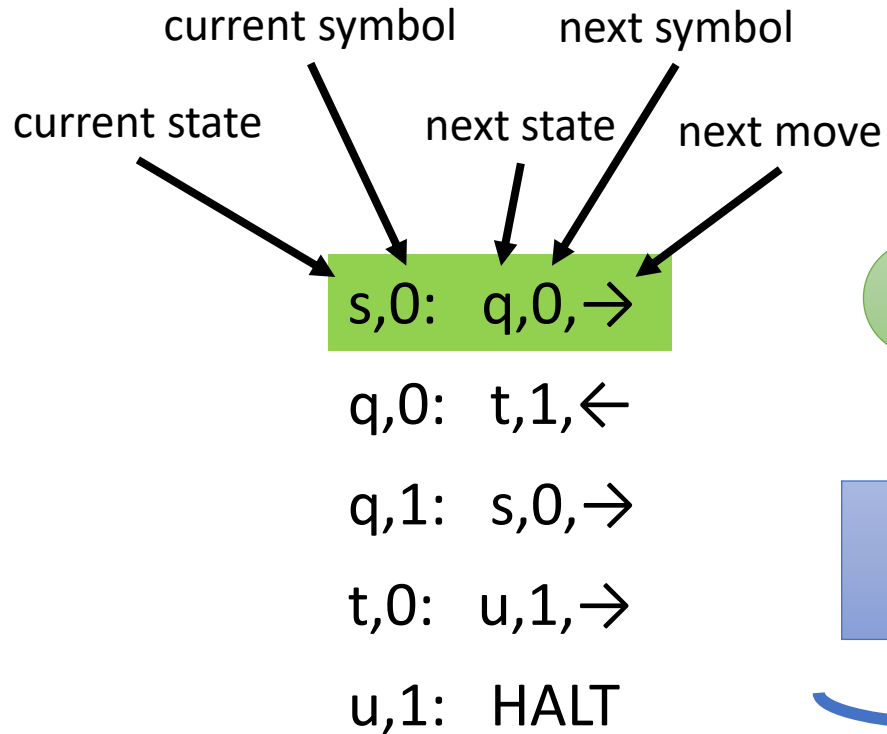
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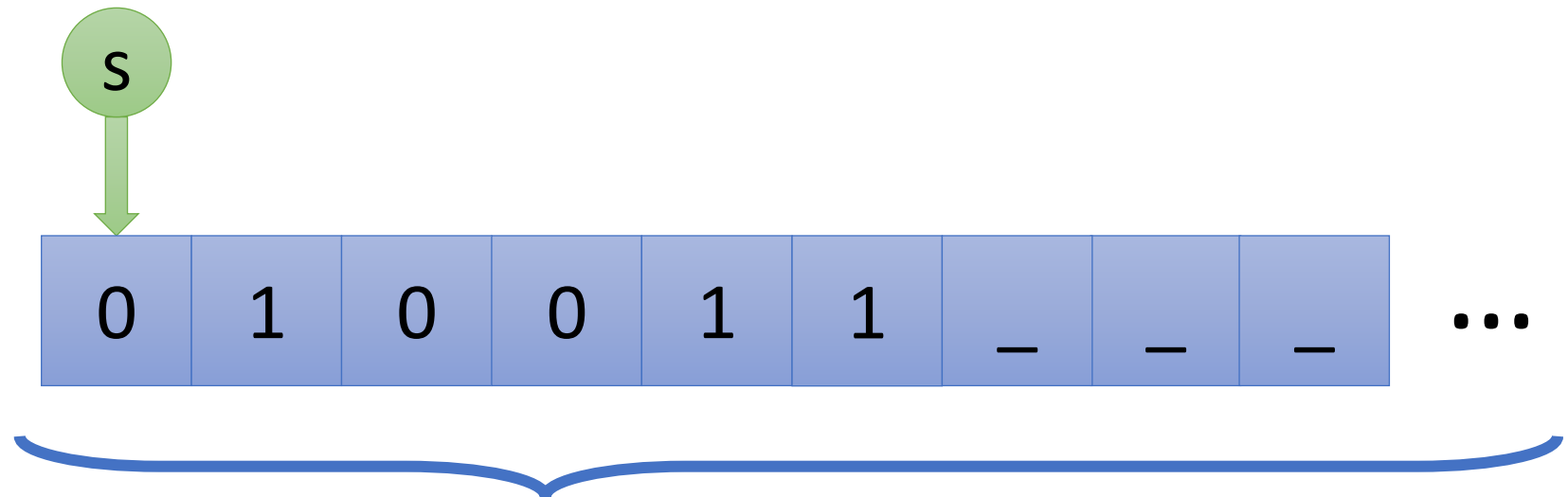
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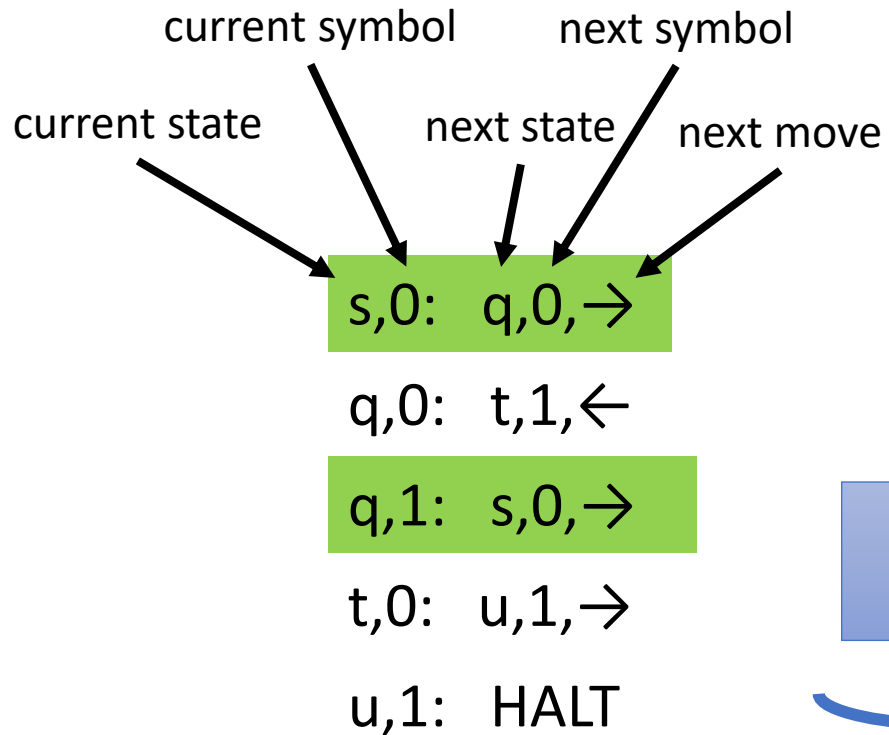


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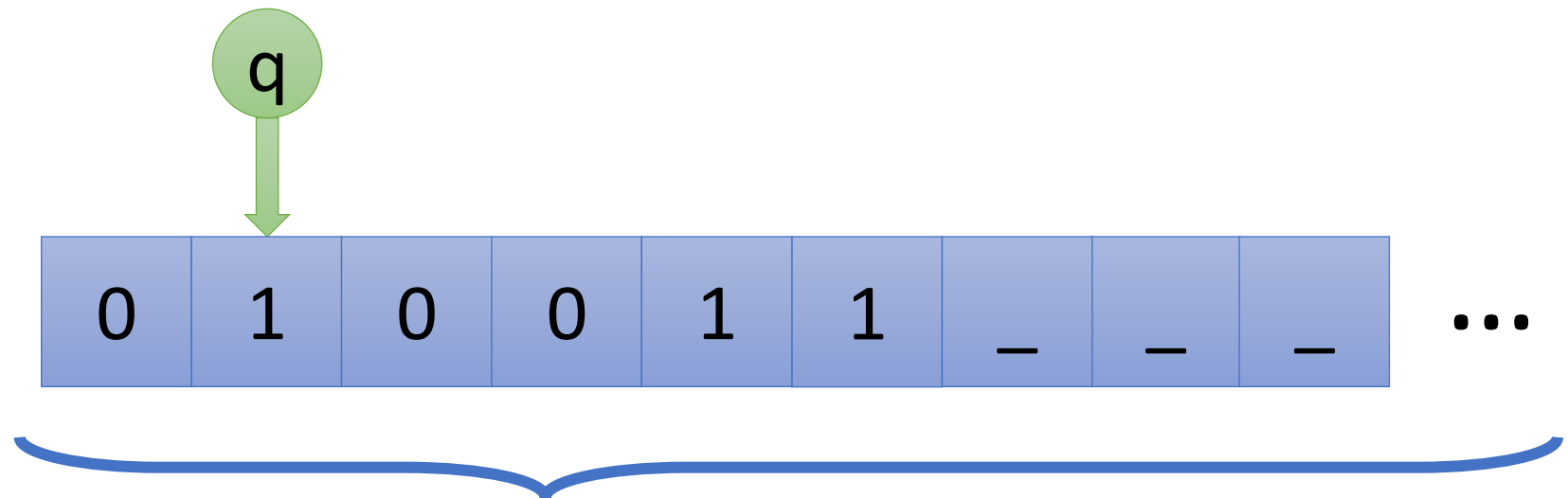
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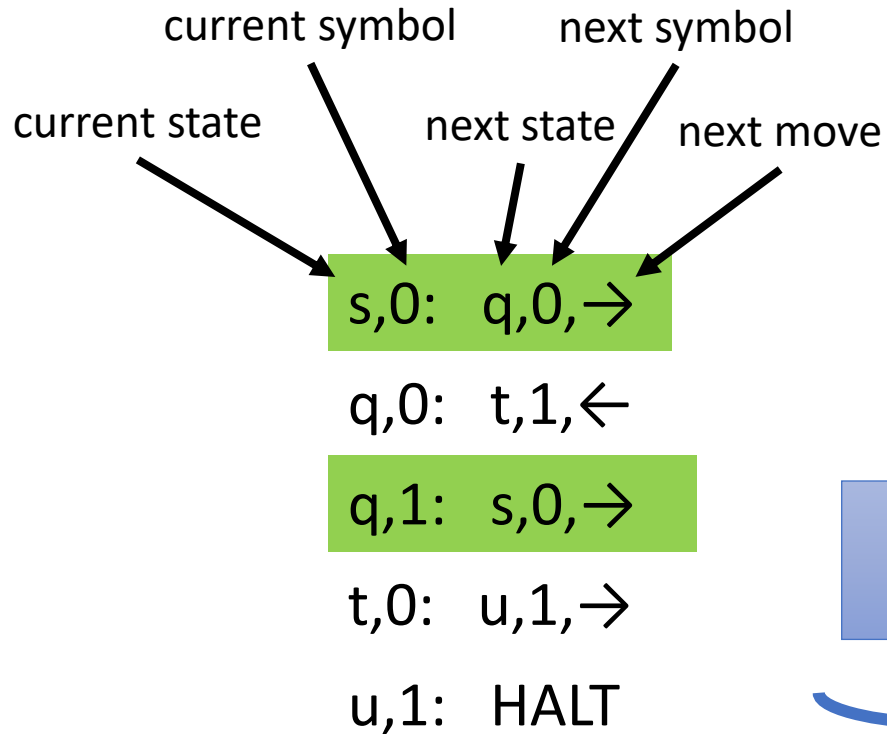


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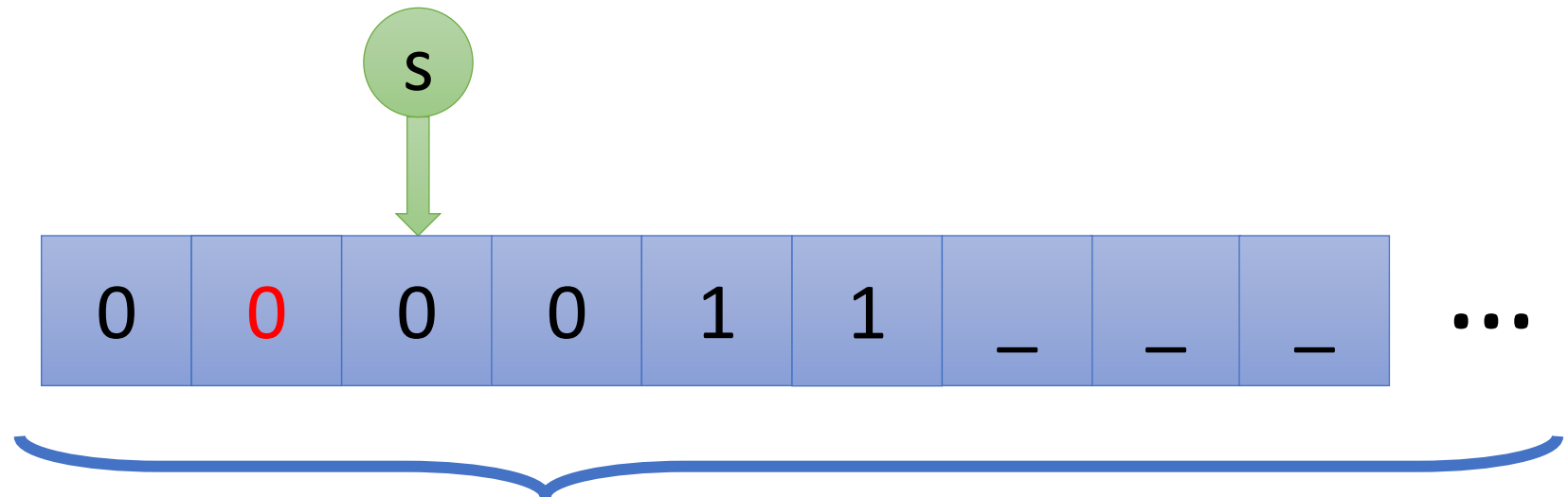
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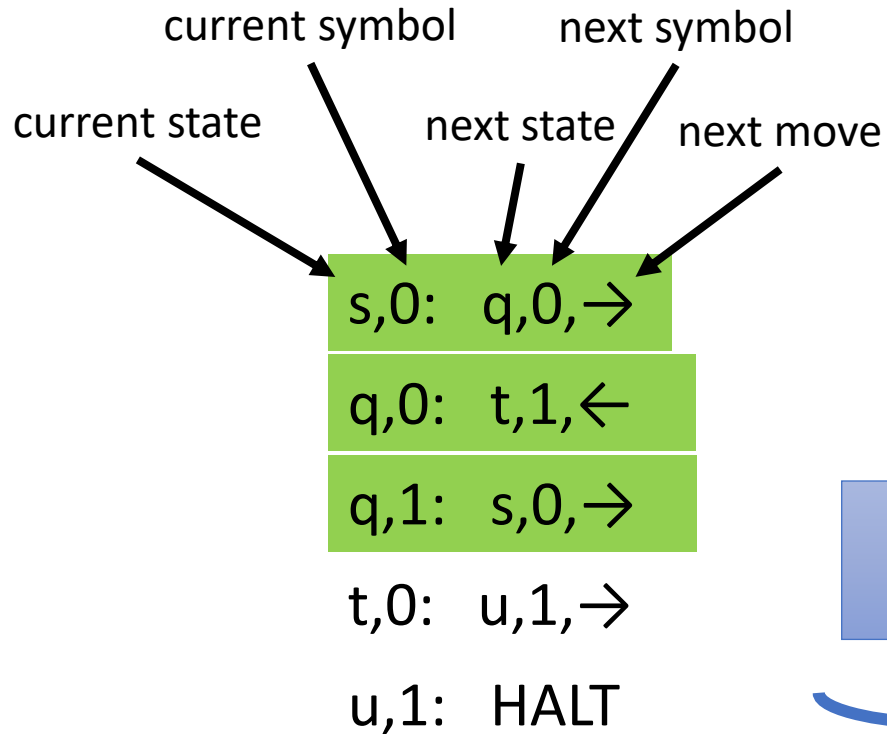
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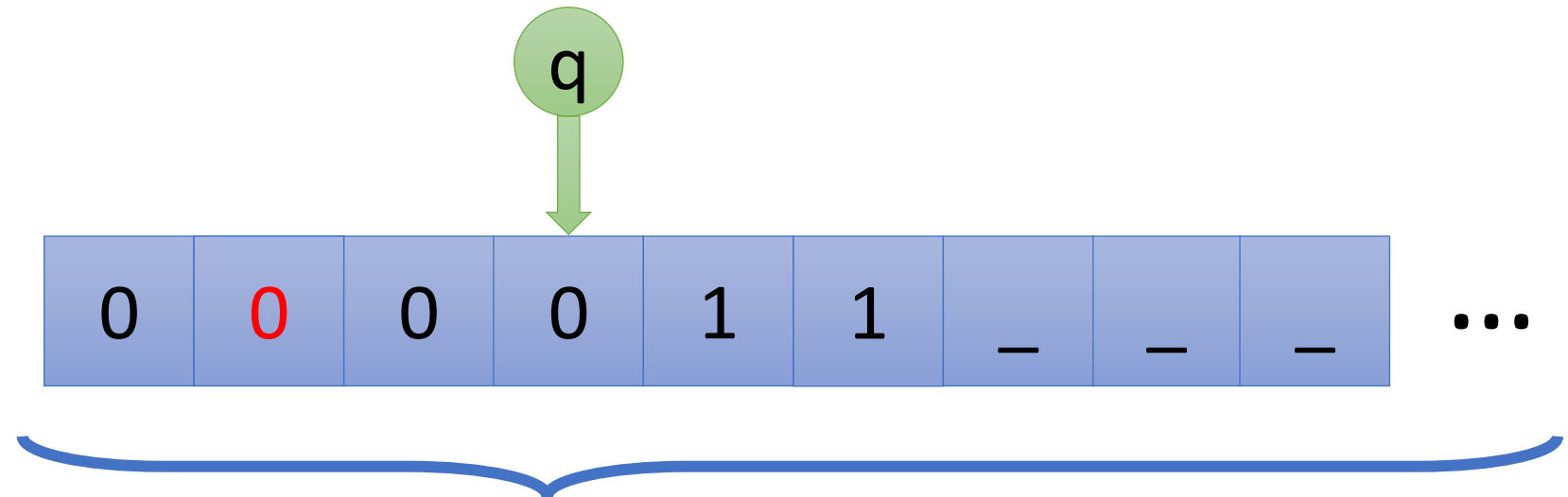
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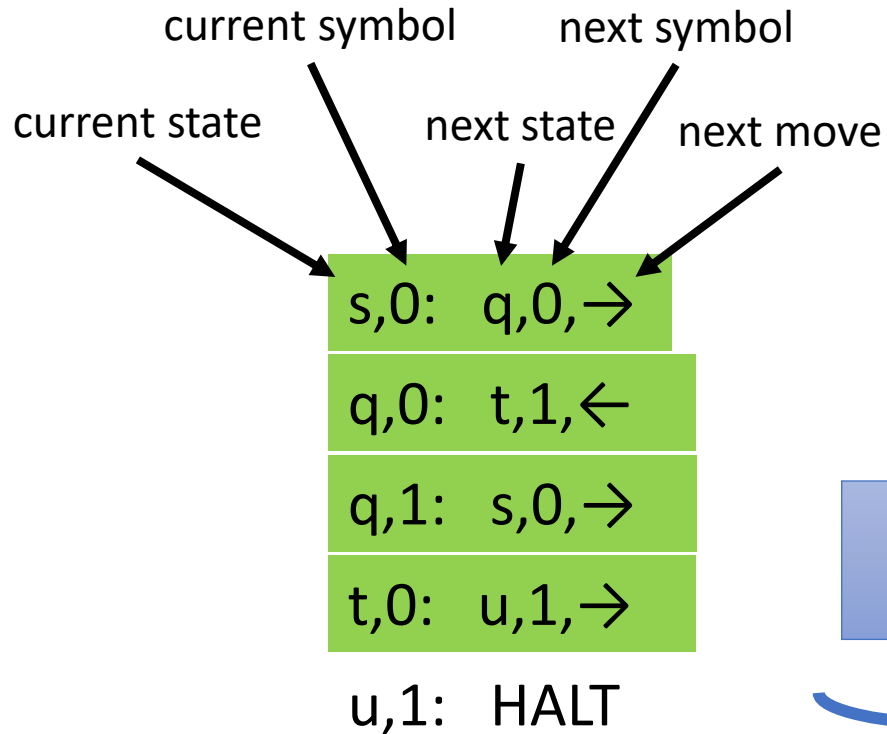
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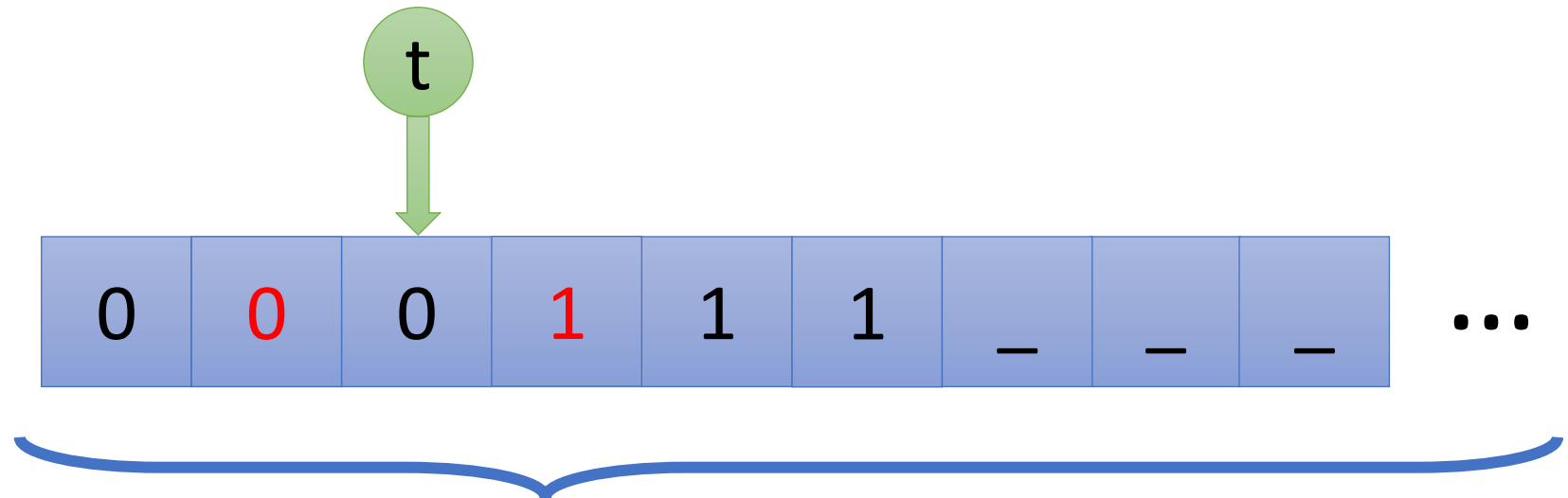
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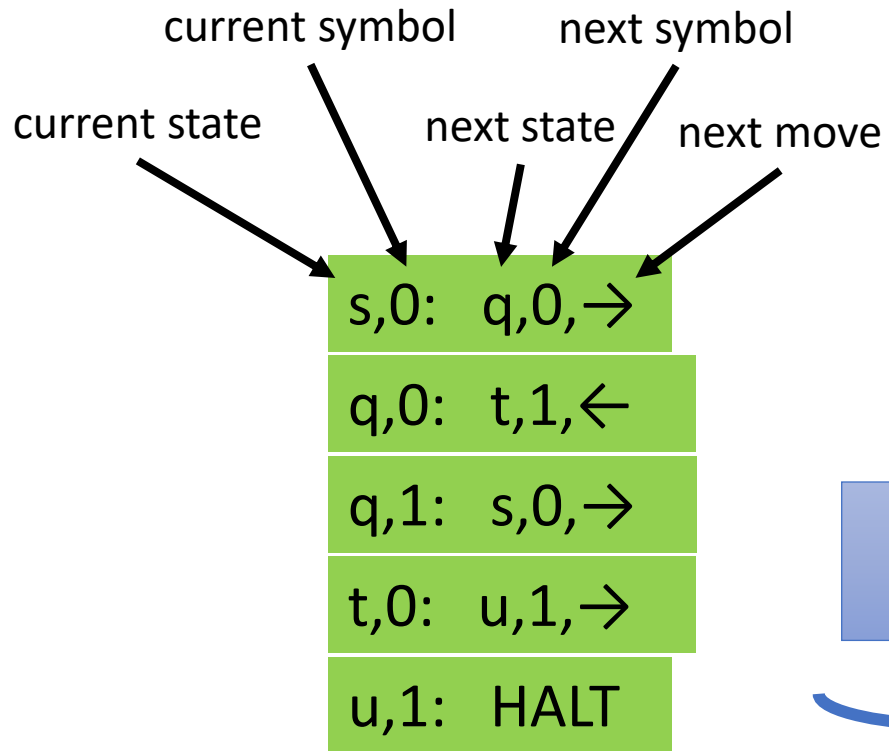
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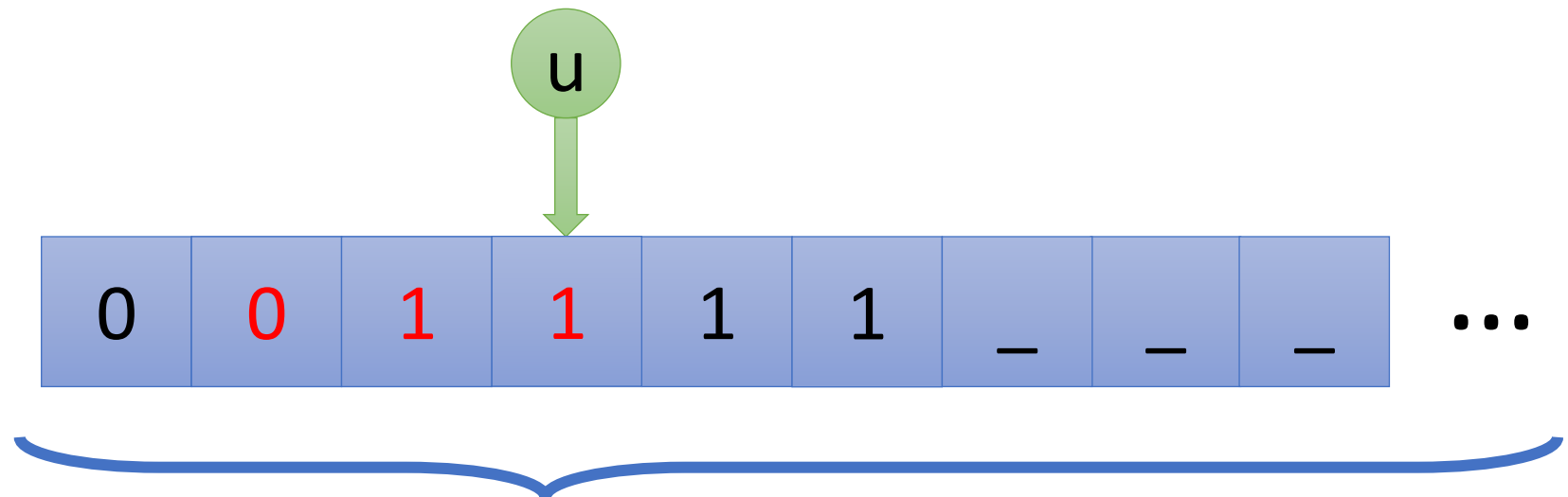
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Tile assembly is Turing-universal

# Tile assembly is Turing-universal

s,0: q,0,→

q,0: t,1,←

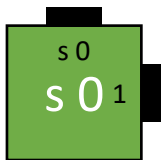
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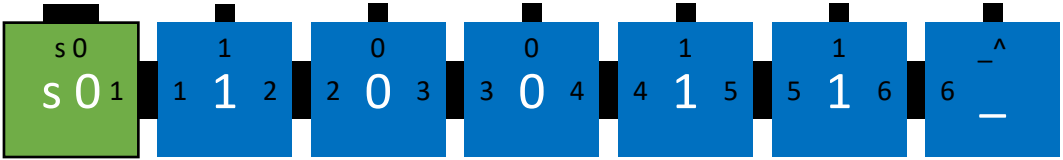
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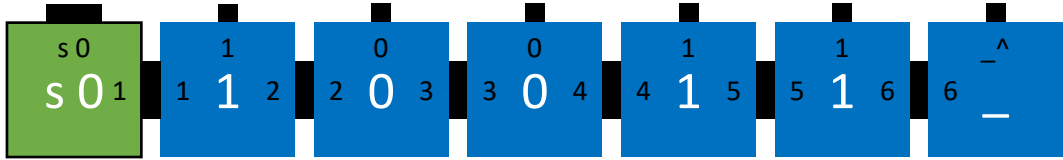
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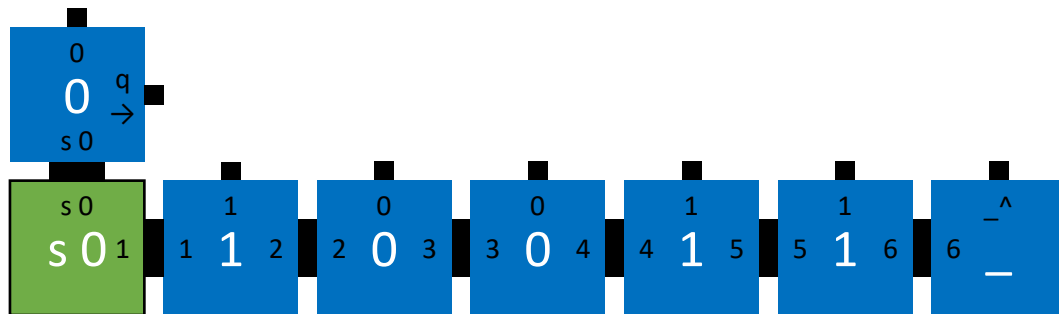
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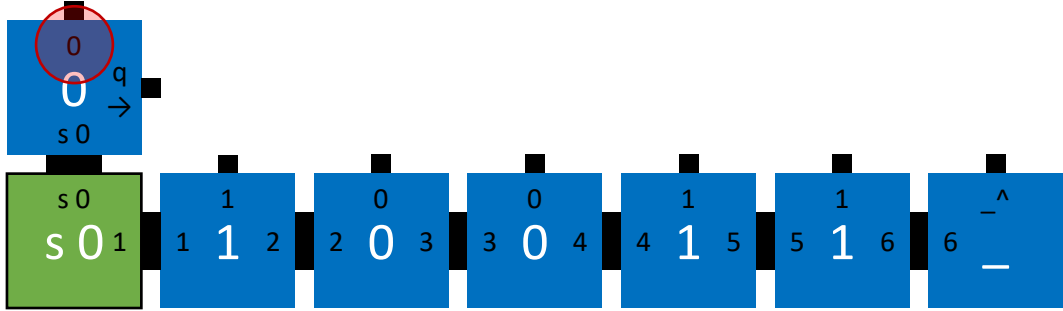
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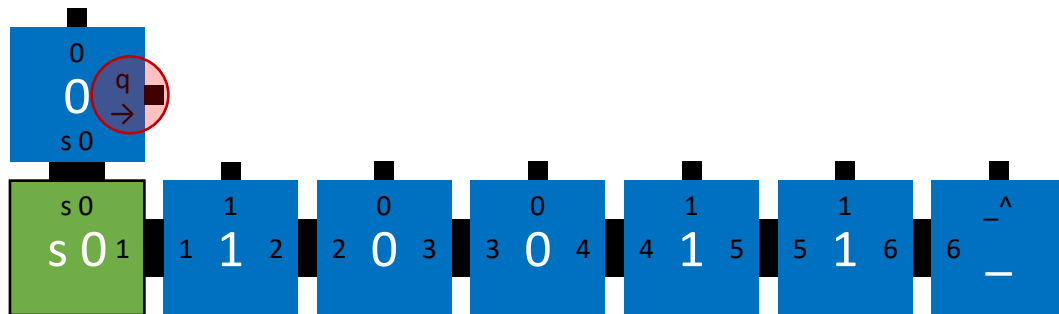
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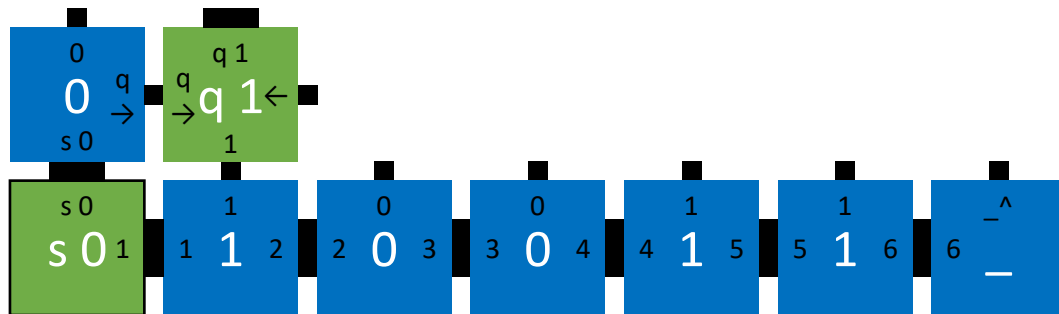
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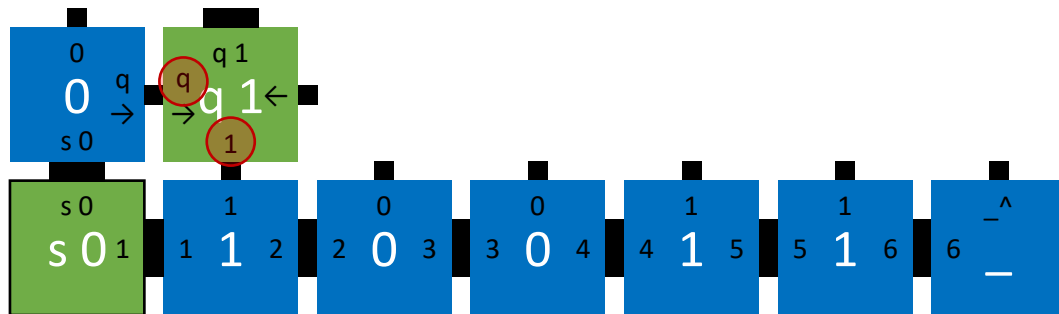
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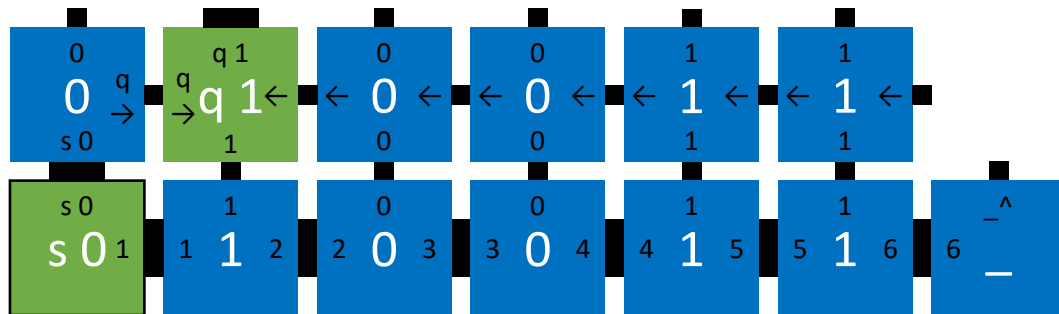
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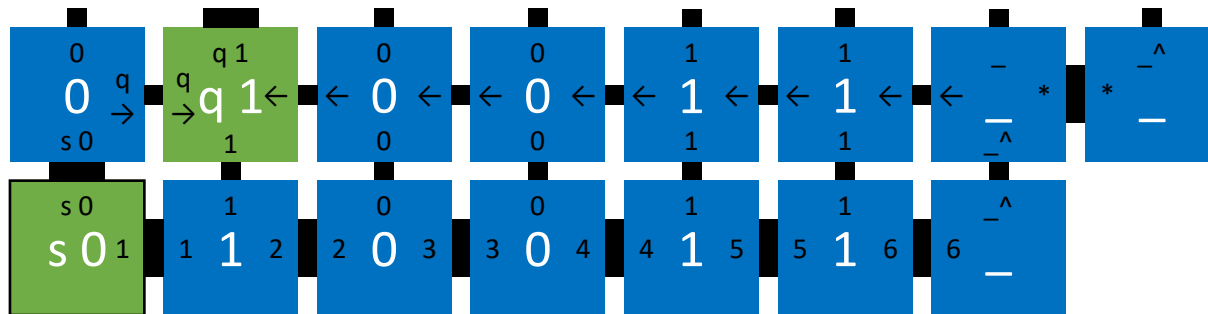
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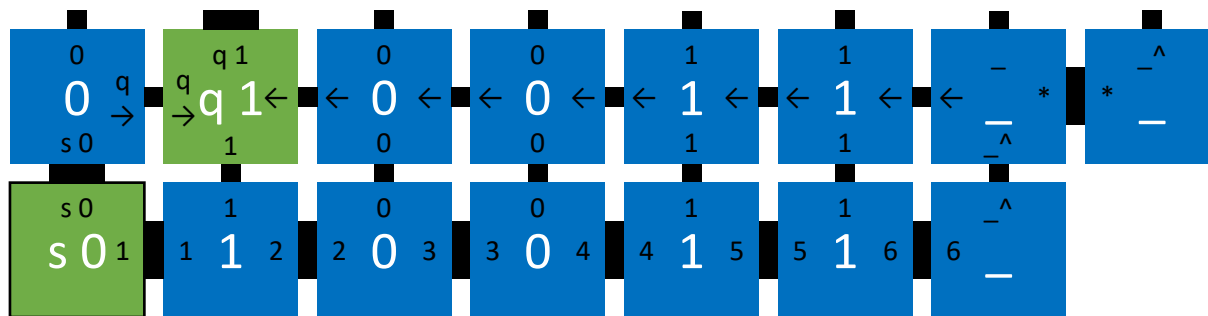
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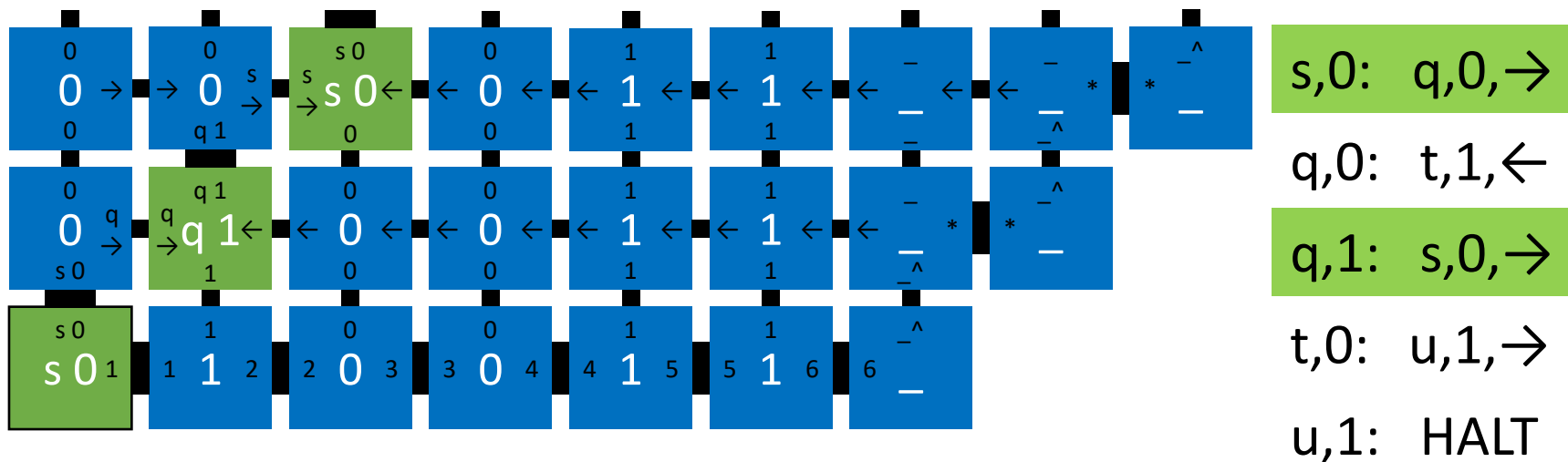
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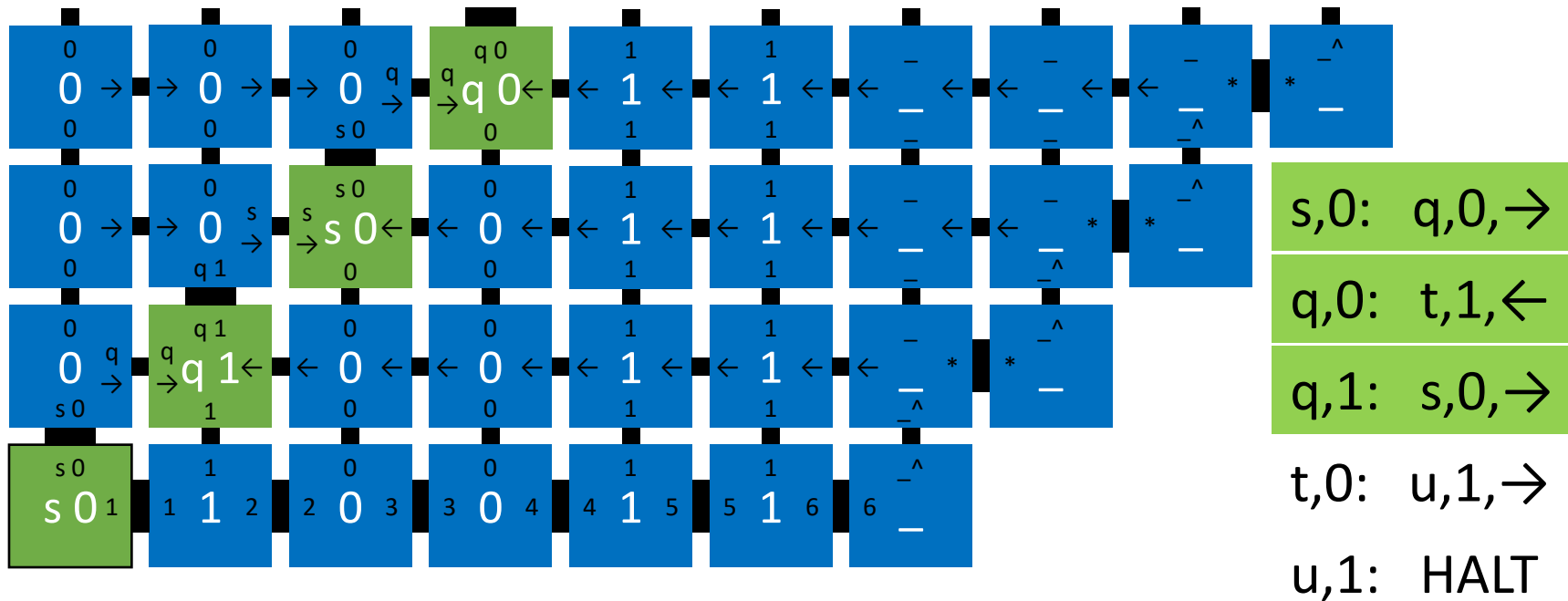
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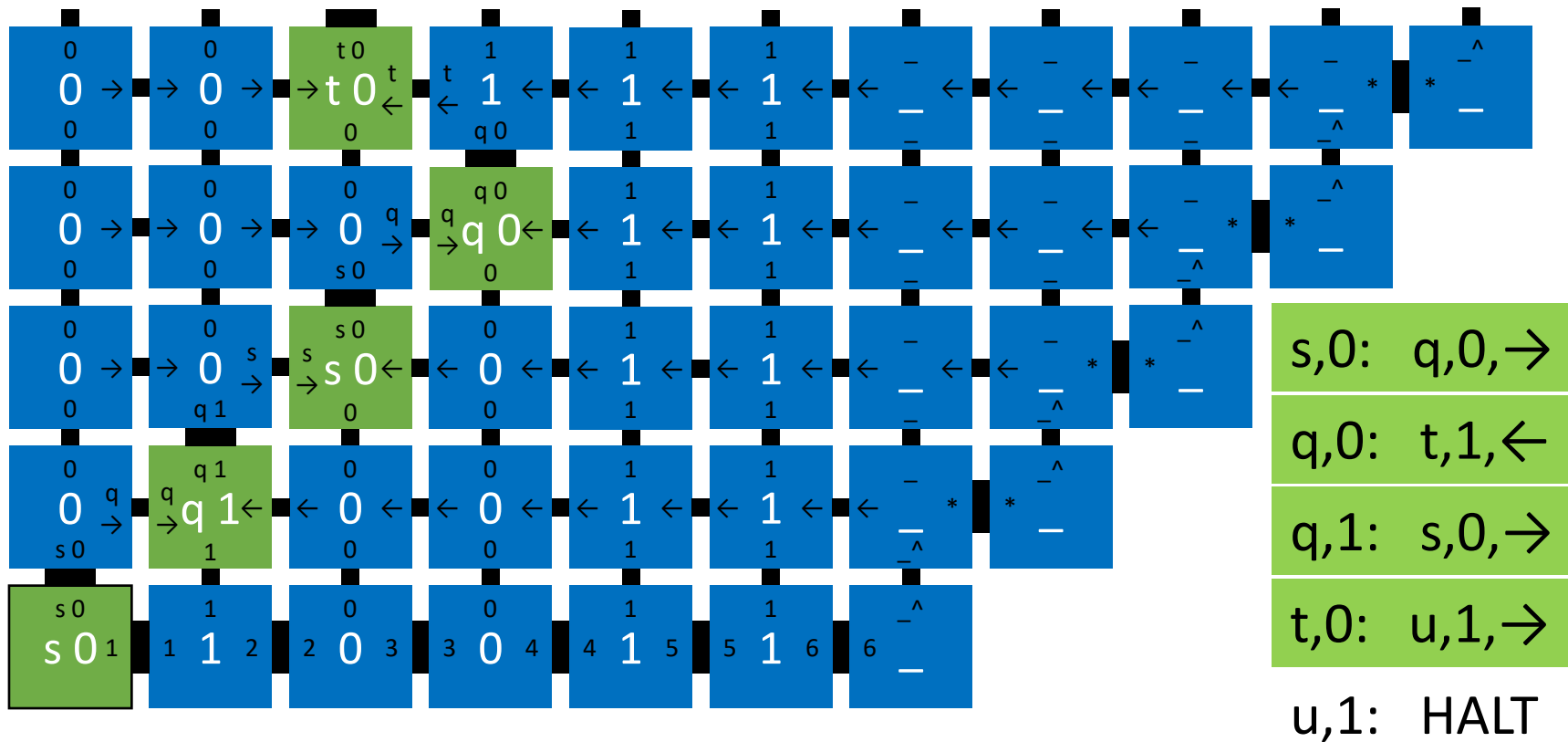
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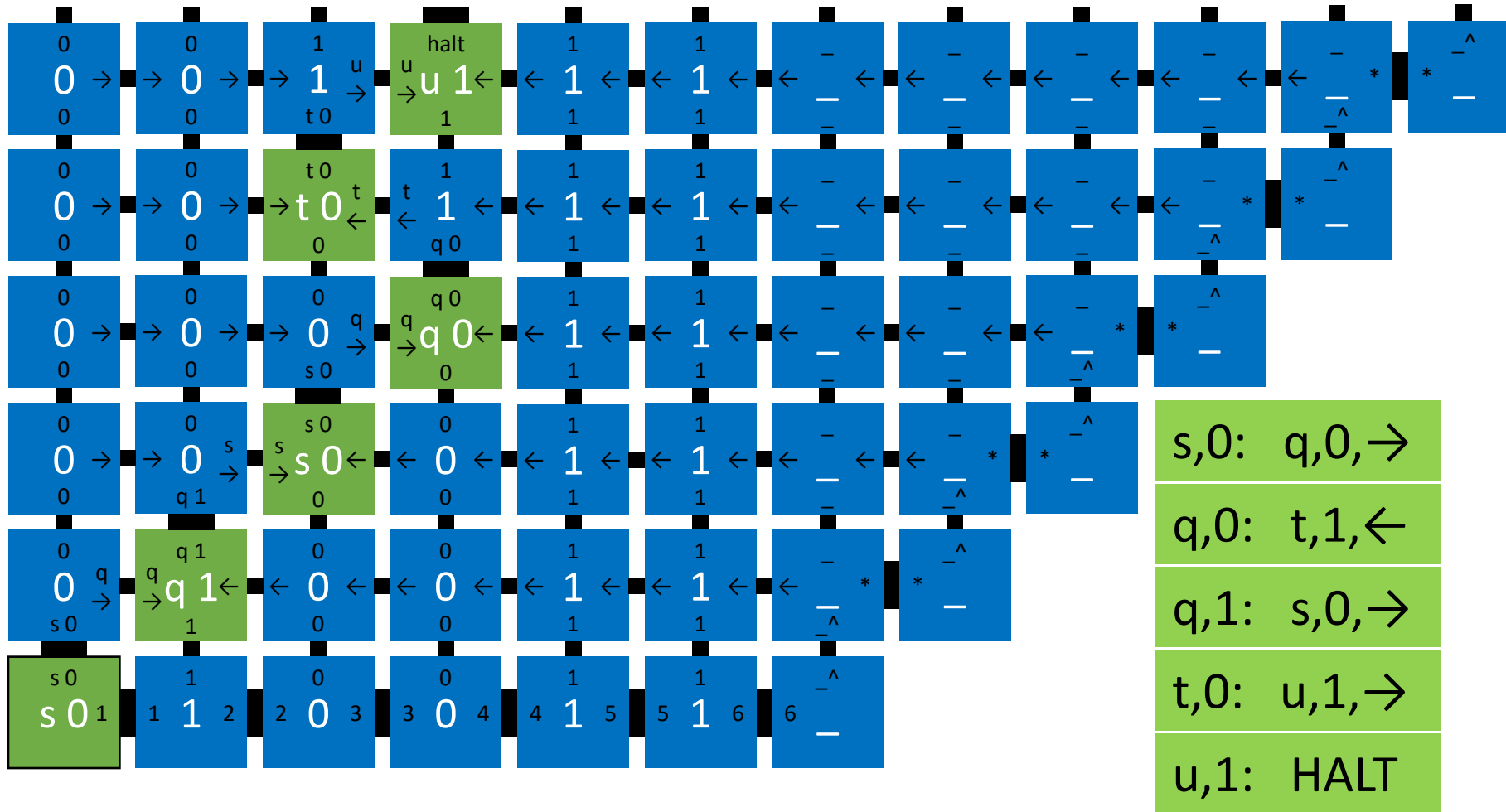
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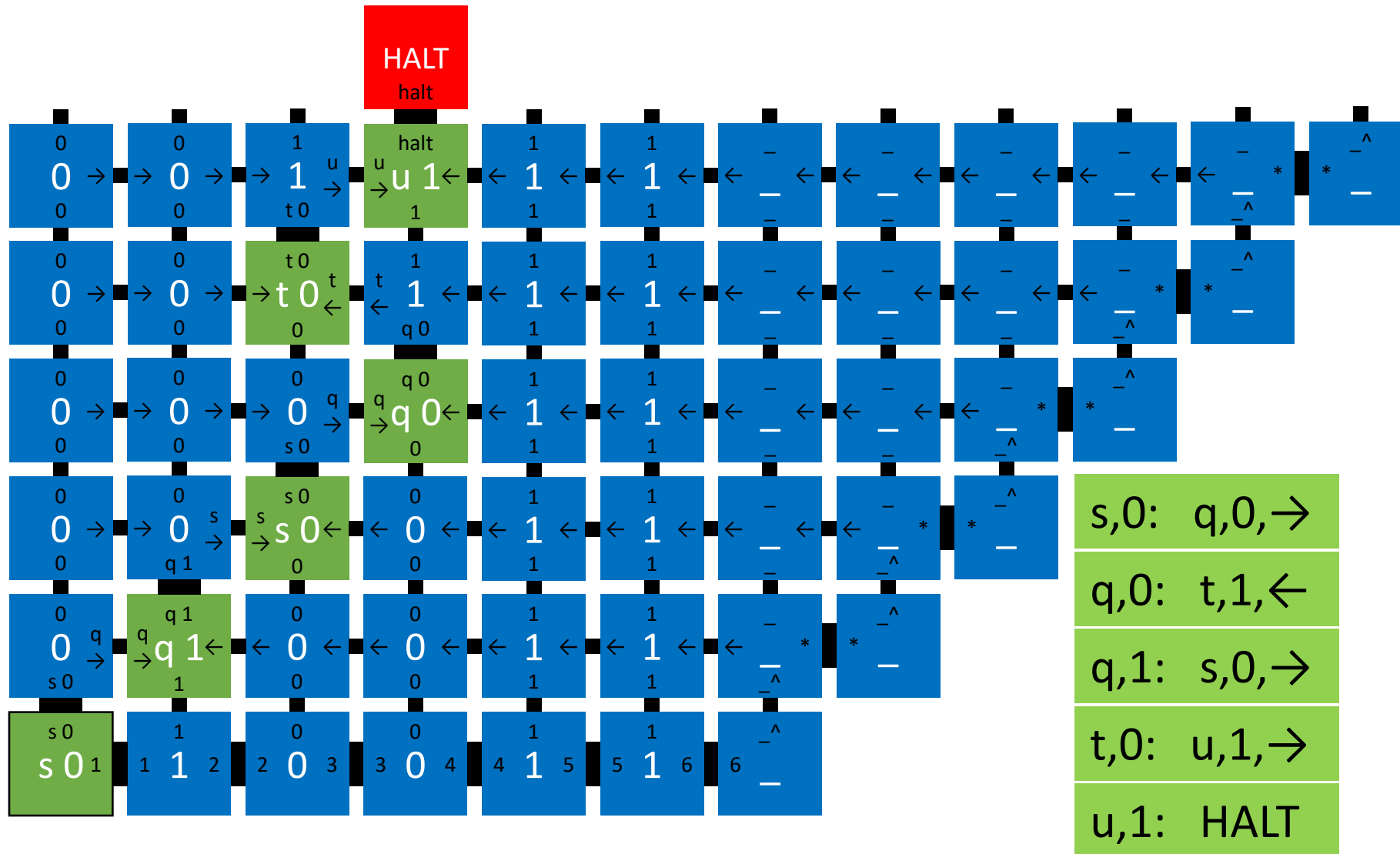
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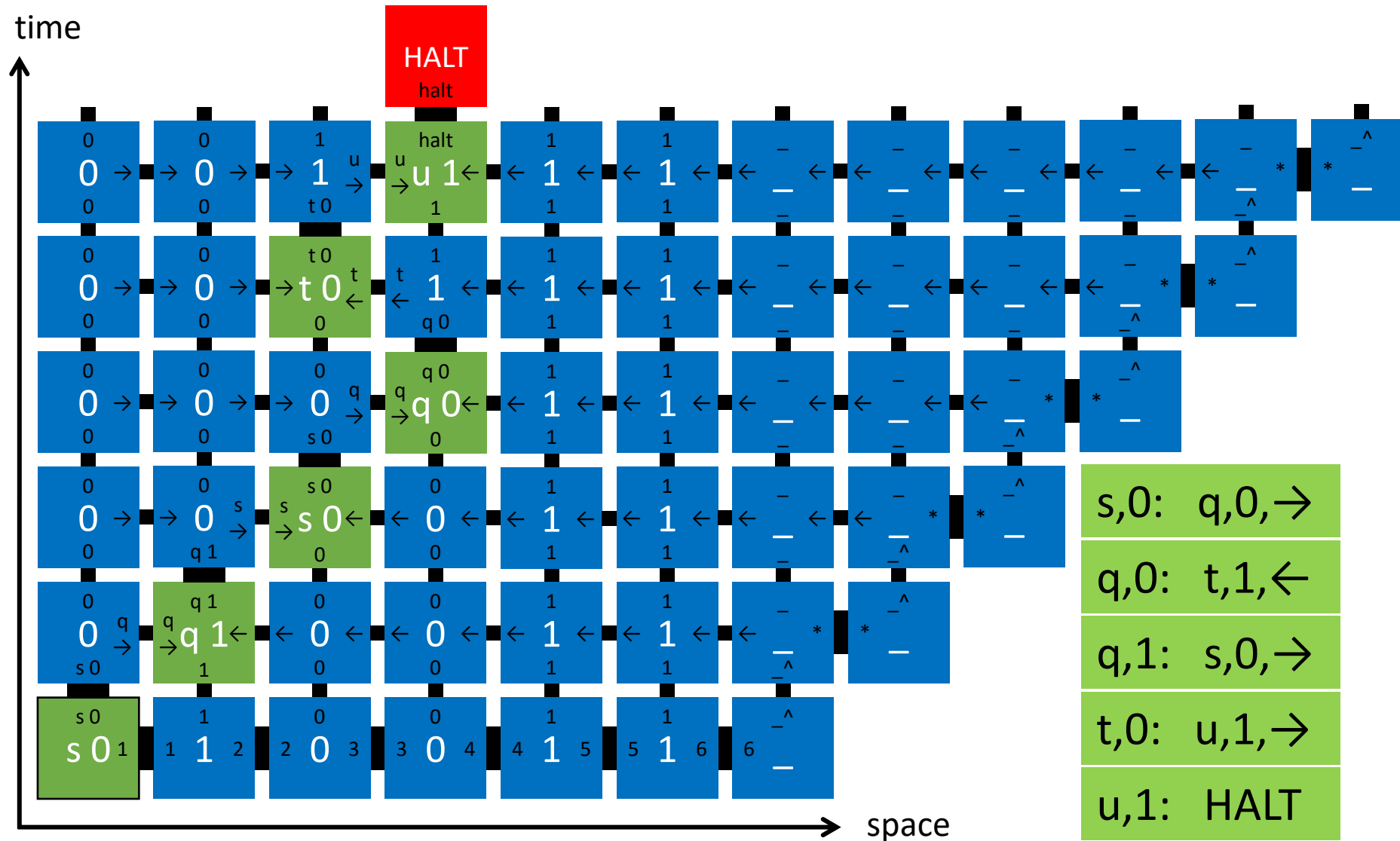


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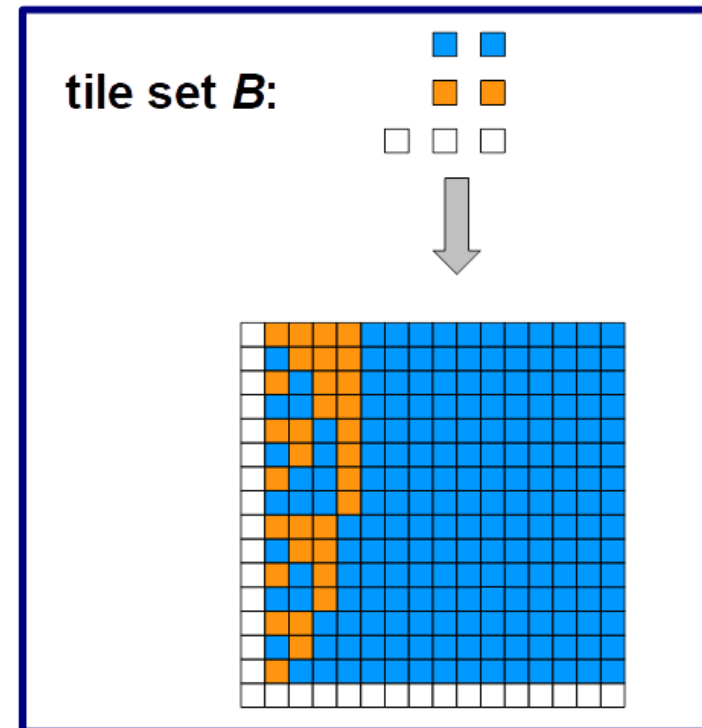
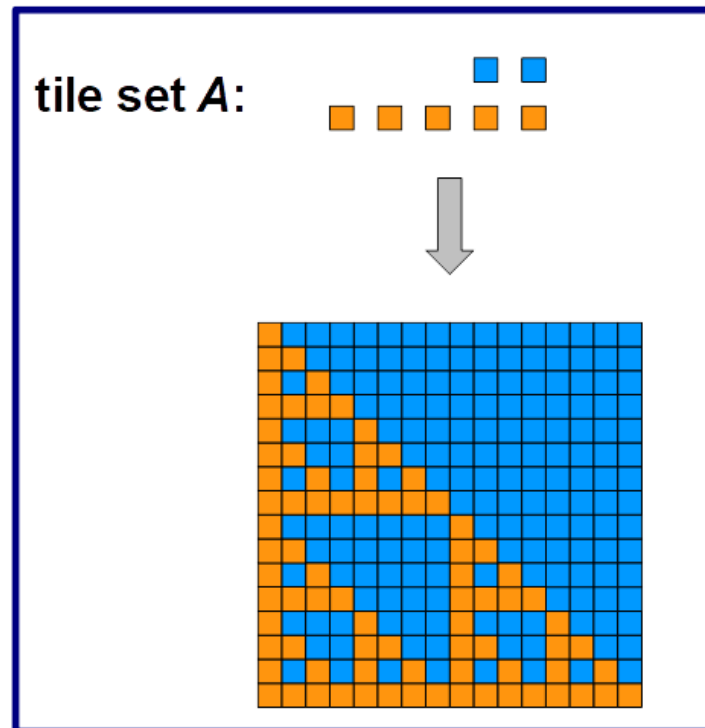


# Tile assembly is Turing-universal



# Putting the *algorithm* in *algorithmic* self-assembly

- **set of tile types** is like a **program**
- **shape** it creates, or **pattern** it paints, is like the **output** of the program



Putting the *algorithm* in *algorithmic* self-assembly

How is a set of tile types **not** like a program?

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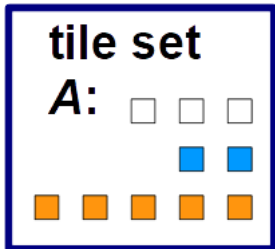
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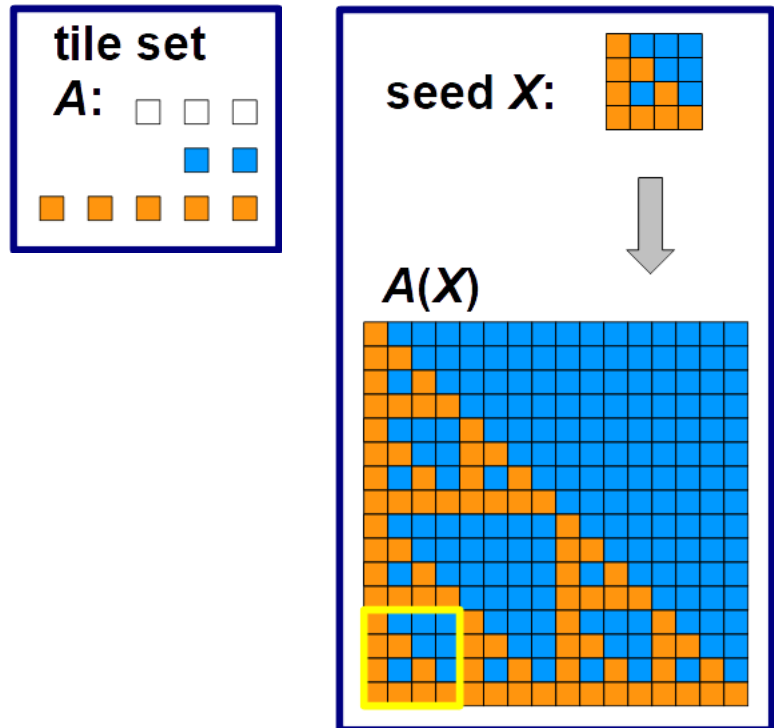
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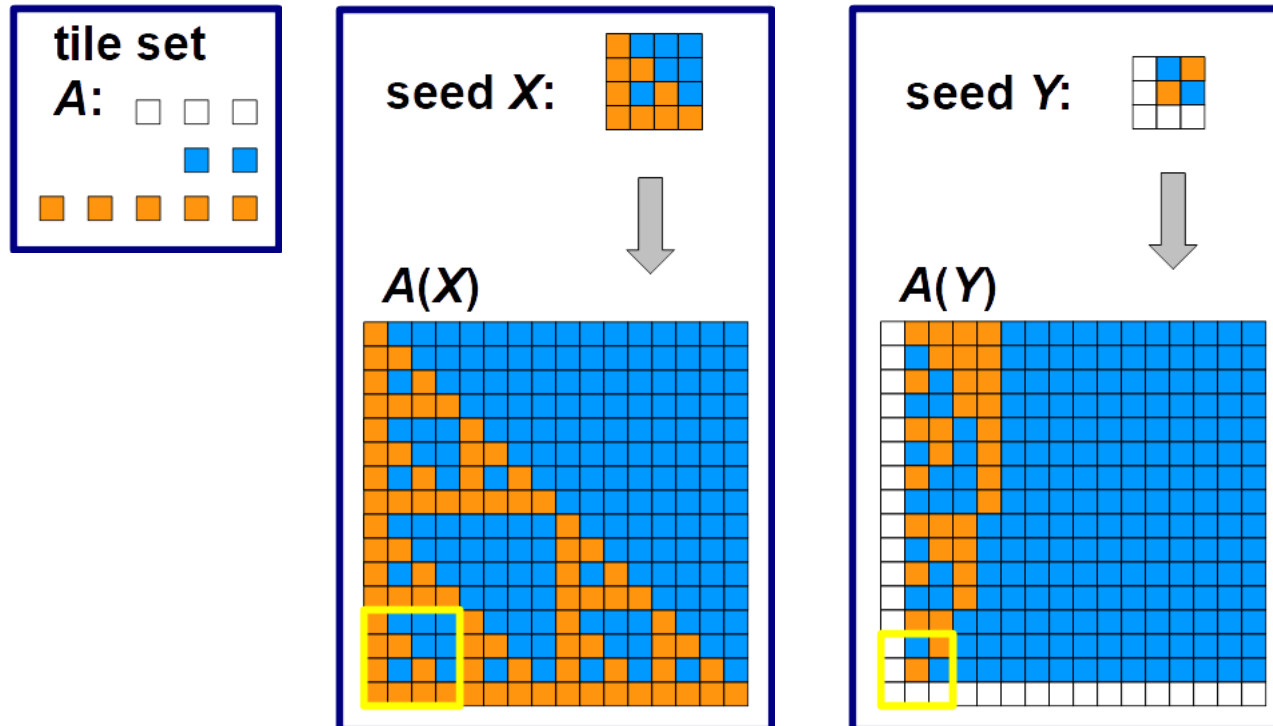
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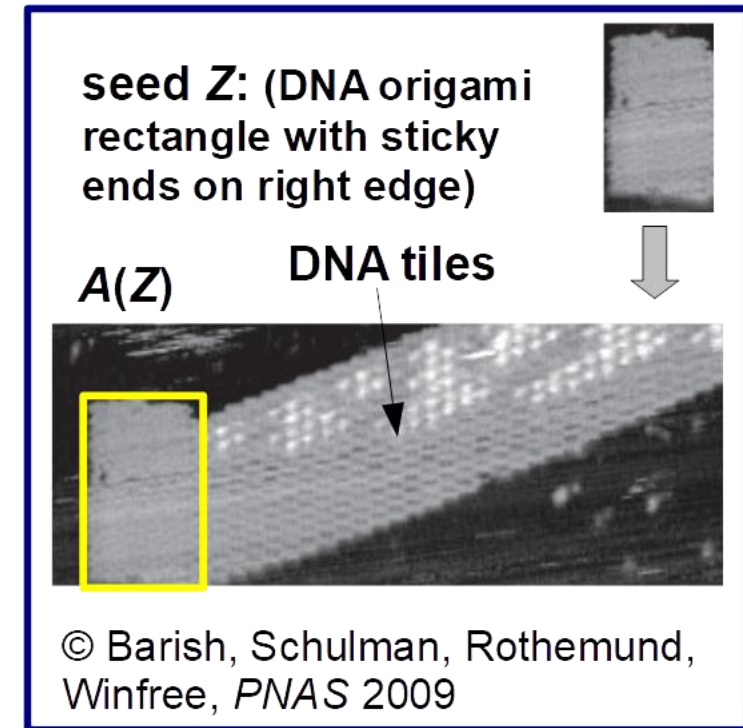
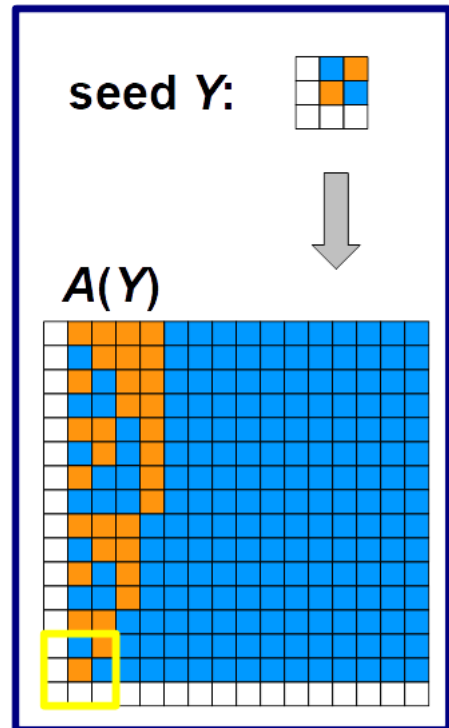
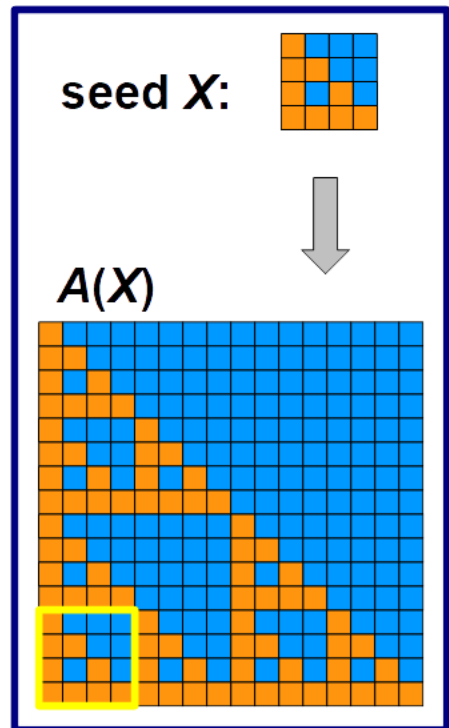
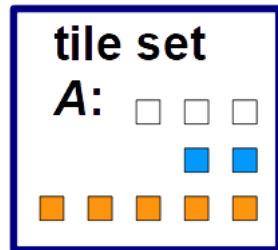




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# Calculating parity of 6-bit string: 1 algorithm, $2^6$ inputs



seed encoding **100101**

seed encoding **110101**

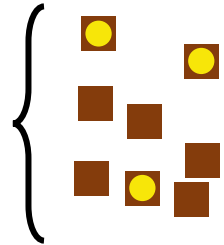


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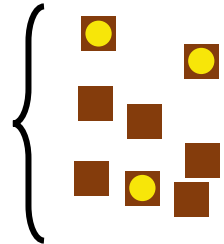


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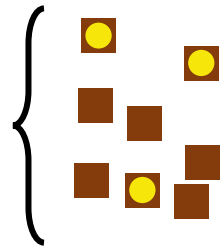


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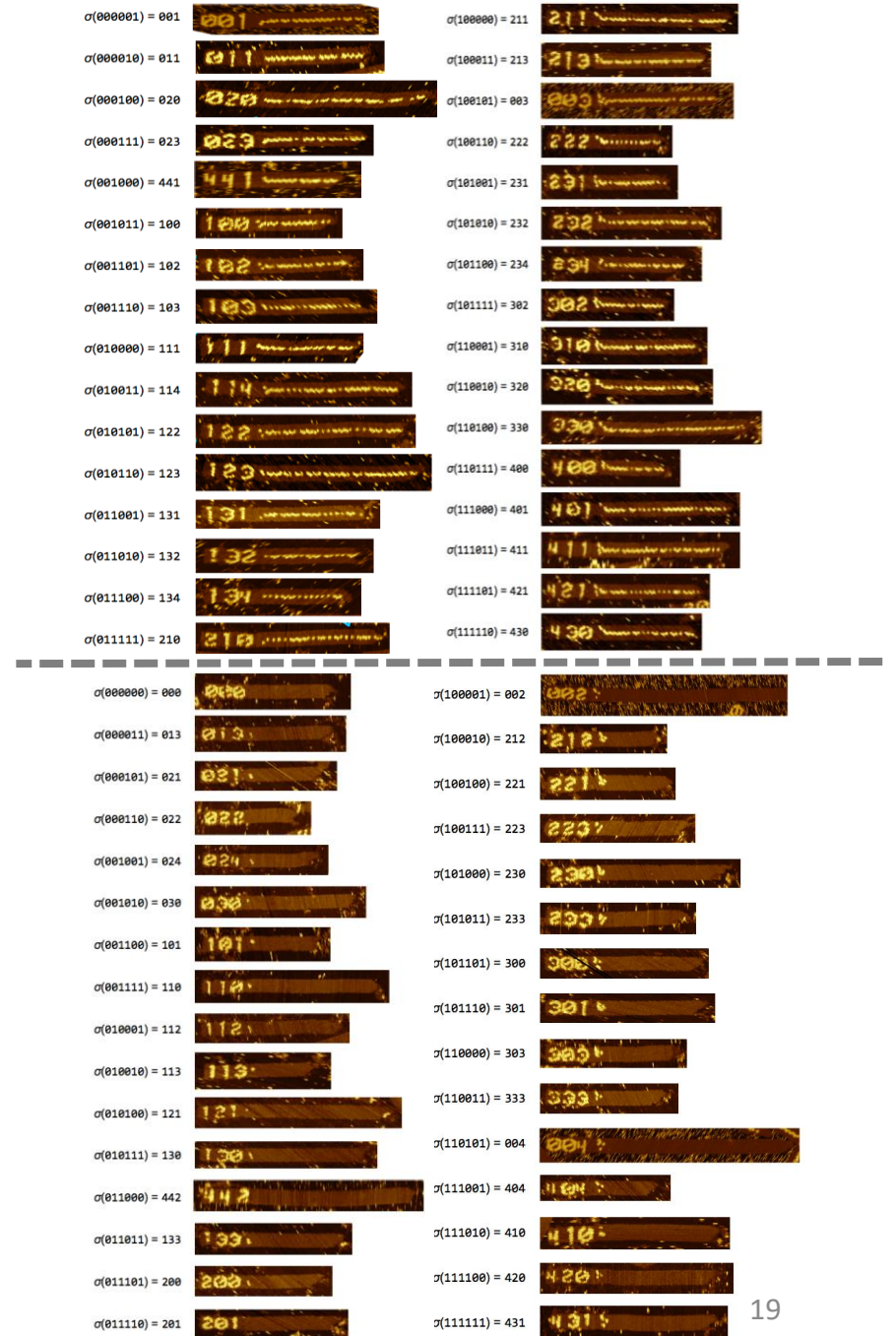
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$2^6$  seeds:



[Iterated Boolean circuit computation via a programmable DNA tile array. Woods, Doty, Myhrvold, Hui, Wu, Yin, Winfree, [in preparation](#), work presented in DNA 23 talk tomorrow by Damien Woods]

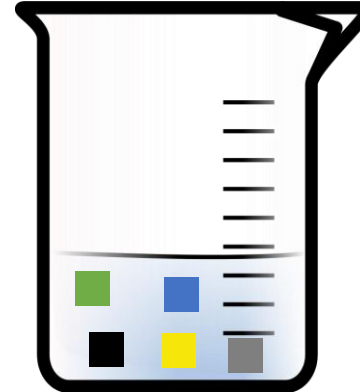
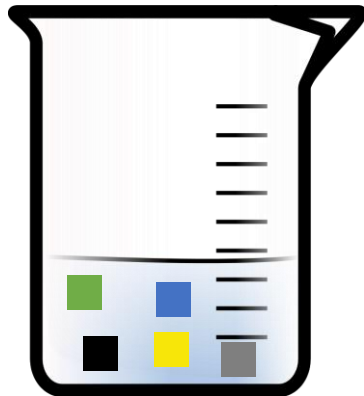
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**Theorem:** There is a single set  $T$  of tile types, so that, for any finite shape  $S$ , from an appropriately chosen seed  $\sigma_S$  “encoding”  $S$ ,  $T$  self-assembles  $S$ .

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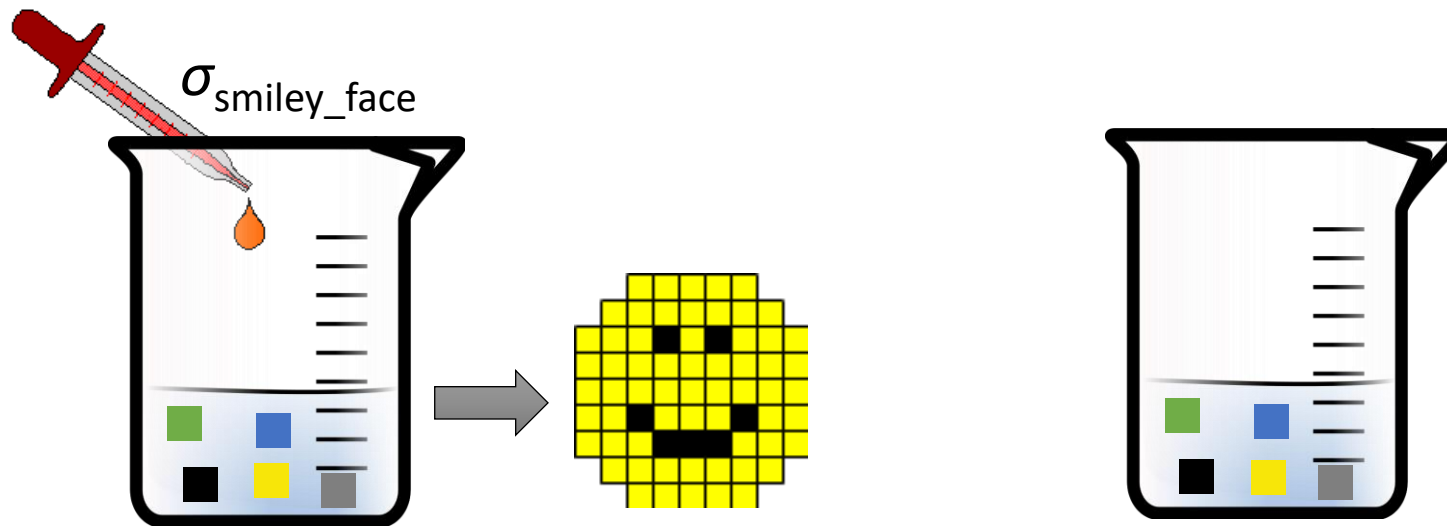
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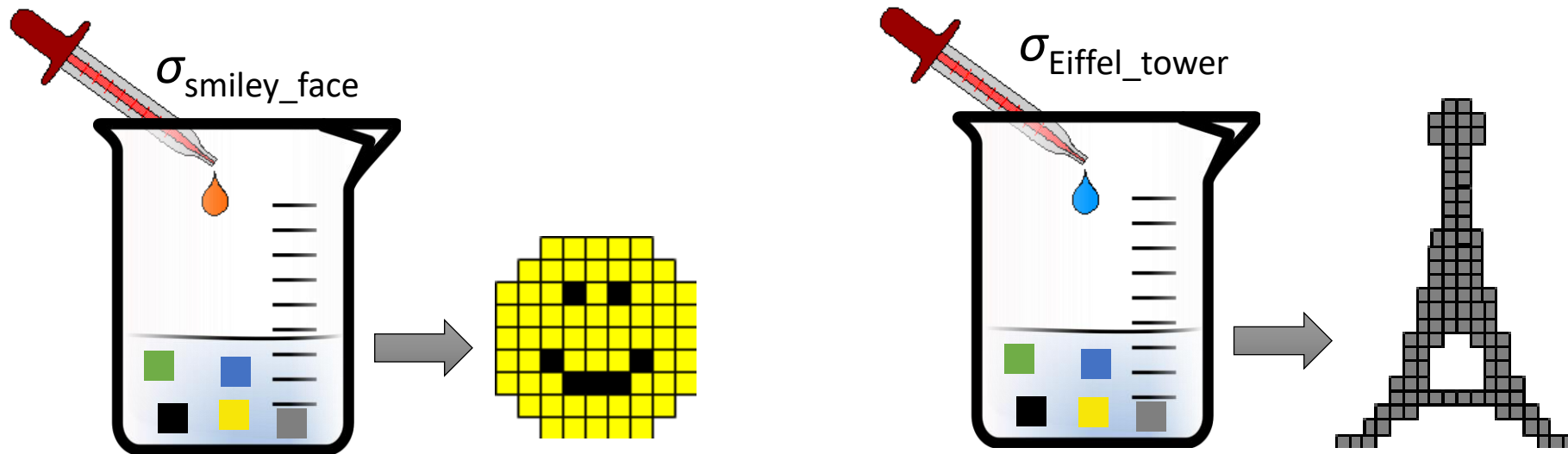
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[Complexity of Self-Assembled Shapes. Soloveichik and Winfree, SIAM Journal on Computing 2007]

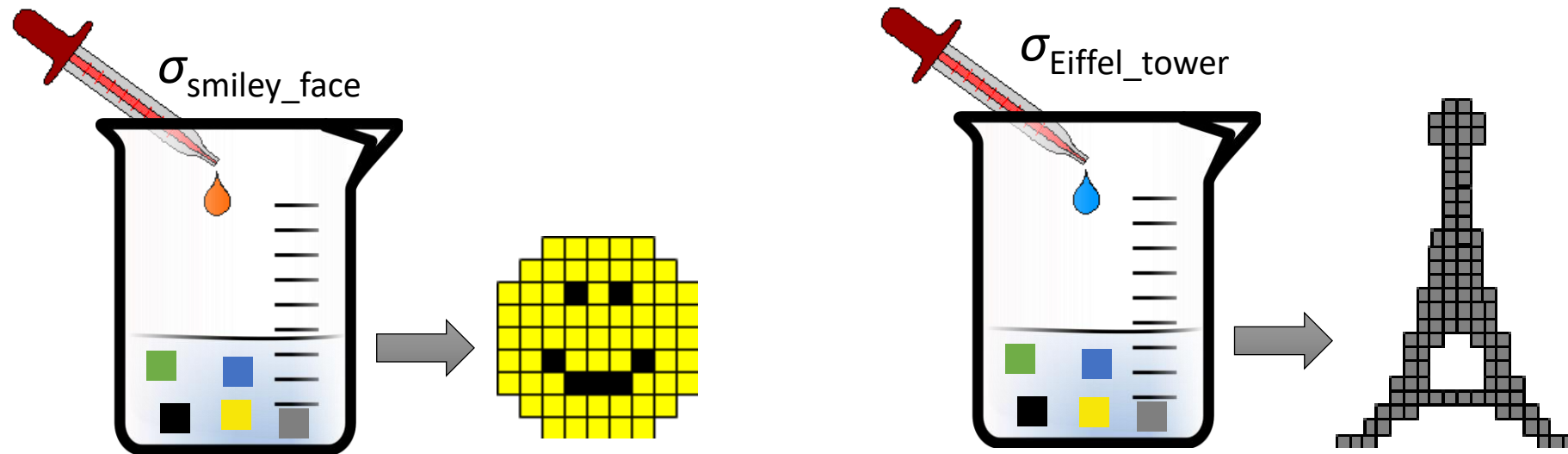
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These tiles are **universally programmable** for building any shape.

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  - possibly, monomer can move



# Active self-assembly at DNA 23

- Marta Andrés Arroyo, Sarah Cannon, Joshua J. Daymude, Dana Randall, and Andréa W. Richa. *A Stochastic Approach to Shortcut Bridging in Programmable Matter*
- Yen-Ru Chin, Jui-Ting Tsai and Ho-Lin Chen. *A Minimal Requirement for Self-Assembly of Lines in Polylogarithmic Time*

# A Stochastic Approach to Shortcut Bridging in Programmable Matter

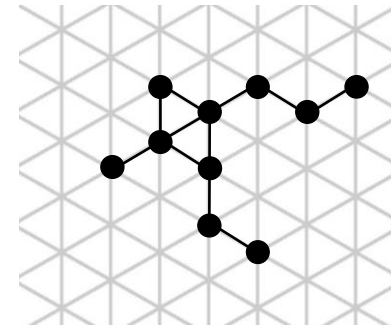
Marta Andrés Arroyo, Sarah Cannon, Joshua J. Daymude, Dana Randall, Andréa W. Richa

## Abstraction of Programmable Matter: **Self-organizing Particle Systems**

A collection of simple computational elements that self-organize to solve system-wide problems of movement, configuration, and coordination via fully distributed, local algorithms.

**Geometric Amoebot Model:** Particles move on the triangular lattice.

- Asynchronous,
- Each has constant-size memory,
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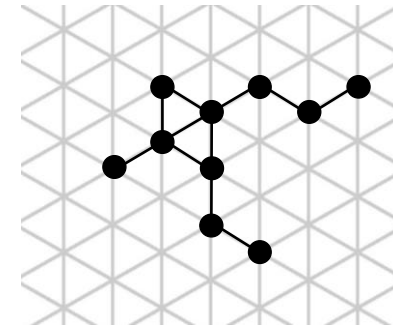
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(Mostly) deterministic algorithms exist for: Leader election, Shape formation (triangle, hexagon, etc.), Infinite object coating. (See [sops.engineering.asu.edu](http://sops.engineering.asu.edu)).

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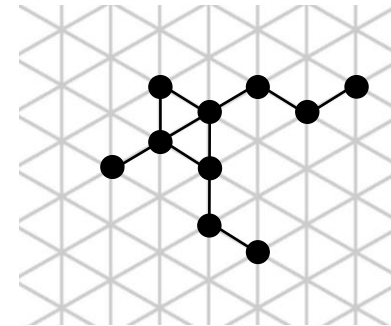
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- Asynchronous,
- Each has constant-size memory,
- Each can communicate only with neighboring particles,
- There is no common orientation, only common chirality,
- Often desirable that the system stays connected.



(Mostly) deterministic algorithms exist for: Leader election, Shape formation (triangle, hexagon, etc.), Infinite object coating. (See [sops.engineering.asu.edu](https://sops.engineering.asu.edu)).

Stochastic algorithms exist for:

- **Compression:** gathering a particle system together as tightly as possible.
  - Often found in natural systems.
  - Approach is decentralized, self-stabilizing, and oblivious (no leader necessary).
  - Uses a Markov chain to derive a local algorithm.
- **Shortcut bridging** (DNA23): Generalizes the stochastic approach.

# A Stochastic Approach to Shortcut Bridging in Programmable Matter

Marta Andrés Arroyo, Sarah Cannon, Joshua J. Daymude, Dana Randall, Andréa W. Richa

A framework for transforming Markov chains into local, asynchronous distributed algorithms:

## Markov chain algorithm:

Starting at any configuration, repeat:

1. **Pick a random particle.**
2. Choose a random direction.
3. If **certain properties** hold, move in that direction with probability **[.....]**.
4. Otherwise, do nothing.

↖ Depends on application

## Distributed algorithm:

**Each particle** continuously executes:

1. Particle proceeds at **its own processing speed** (possibly **variable**).
2. Choose a random direction.
3. If **certain properties** hold, move in that direction with probability **[.....]**.
4. Otherwise, do nothing.

↖ Poisson clock with individual rate

↖ Depends on application

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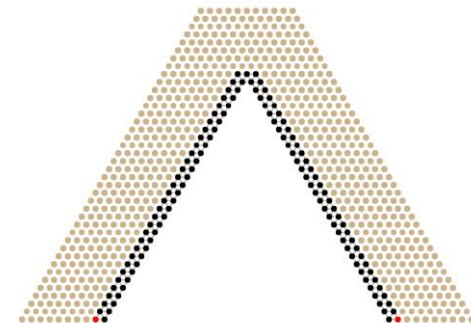
↖ Depends on application

**Shortcut Bridging:** Bridge across a V-shaped gap in a way that balances minimizing paths between endpoints with cost of bridge.

Chris R. Reid, Matthew J. Lutz, Scott Powell, Albert B. Kao, Iain D. Couzin, and Simon Garnier. Army ants dynamically adjust living bridges in response to a cost-benefit trade-off. *Proceedings of the National Academy of Sciences*, 112(49):15113-15118, 2015.



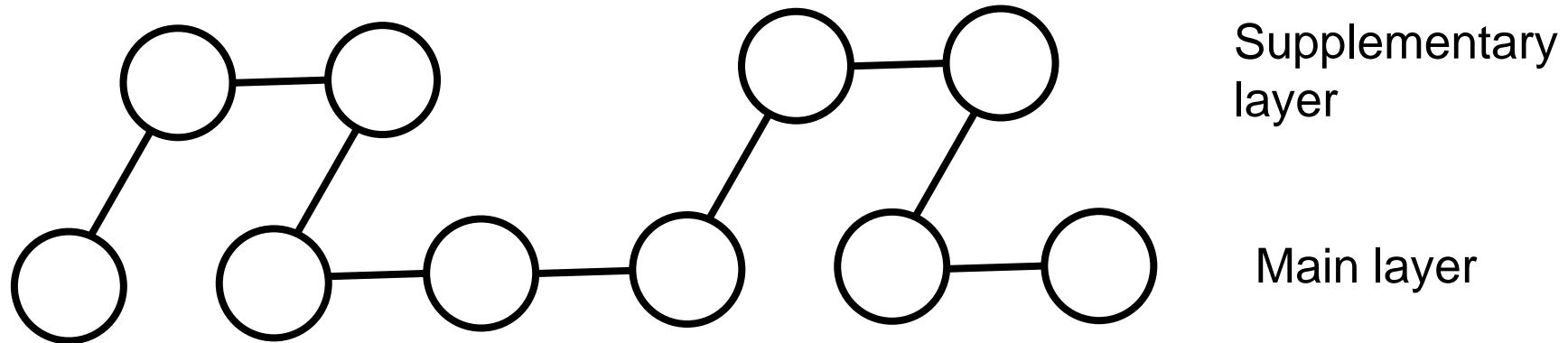
Inspired by ants (Reid et al. 2015)



Our algorithm

# Theorem:

With only one supplementary layer,



if each nubot can only perform one state change, then the main layer can only grow **linearly**.

[Yen-Ru Chin, Jui-Ting Tsai and Ho-Lin Chen. A Minimal Requirement for Self-Assembly of Lines in Polylogarithmic Time, *DNA 23*]

# Theorem:

Simple extensions allow exponential growth:

- Two supplementary layers

or

- Disappearance does not require a state change

[Yen-Ru Chin, Jui-Ting Tsai and Ho-Lin Chen. A Minimal Requirement for Self-Assembly of Lines in Polylogarithmic Time, *DNA* 23]

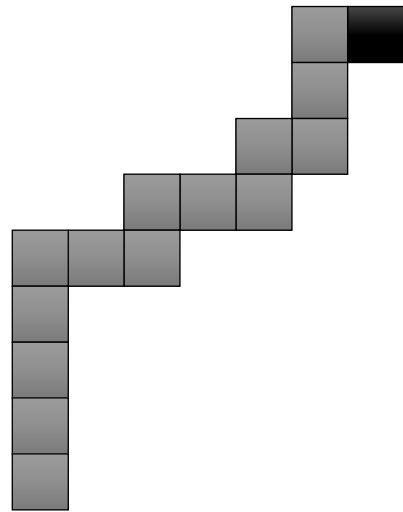


# Non-cooperative binding

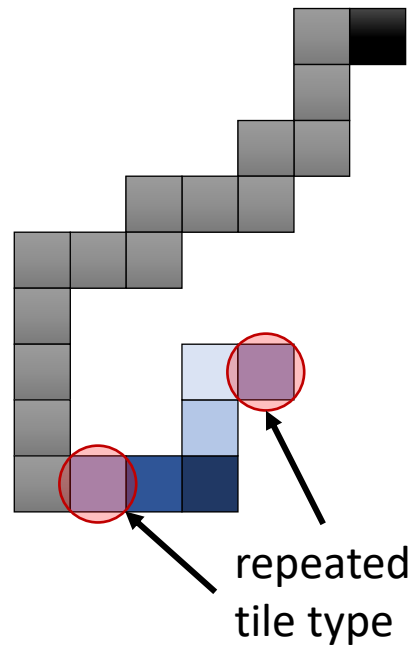
# Non-cooperative binding



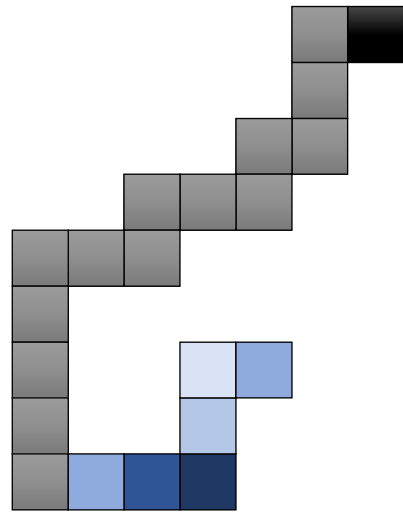
# Non-cooperative binding



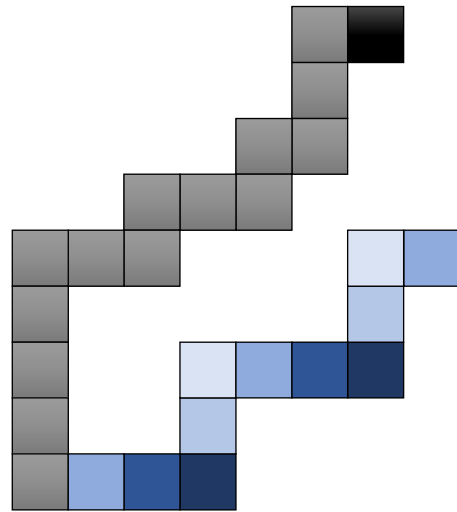
# Non-cooperative binding



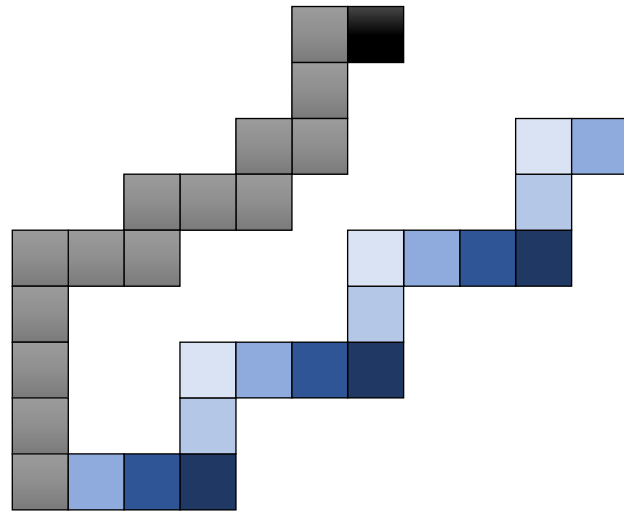
# Non-cooperative binding



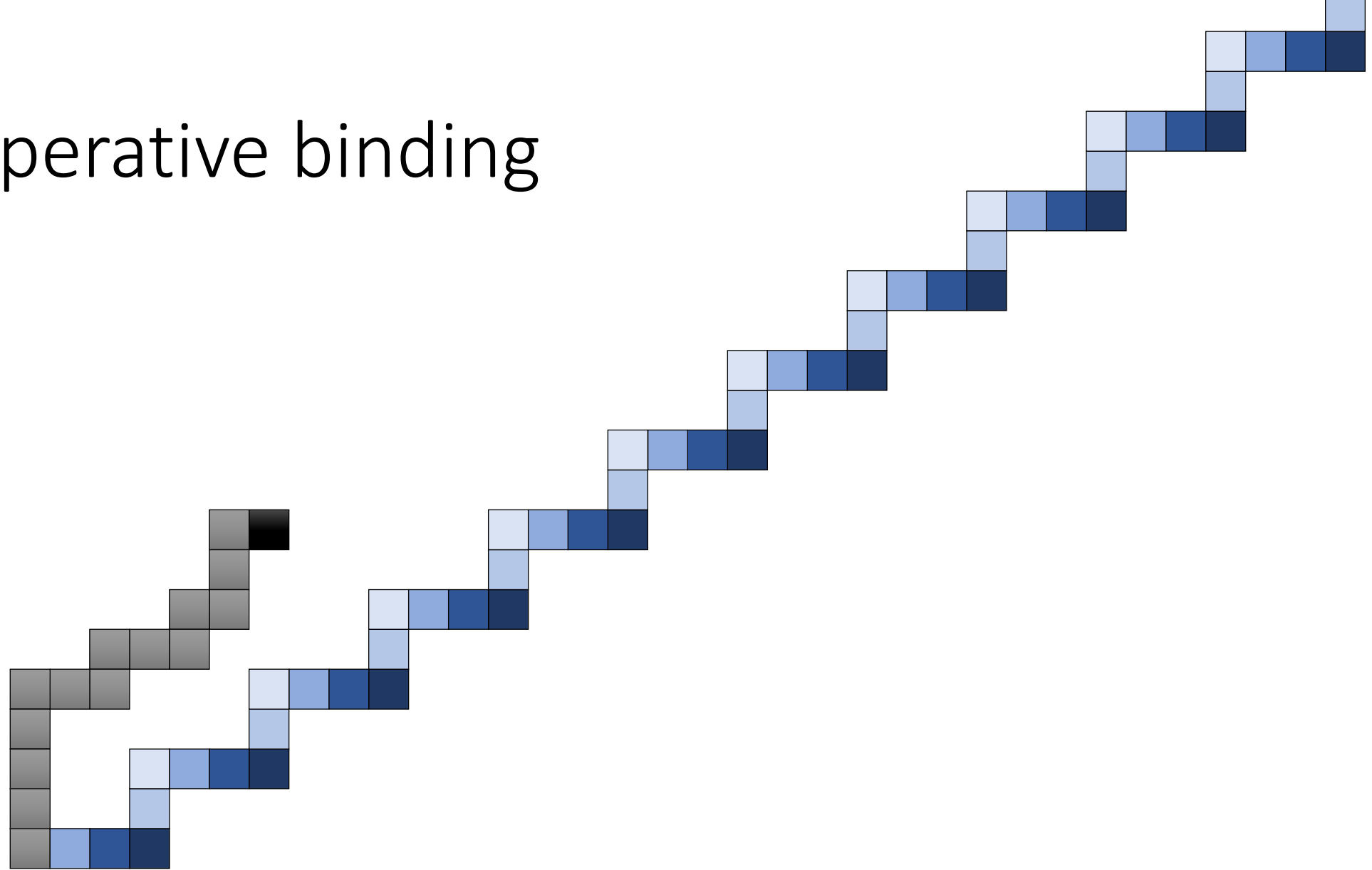
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# Non-cooperative binding

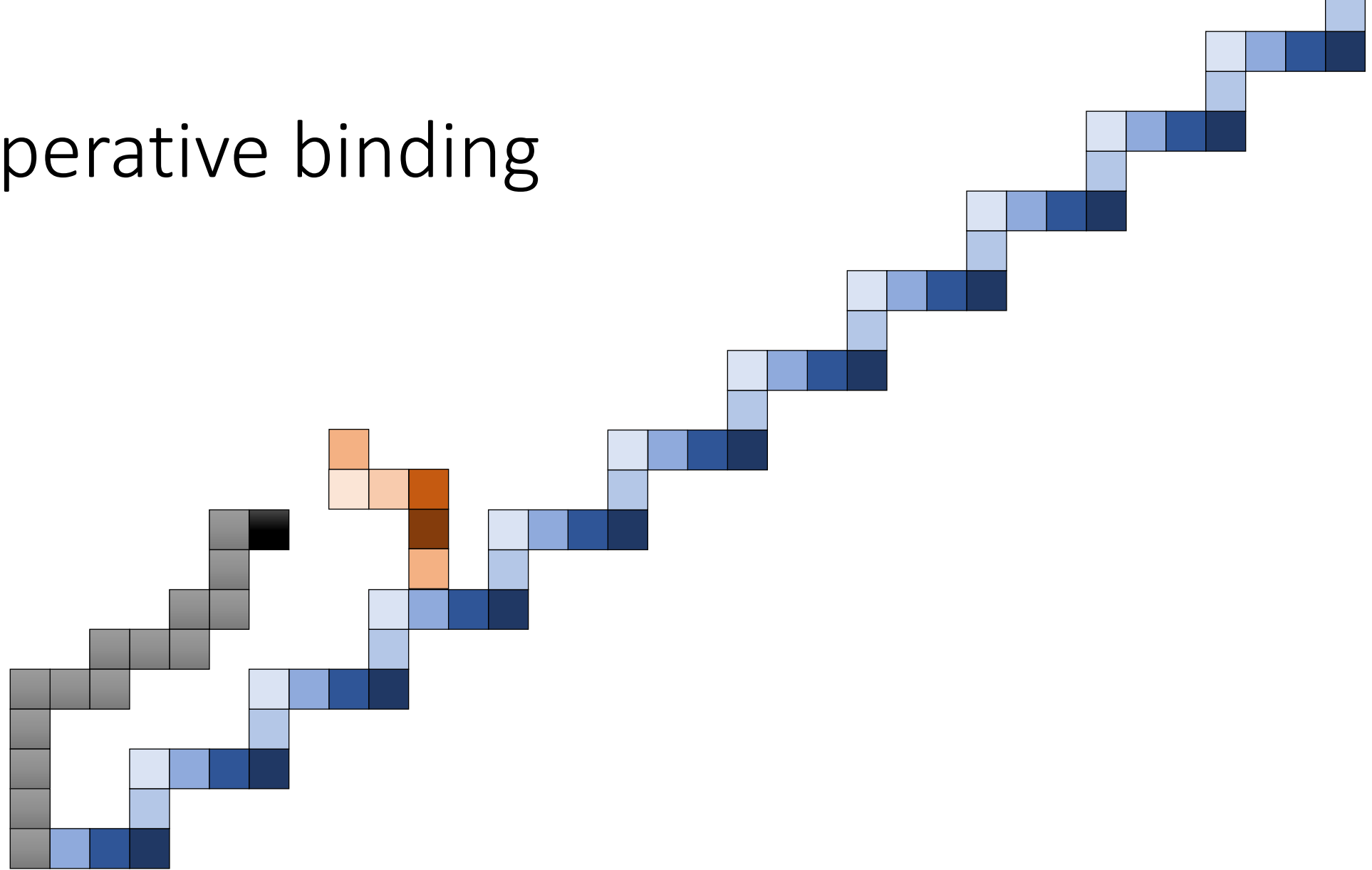


# Non-cooperative binding

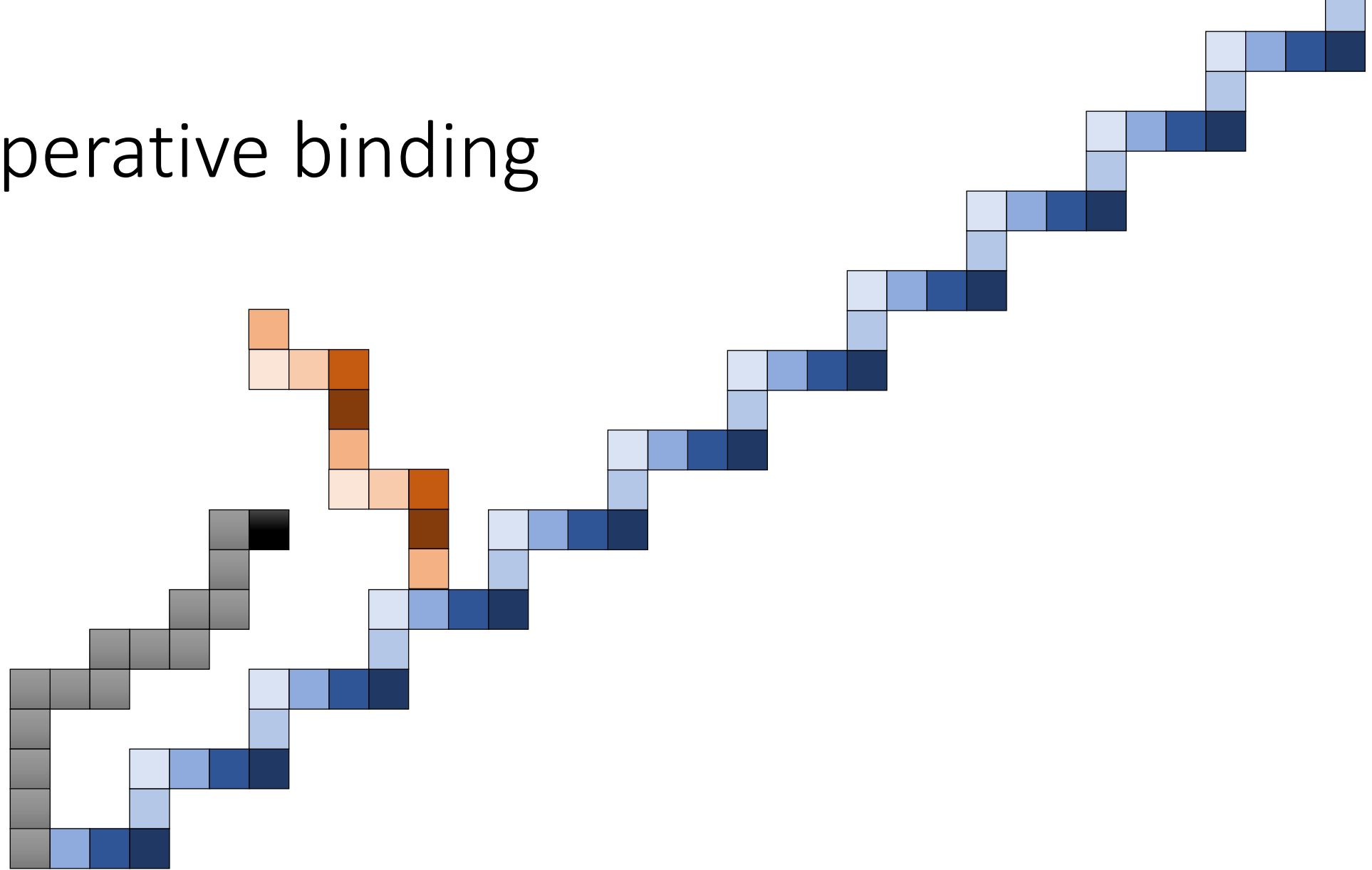




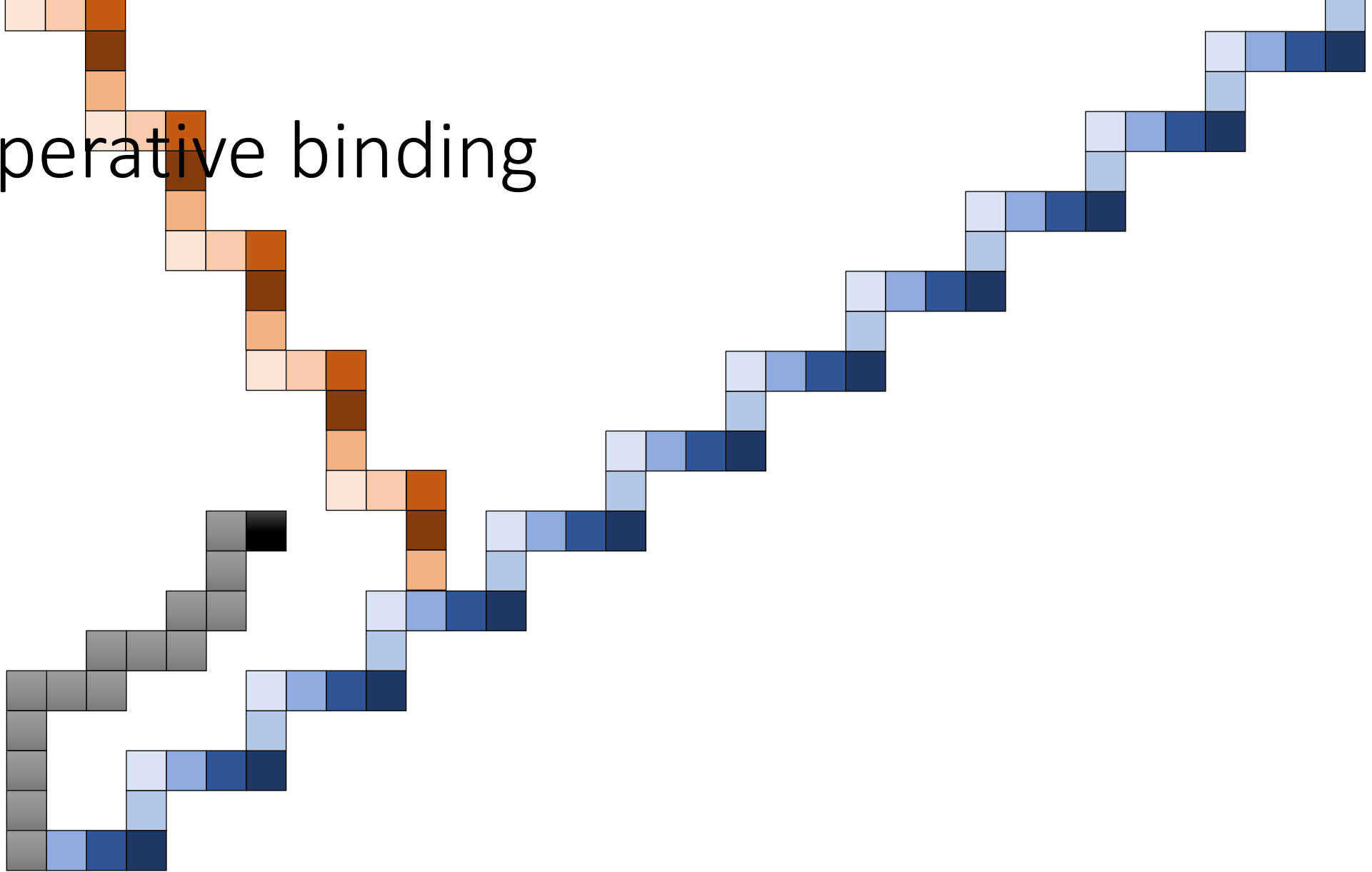
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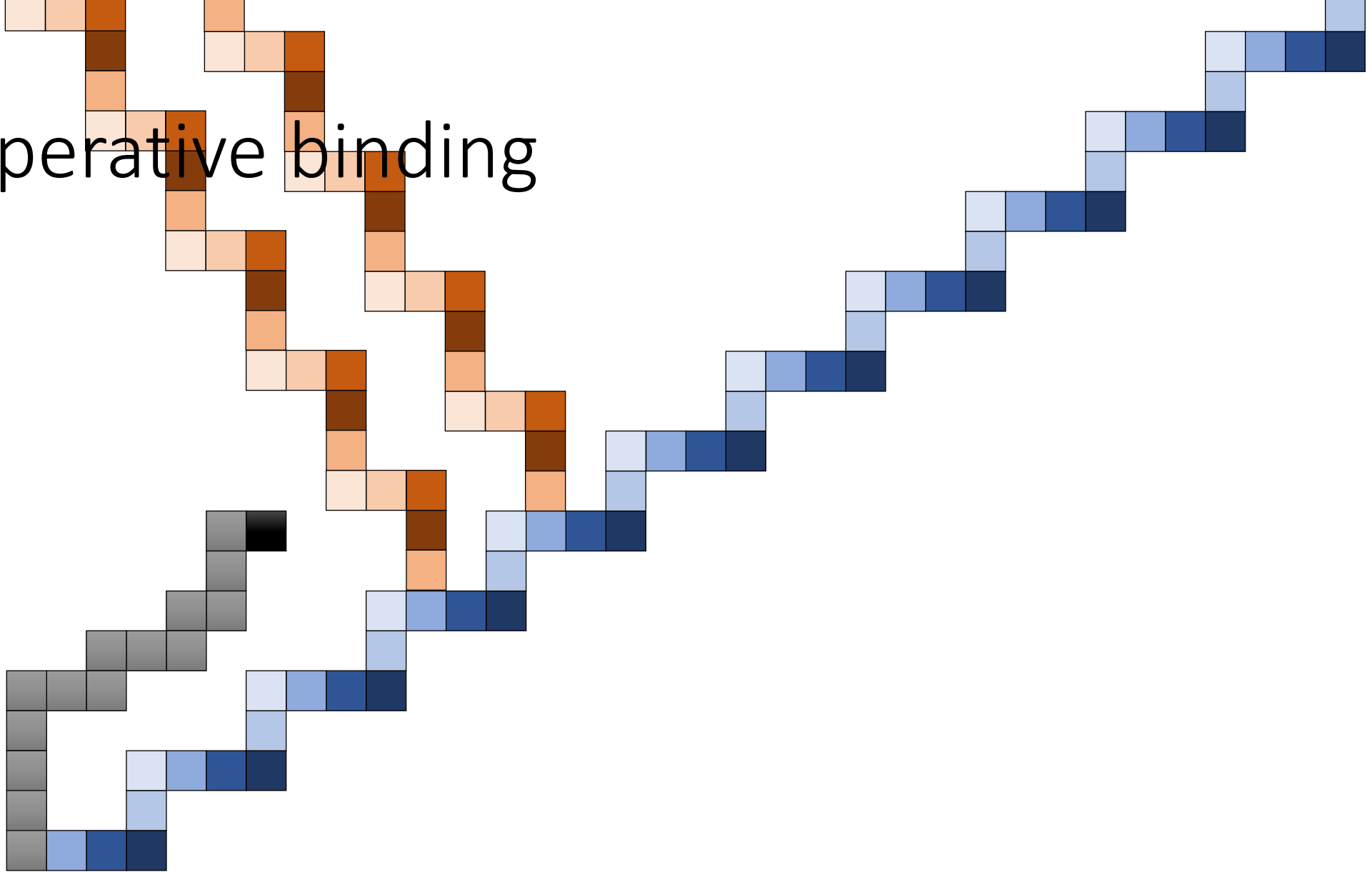
# Non-cooperative binding



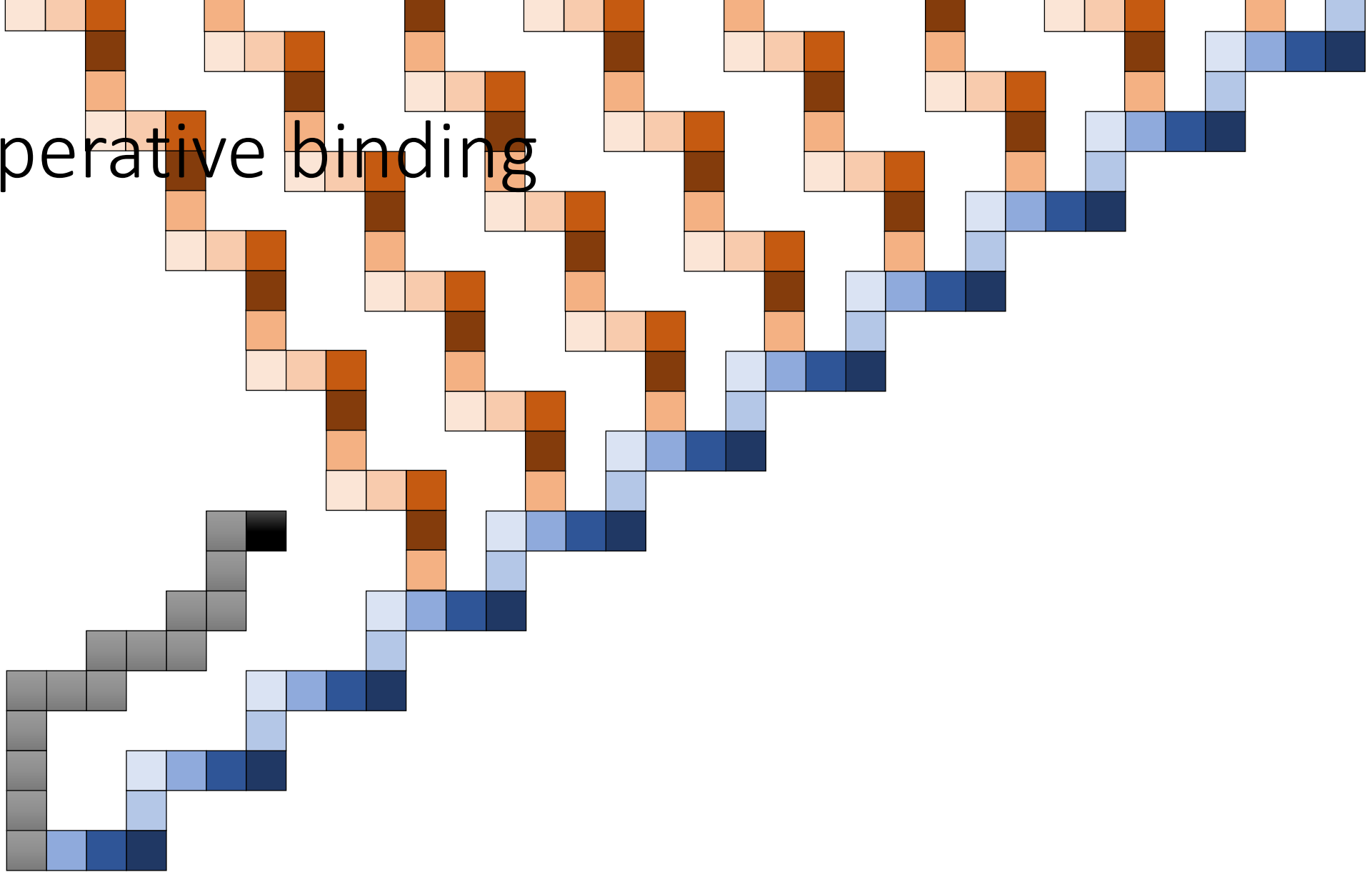
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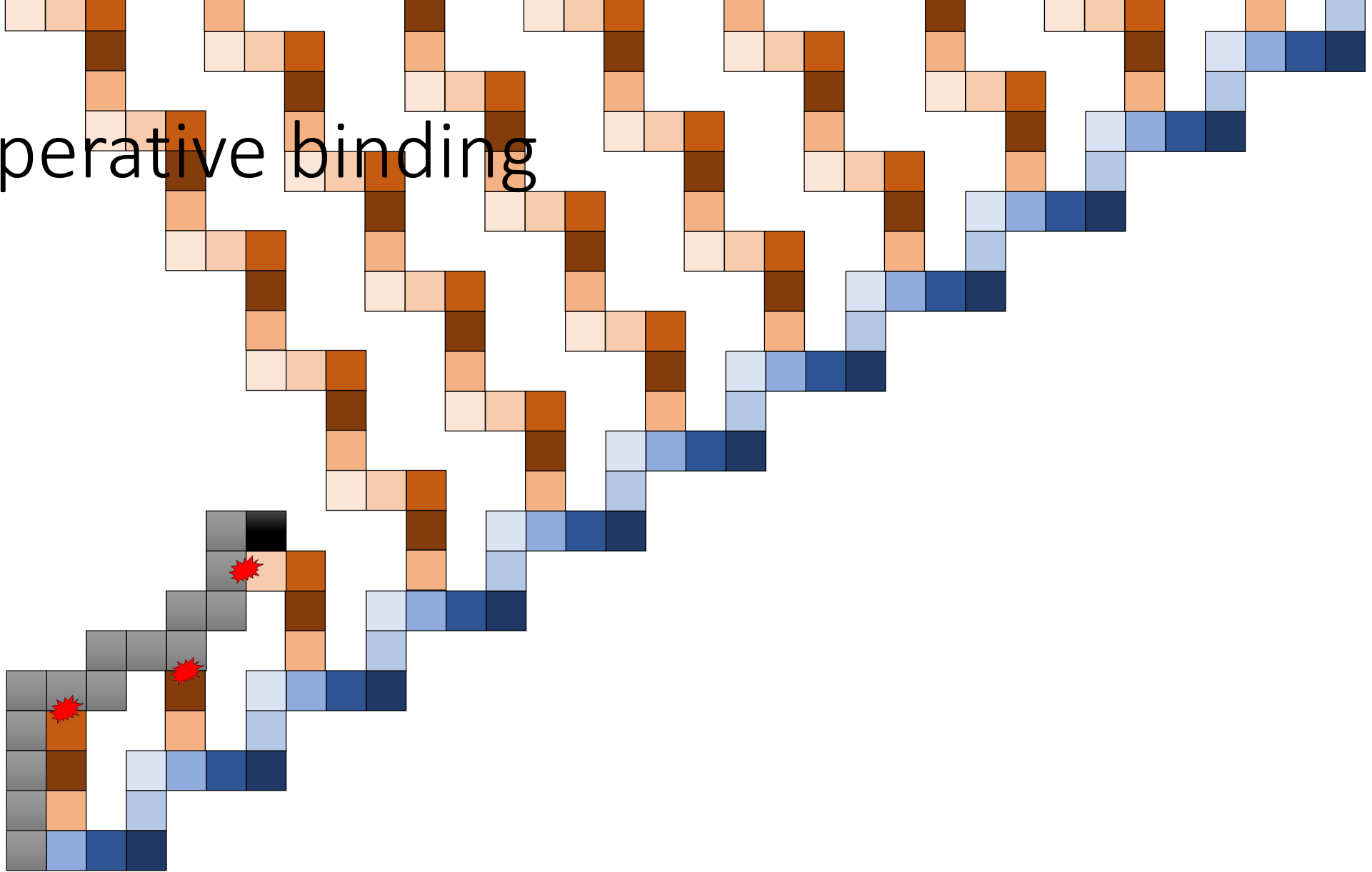
# Non-cooperative binding



# Non-cooperative binding



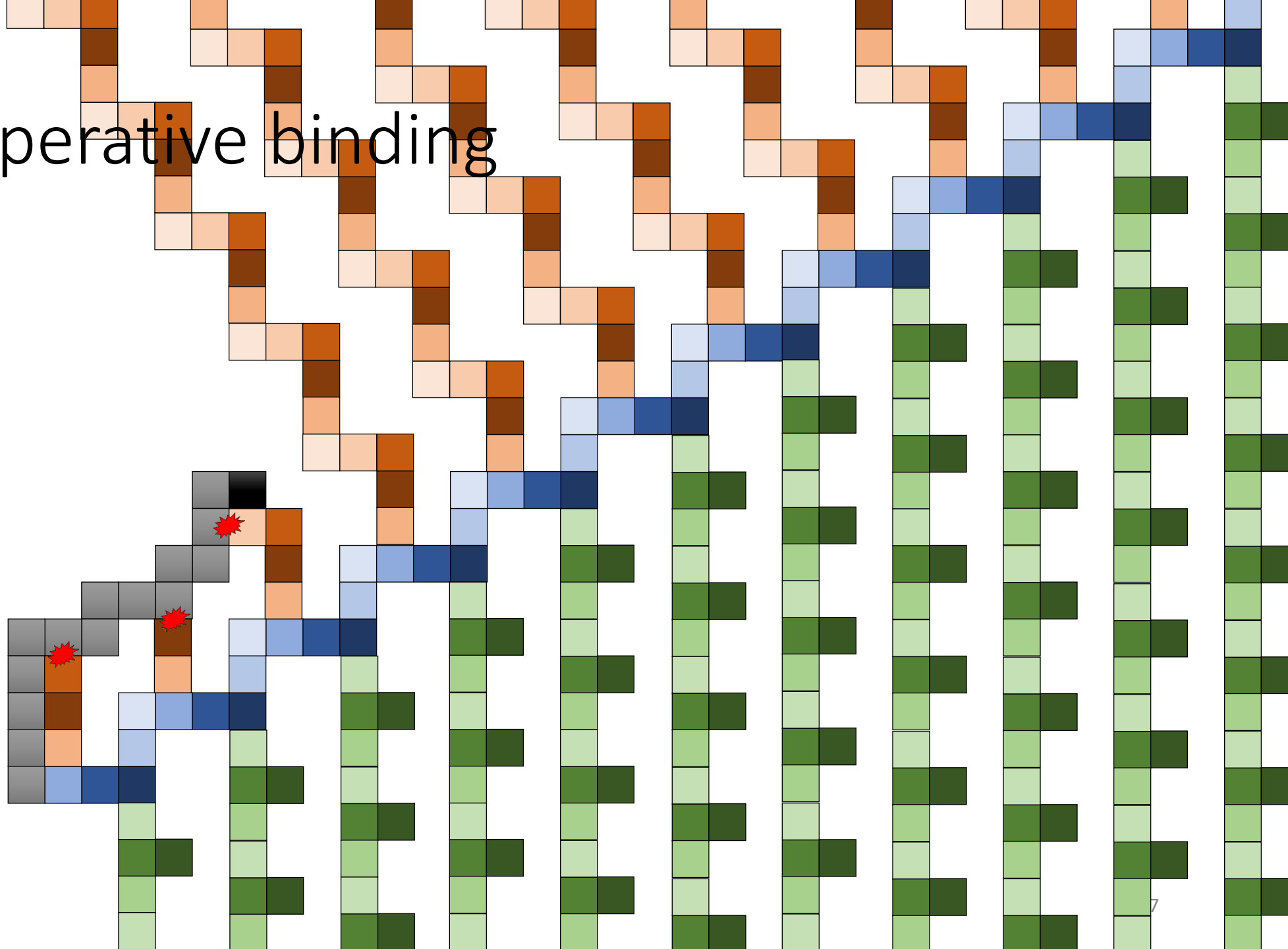
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# Non-cooperative binding



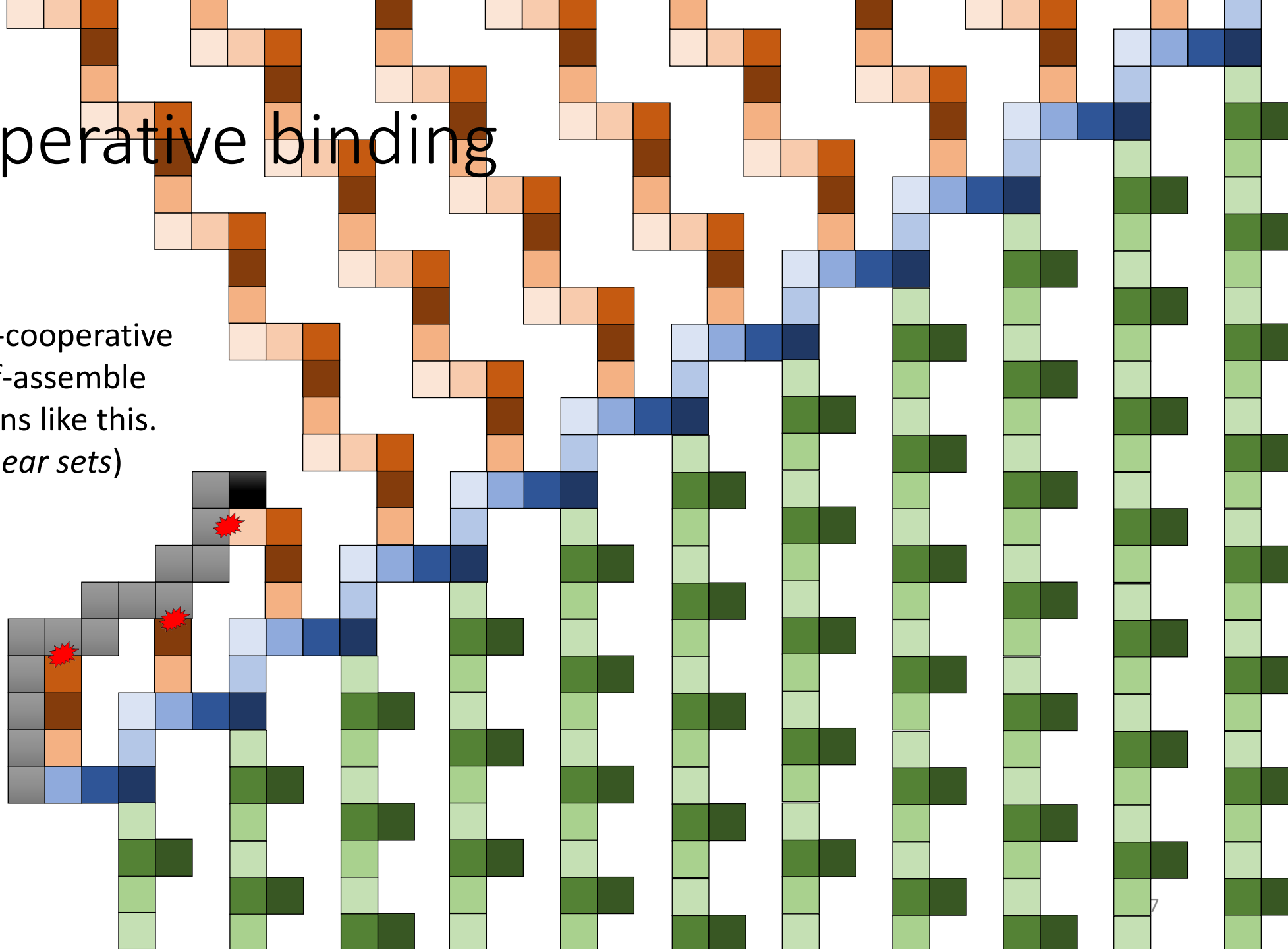
# Non-cooperative binding





# Non-cooperative binding

**Conjecture:** Non-cooperative tiles can only self-assemble “periodic” patterns like this.  
(formally, *semilinear sets*)

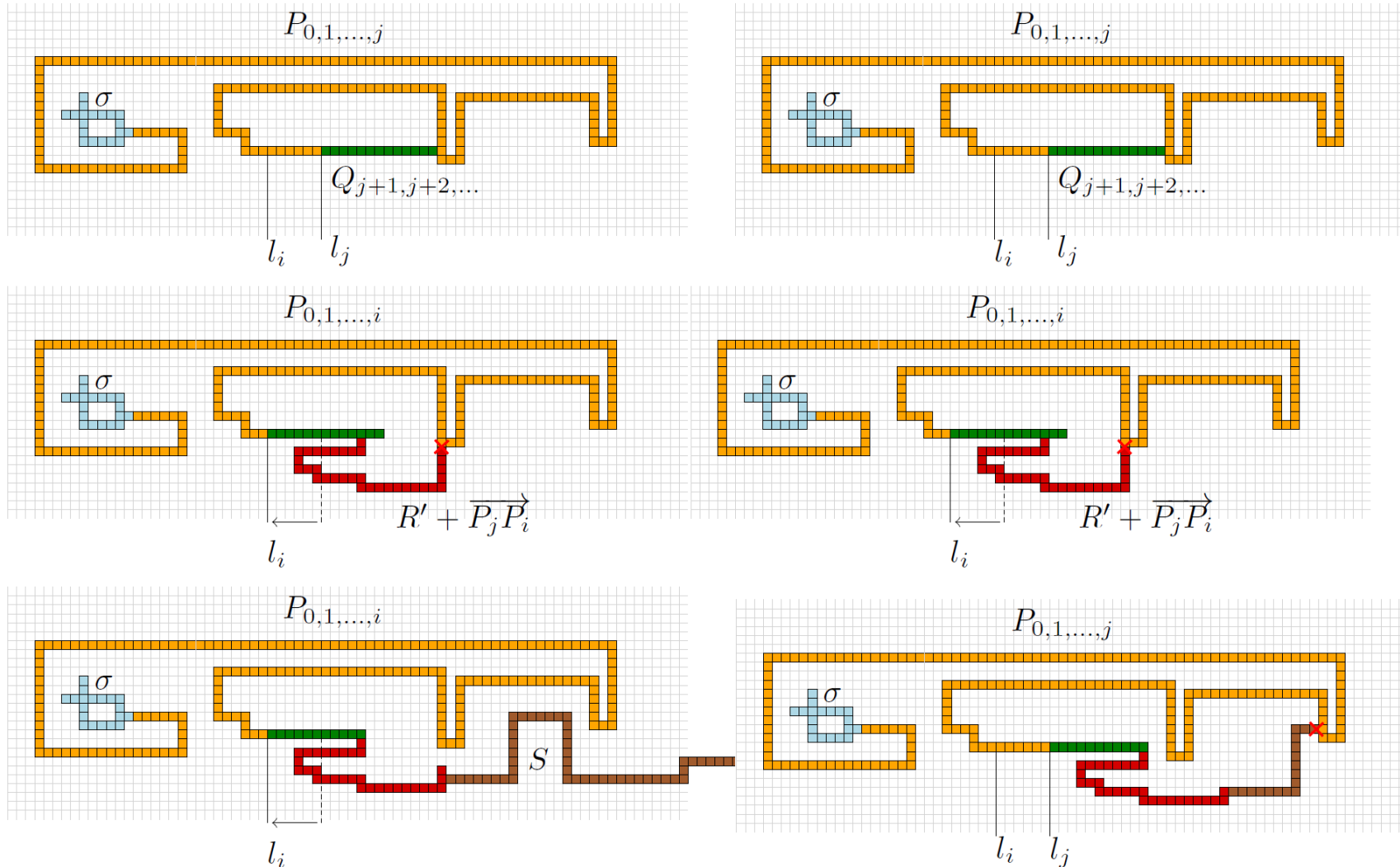


# Non-cooperative binding at DNA 23

- Pierre-Étienne Meunier and Damien Woods, *The non-cooperative tile assembly model is not intrinsically universal or capable of bounded Turing machine simulation*

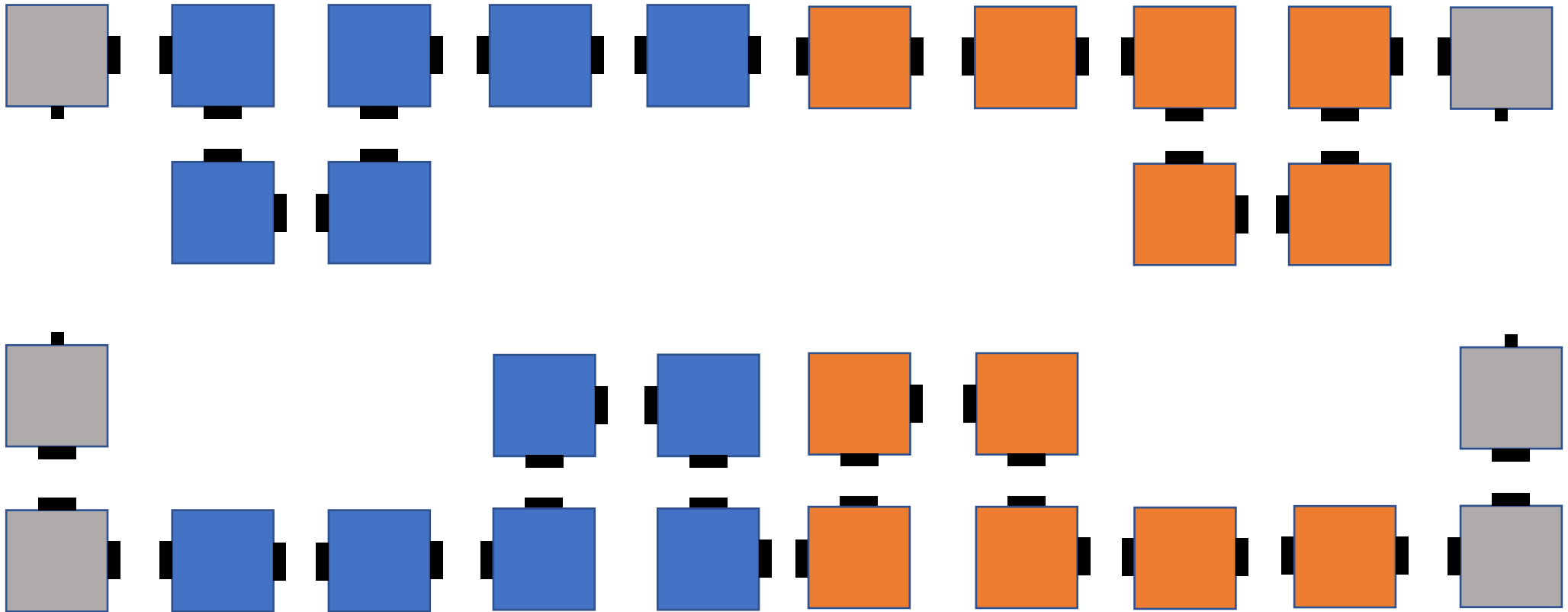
# Temperature 1 does not simulate itself

Pierre-Étienne Meunier and Damien Woods

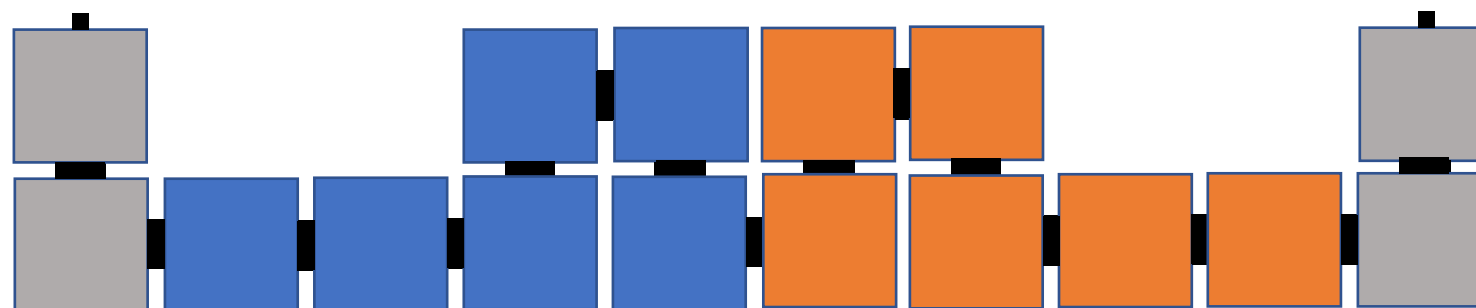
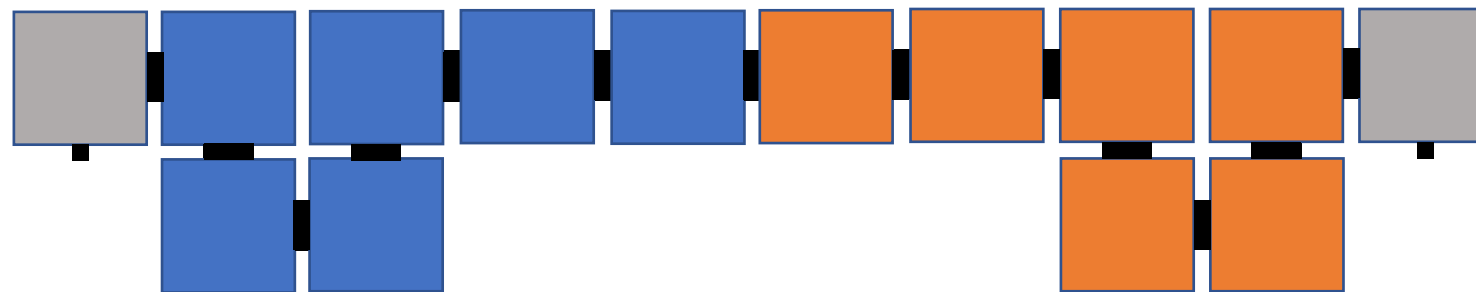


... and much more on our poster!

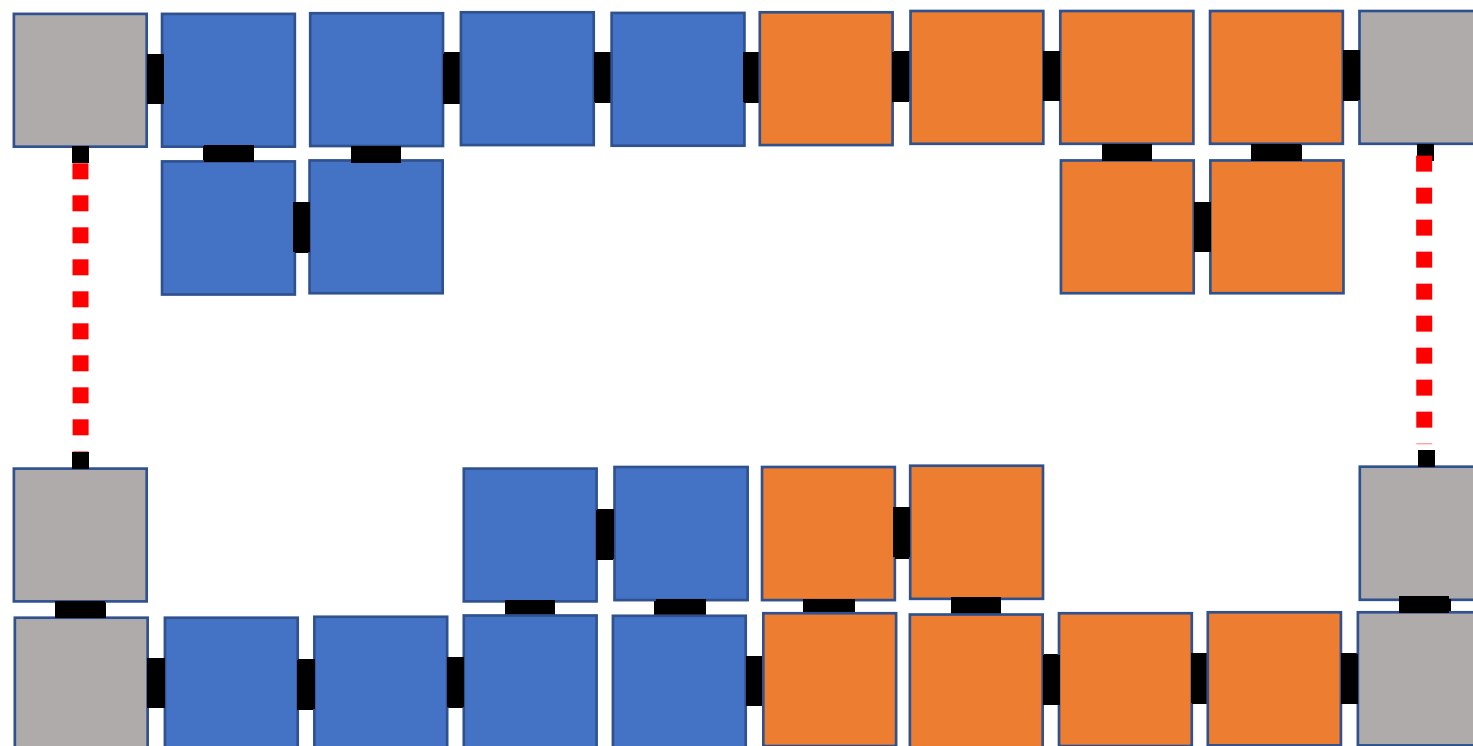
# Hierarchical self-assembly



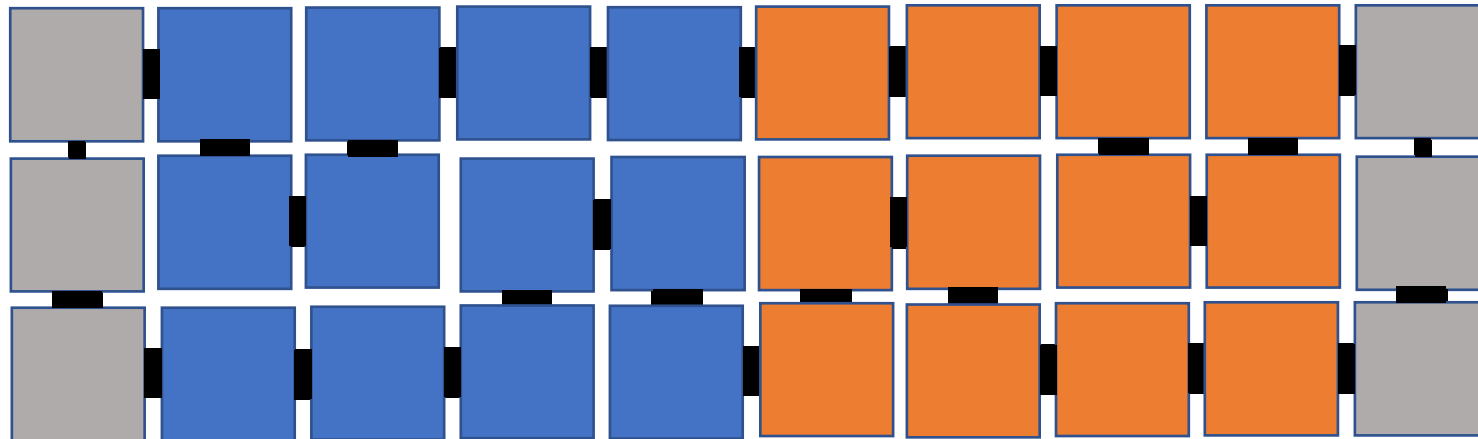
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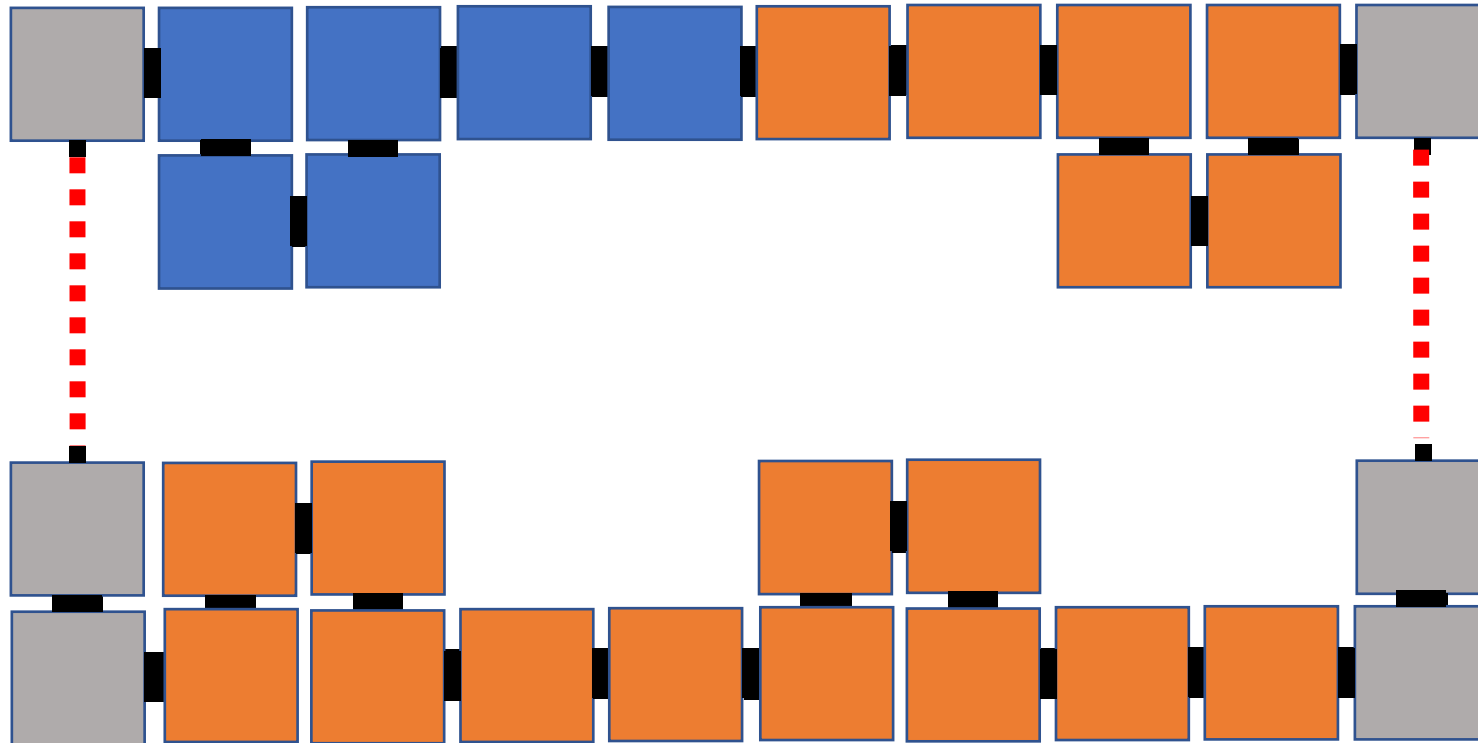
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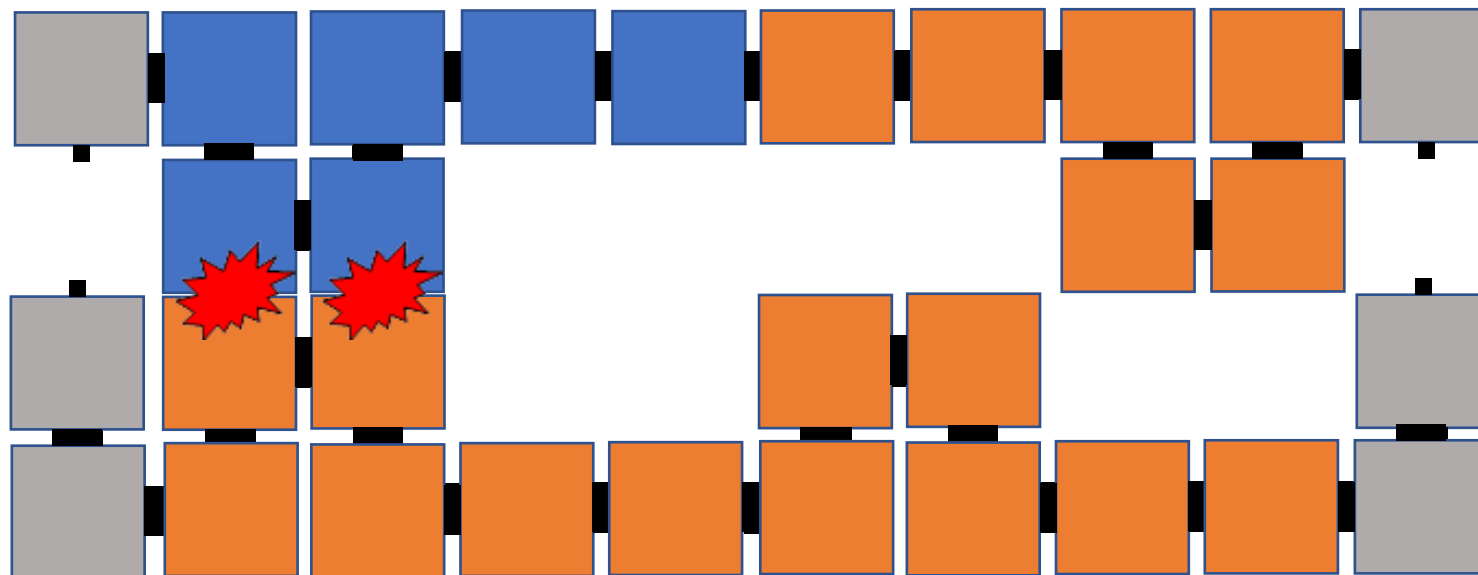


# Hierarchical self-assembly





# Hierarchical self-assembly



# Hierarchical self-assembly at DNA 23

- Robert Schweller, Andrew Winslow, and Tim Wylie, *Complexities for high temperature two-handed tile self-assembly*

# Thank you!

Questions?