



FRACTALS, REACHABILITY, AND COMPUTATION IN MODELS OF DNA SELF- ASSEMBLY AND CHEMICAL REACTION NETWORKS

by: Ryan Knobel



Advisors

- Dr. Tim Wylie (Chair)
- Dr. Robert Schweller
- Dr. Bin Fu
- Dr. Austin Luchsinger



Coauthors

- Michael Alanis
- Divya Bajaj
- Josh Brunner
- Jose-Luis Castellanos
- Michael Coulombe
- Erik Demaine
- Jenny Diomidova
- Tim Gomez
- Elise Grizzel
- Asher Haun
- Markus Hecher
- Jayson Lynch
- Aiden Massie
- Juan Manuel Perez
- Tom Peters
- Rene Reyes
- Andrew Rodriguez
- Marco Rodriguez
- Adrian Salinas
- Pablo Santos
- Ramiro Santos



Overview

1. Building Fractals in Seeded Tile Automata
2. Reachability in Chemical Reaction Networks
3. Game Complexity

Fractals in Seeded Tile Automata



Fractals in Seeded TA

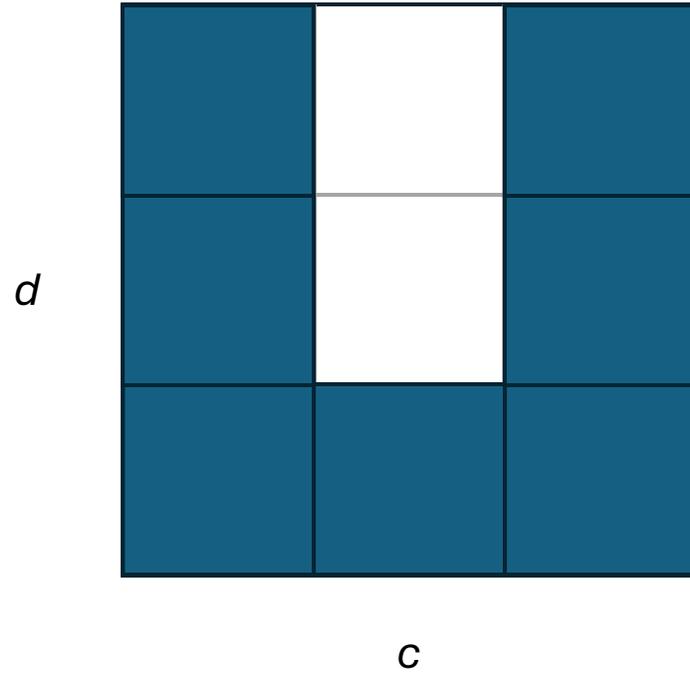
▣

Authors: Asher Haun, **Ryan Knobel**, Adrian Salinas, Ramiro Santos,
Robert Schweller, Timothy Wylie

Discrete Self-Similar Fractals

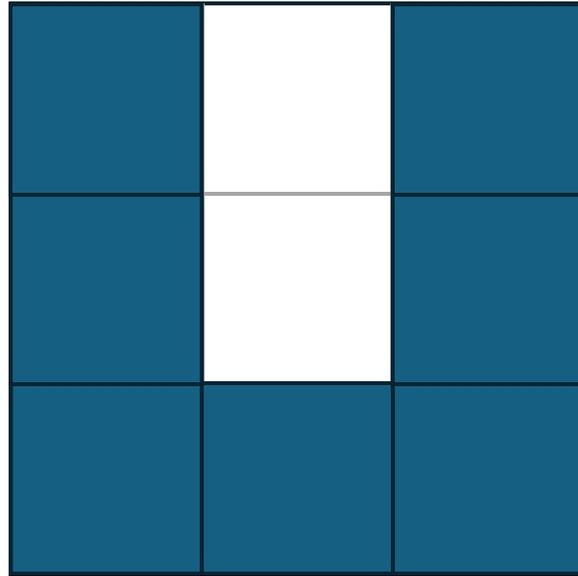
What are they?

Generator



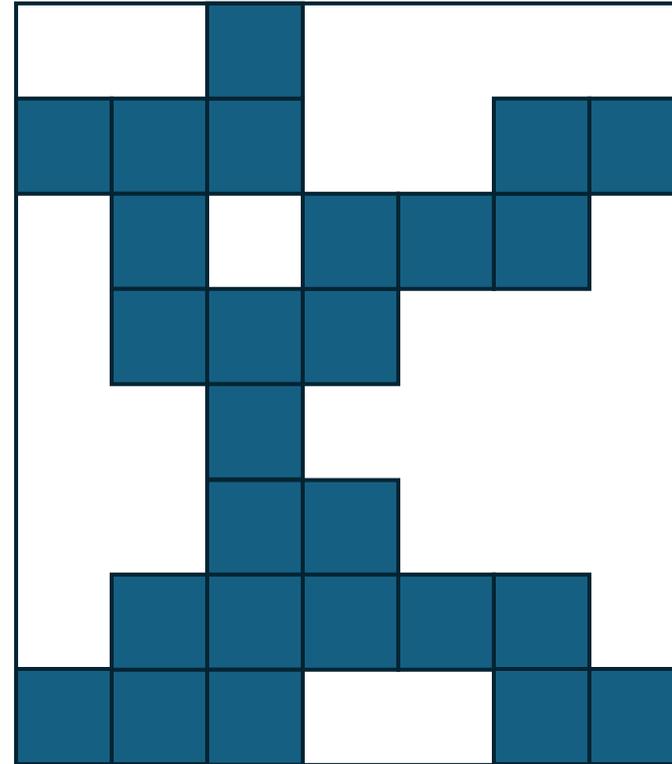
Generator

1. Connected



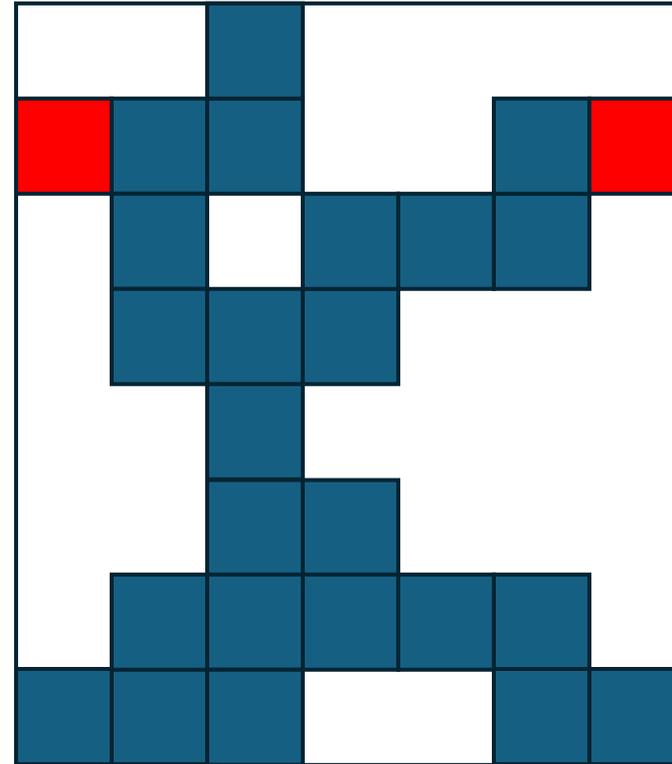
Generator

1. Connected
2. Feasible



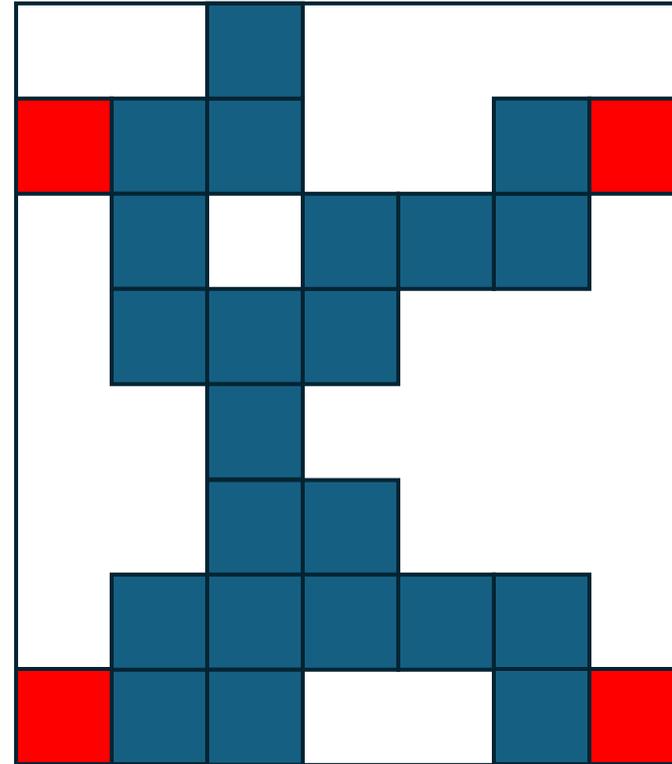
Generator

1. Connected
2. Feasible



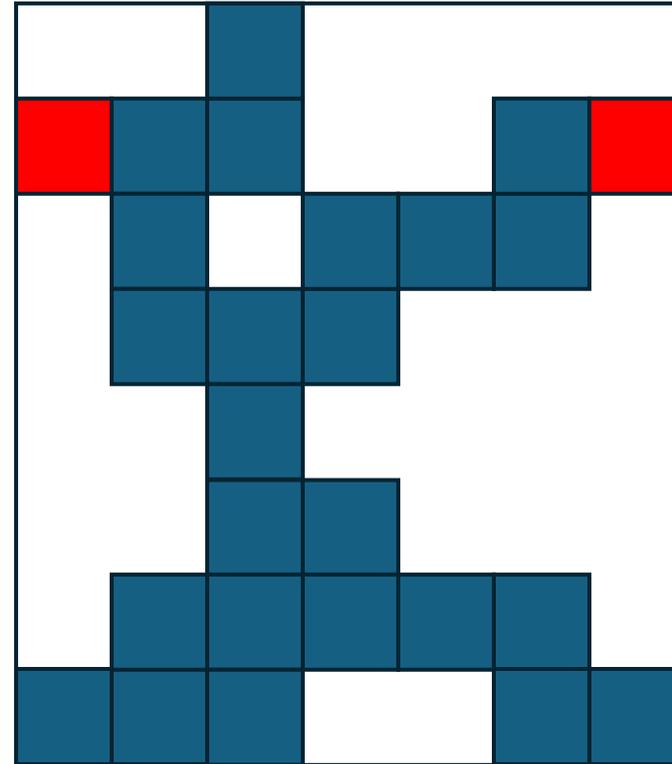
Generator

1. Connected
2. Feasible



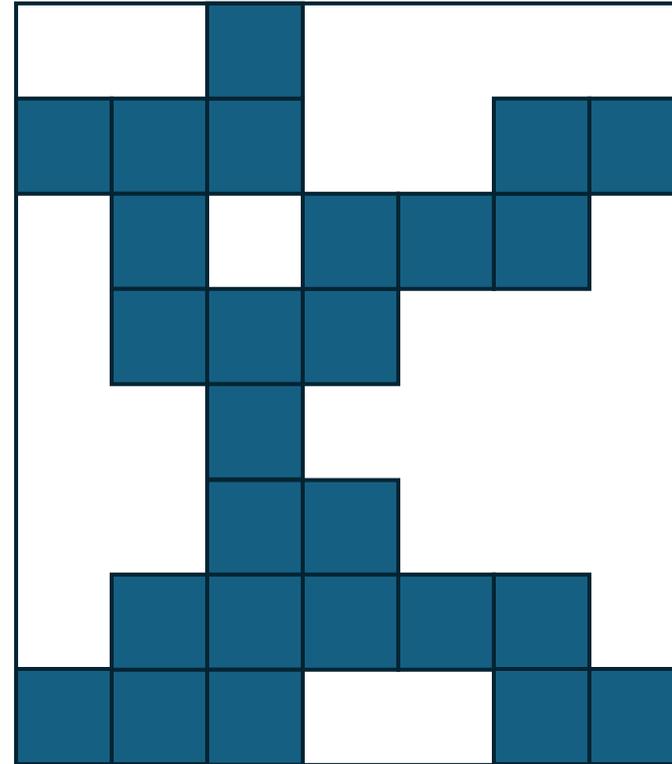
Generator

1. Connected
2. Feasible



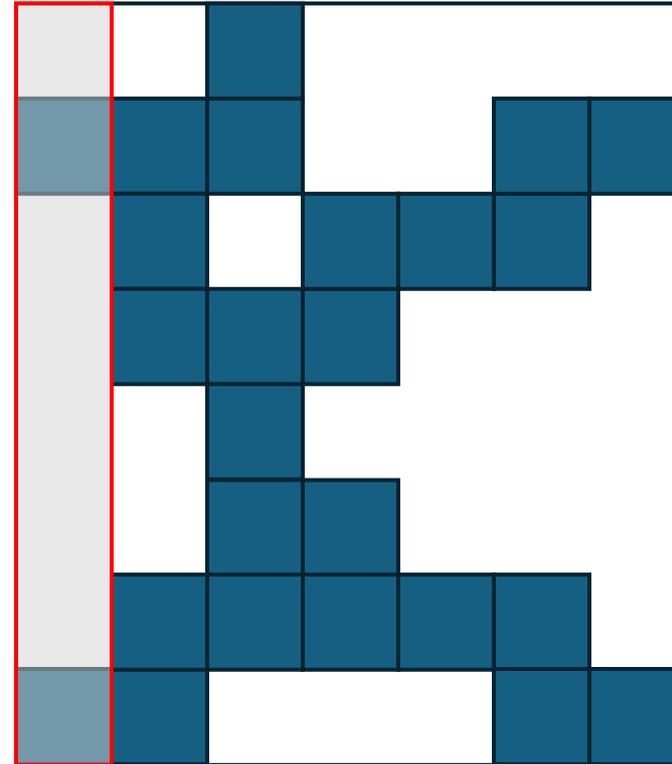
Generator

1. Connected
2. Feasible



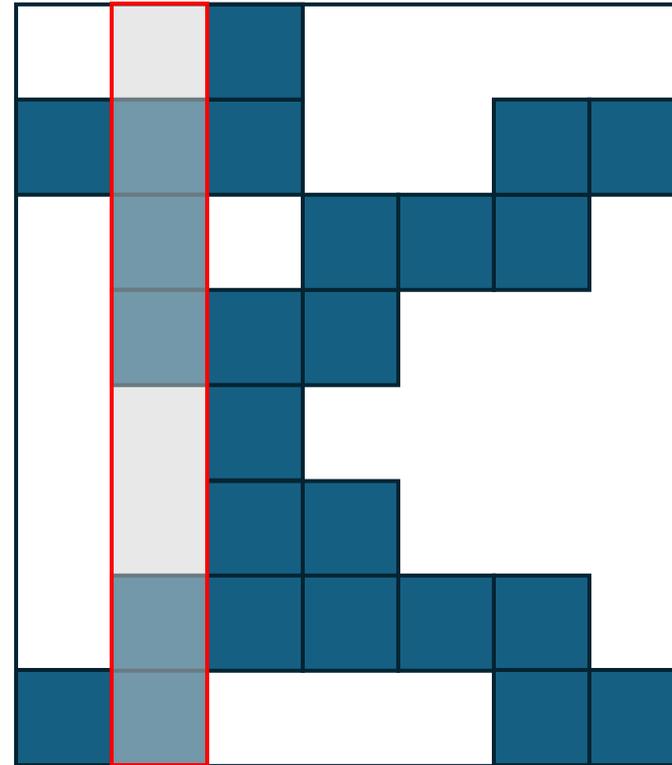
Generator

1. Connected
2. Feasible



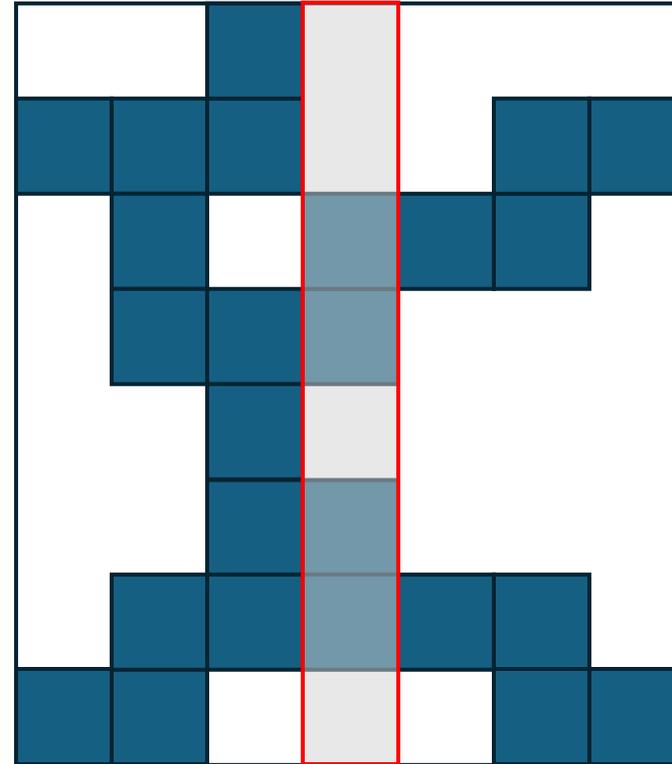
Generator

1. Connected
2. Feasible



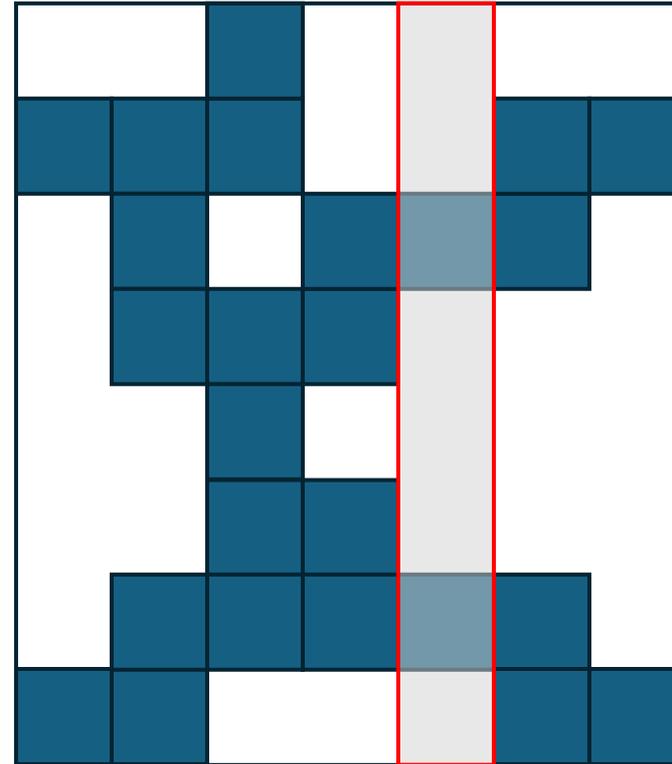
Generator

1. Connected
2. Feasible



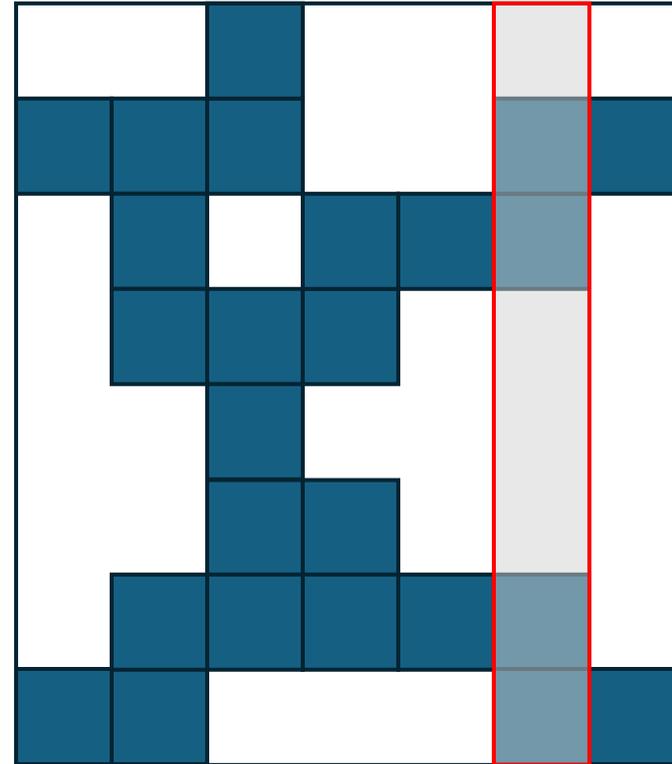
Generator

1. Connected
2. Feasible



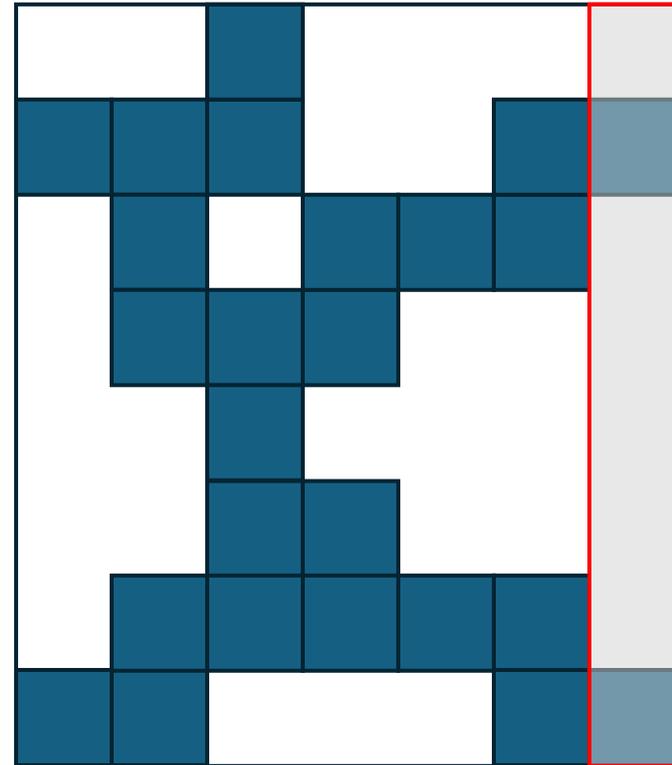
Generator

1. Connected
2. Feasible



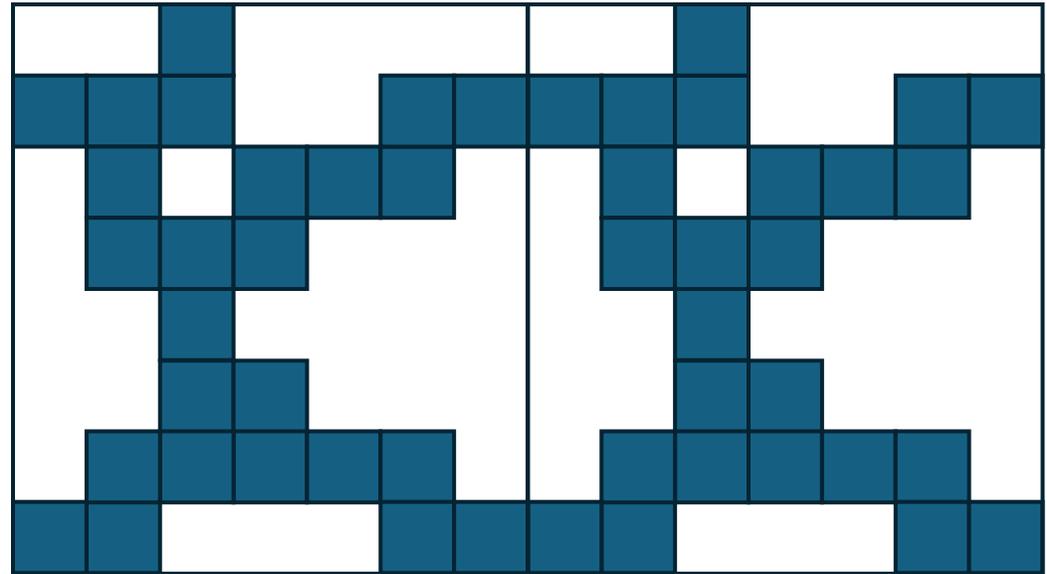
Generator

1. Connected
2. Feasible



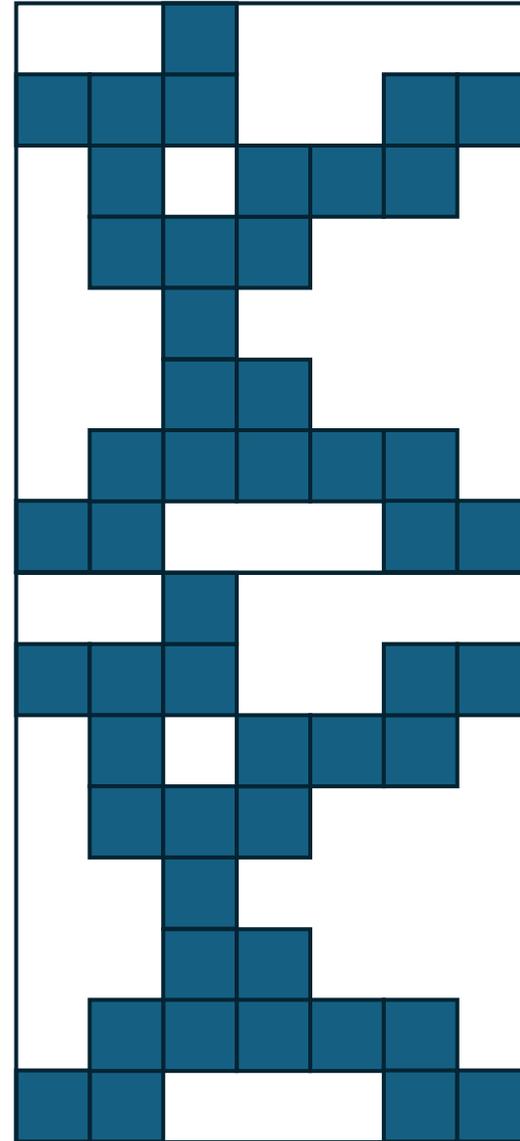
Generator

1. Connected
2. Feasible

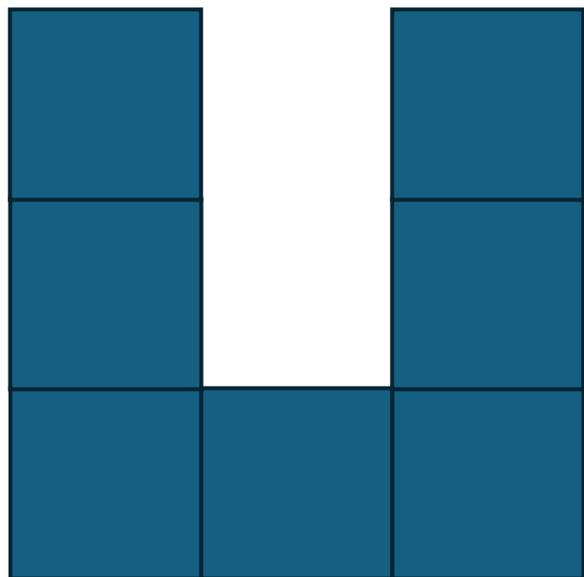


Generator

1. Connected
2. Feasible

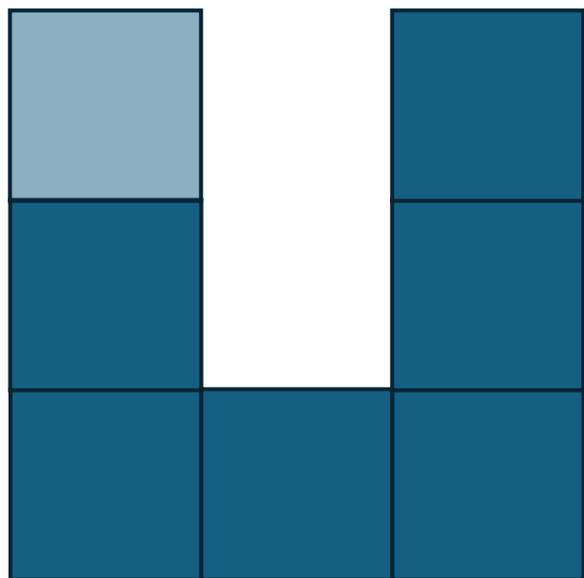


Discrete Self-Similar Fractal

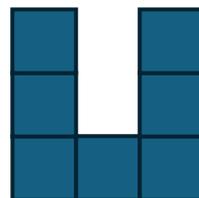


Stage 1

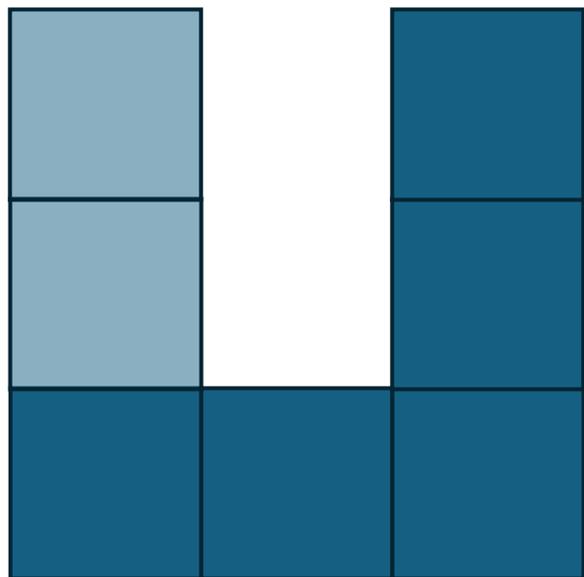
Discrete Self-Similar Fractal



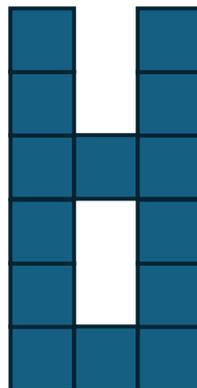
Stage 1



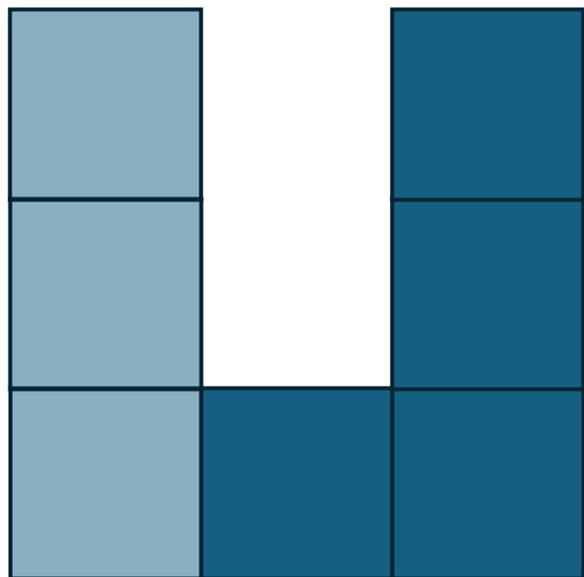
Discrete Self-Similar Fractal



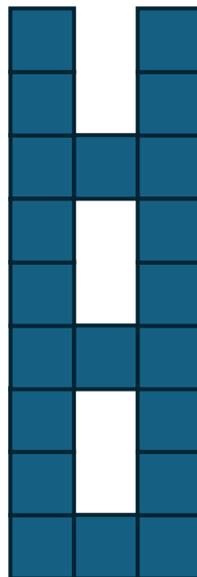
Stage 1



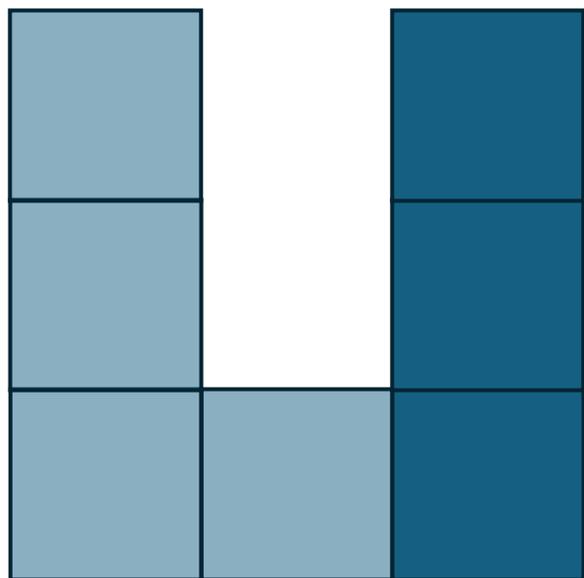
Discrete Self-Similar Fractal



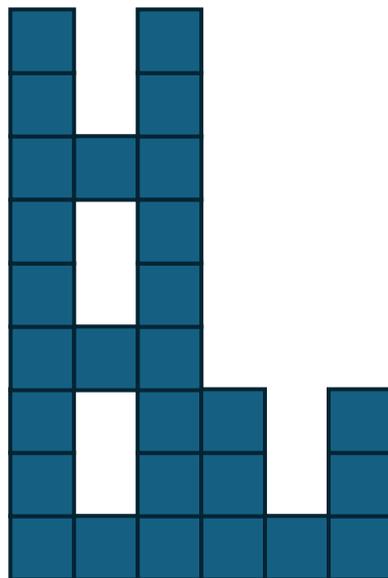
Stage 1



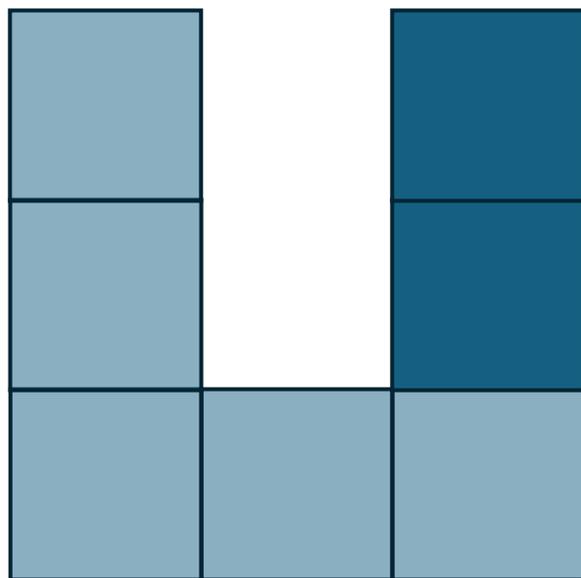
Discrete Self-Similar Fractal



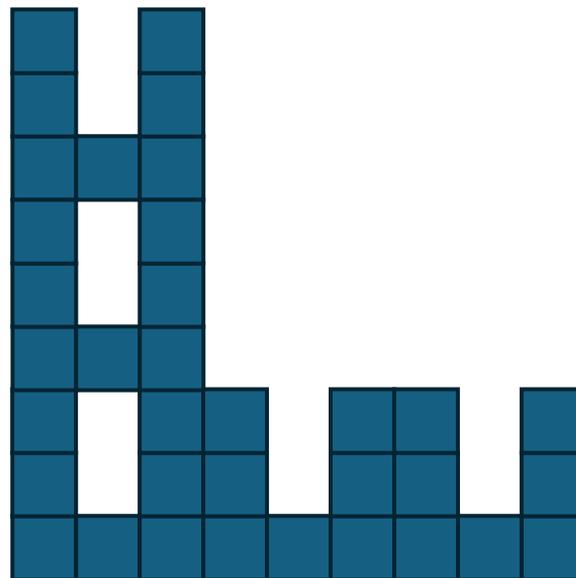
Stage 1



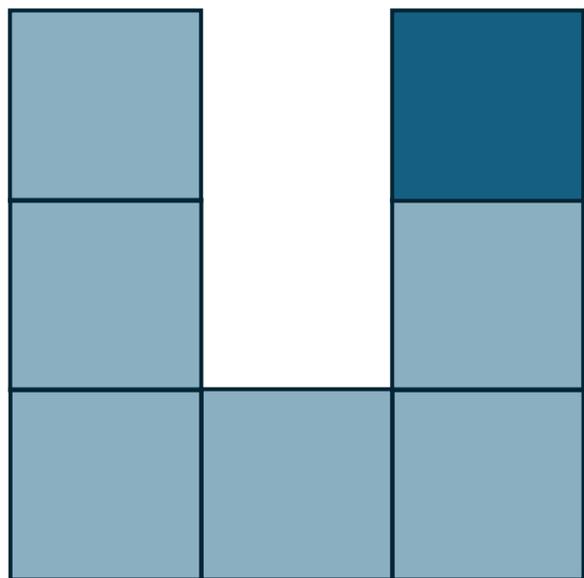
Discrete Self-Similar Fractal



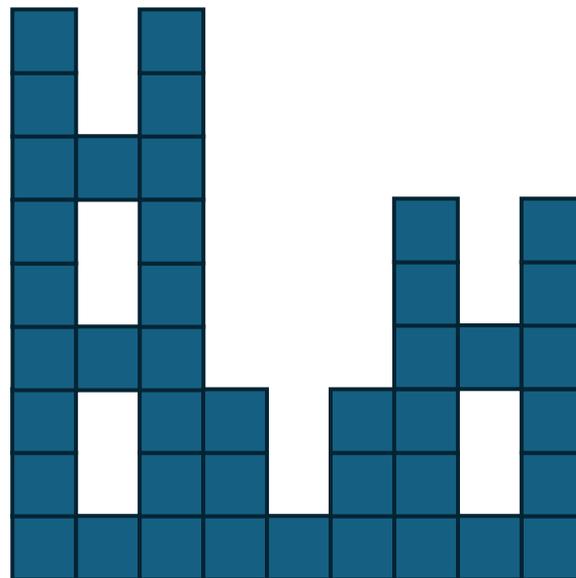
Stage 1



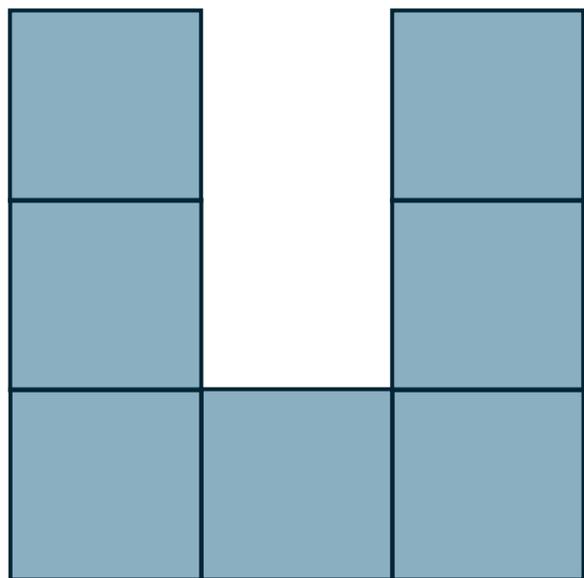
Discrete Self-Similar Fractal



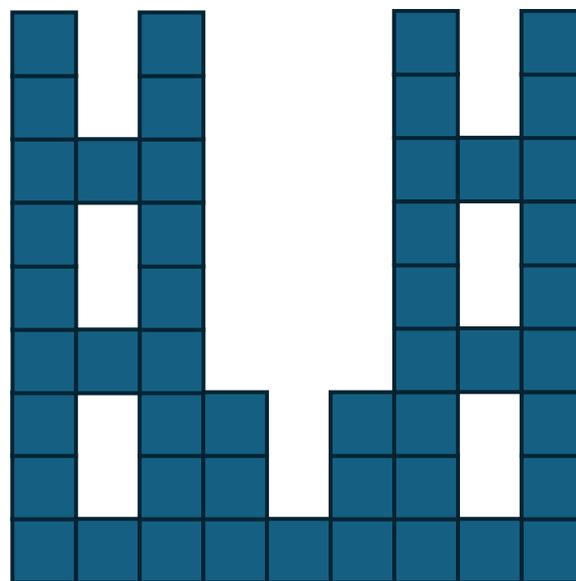
Stage 1



Discrete Self-Similar Fractal

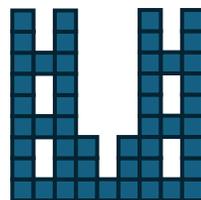
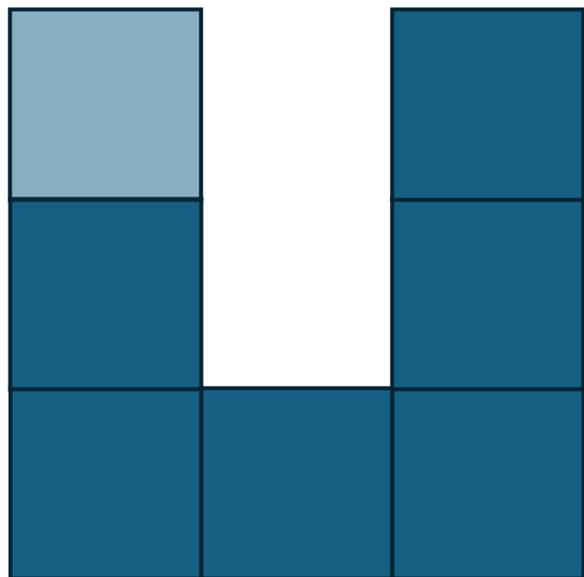


Stage 1

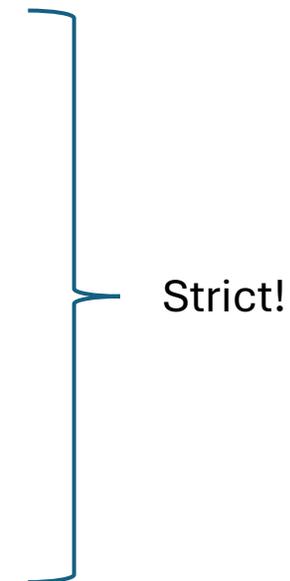
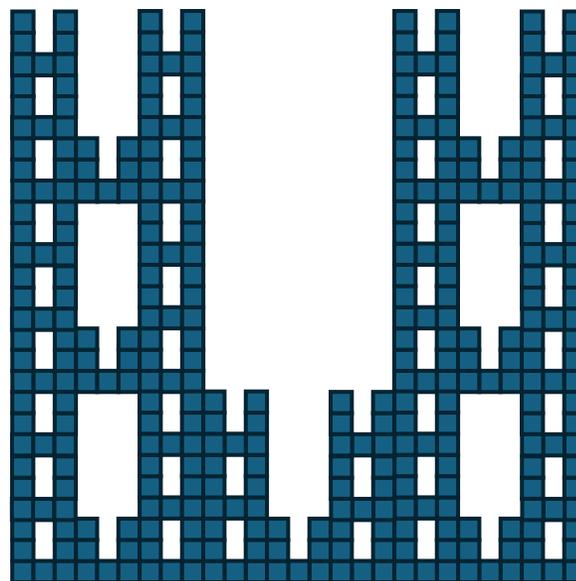
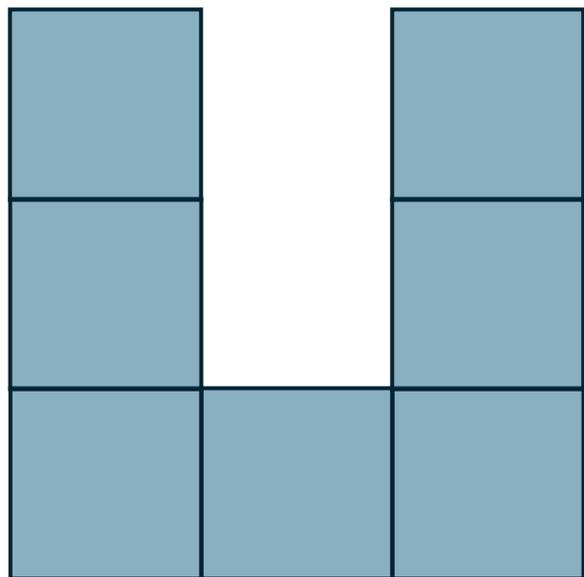


Stage 2

Discrete Self-Similar Fractal

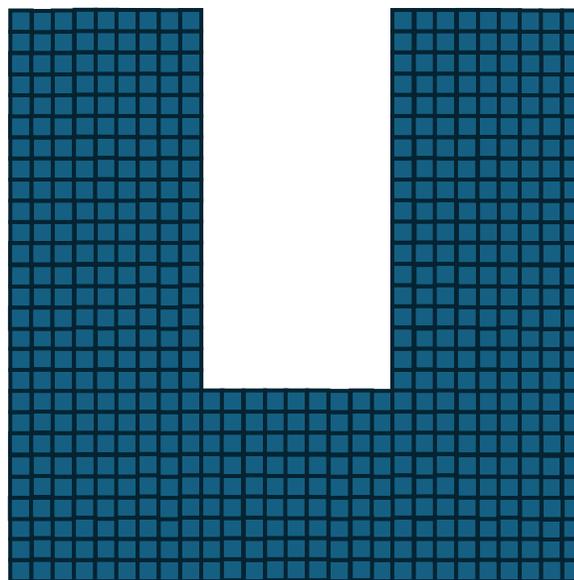
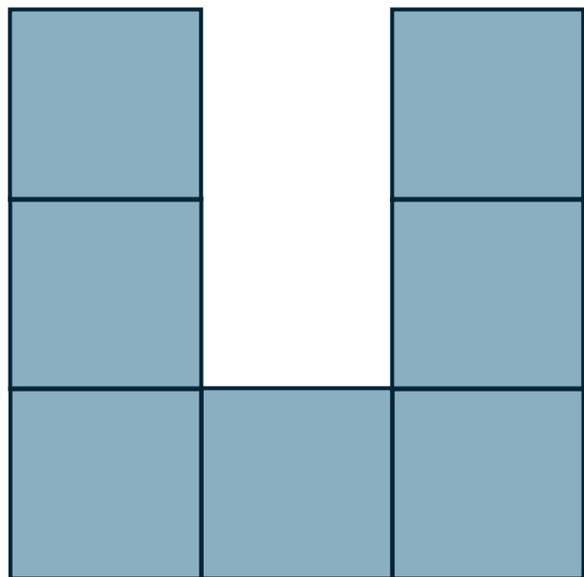


Discrete Self-Similar Fractal

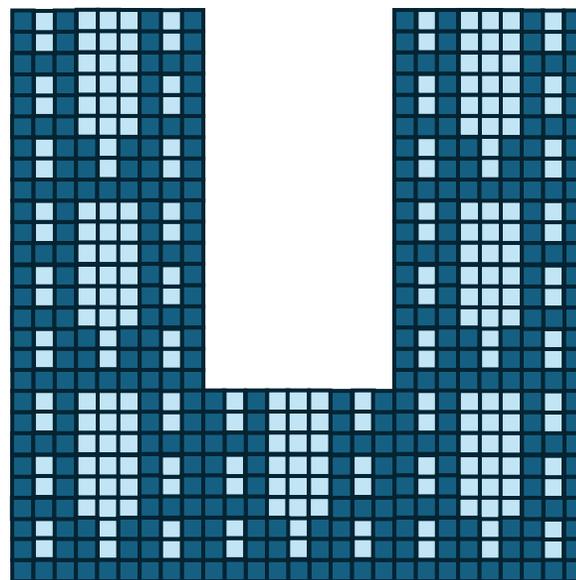
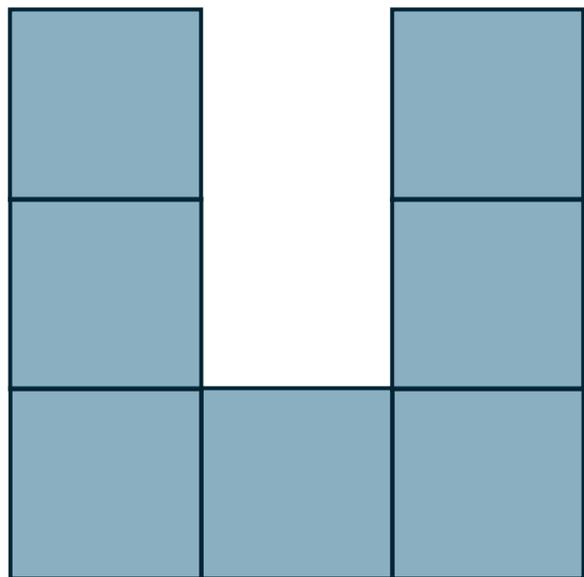


Stage 3

Discrete Self-Similar Fractal



Discrete Self-Similar Fractal



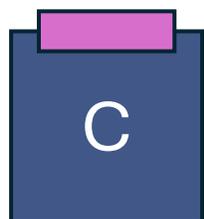
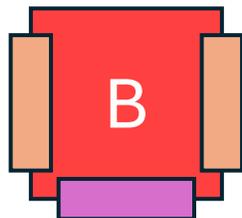
Weak!

Previous Work

Why is this important?

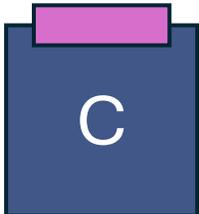
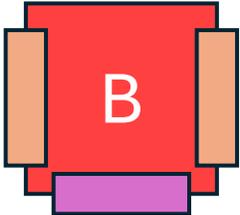
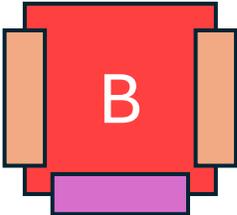
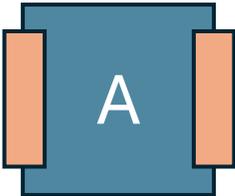
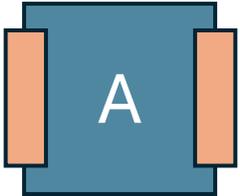
Tile Self-Assembly

Tiles:



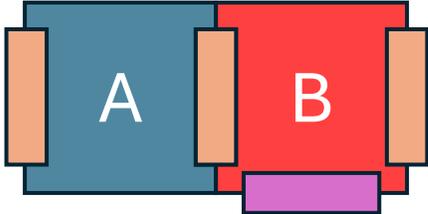
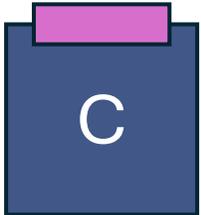
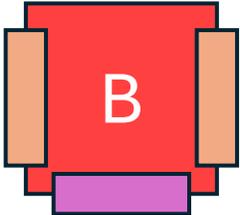
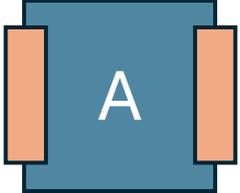
Tile Self-Assembly

Tiles:



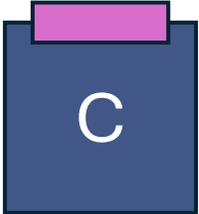
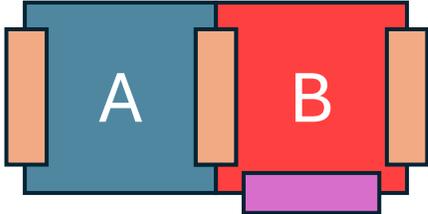
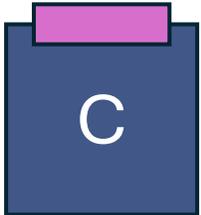
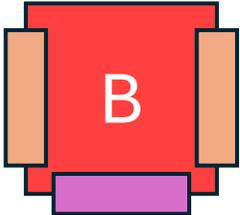
Tile Self-Assembly

Tiles:



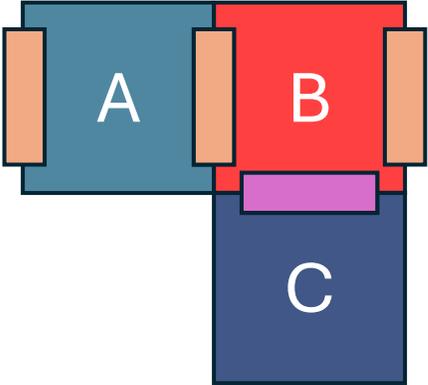
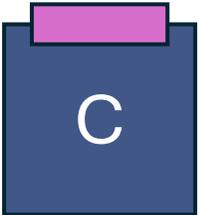
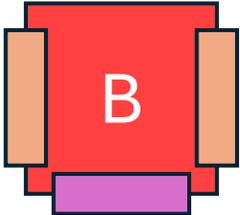
Tile Self-Assembly

Tiles:



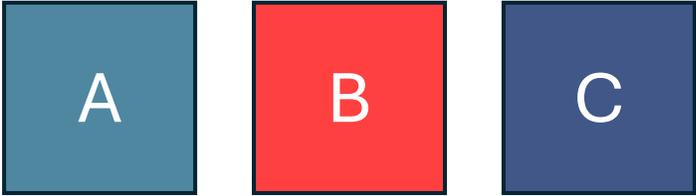
Tile Self-Assembly

Tiles:

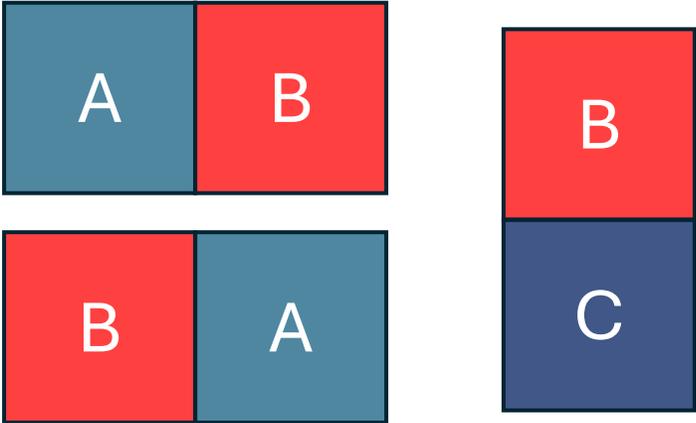


Tile Self-Assembly

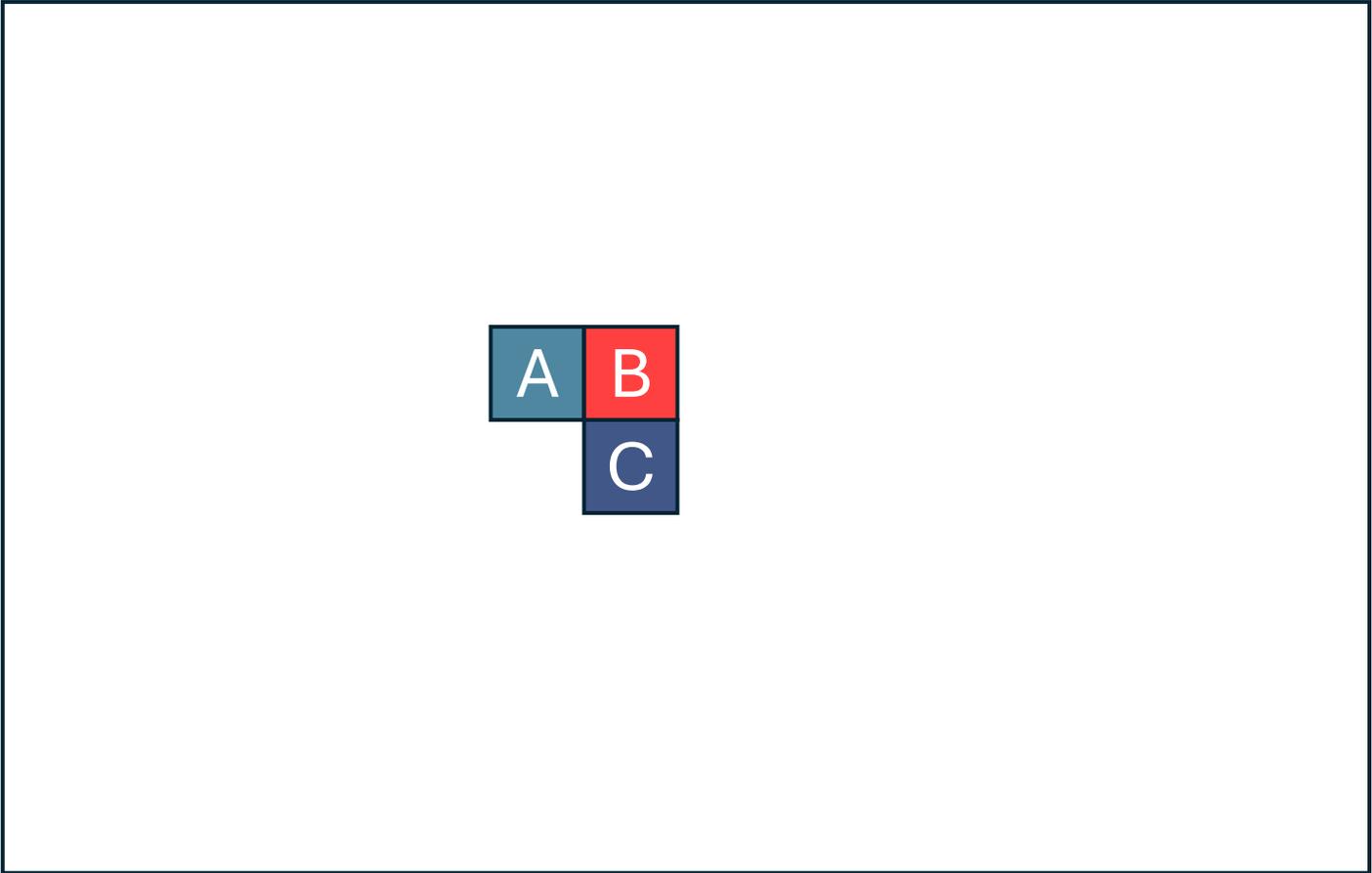
Tiles:



Affinities:

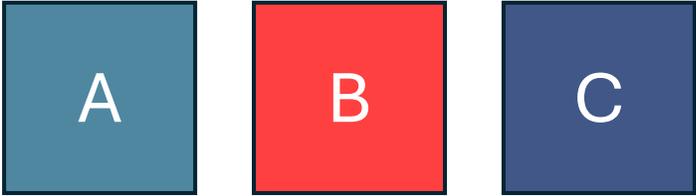


System:

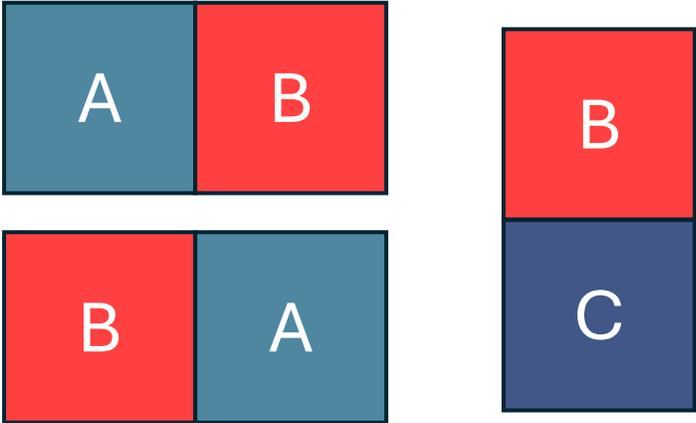


Tile Self-Assembly

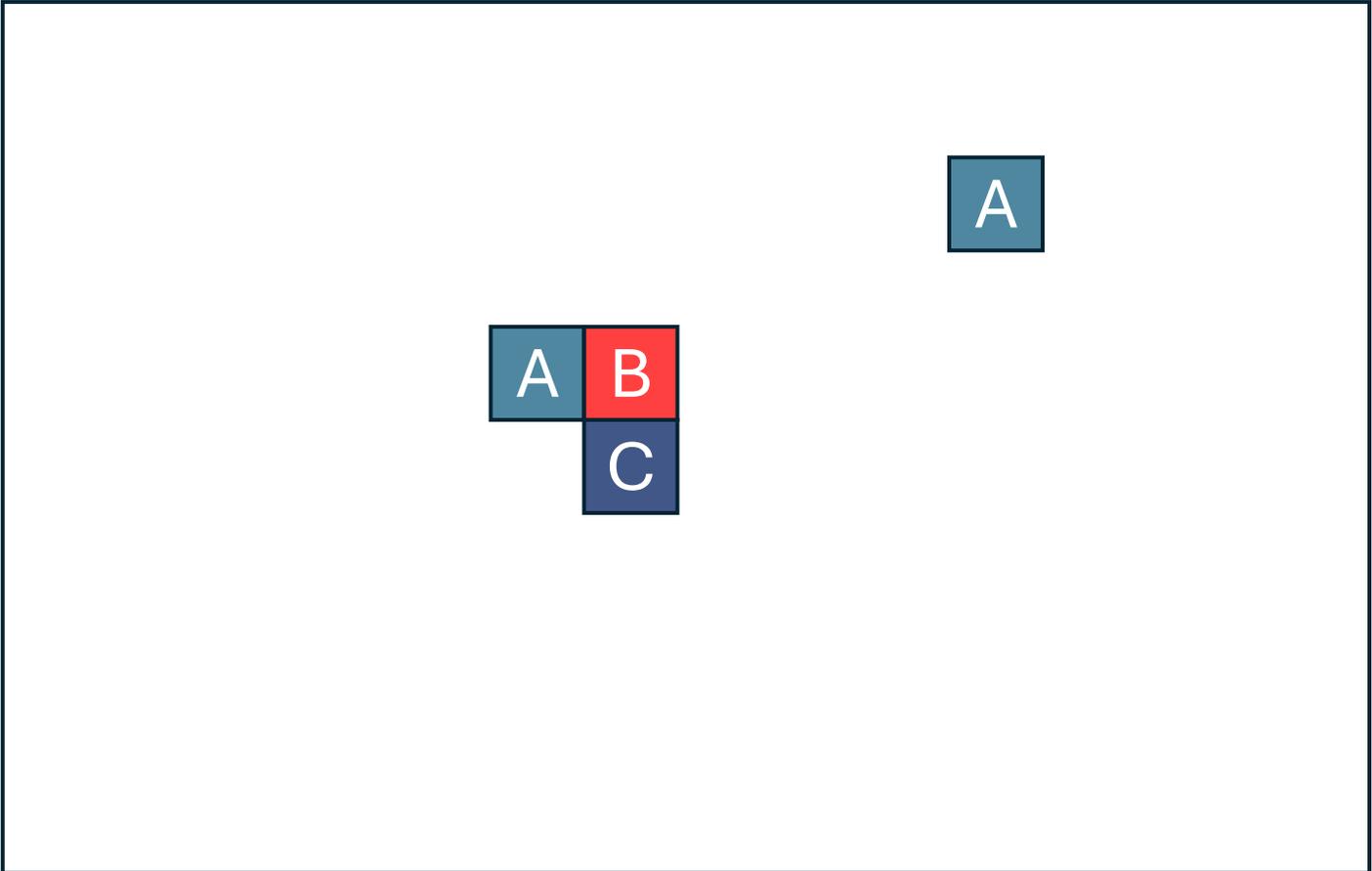
Tiles:



Affinities:

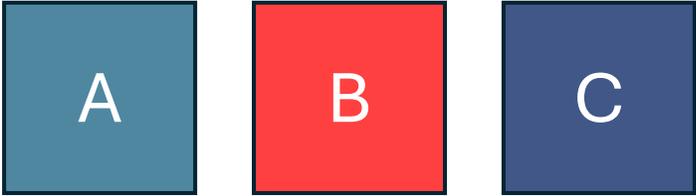


System:

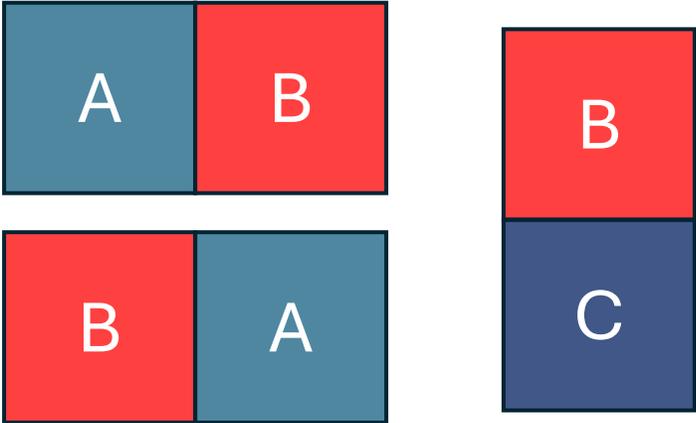


Tile Self-Assembly

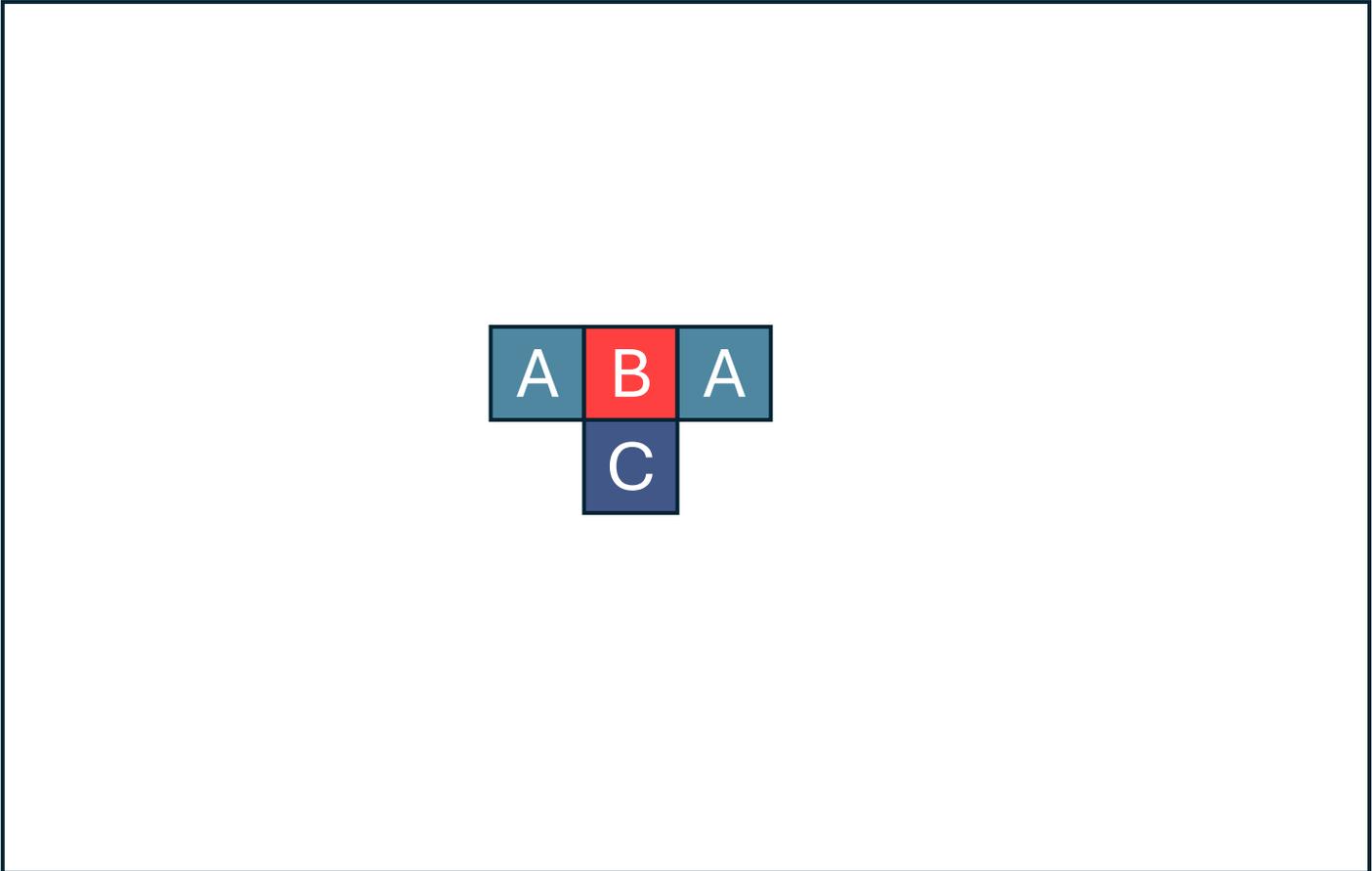
Tiles:



Affinities:

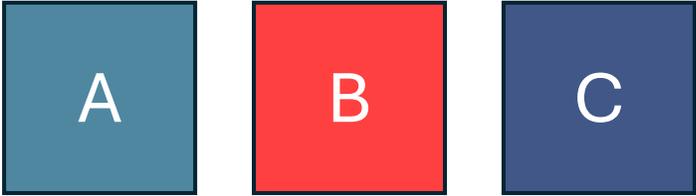


System:

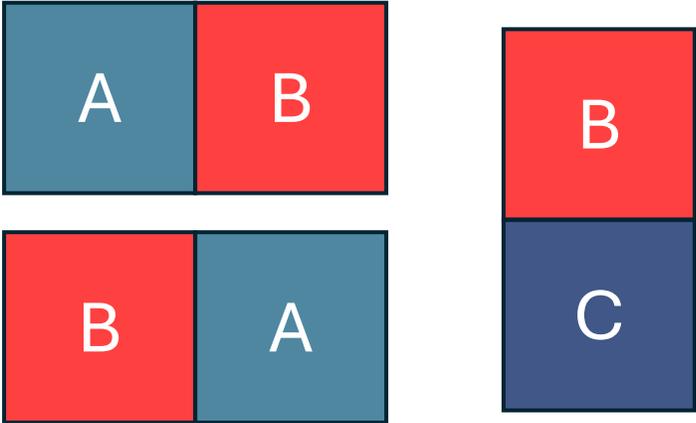


Tile Self-Assembly

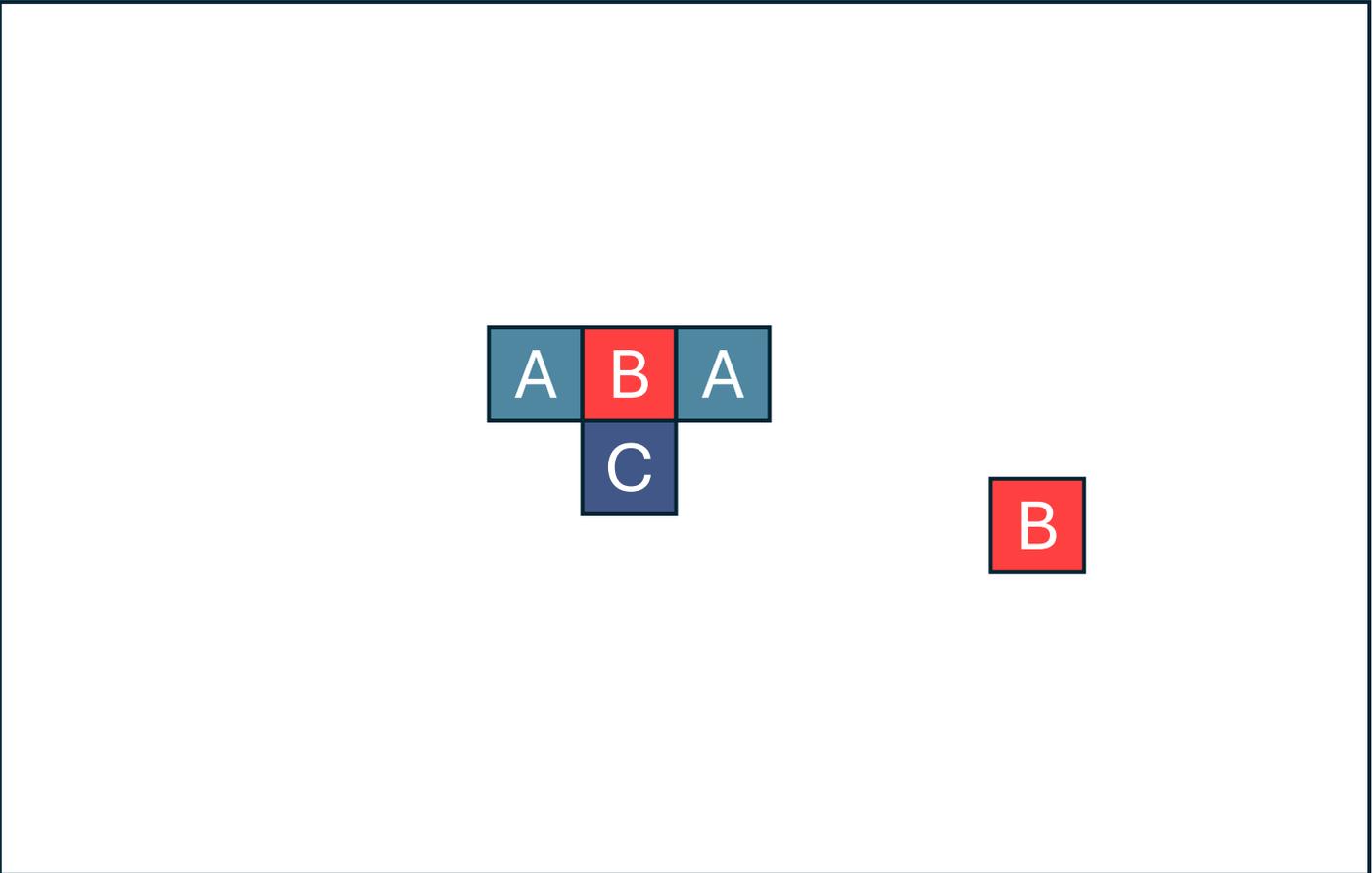
Tiles:



Affinities:



System:

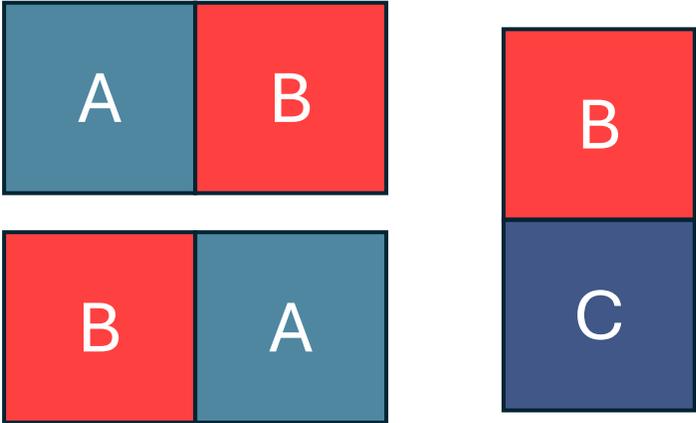


Tile Self-Assembly

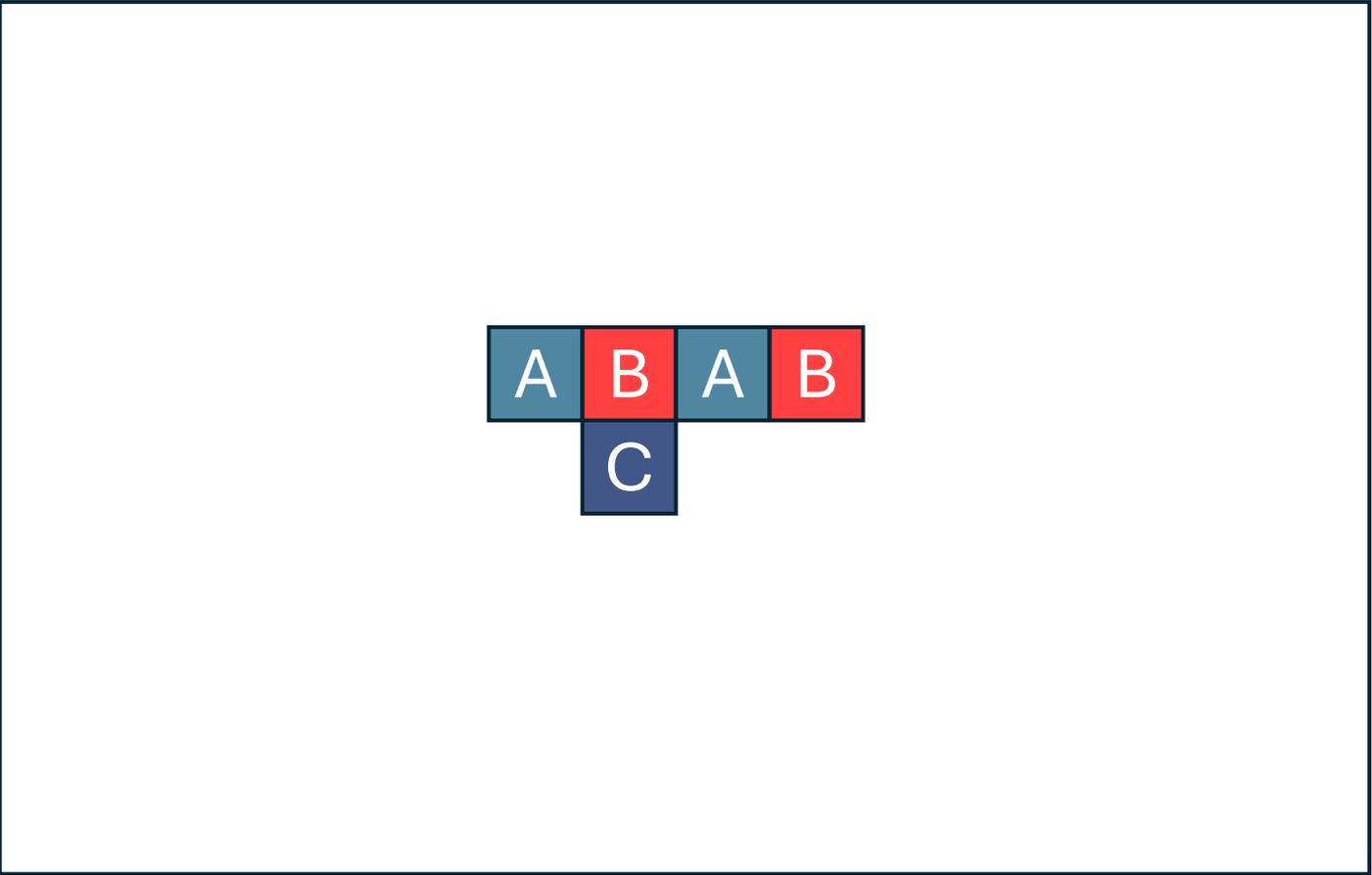
Tiles:



Affinities:



System:

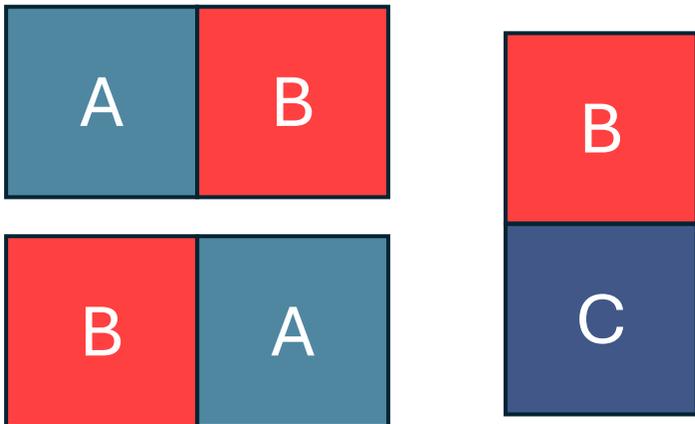


Tile Self-Assembly

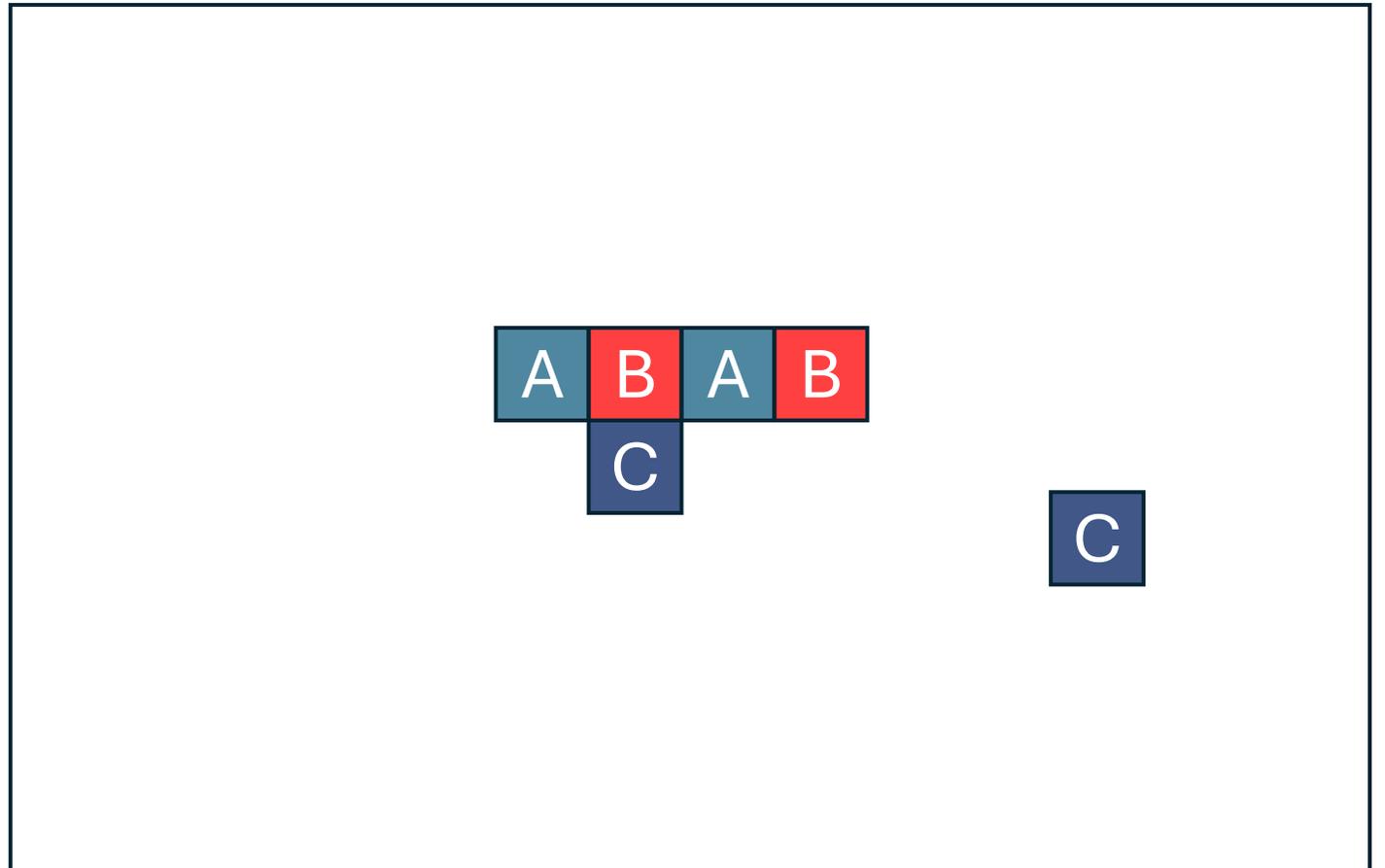
Tiles:



Affinities:



System:

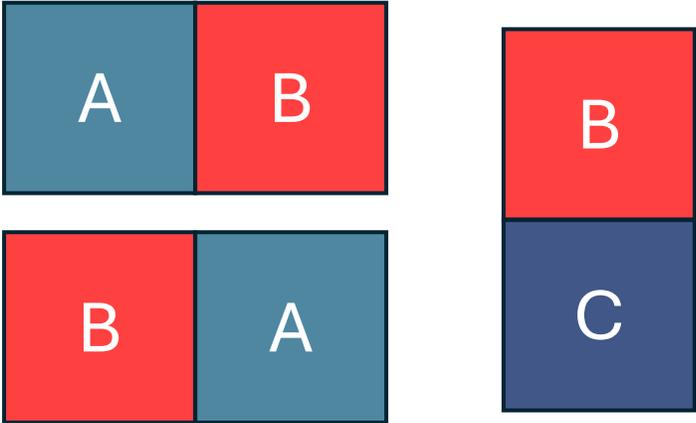


Tile Self-Assembly

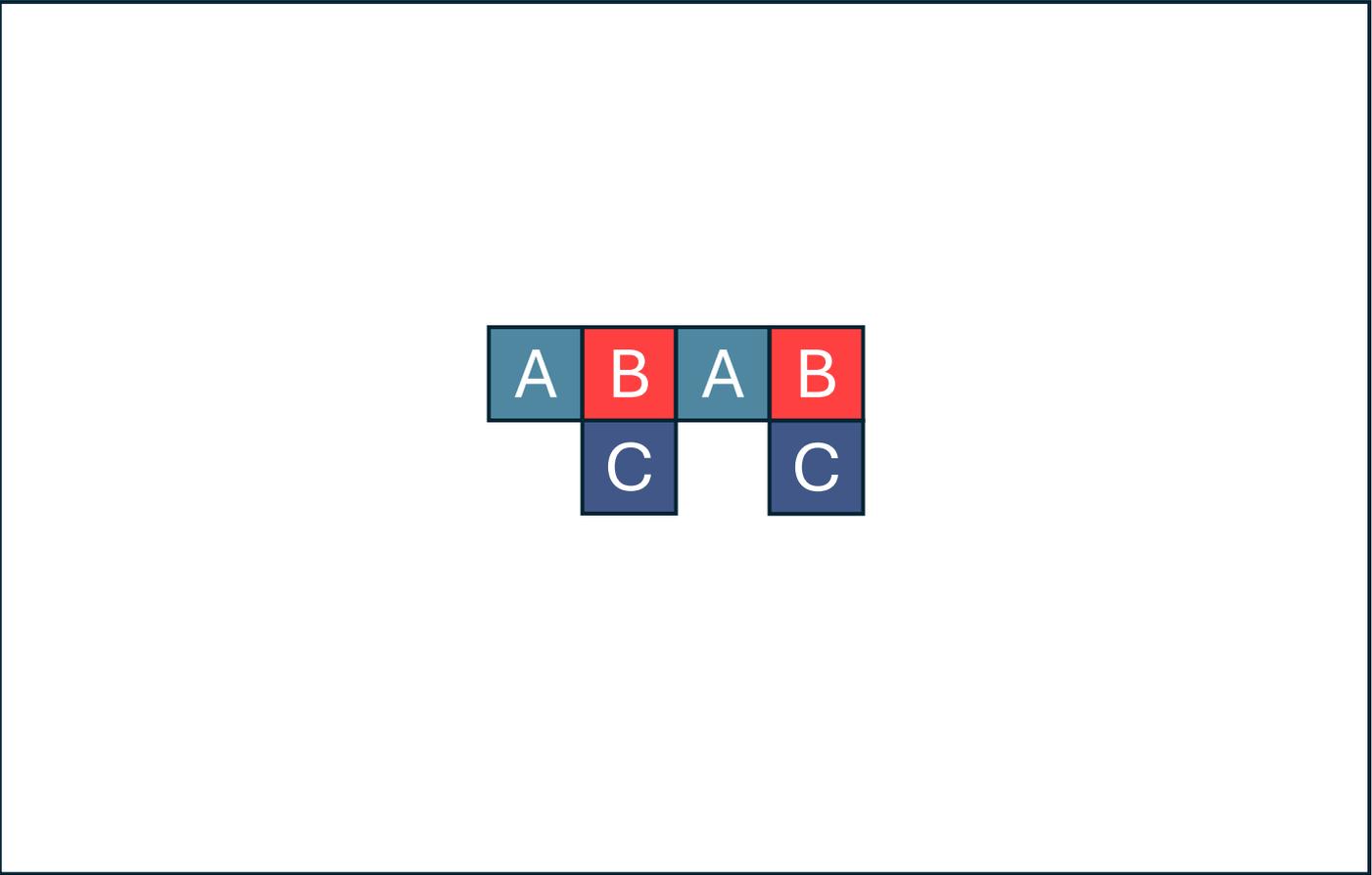
Tiles:



Affinities:



System:



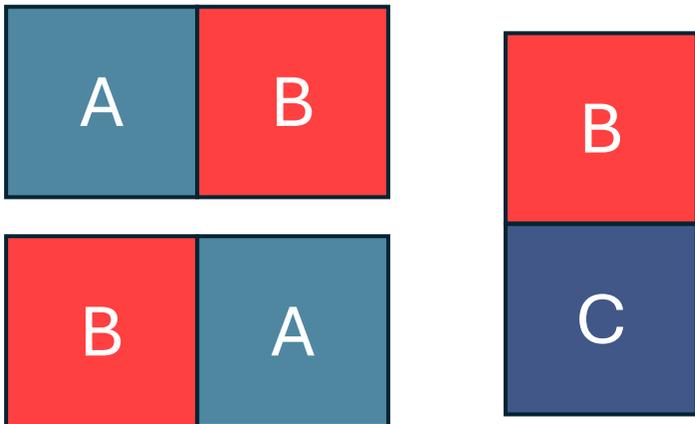
The aTAM (abstract Tile Assembly Model)

Tiles:

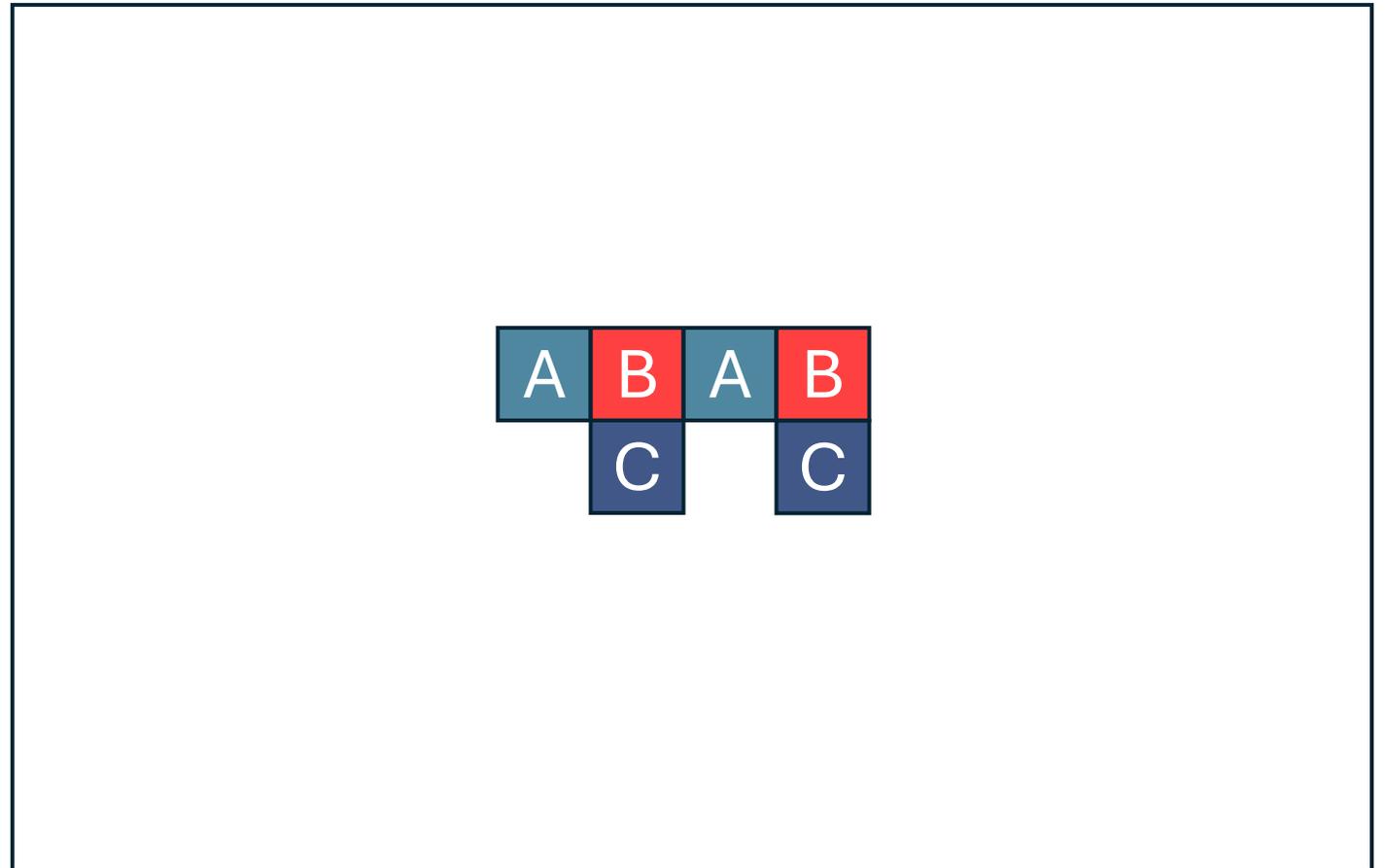


Affinities:

Temperature: τ



System:



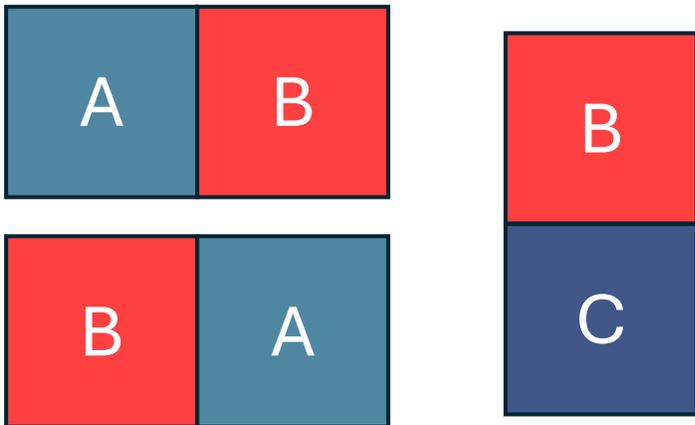
The aTAM (abstract Tile Assembly Model)

Tiles:

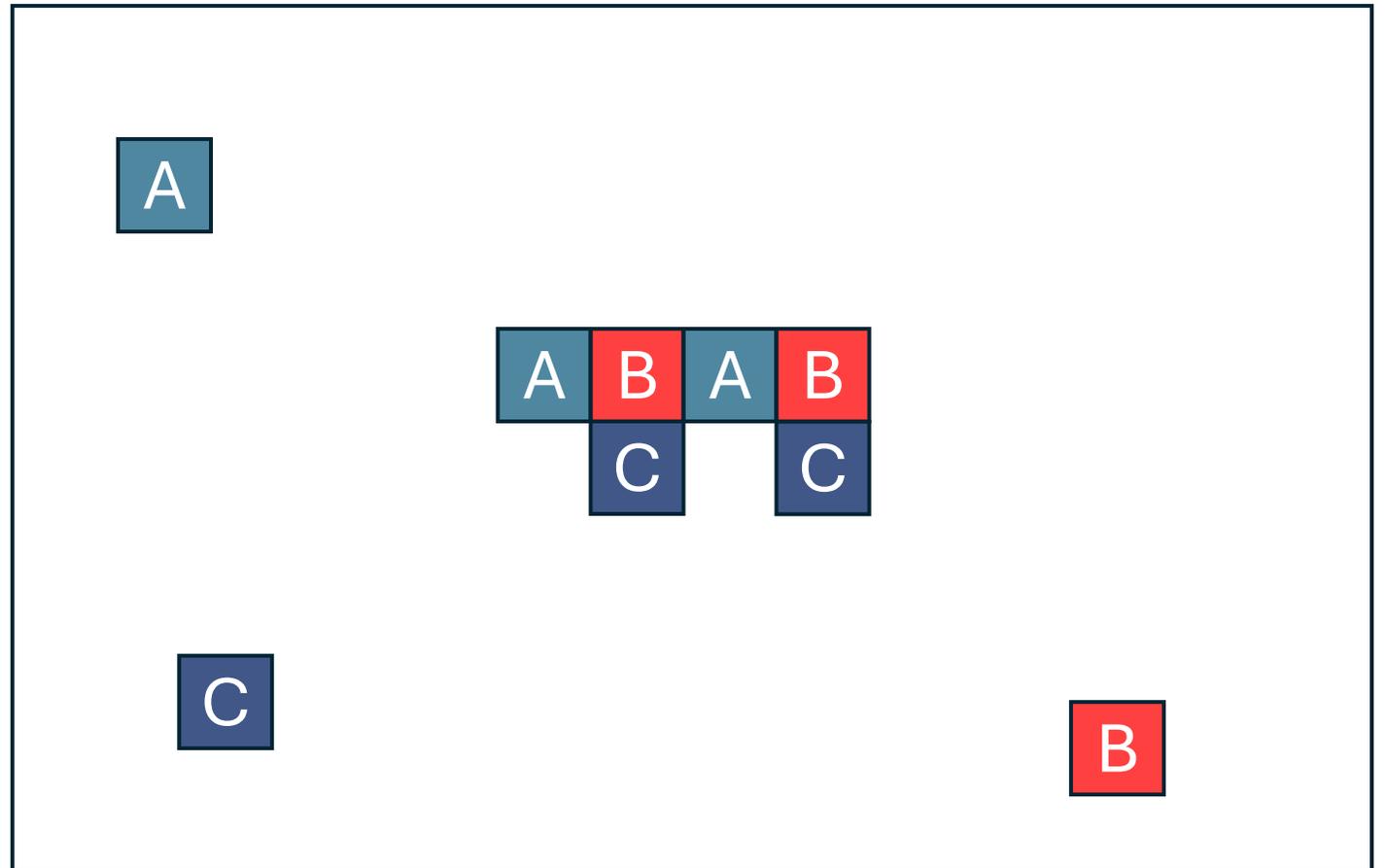


Affinities:

Temperature: τ



System:



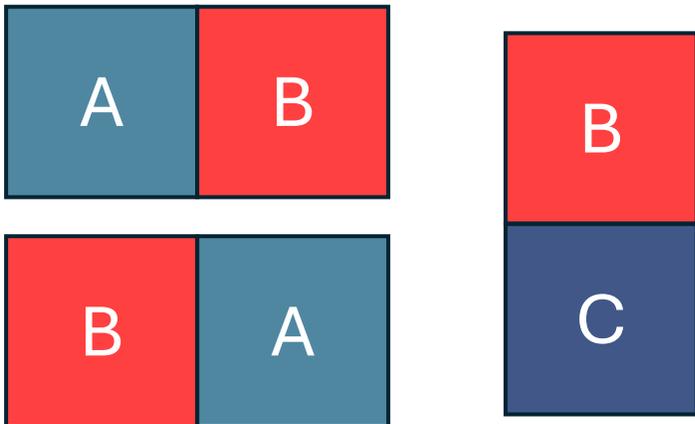
The aTAM (abstract Tile Assembly Model)

Tiles:

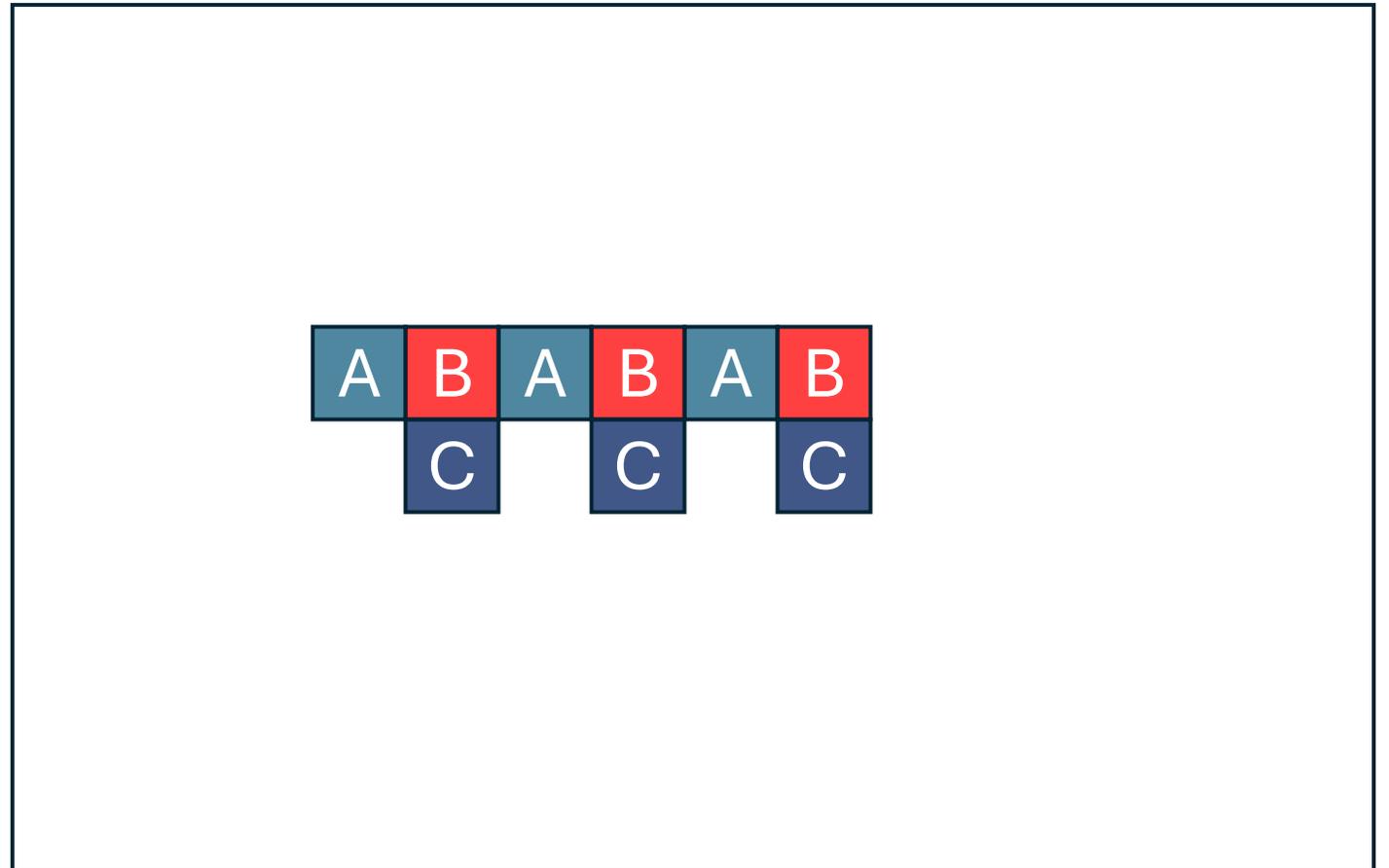


Affinities:

Temperature: τ

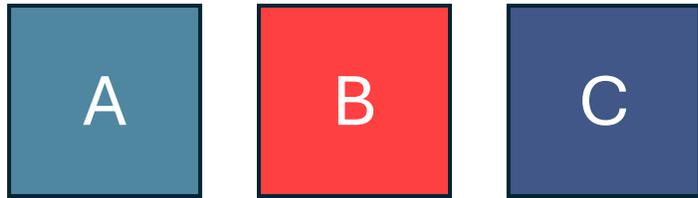


System:



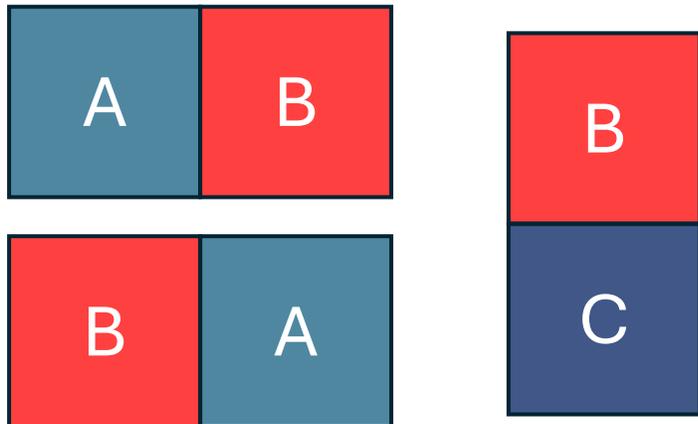
The aTAM (abstract Tile Assembly Model)

Tiles:

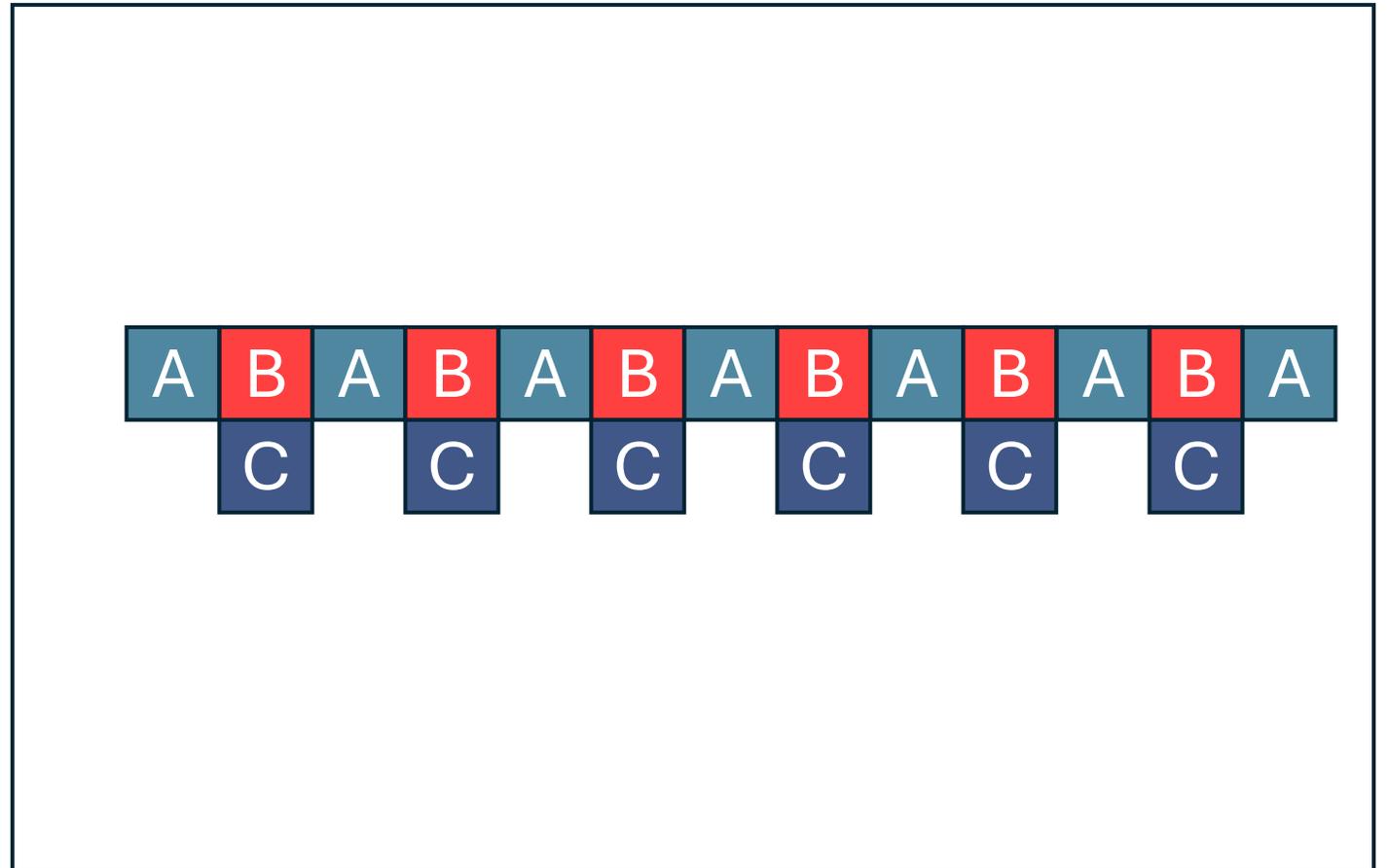


Affinities:

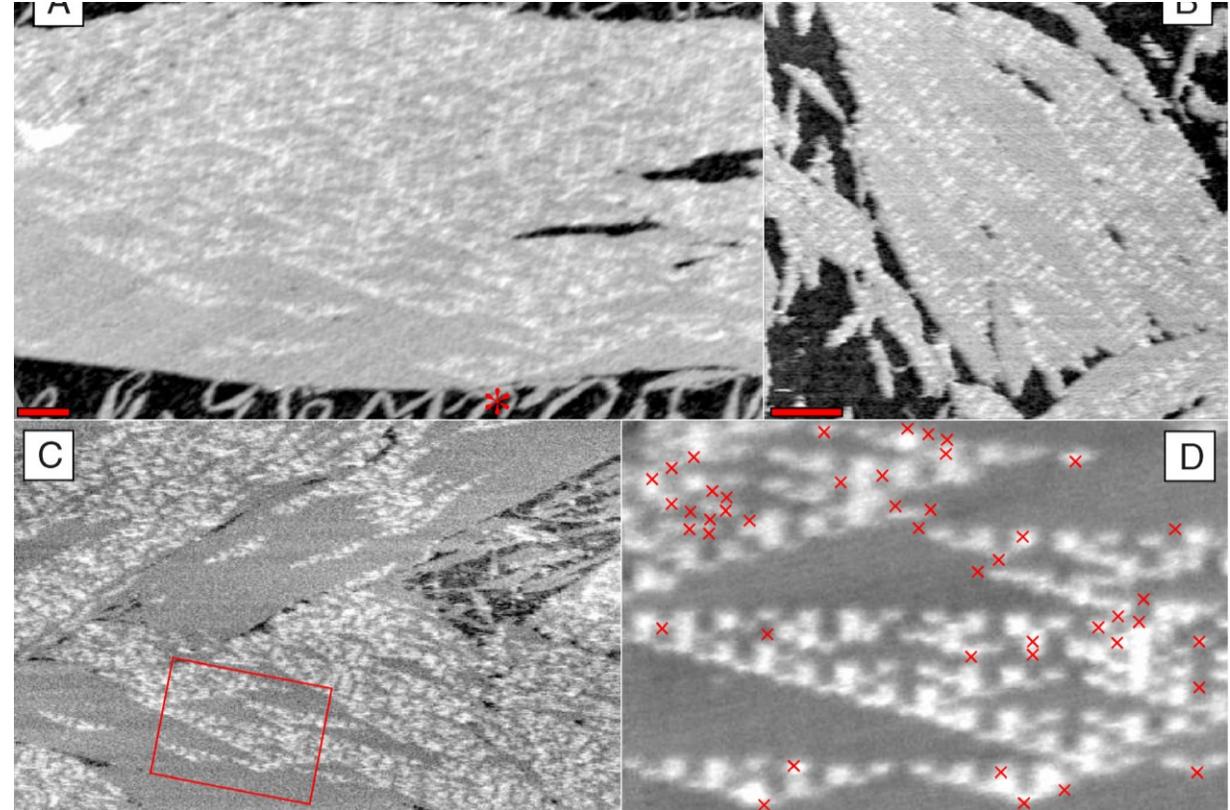
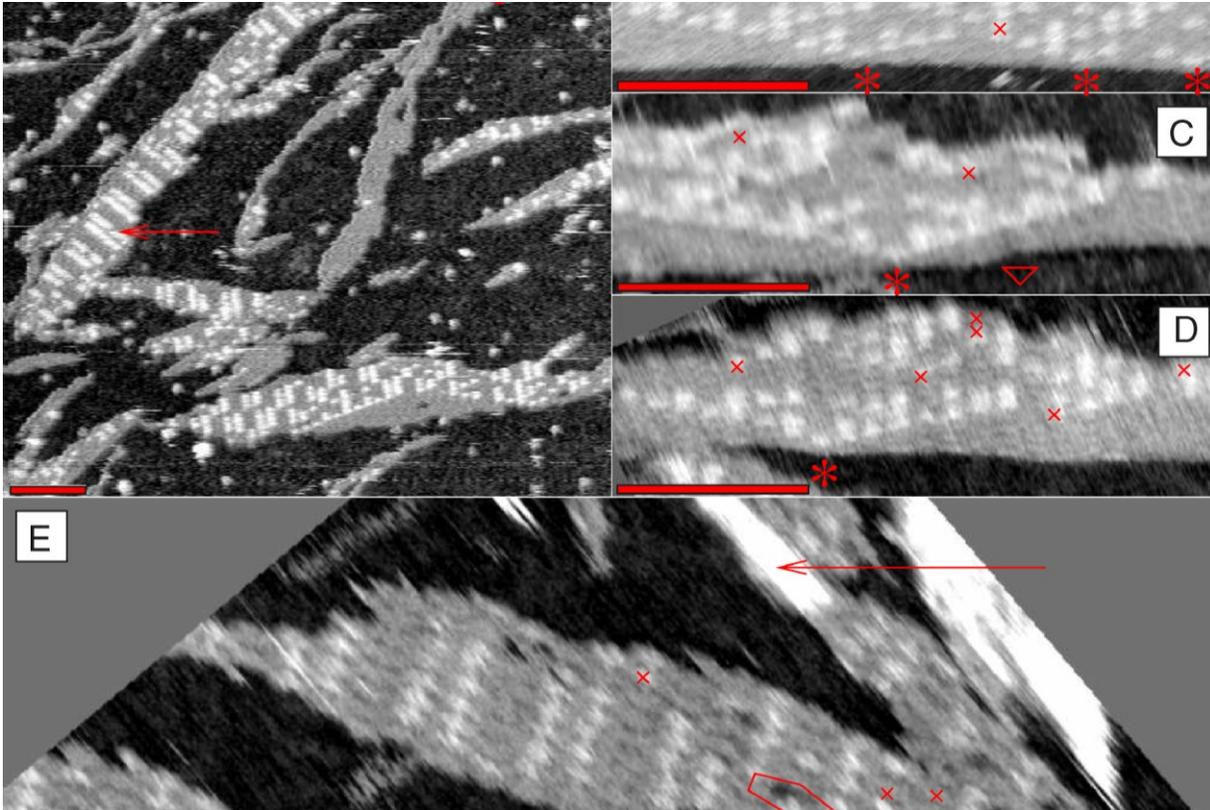
Temperature: τ



System:



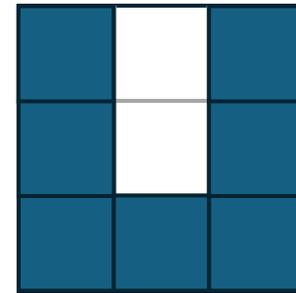
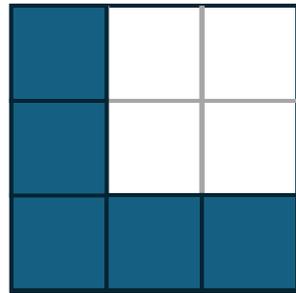
What is known (aTAM)



Rothemund PWK, Papadakis N, Winfree E (2004) Algorithmic Self-Assembly of DNA Sierpinski Triangles. PLoS Biol 2(12): e424.

What is known (aTAM)

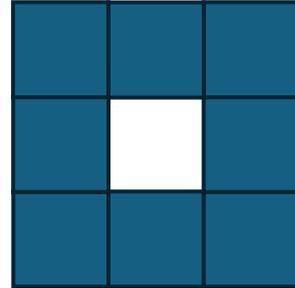
- **2010** [M. J. Patitz, S. M. Summers. Self-assembly of discrete self-similar fractals]:
 1. Any “L” shape does not strictly self assemble in the aTAM (any temp)
 2. No fractal weakly self assembles at temperature 1
 3. “Nice” fractals can be weakly self assembled at higher temps



- **2025** [F. Becker, D. Hader, M. J. Patitz. Strict self-assembly of discrete self-similar fractals in the abstract tile-assembly model]:
 1. A full characterization of which DSSFs are buildable in the aTAM.

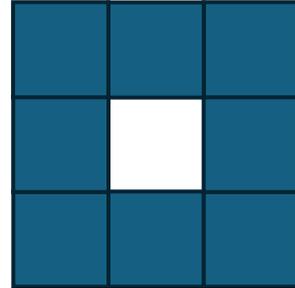
Variations of the aTAM

- 2HAM (2-Handed Assembly Model):
 1. 2 different assemblies can attach
 2. Can finitely assemble a larger class of shapes
- STAM (Signal-Passing Tile Assembly Model):
 1. Glues can turn “on” and “off”
 2. Detachment is allowed



Variations of the aTAM

- 2HAM (2-Handed Assembly Model):
 1. 2 different assemblies can attach
 2. Can finitely assemble a larger class of shapes
- STAM (Signal-Passing Tile Assembly Model):
 1. Glues can turn “on” and “off”
 2. Detachment is allowed
 3. Any arbitrary fractal is buildable
 4. Without detachments, some shapes impossible



A Comparison

	aTAM	2HAM	STAM
Description	<ul style="list-style-type: none">- Single tile attachments- No detachments- Fixed glues	<ul style="list-style-type: none">- Up to 2 assembly attachments- No detachments- Fixed glues	<ul style="list-style-type: none">- Up to 2 assembly attachments- Detachments- Glues turn on/off
Results	<ul style="list-style-type: none">- No fractals weakly buildable (temp 1)- Some fractals not strictly buildable (temp > 1)	<ul style="list-style-type: none">- Finitely assemble larger class of shapes- Still some non-buildable fractals	<ul style="list-style-type: none">- All fractals strictly buildable- Without detachment: some impossible fractals

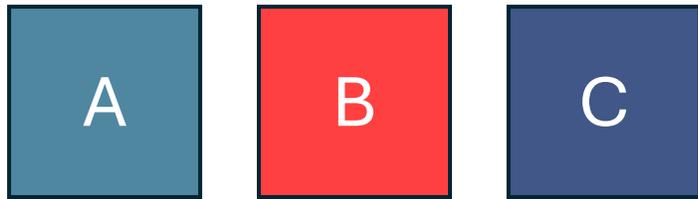
Question: What if adjacent tiles can infinitely change states?

Seeded Tile Automata

What is the model?

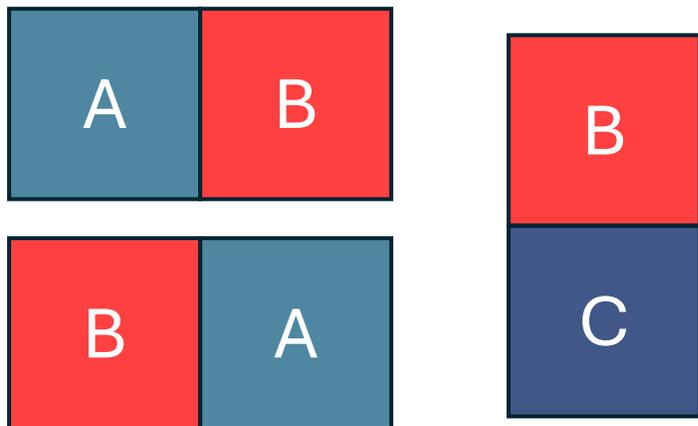
Seeded TA

Tiles:

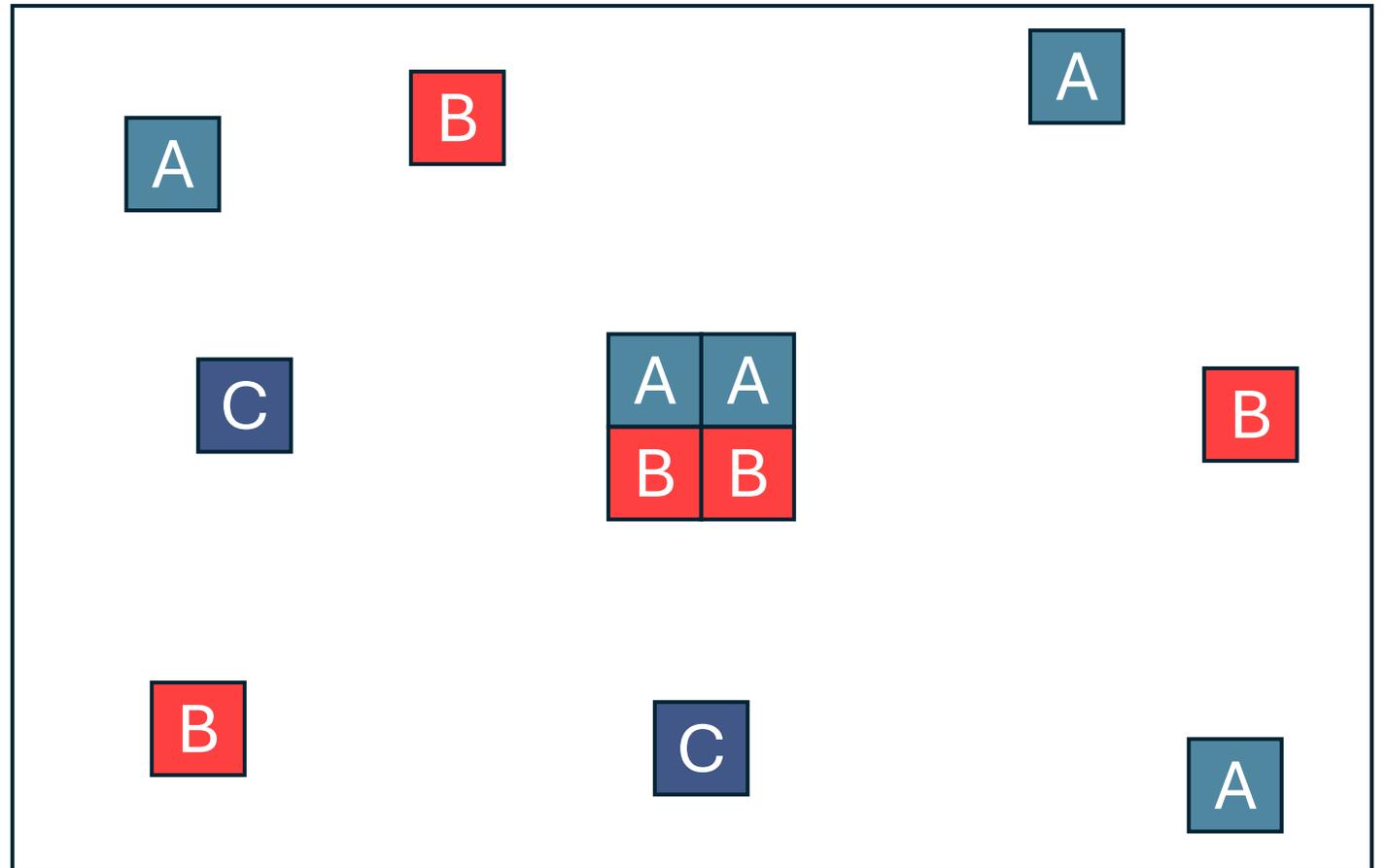


Affinities:

Temperature: τ

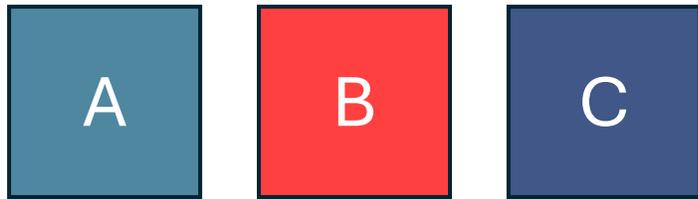


System:



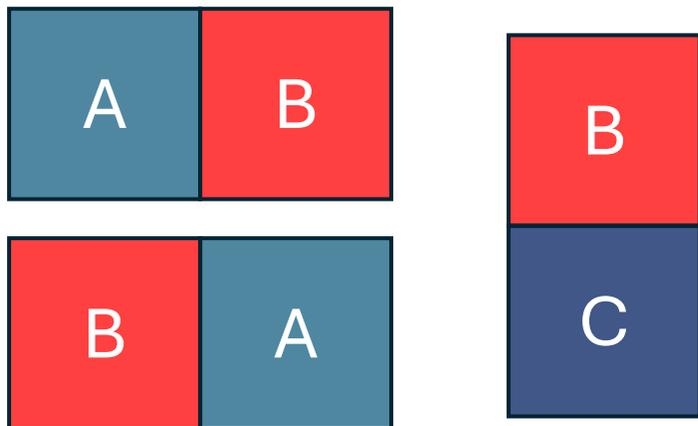
Seeded TA

Tiles:

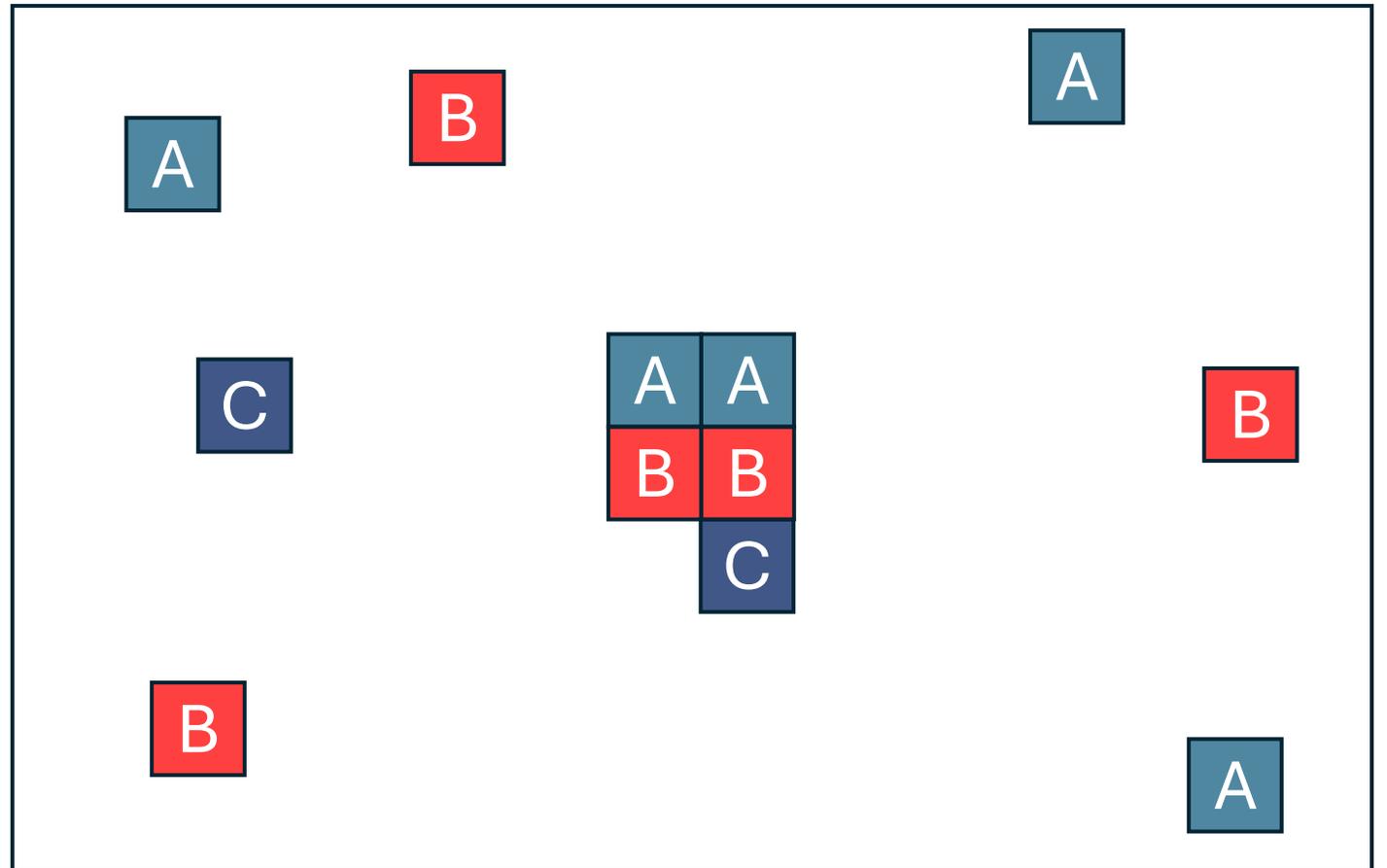


Affinities:

Temperature: τ



System:



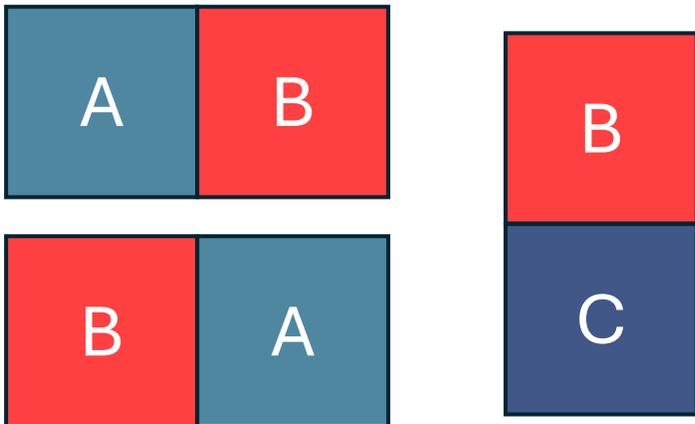
Seeded TA

Tiles:

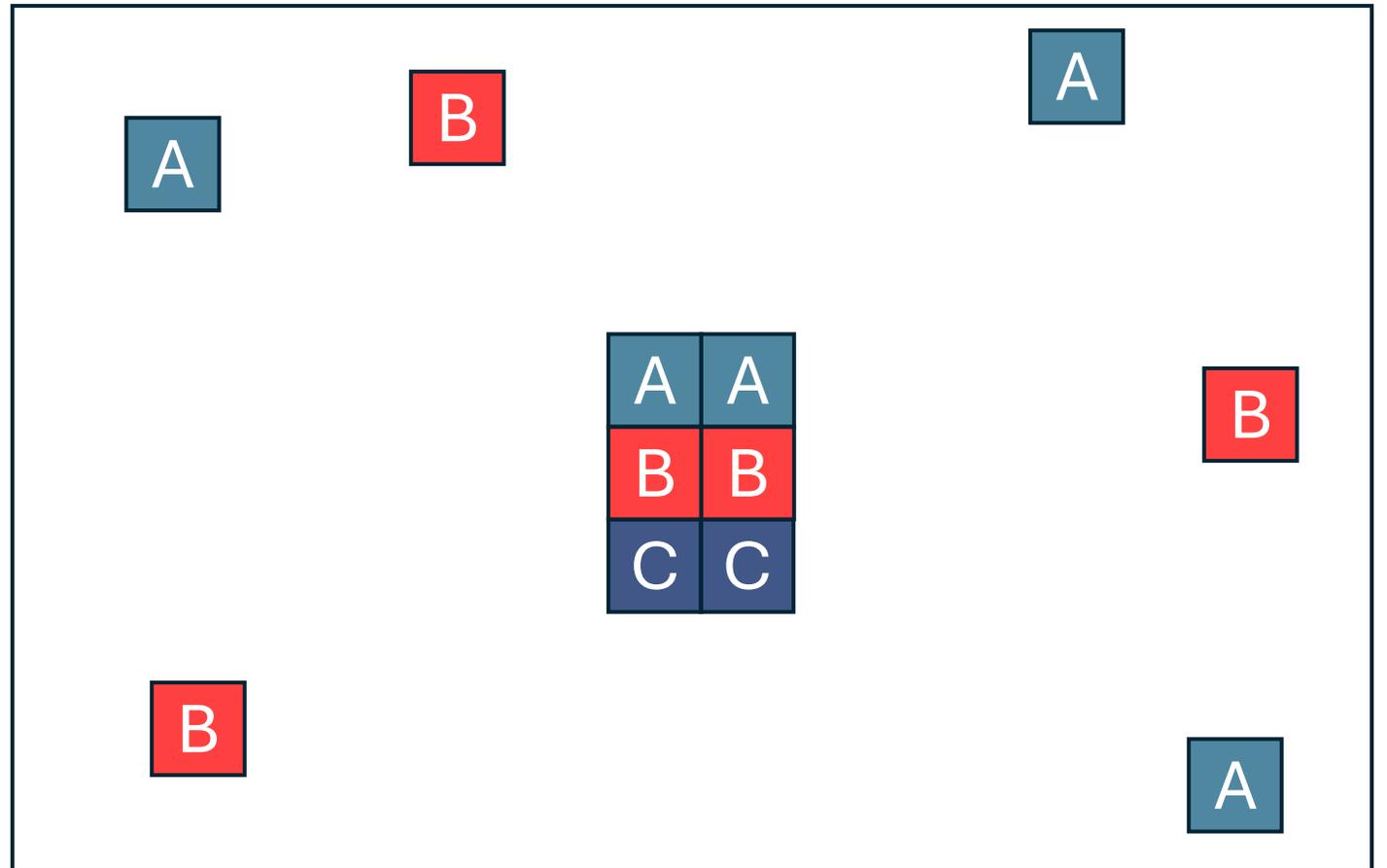


Affinities:

Temperature: τ



System:



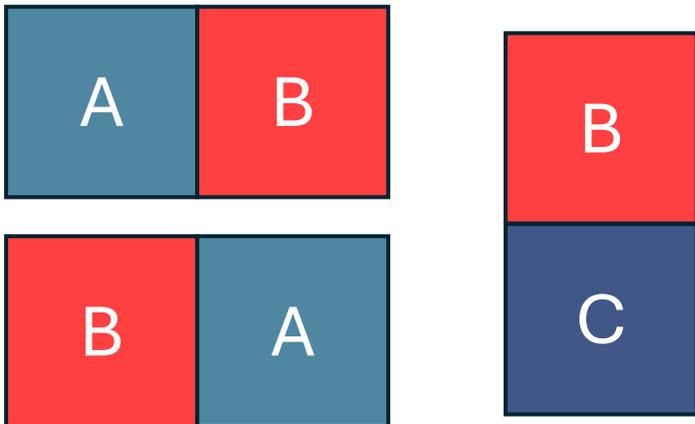
Seeded TA

Tiles:

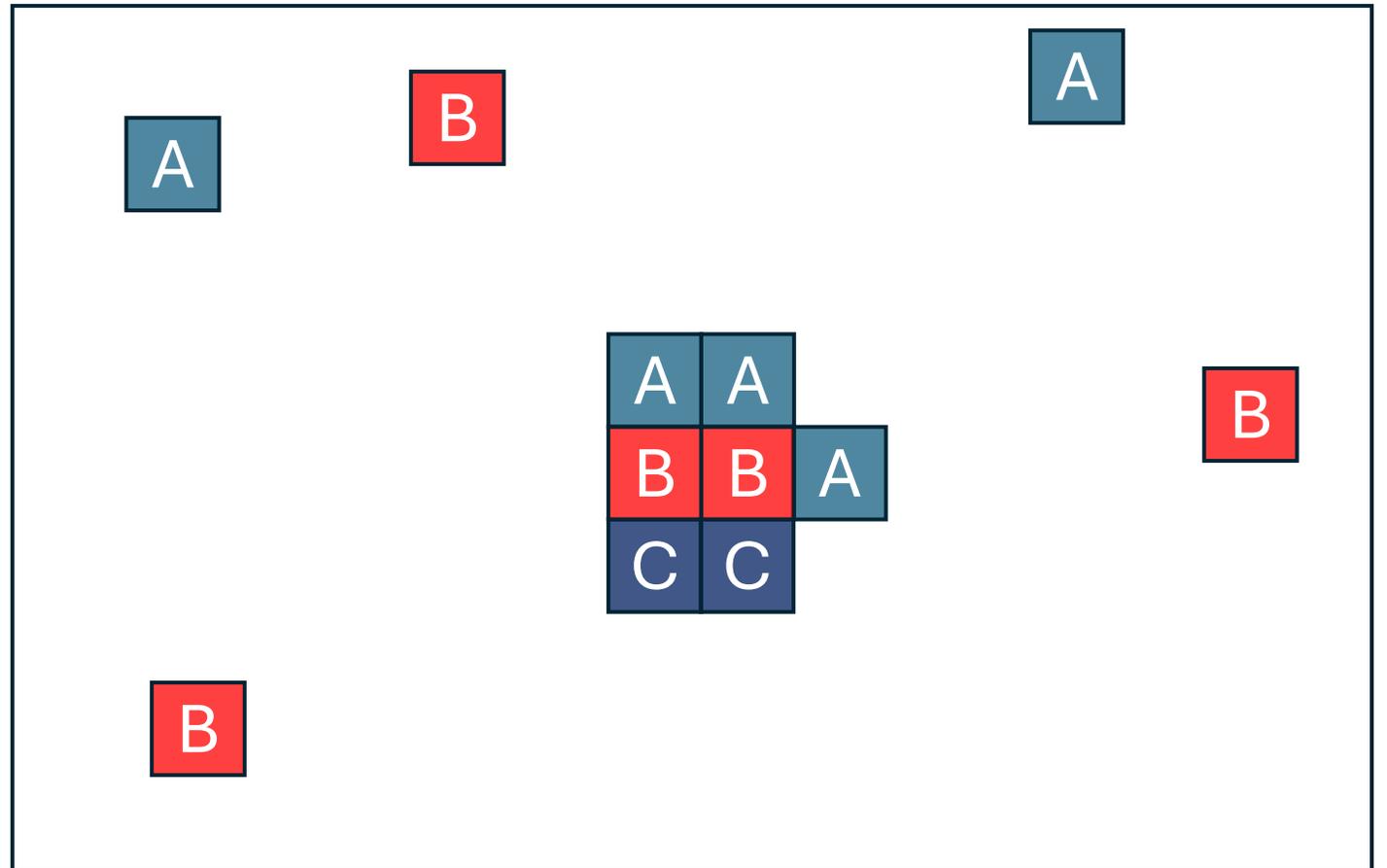


Affinities:

Temperature: τ

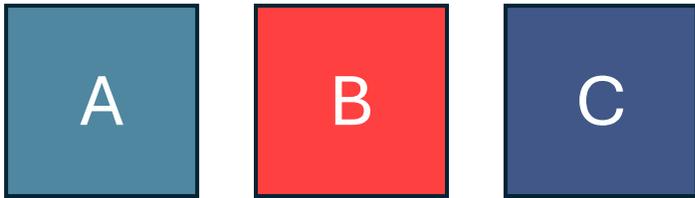


System:



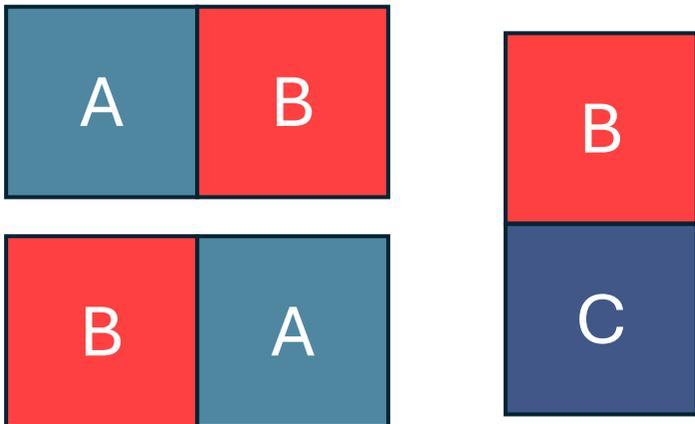
Seeded TA

Tiles:

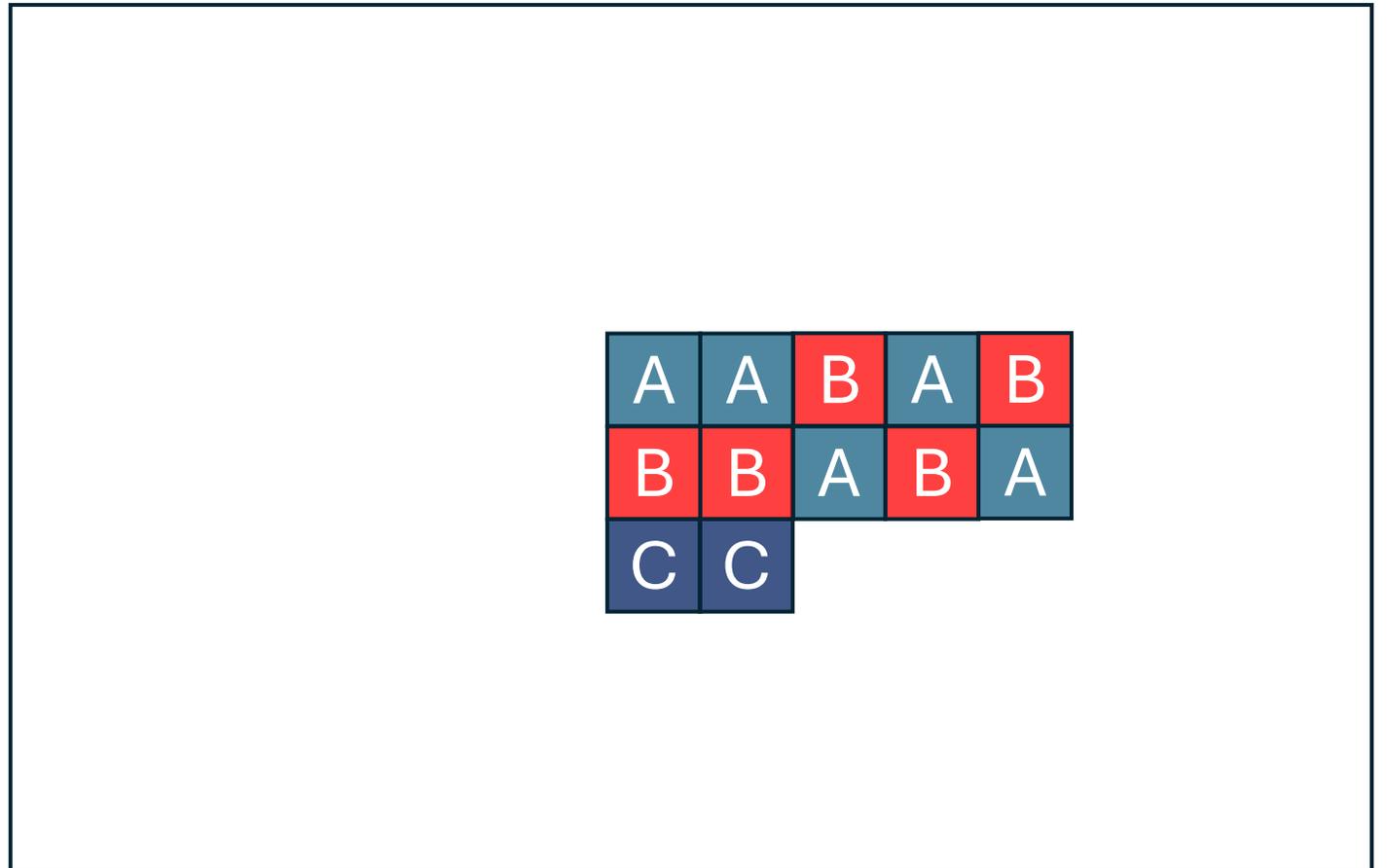


Affinities:

Temperature: τ

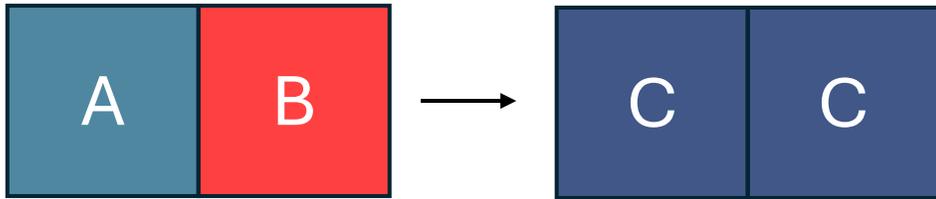


System:



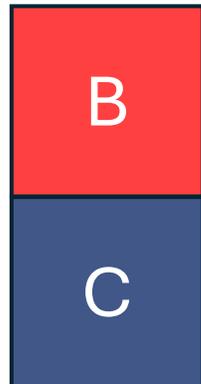
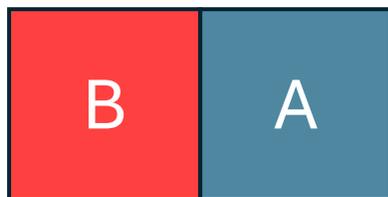
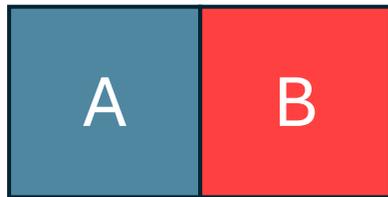
Seeded TA

Transitions:

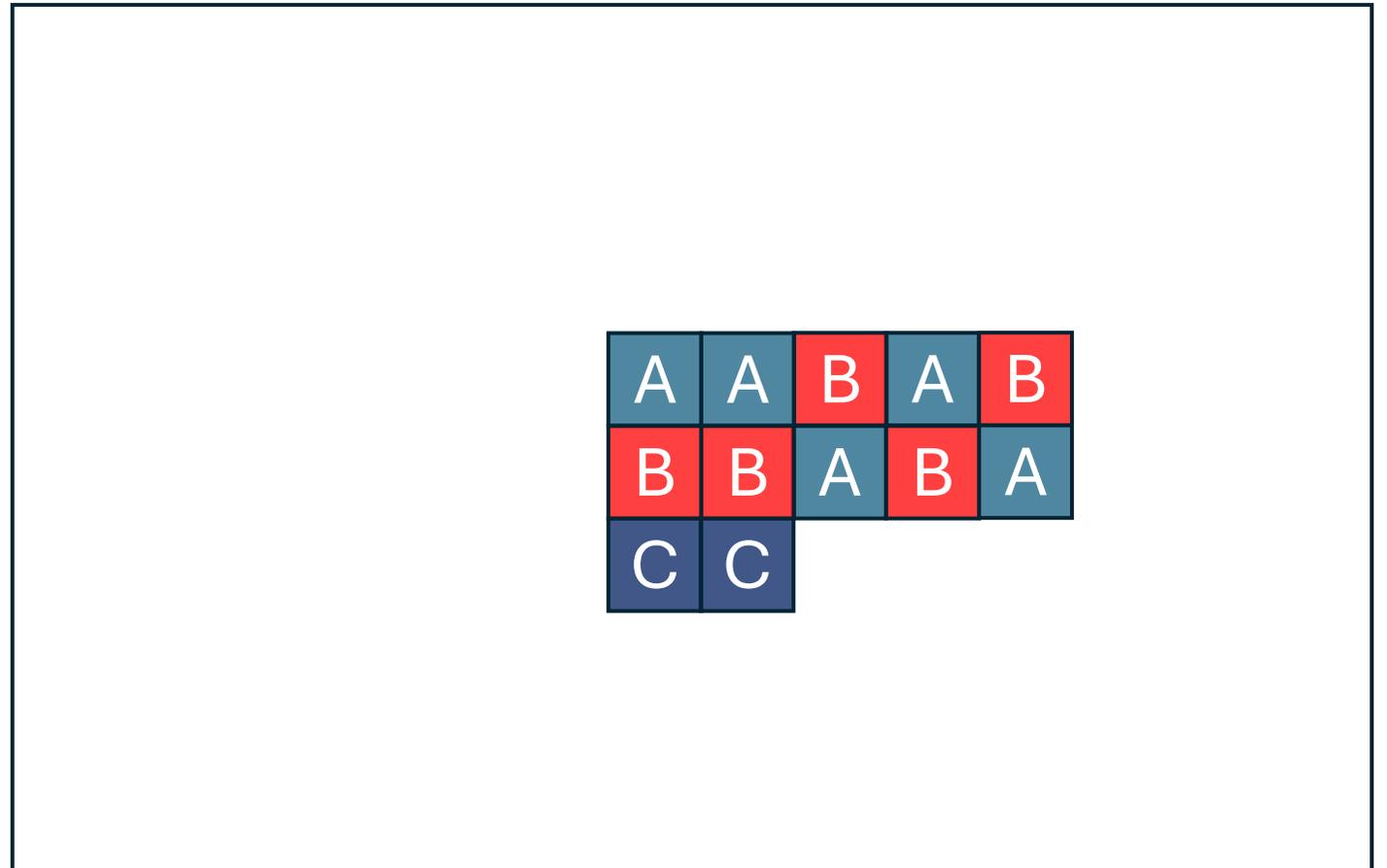


Affinities:

Temperature: τ

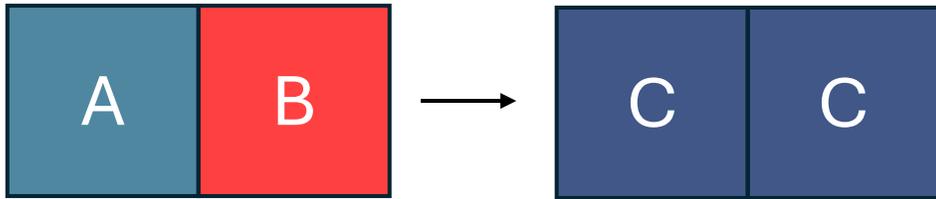


System:



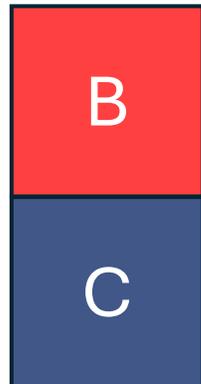
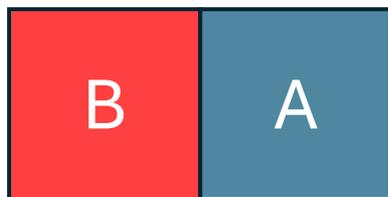
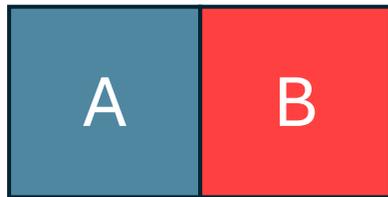
Seeded TA

Transitions:

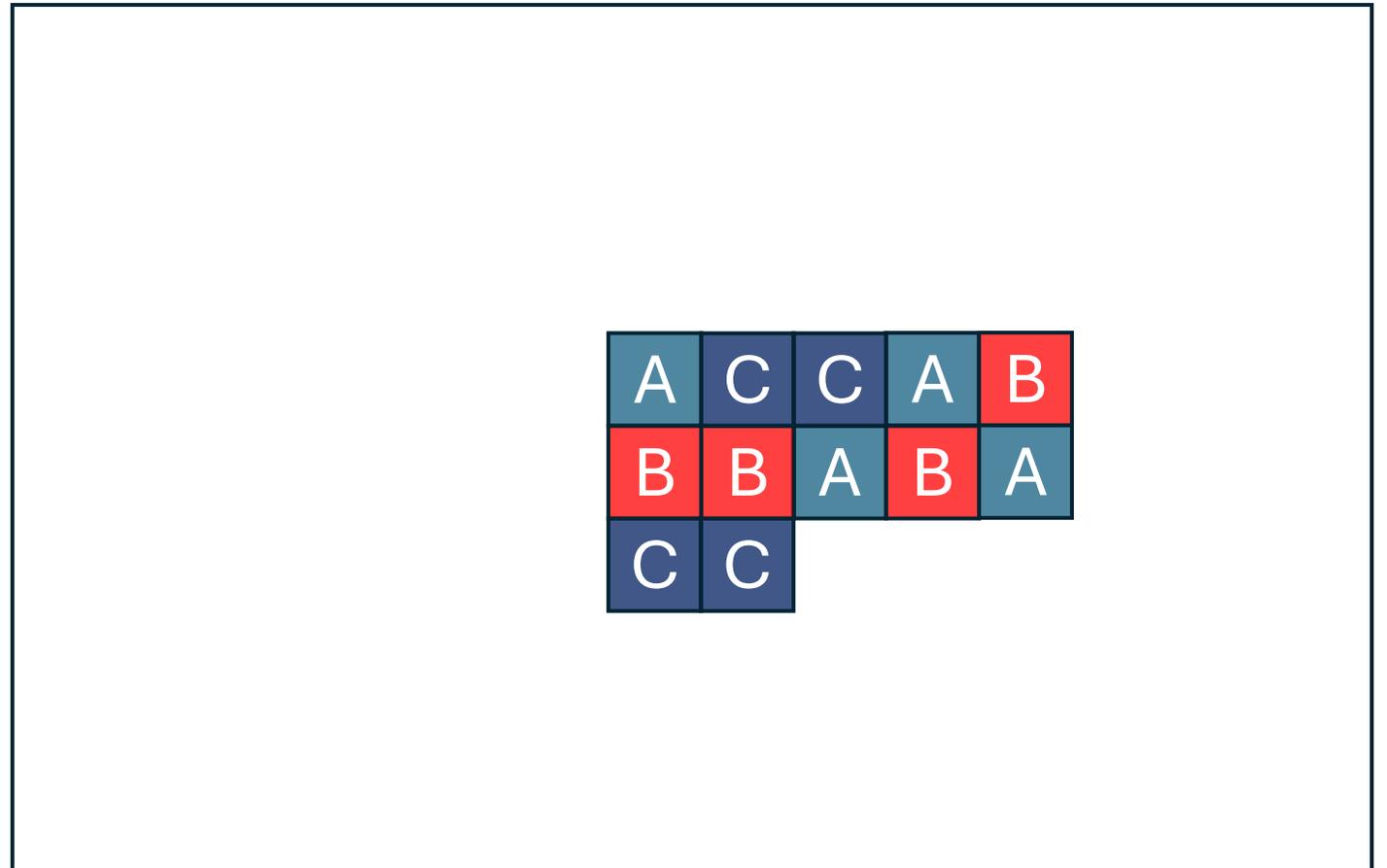


Affinities:

Temperature: τ

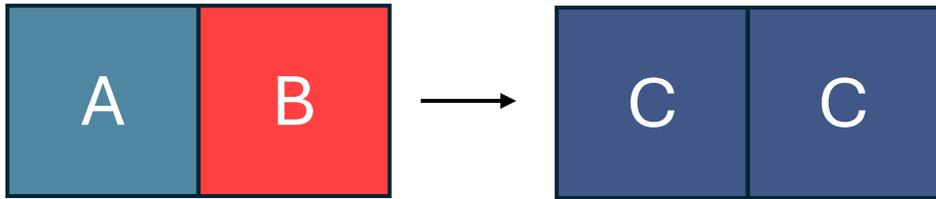


System:



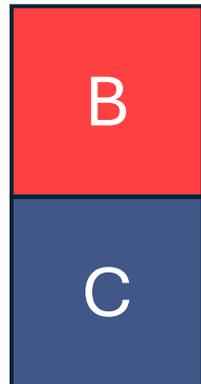
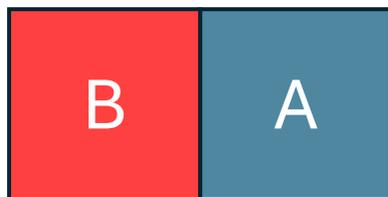
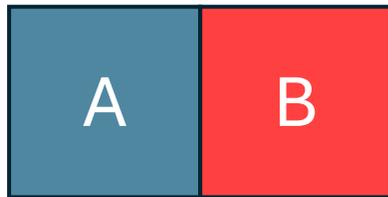
Seeded TA

Transitions:

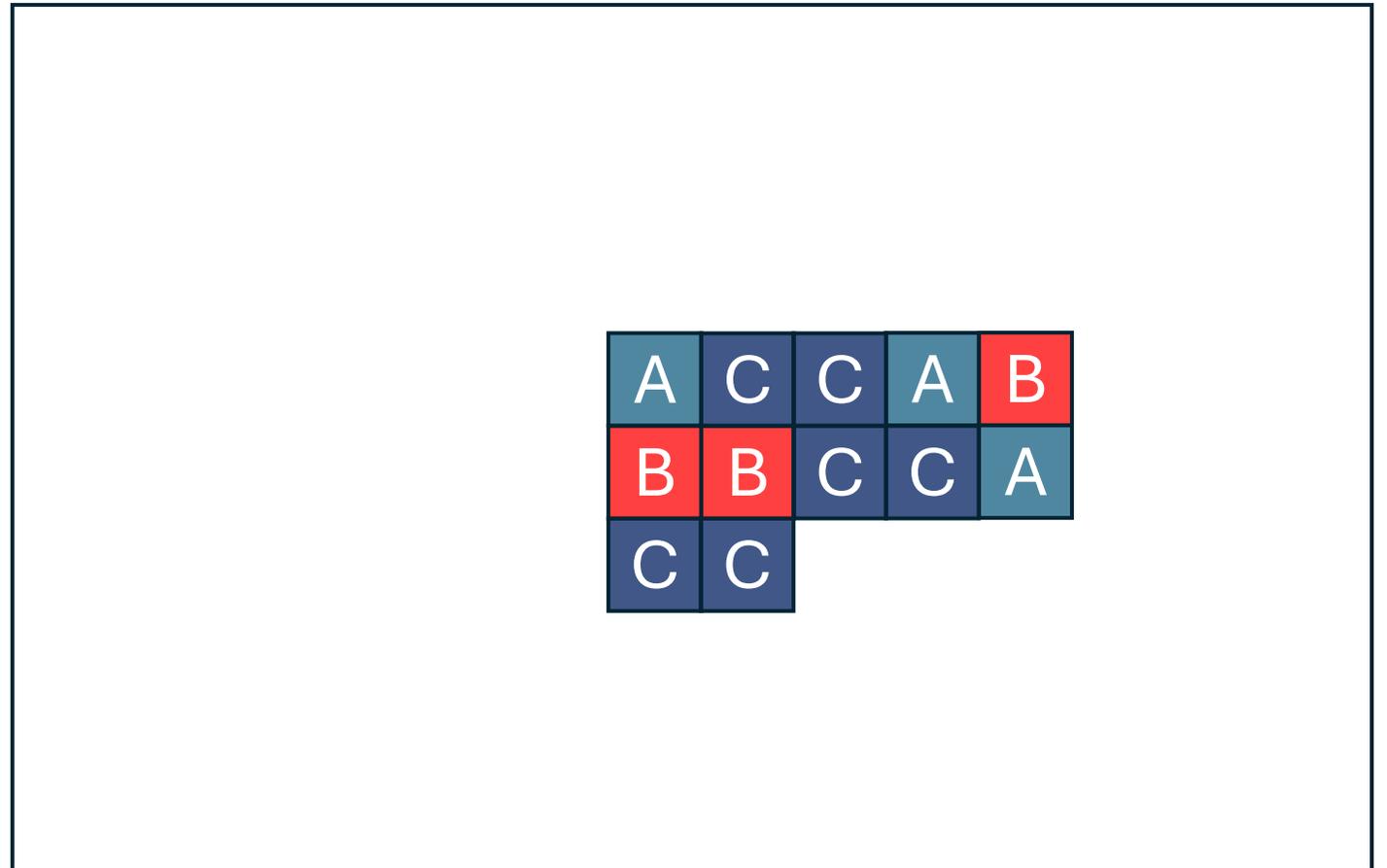


Affinities:

Temperature: τ

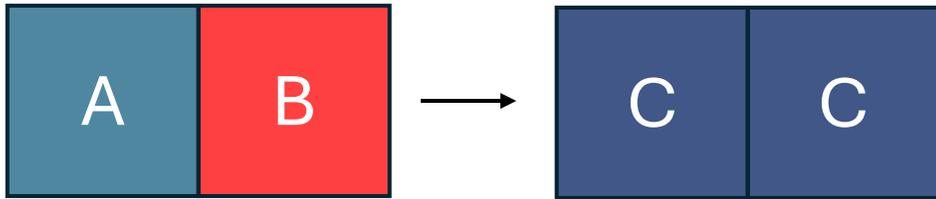


System:



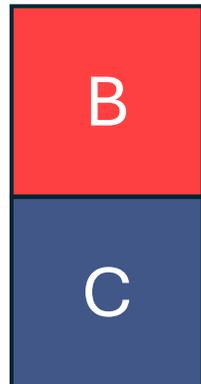
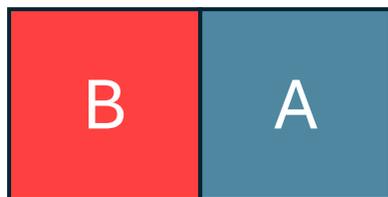
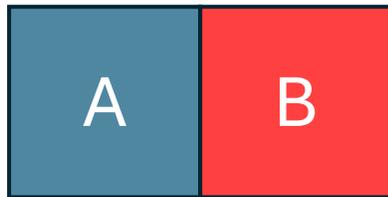
Seeded TA

Transitions:

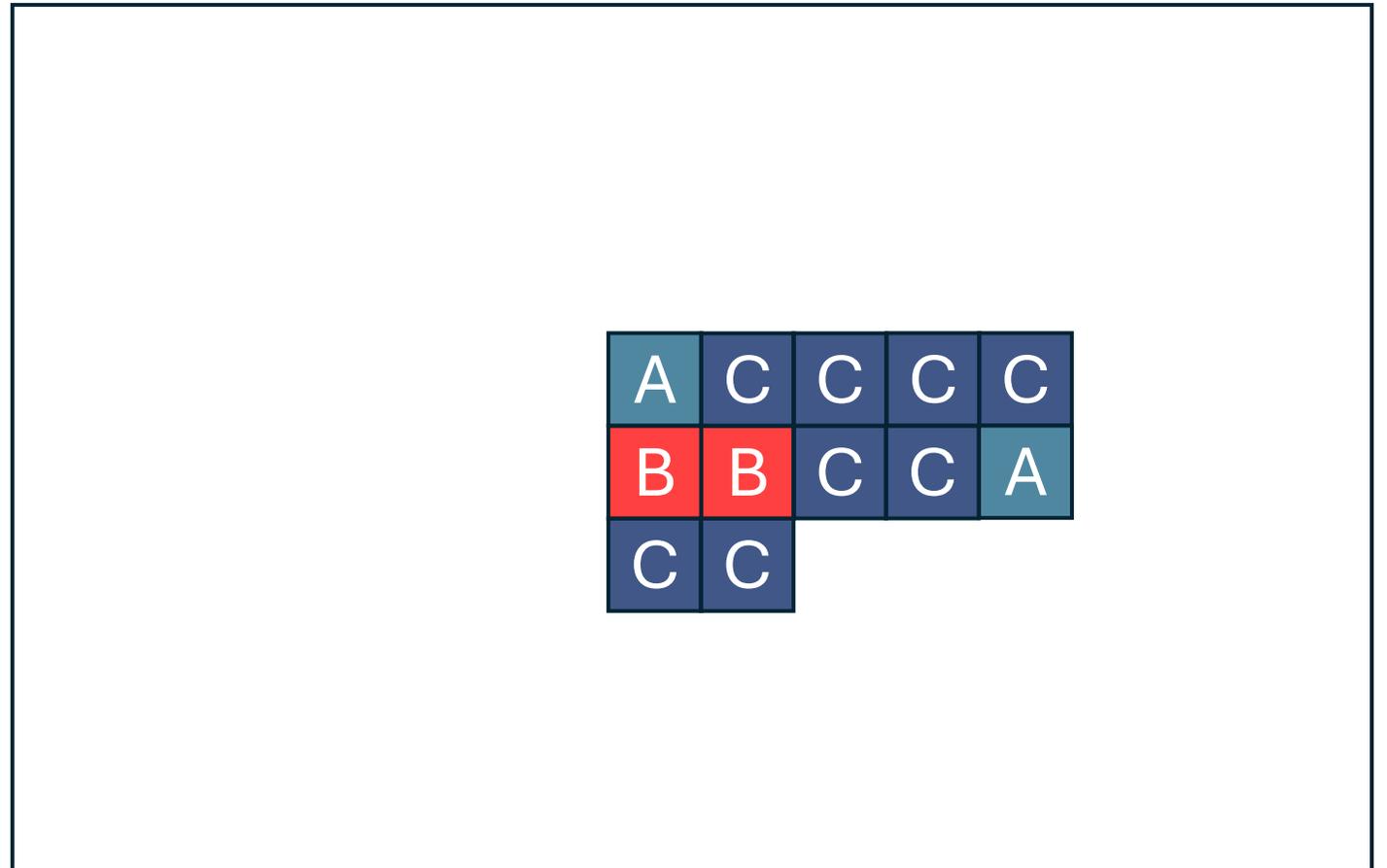


Affinities:

Temperature: τ



System:



What is known

	aTAM	2HAM	STAM	Seeded TA
Description	<ul style="list-style-type: none"> - Single tile attachments - No detachments - Fixed glues 	<ul style="list-style-type: none"> - Up to 2 assembly attachments - No detachments - Fixed glues 	<ul style="list-style-type: none"> - Up to 2 assembly attachments - Detachments - Glues turn on/off 	<ul style="list-style-type: none"> - Single tile attachments - No detachments - Transitions
Results	<ul style="list-style-type: none"> - No fractals weakly buildable (temp 1) - Some fractals not strictly buildable (temp > 1) 	<ul style="list-style-type: none"> - Finitely assemble larger class of shapes - Still some non-buildable fractals 	<ul style="list-style-type: none"> - All fractals strictly buildable - Without detachment: some impossible fractals 	<ul style="list-style-type: none"> - Fractals with generators that have a Ham-path are strictly buildable (temp 1)

Our Contribution

	aTAM	2HAM	STAM	Seeded TA
Description	<ul style="list-style-type: none"> - Single tile attachments - No detachments - Fixed glues 	<ul style="list-style-type: none"> - Up to 2 assembly attachments - No detachments - Fixed glues 	<ul style="list-style-type: none"> - Up to 2 assembly attachments - Detachments - Glues turn on/off 	<ul style="list-style-type: none"> - Single tile attachments - No detachments - Transitions
Results	<ul style="list-style-type: none"> - No fractals weakly buildable (temp 1) - Some fractals not strictly buildable (temp > 1) 	<ul style="list-style-type: none"> - Finitely assemble larger class of shapes - Still some non-buildable fractals 	<ul style="list-style-type: none"> - All fractals strictly buildable - Without detachment: some impossible fractals 	<ul style="list-style-type: none"> - Fractals with generators that have a Ham-path are strictly buildable (temp 1)

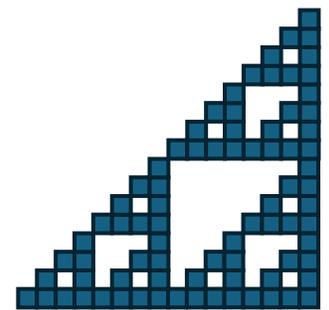
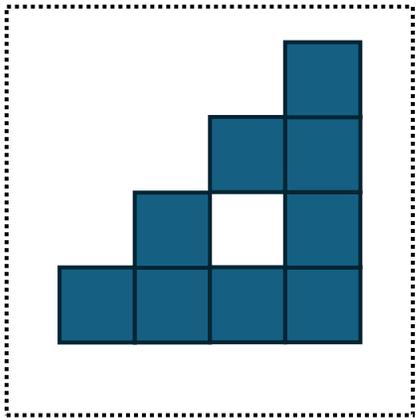
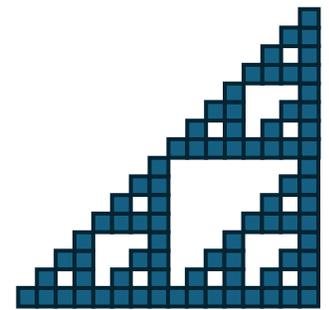
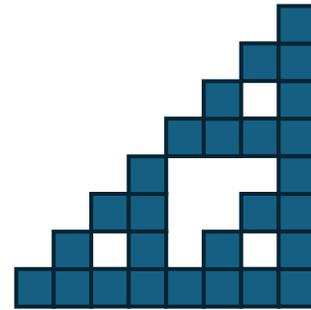
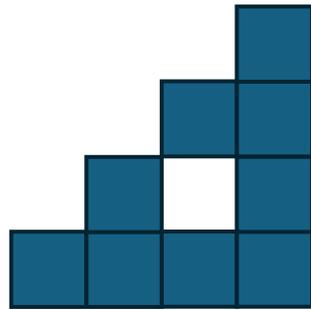
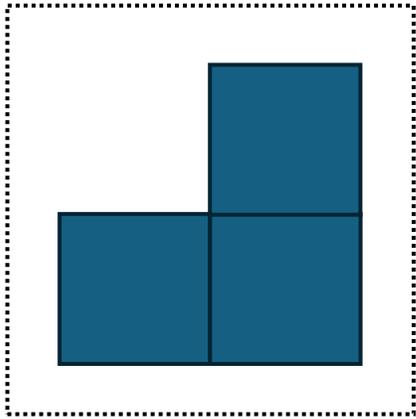
Our Contribution

	aTAM	2HAM	STAM	Seeded TA
Description	<ul style="list-style-type: none"> - Single tile attachments - No detachments - Fixed glues 	<ul style="list-style-type: none"> - Up to 2 assembly attachments - No detachments - Fixed glues 	<ul style="list-style-type: none"> - Up to 2 assembly attachments - Detachments - Glues turn on/off 	<ul style="list-style-type: none"> - Single tile attachments - No detachments - Transitions
Results	<ul style="list-style-type: none"> - No fractals weakly buildable (temp 1) - Some fractals not strictly buildable (temp > 1) 	<ul style="list-style-type: none"> - Finitely assemble larger class of shapes - Still some non-buildable fractals 	<ul style="list-style-type: none"> - All fractals strictly buildable - Without detachment: some impossible fractals 	<ul style="list-style-type: none"> - ALL fractals are strictly buildable (temp 1) - There exists a single system that does so

The Construction

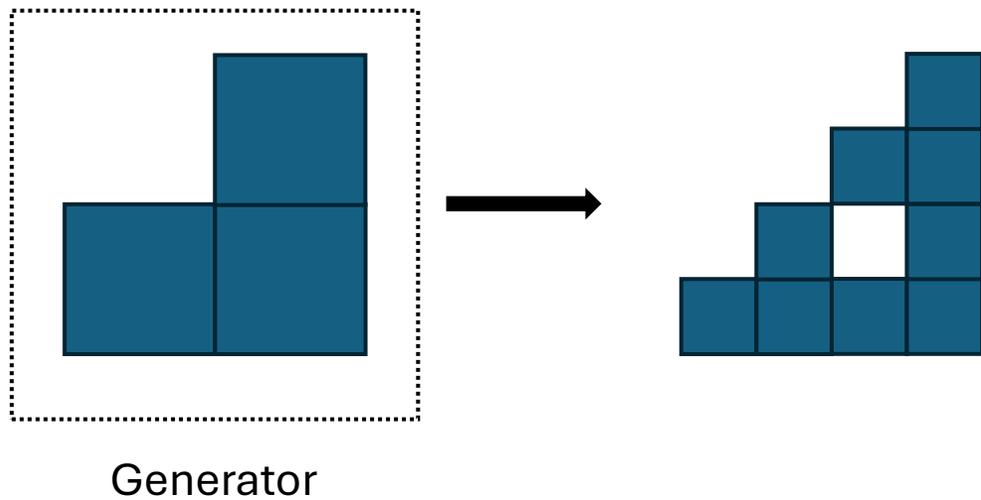
How did we do it?

Important Observation

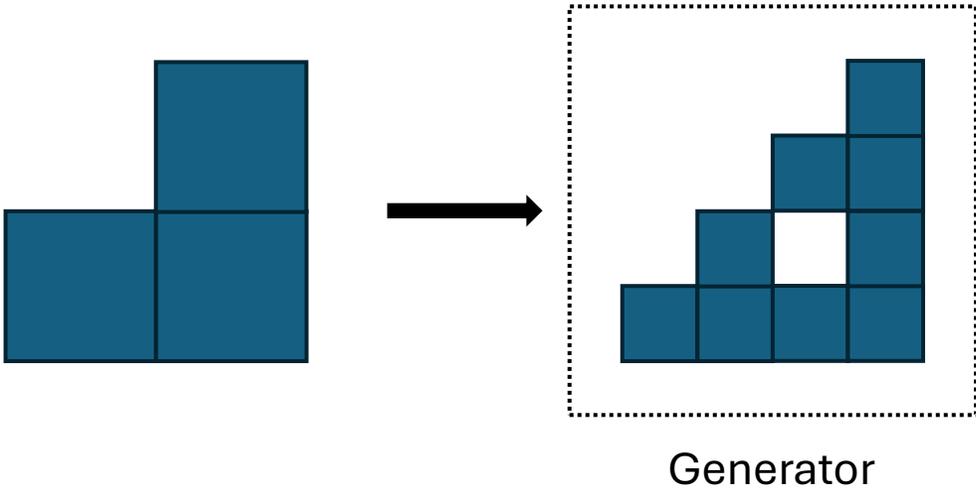


Generators

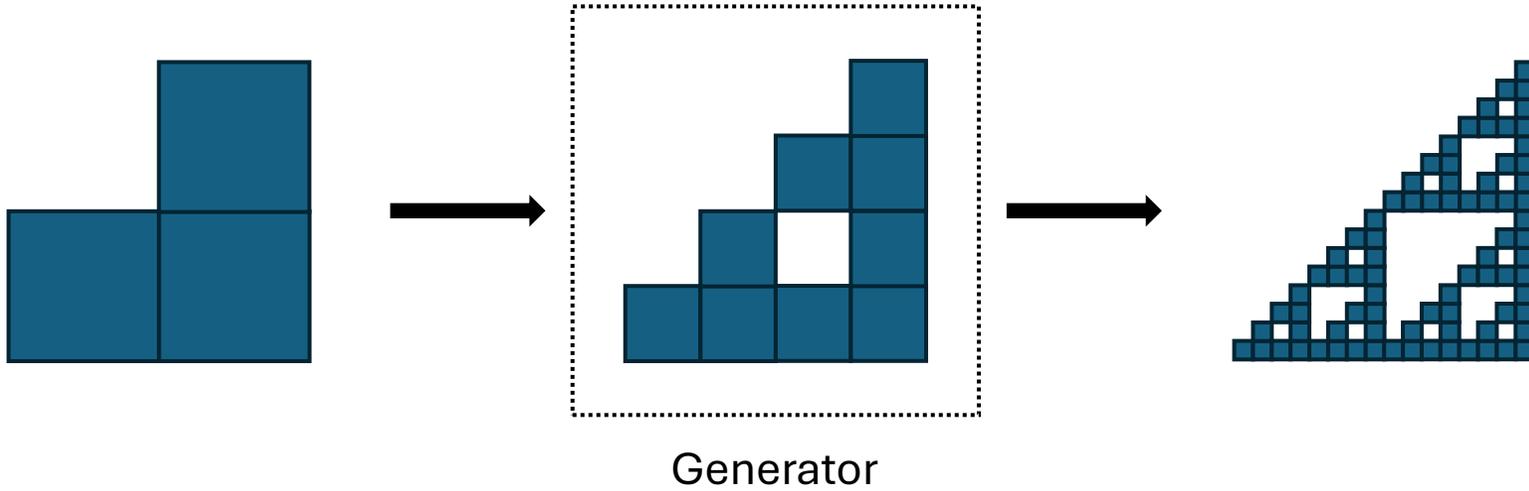
Important Observation



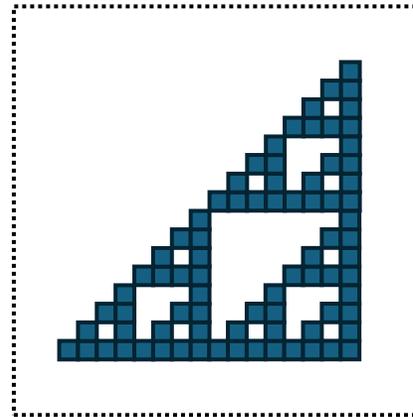
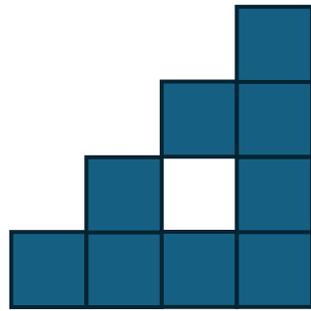
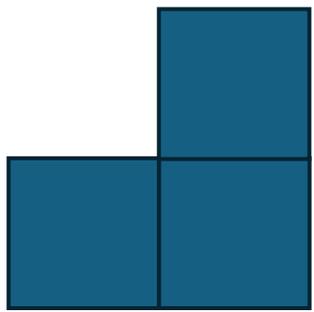
Important Observation



Important Observation



Important Observation

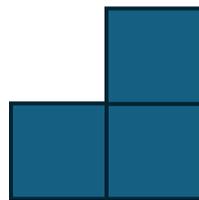
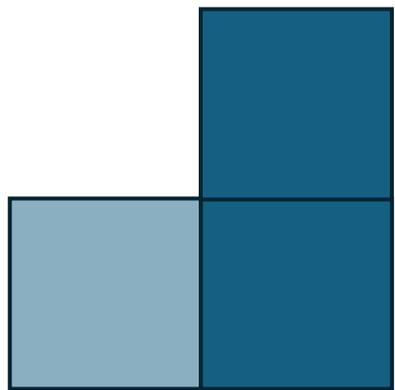


Generator

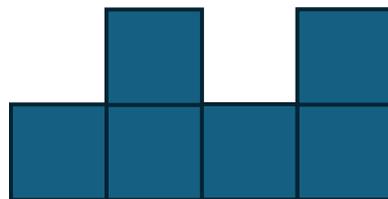
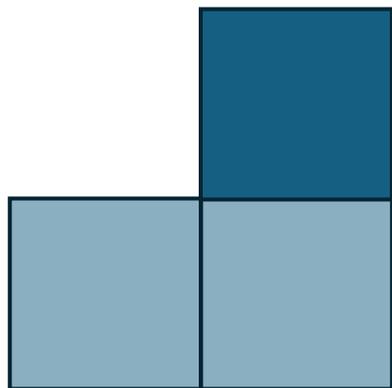


...

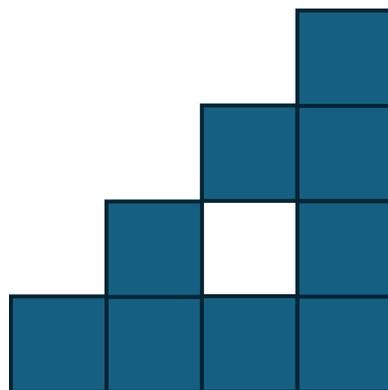
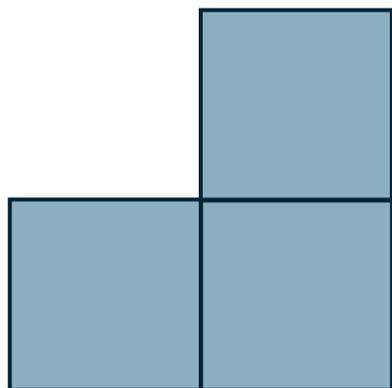
High Level Idea



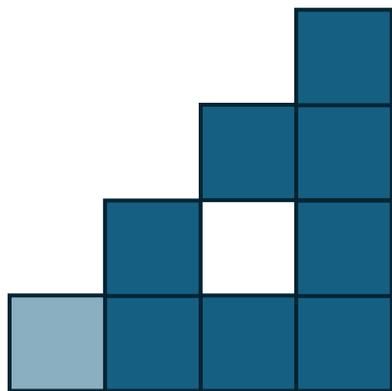
High Level Idea



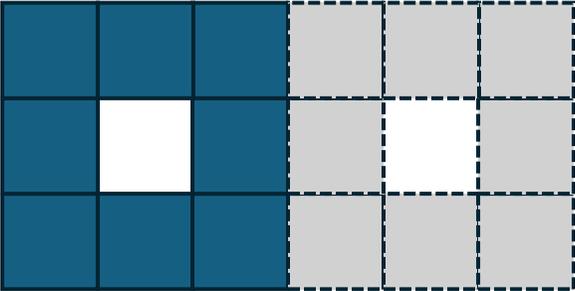
High Level Idea



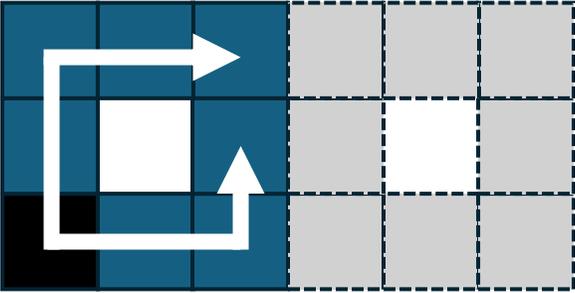
High Level Idea



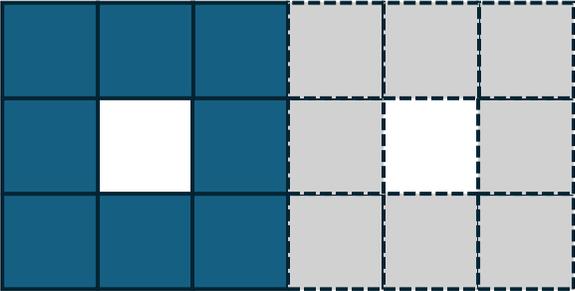
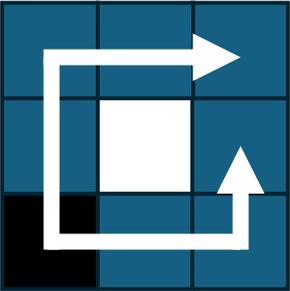
Step 1: Devising an Order



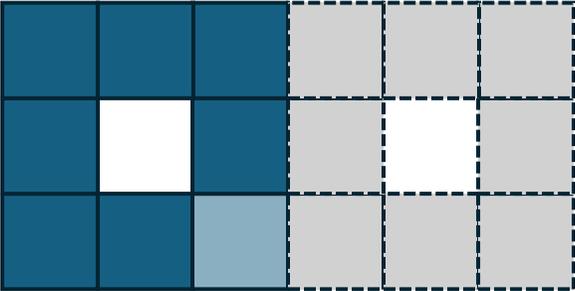
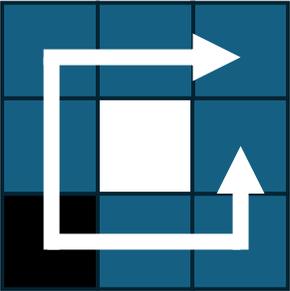
Step 1: Devising an Order



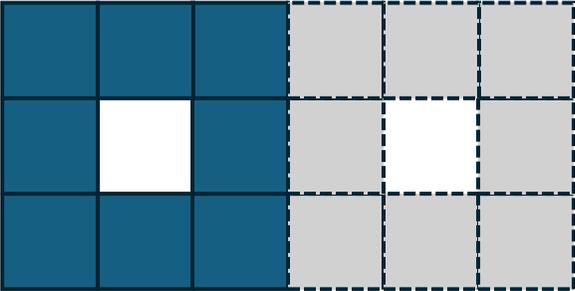
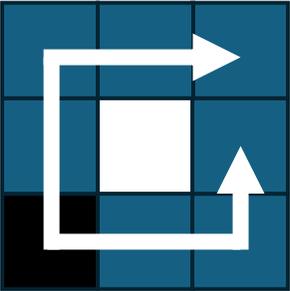
Step 2: A Copying Procedure



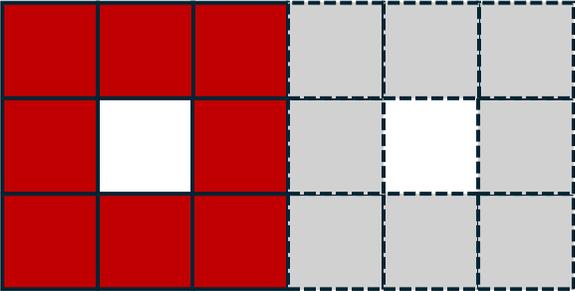
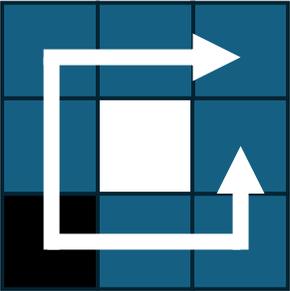
Step 2: A Copying Procedure



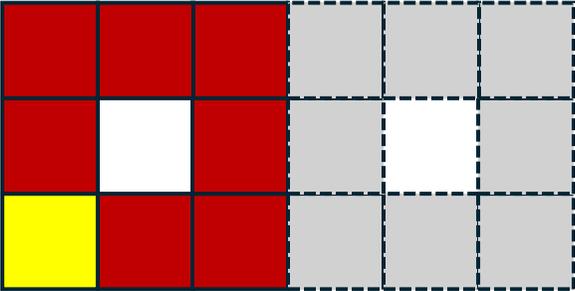
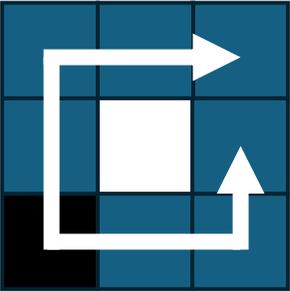
Step 2: A Copying Procedure



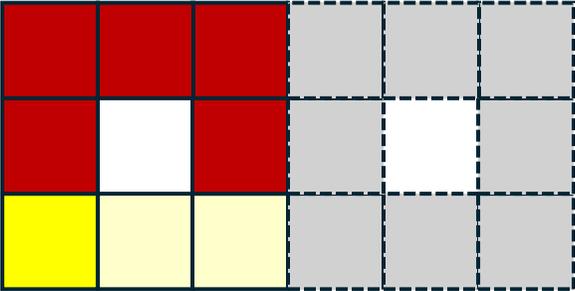
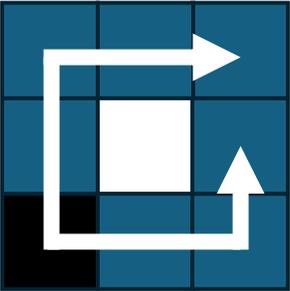
Step 2: A Copying Procedure



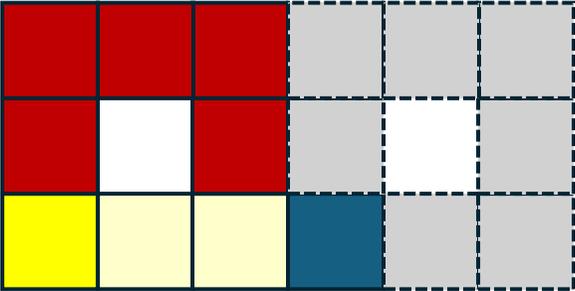
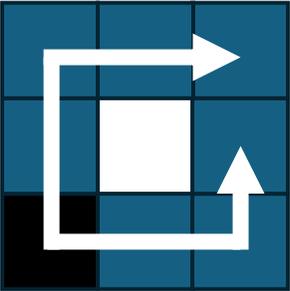
Step 2: A Copying Procedure



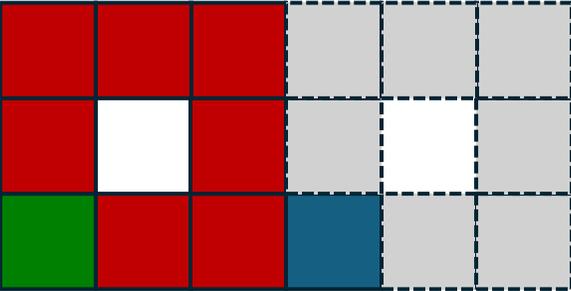
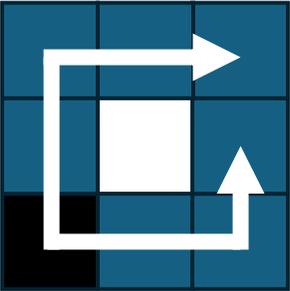
Step 2: A Copying Procedure



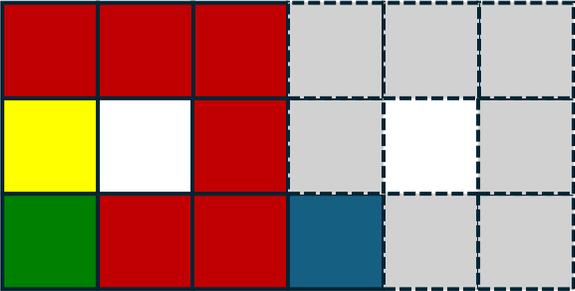
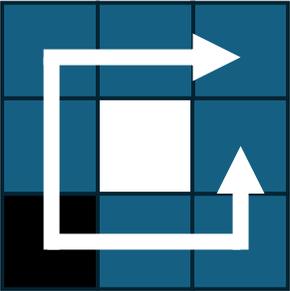
Step 2: A Copying Procedure



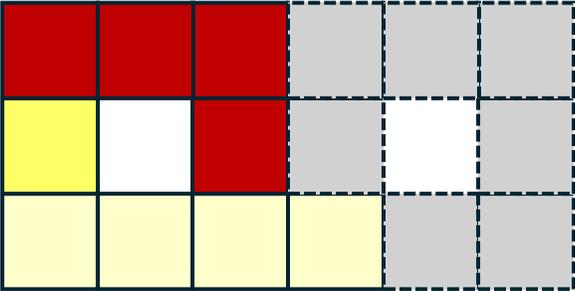
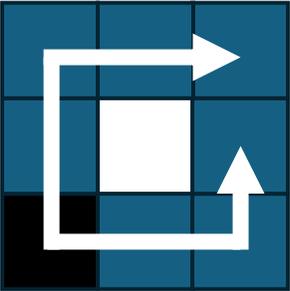
Step 2: A Copying Procedure



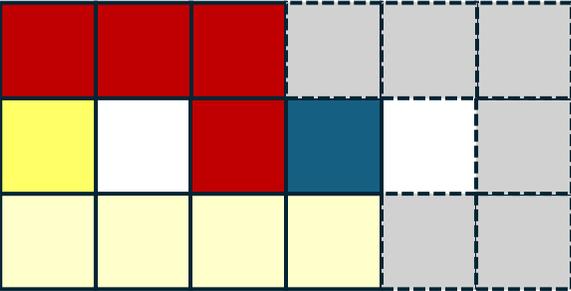
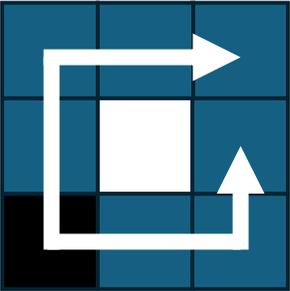
Step 2: A Copying Procedure



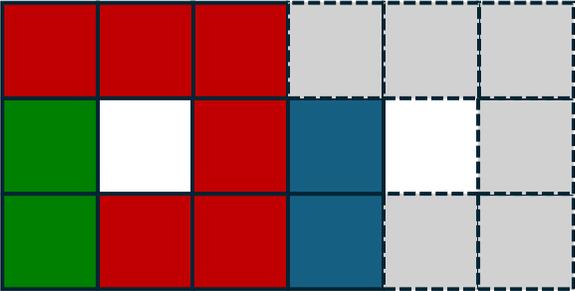
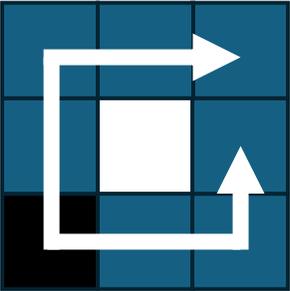
Step 2: A Copying Procedure



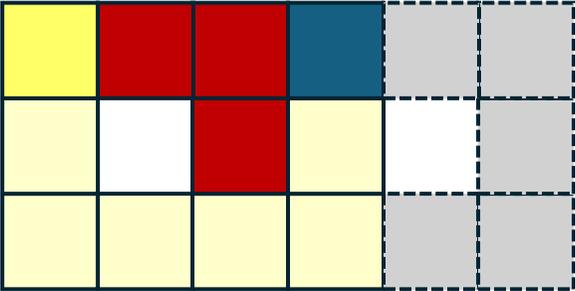
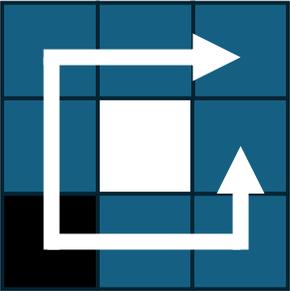
Step 2: A Copying Procedure



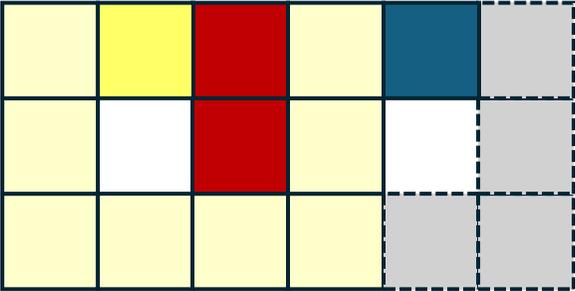
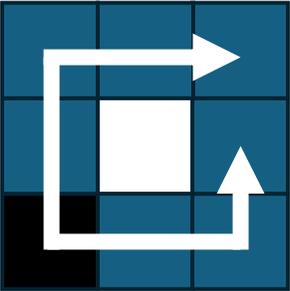
Step 2: A Copying Procedure



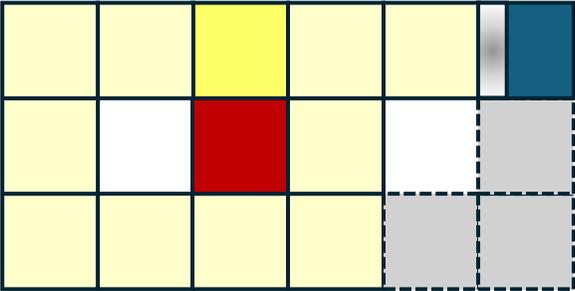
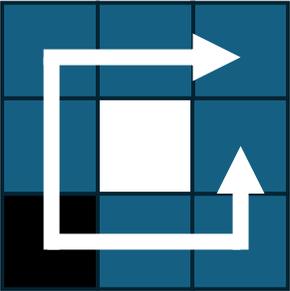
Step 2: A Copying Procedure



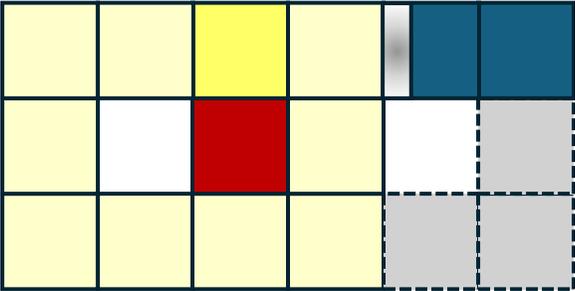
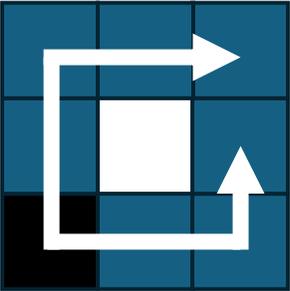
Step 2: A Copying Procedure



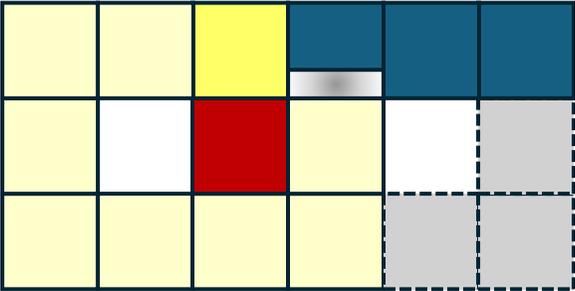
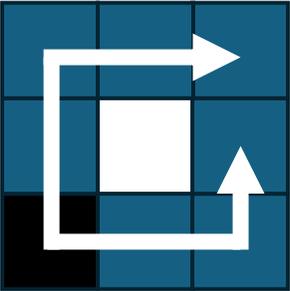
Step 2: A Copying Procedure



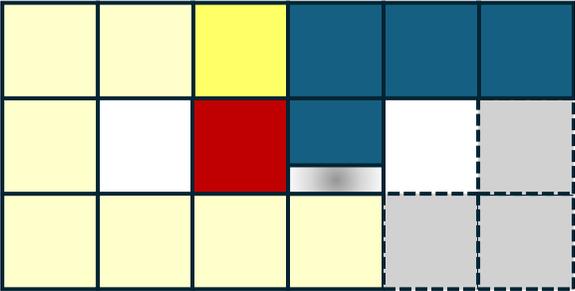
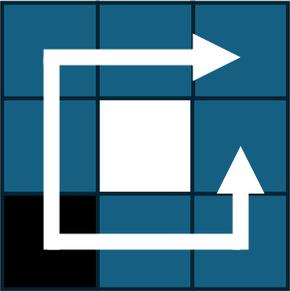
Step 2: A Copying Procedure



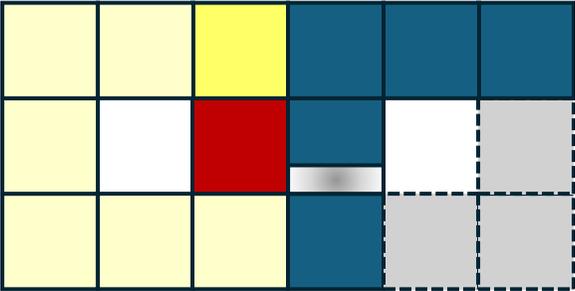
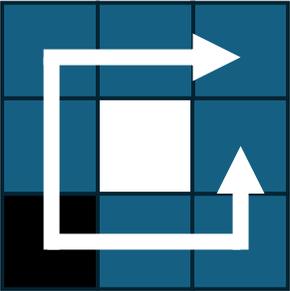
Step 2: A Copying Procedure



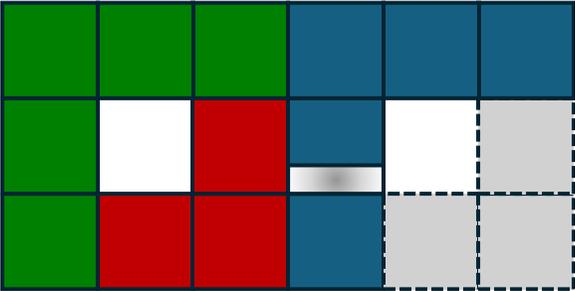
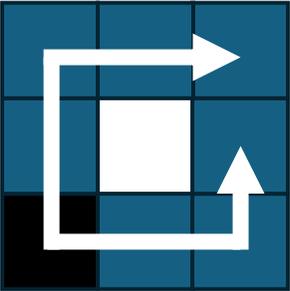
Step 2: A Copying Procedure



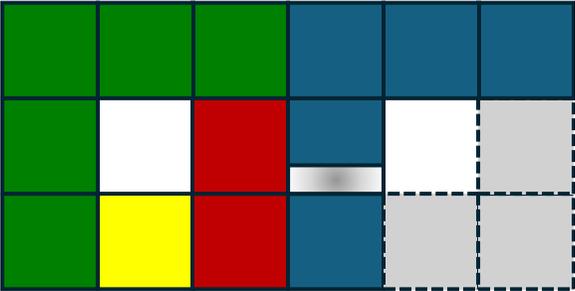
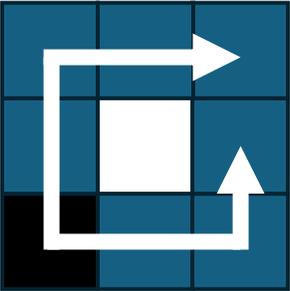
Step 2: A Copying Procedure



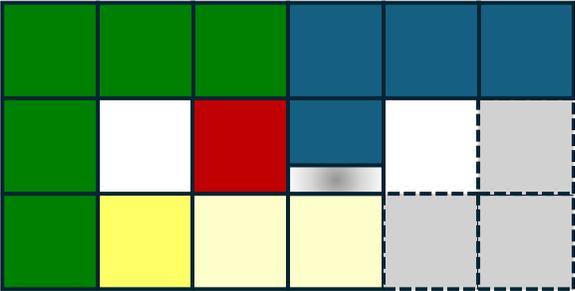
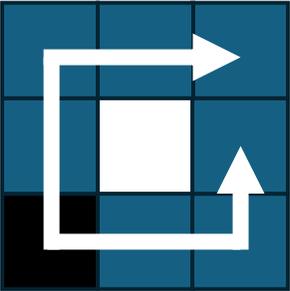
Step 2: A Copying Procedure



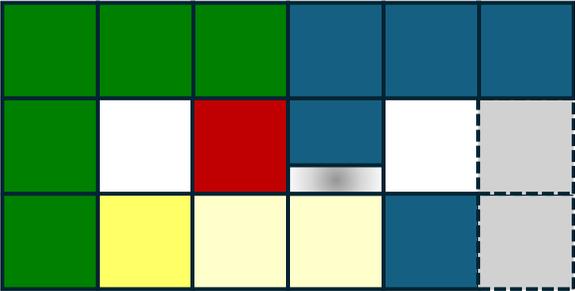
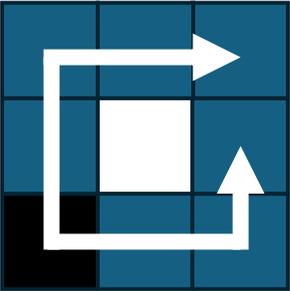
Step 2: A Copying Procedure



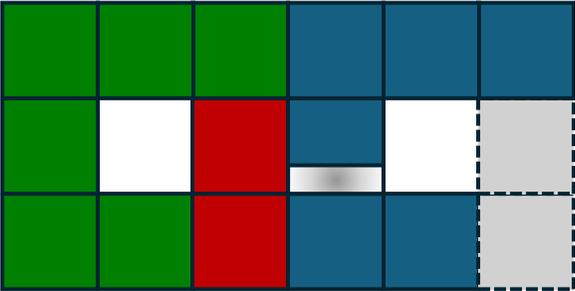
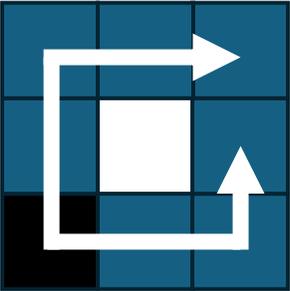
Step 2: A Copying Procedure



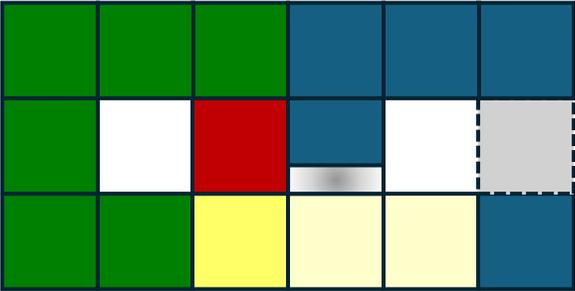
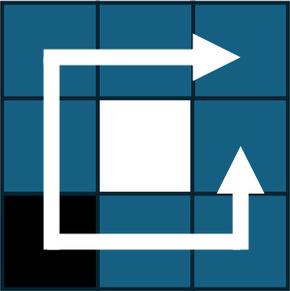
Step 2: A Copying Procedure



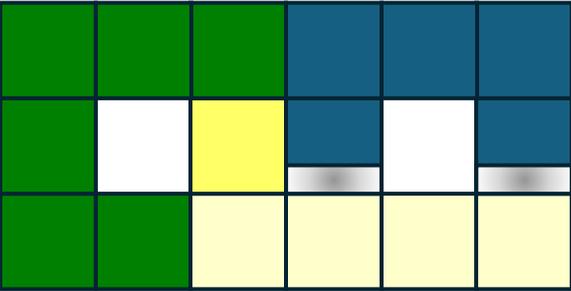
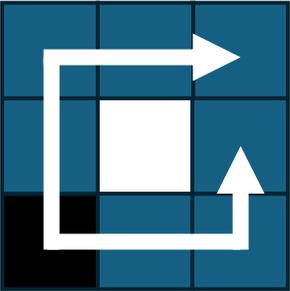
Step 2: A Copying Procedure



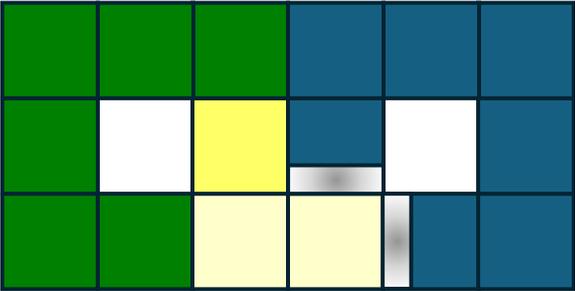
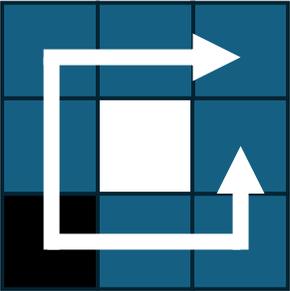
Step 2: A Copying Procedure



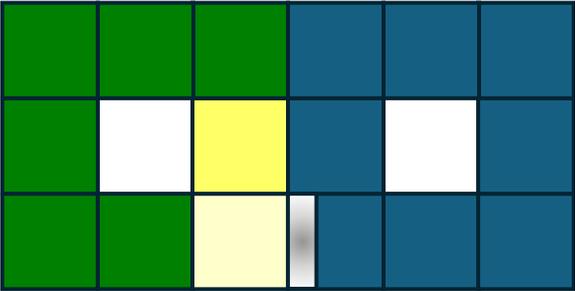
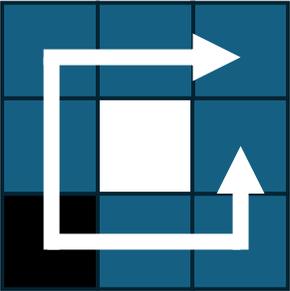
Step 2: A Copying Procedure



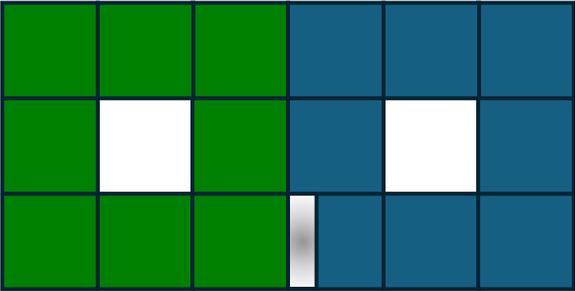
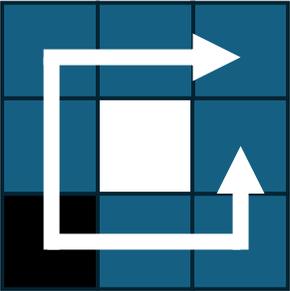
Step 2: A Copying Procedure



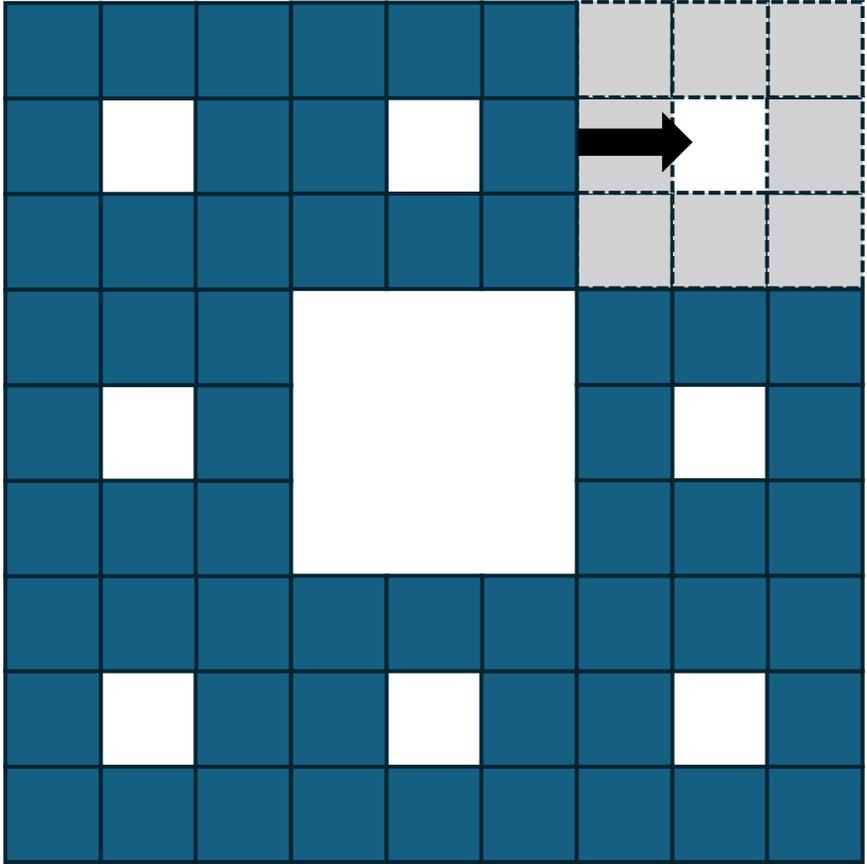
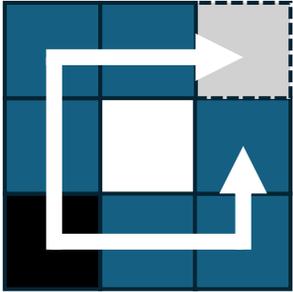
Step 2: A Copying Procedure



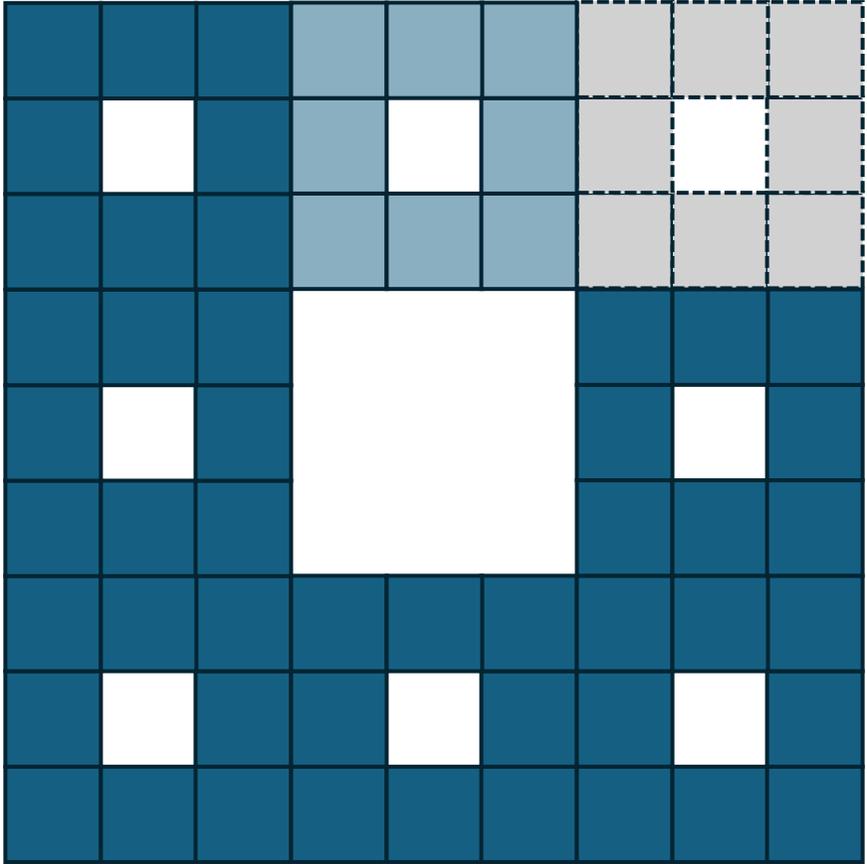
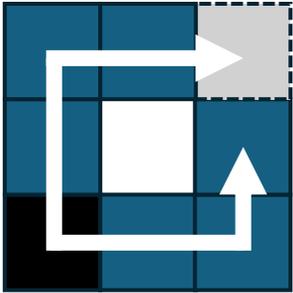
Step 2: A Copying Procedure



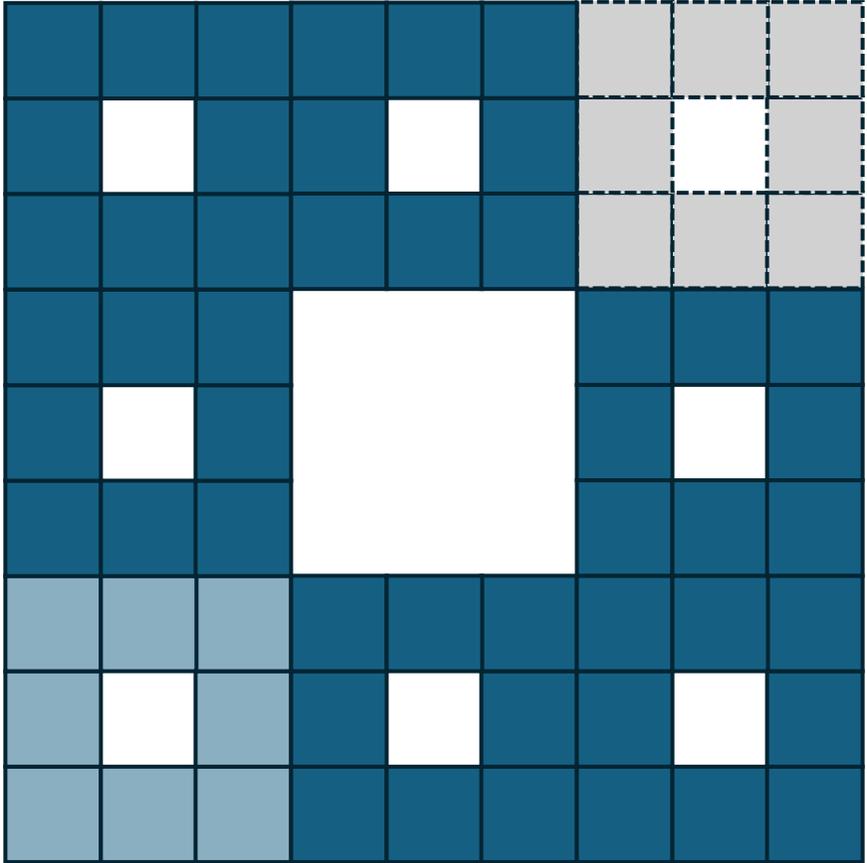
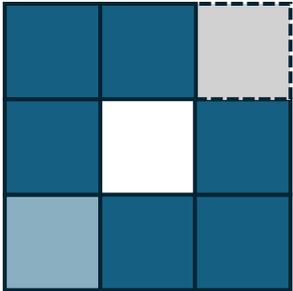
Step 3: Growing the Full Assembly



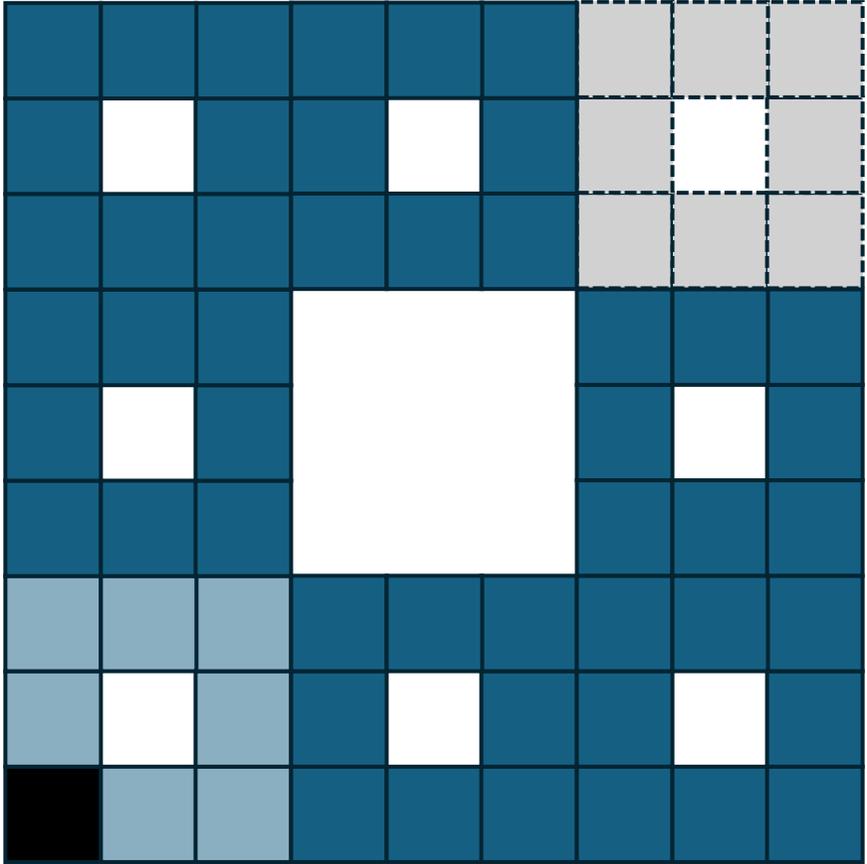
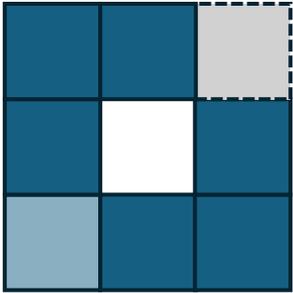
Step 3: Growing the Full Assembly



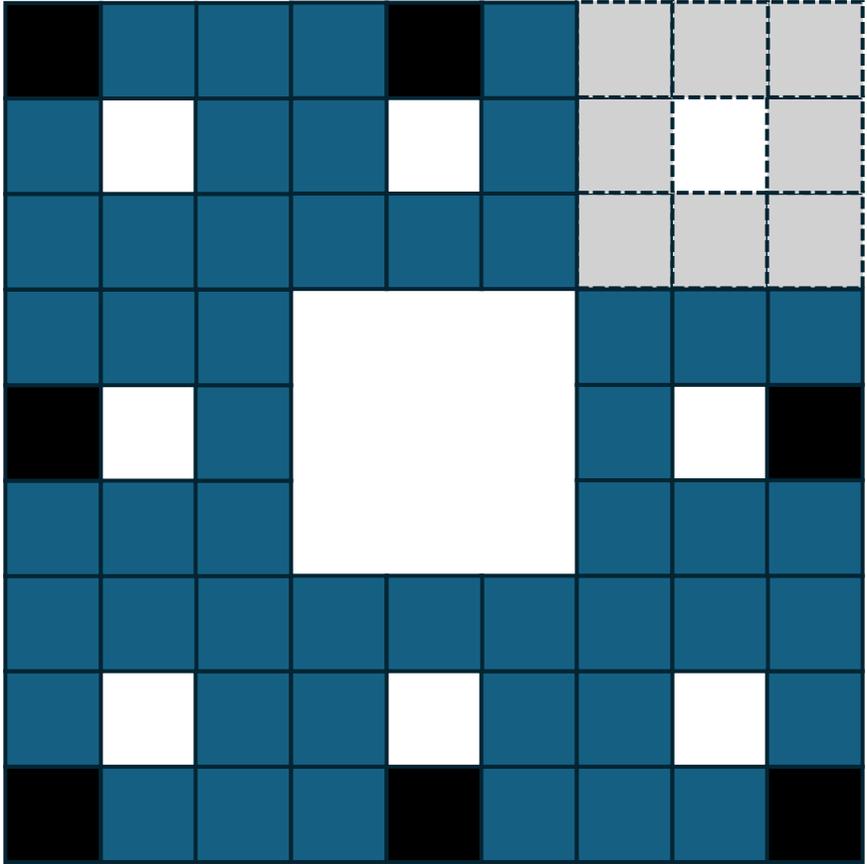
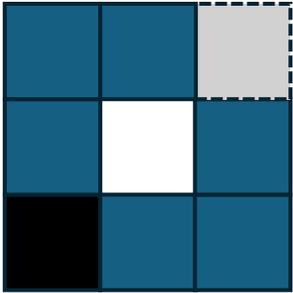
Step 3: Growing the Full Assembly



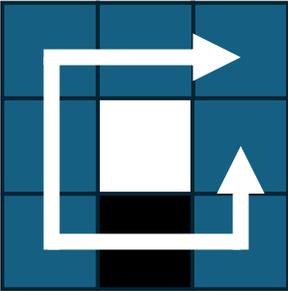
Step 3: Growing the Full Assembly



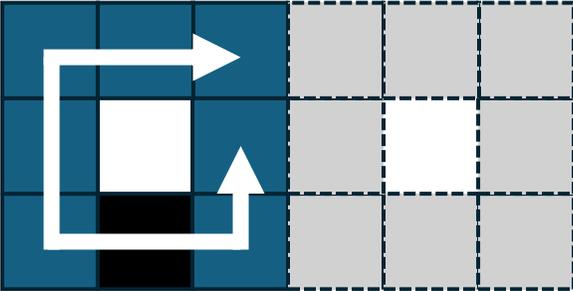
Step 3: Growing the Full Assembly



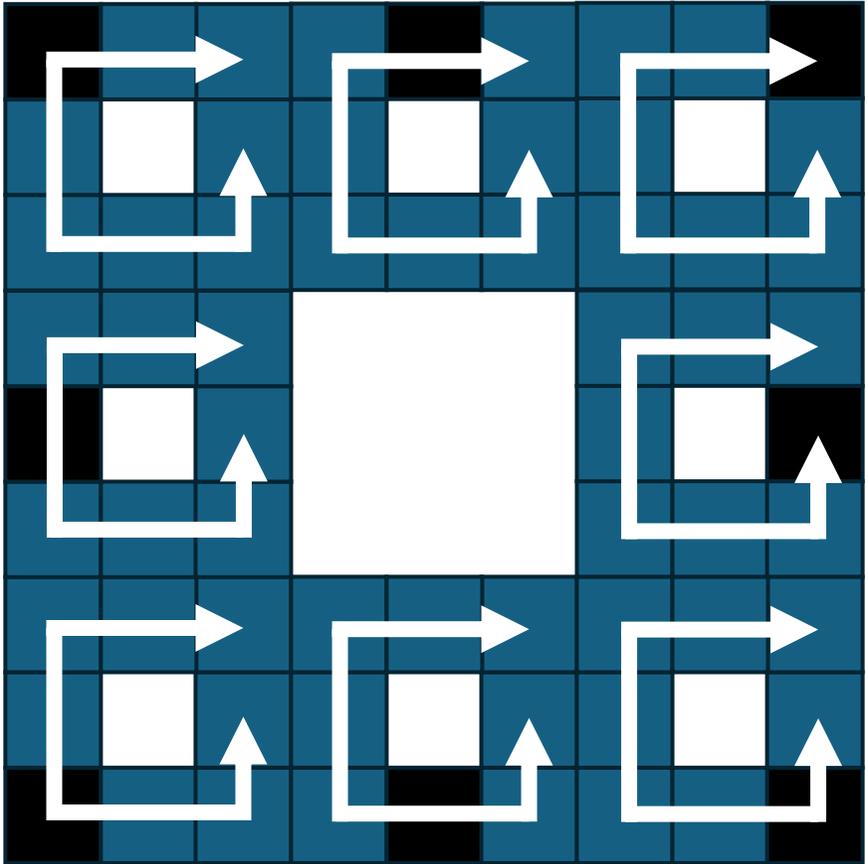
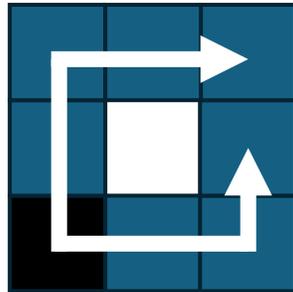
Step 3: Growing the Full Assembly



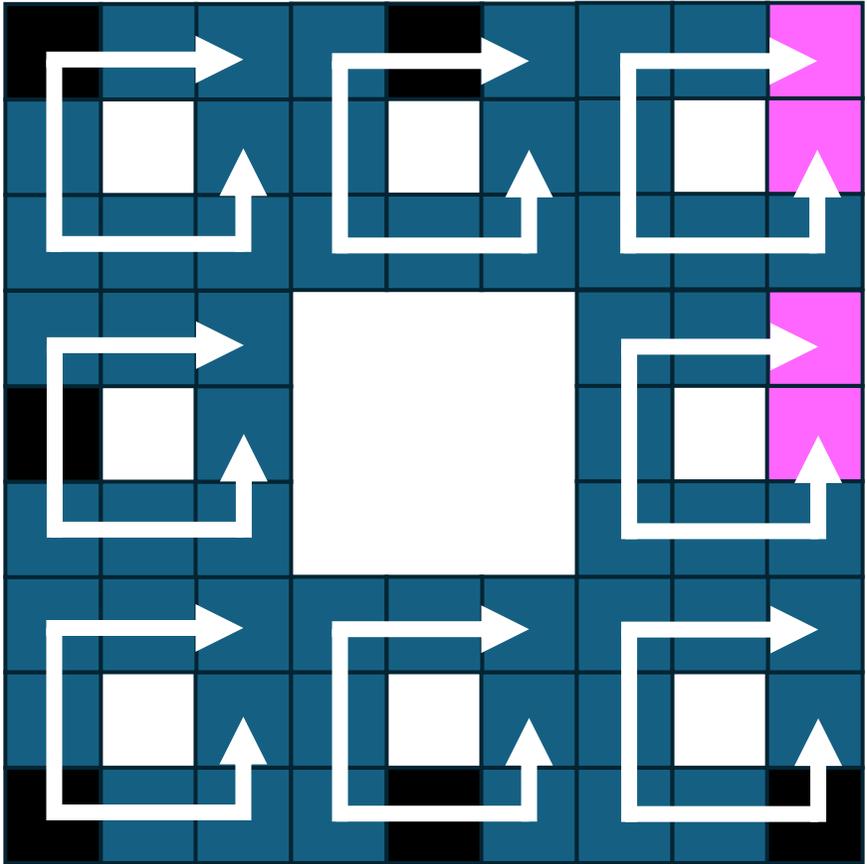
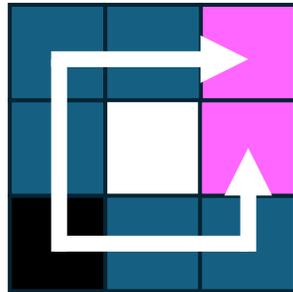
Step 3: Growing the Full Assembly



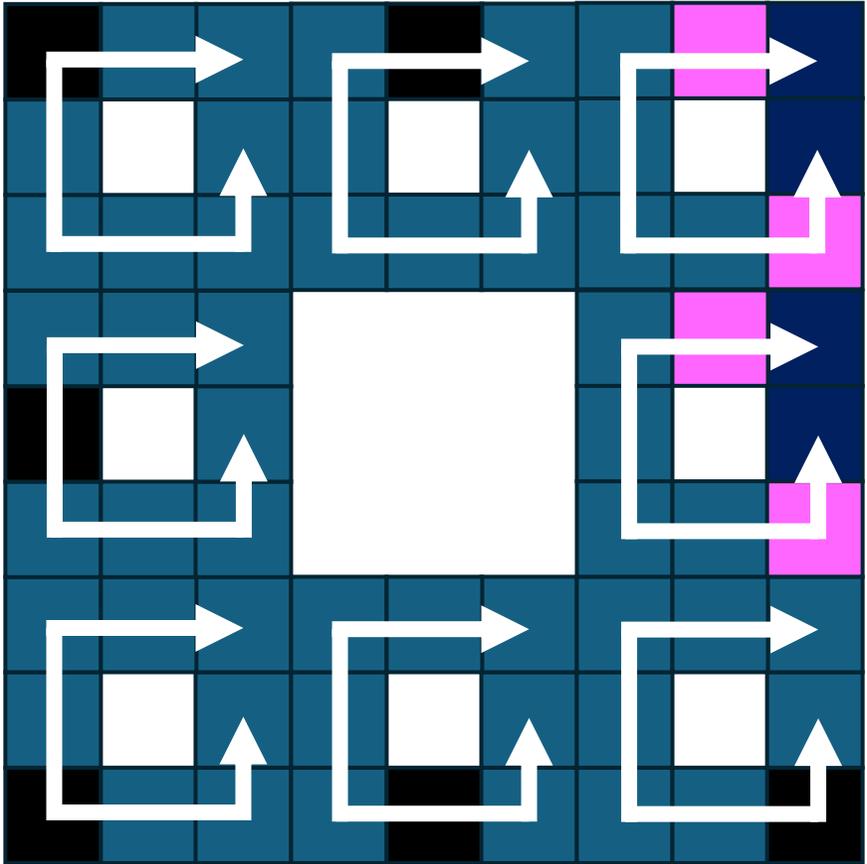
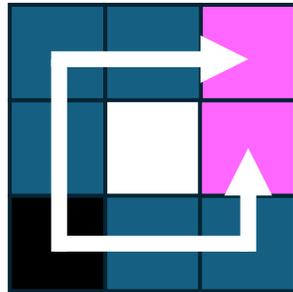
Step 4: Resetting



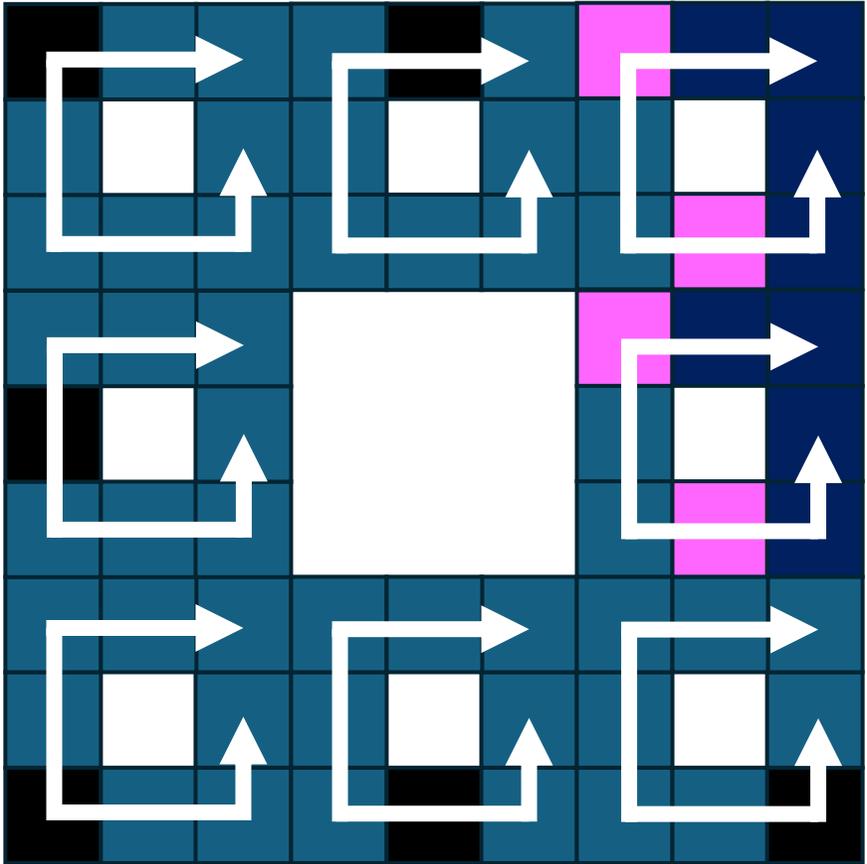
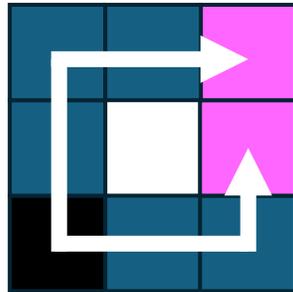
Step 4: Resetting



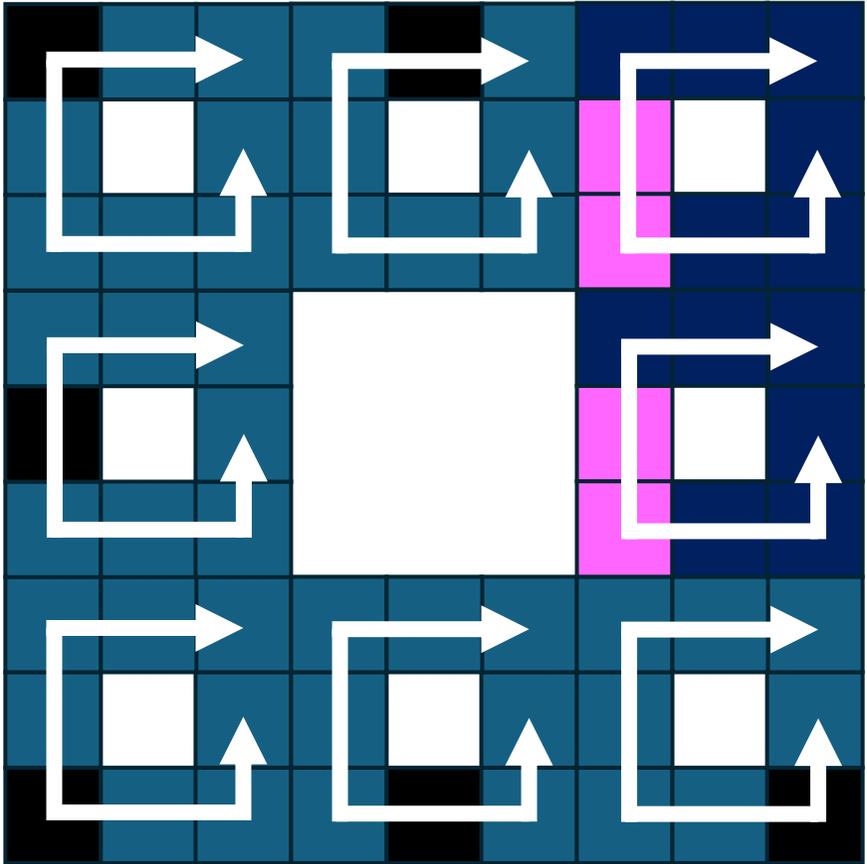
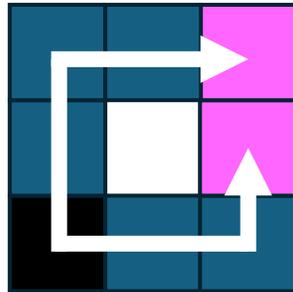
Step 4: Resetting



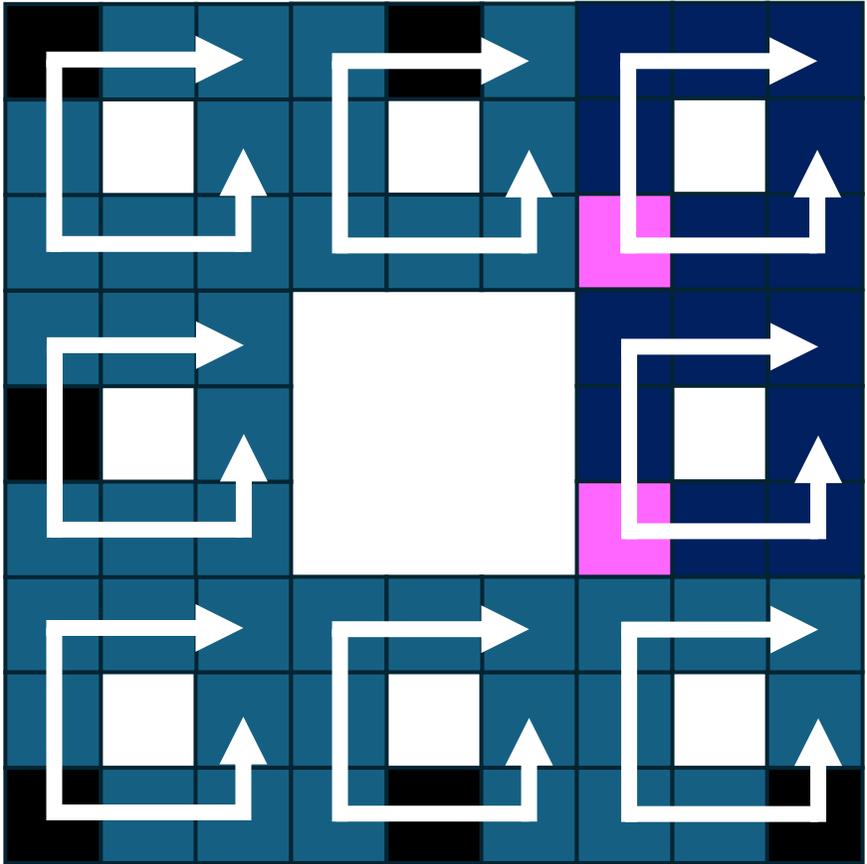
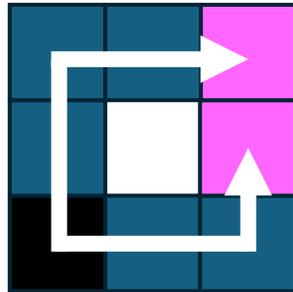
Step 4: Resetting



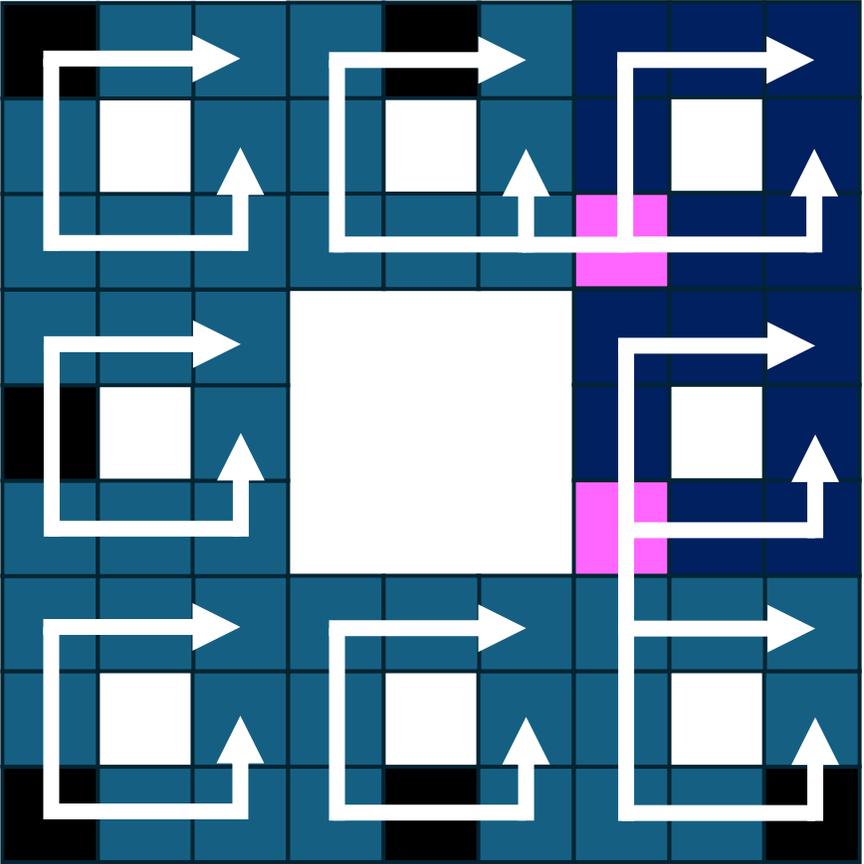
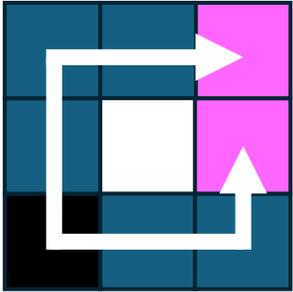
Step 4: Resetting



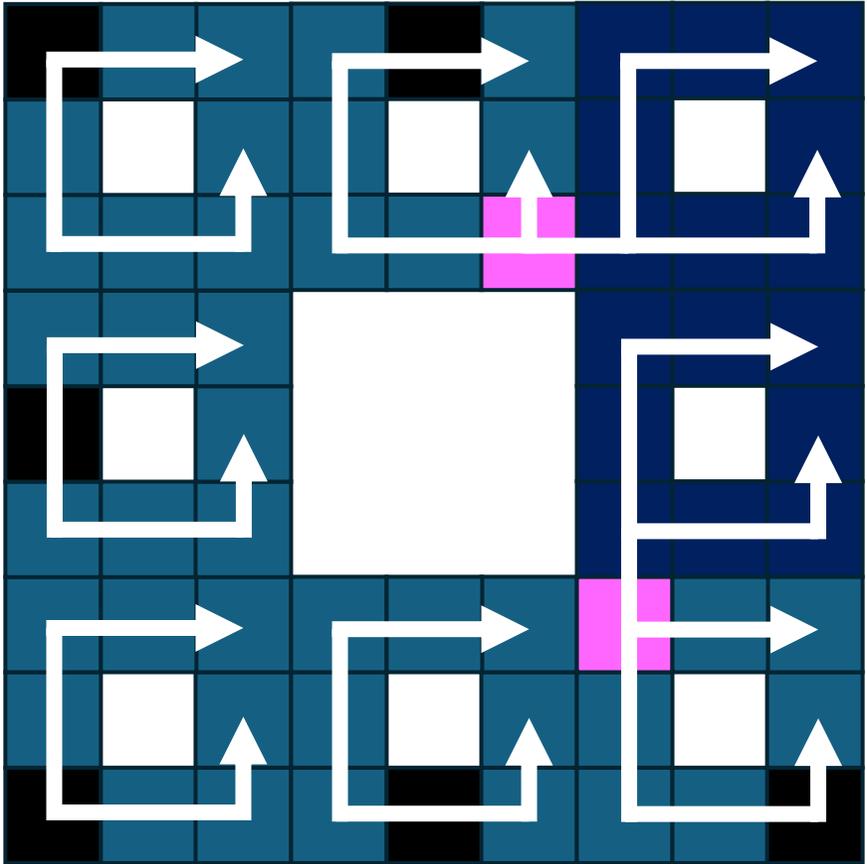
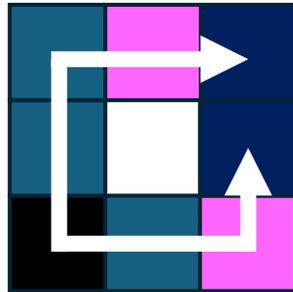
Step 4: Resetting



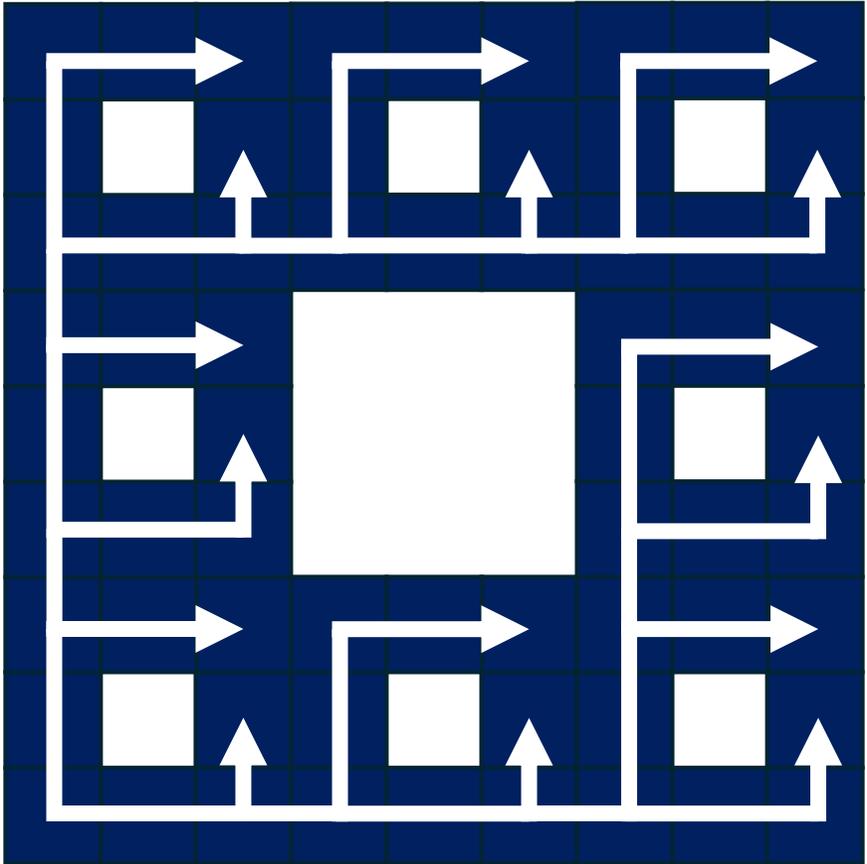
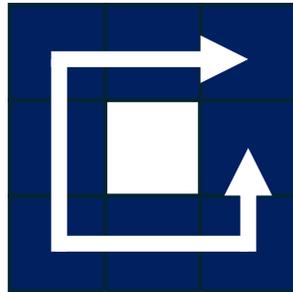
Step 4: Resetting



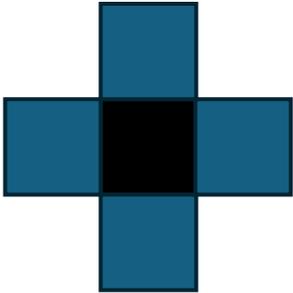
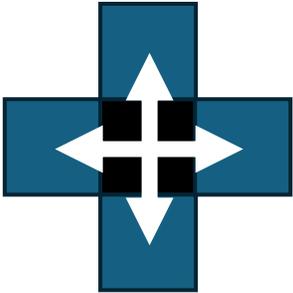
Step 4: Resetting



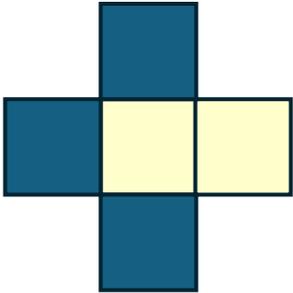
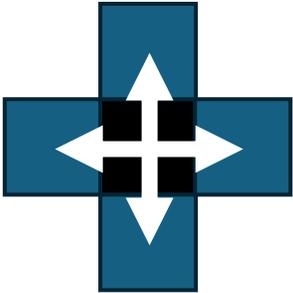
Step 4: Resetting



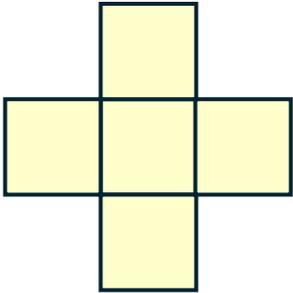
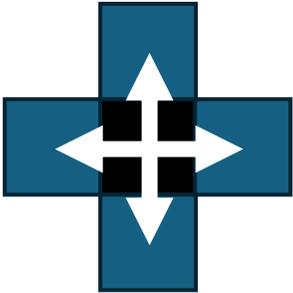
Synchronization



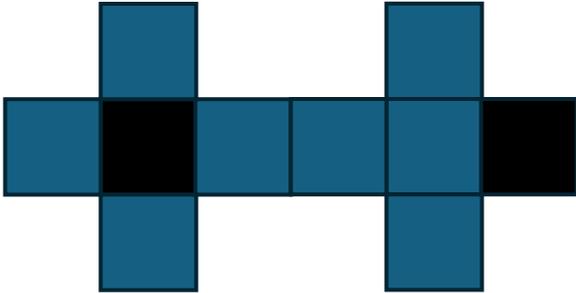
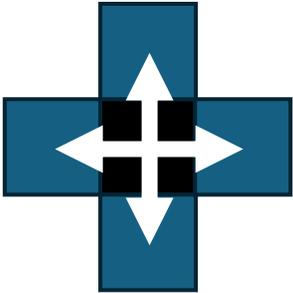
Synchronization



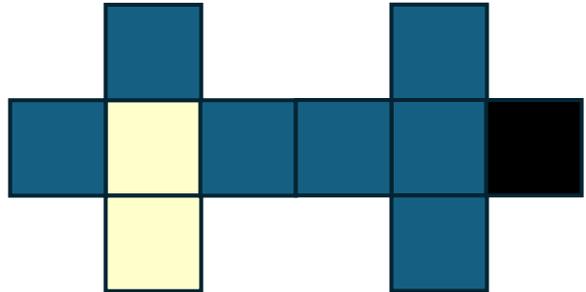
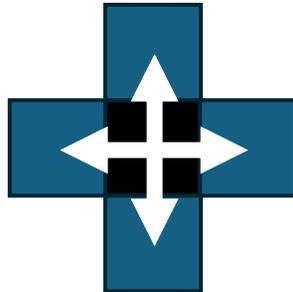
Synchronization



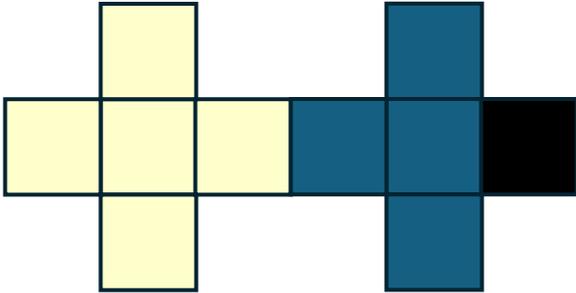
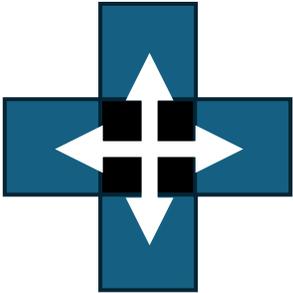
Synchronization



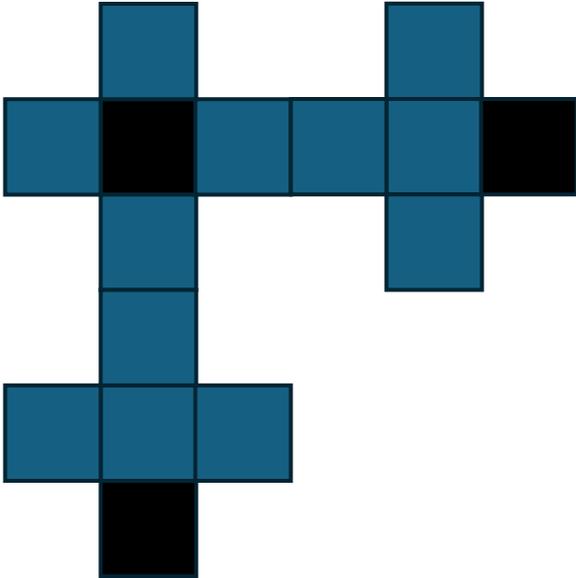
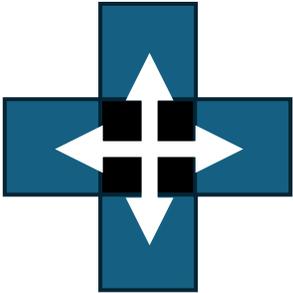
Synchronization



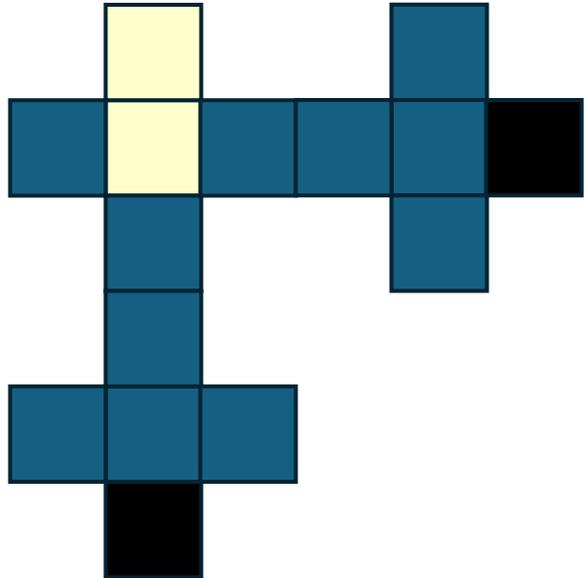
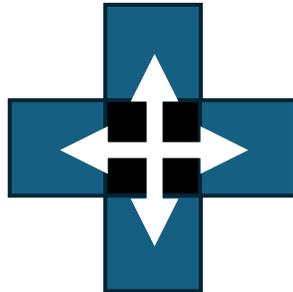
Synchronization



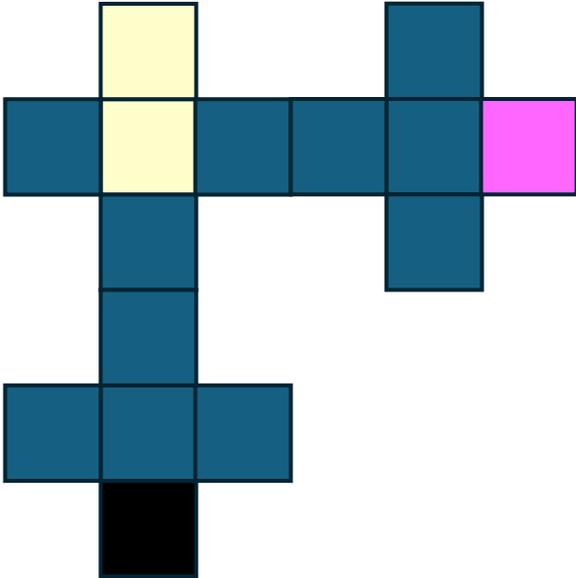
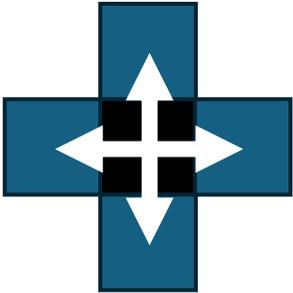
Synchronization



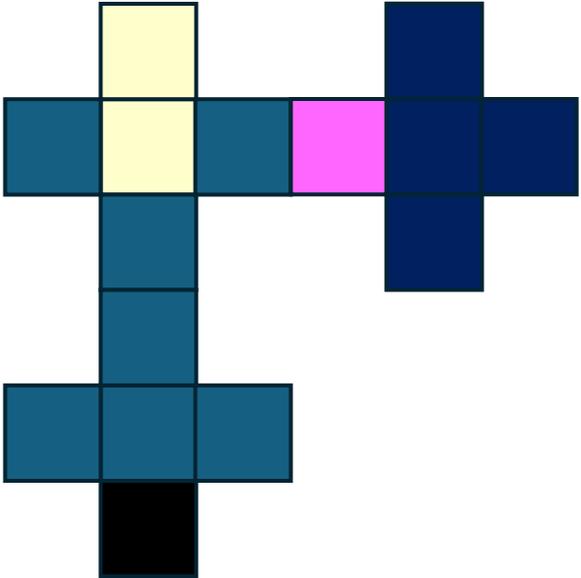
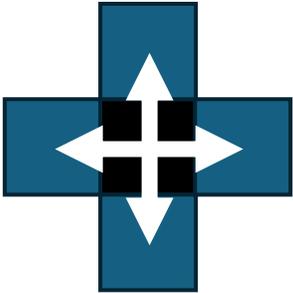
Synchronization



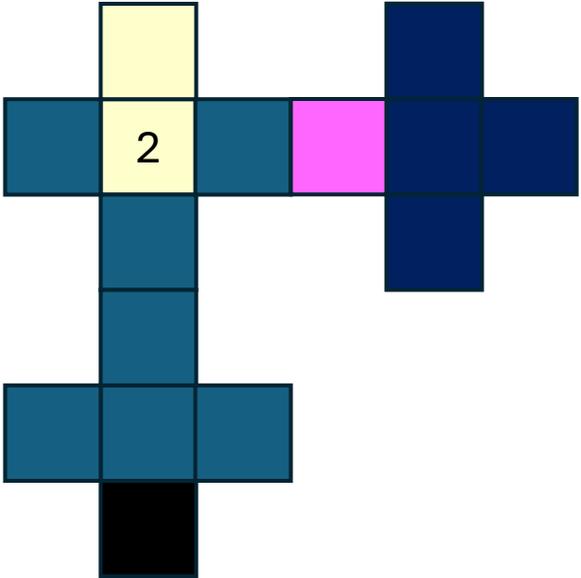
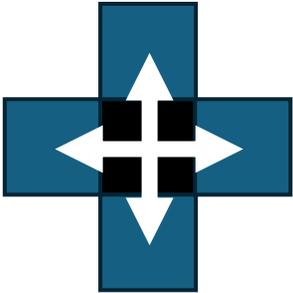
Synchronization



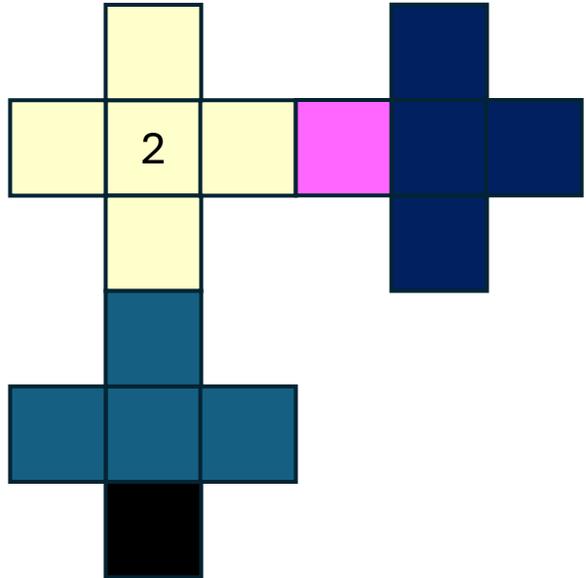
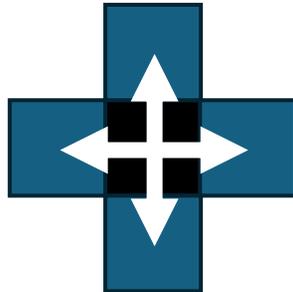
Synchronization



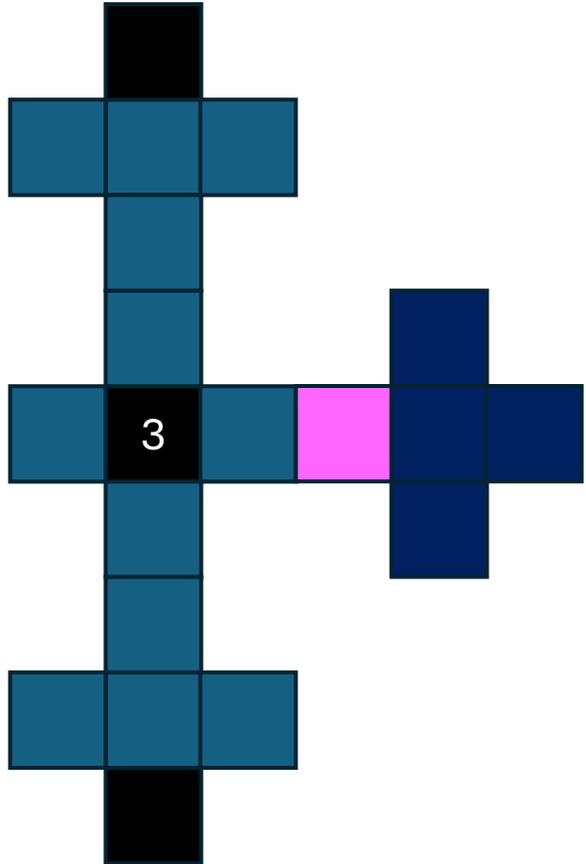
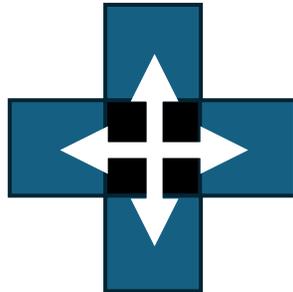
Synchronization



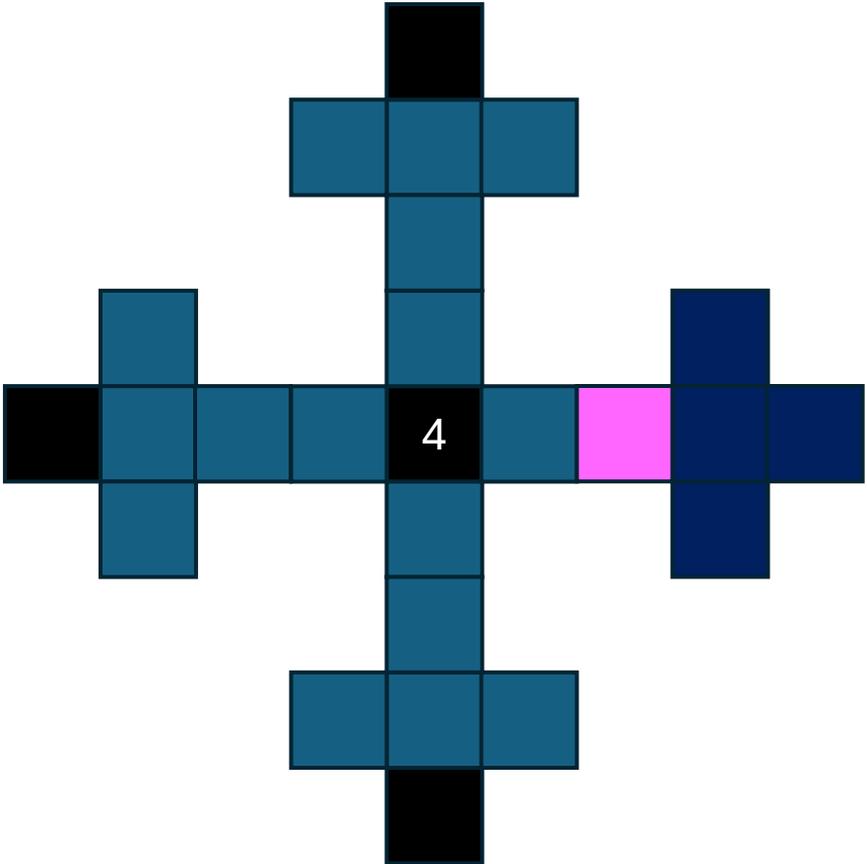
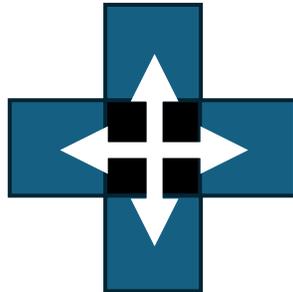
Synchronization



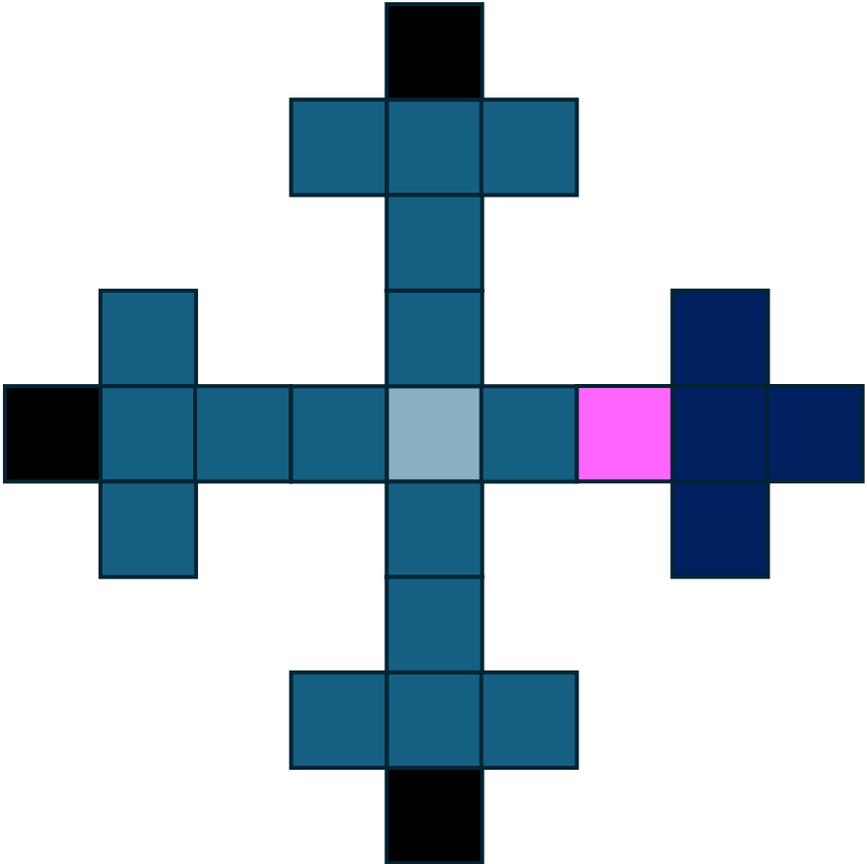
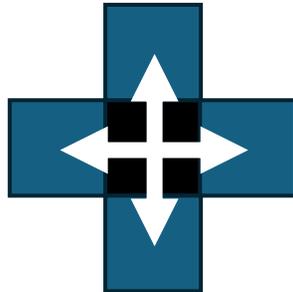
Synchronization



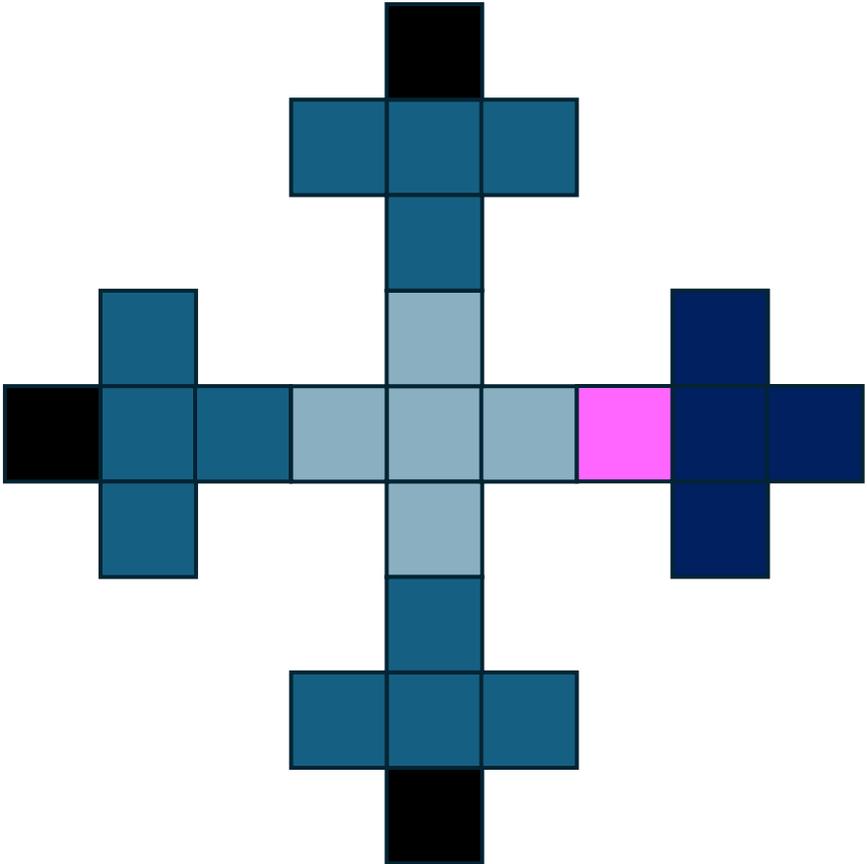
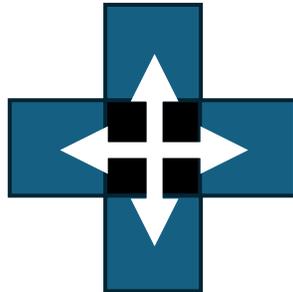
Synchronization



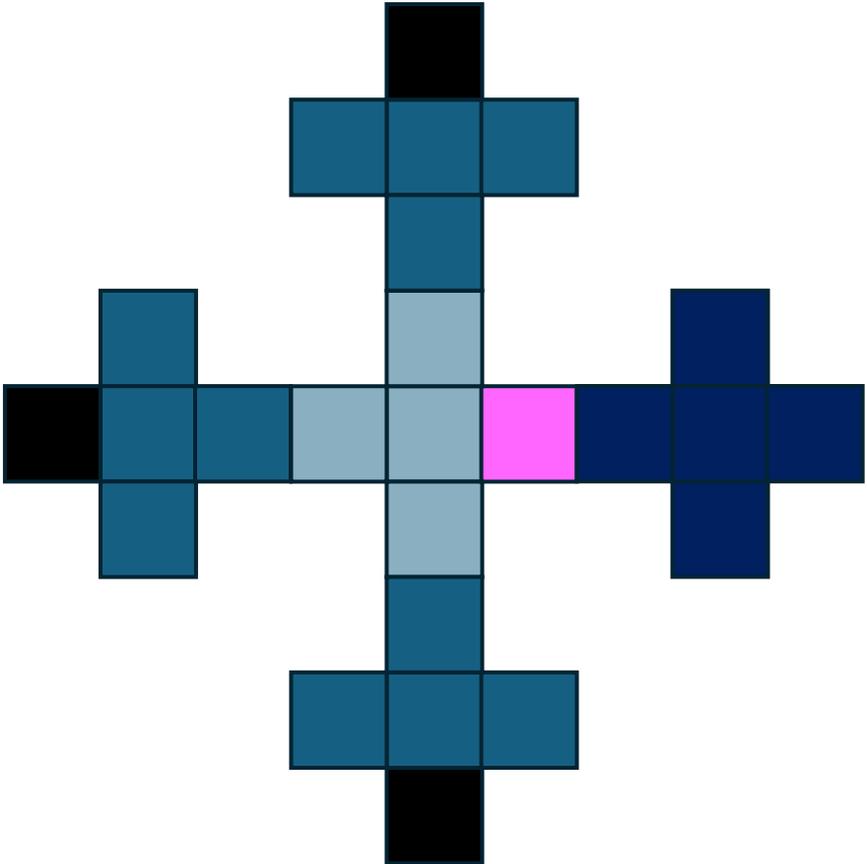
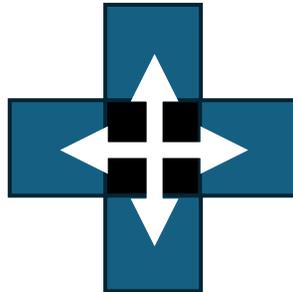
Synchronization



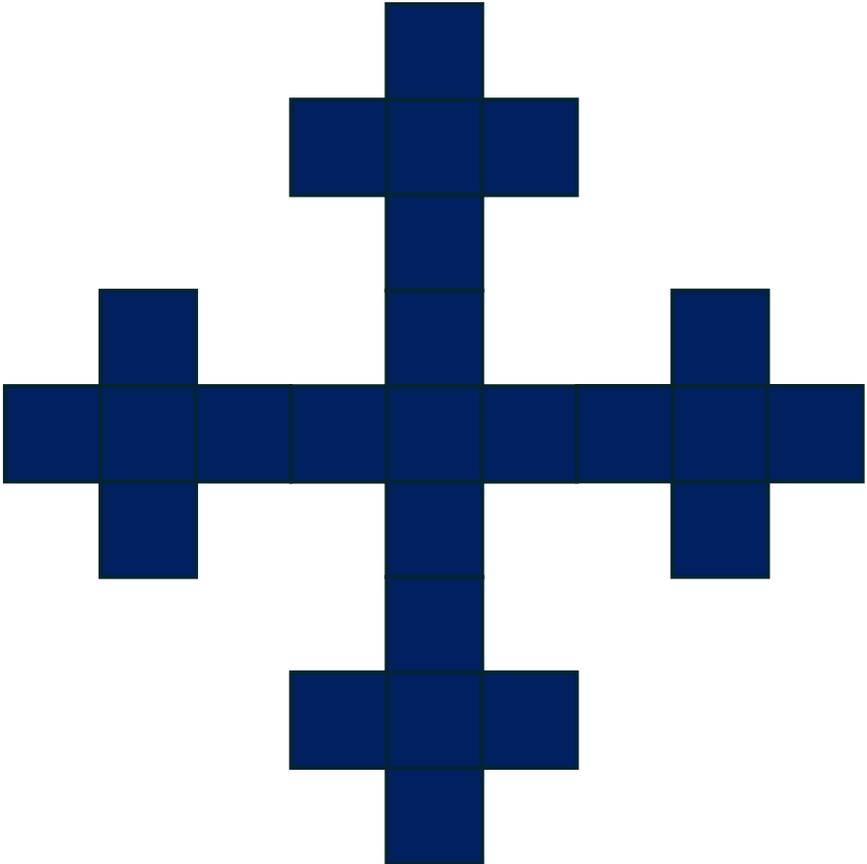
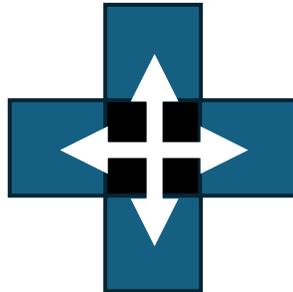
Synchronization



Synchronization



Synchronization



Final Result (Sierpinski Triangle)

Conclusion

What is left?

Conclusion

- All fractals are buildable at temperature 1
- A single system exists that builds all these fractals
- Do higher temperatures allow for more efficient fractal constructions?
- Are there special classes of fractals which can be built with small systems?

Reachability in Chemical Reaction Networks



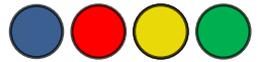
Introduction to the Model

Chemical Reaction Networks

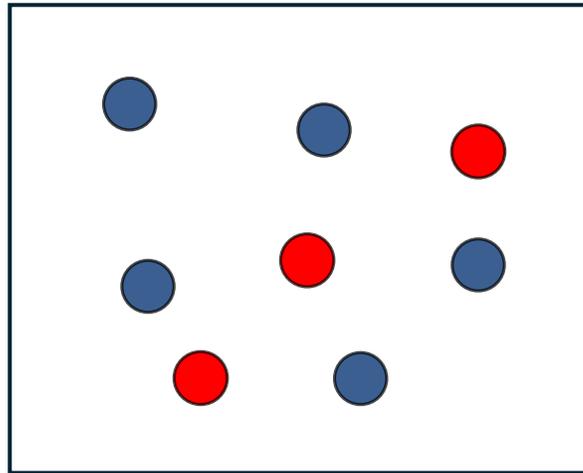
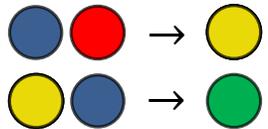
- Ordered pair (Λ, Γ)
 - Λ = Set of input species
 - Γ = Set of rules
- Configuration
 - Length $|\Lambda|$ vector of non-negative integers
 - Represents count of each species

Example CRN System

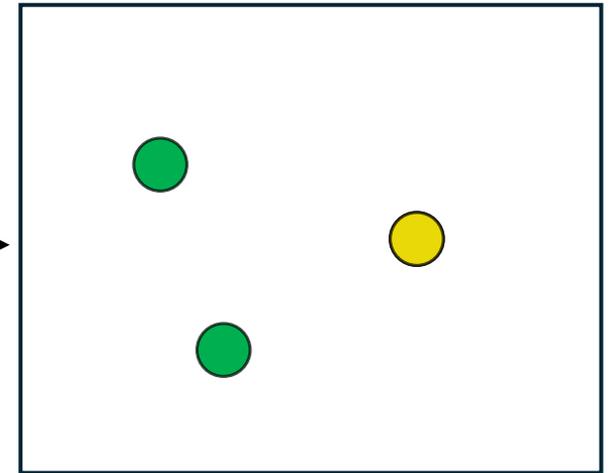
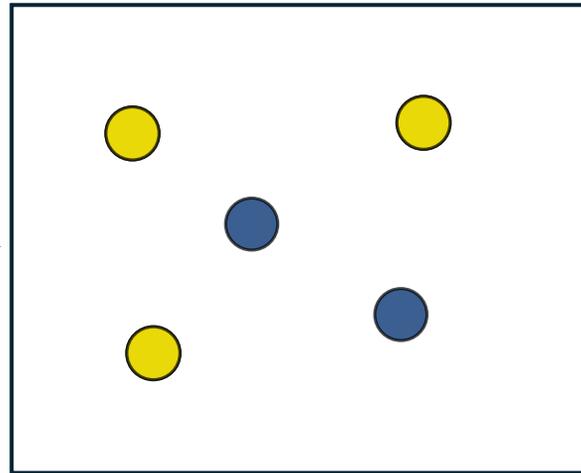
Species:



Rules:



Configuration I:
[5, 3, 0, 0]



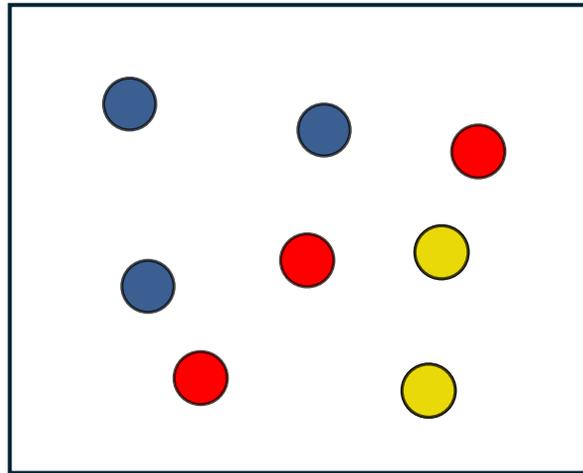
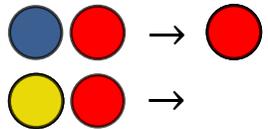
Configuration D:
[0, 0, 1, 2]

Example Void CRN System

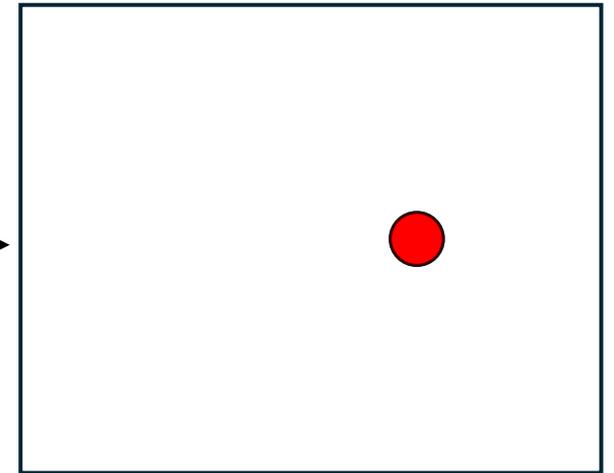
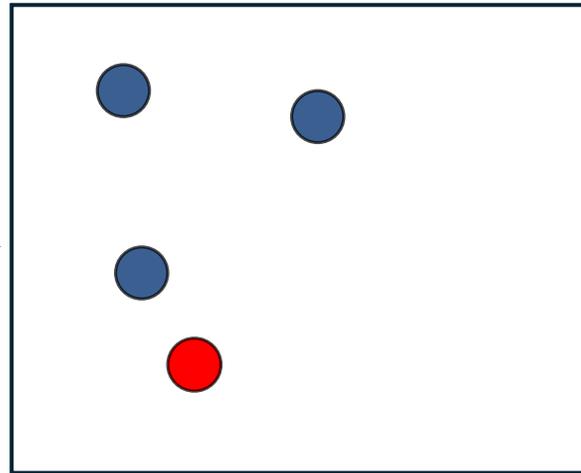
Species:



Rules:



Configuration I:
[3, 3, 2]



Configuration D:
[0, 1, 0]

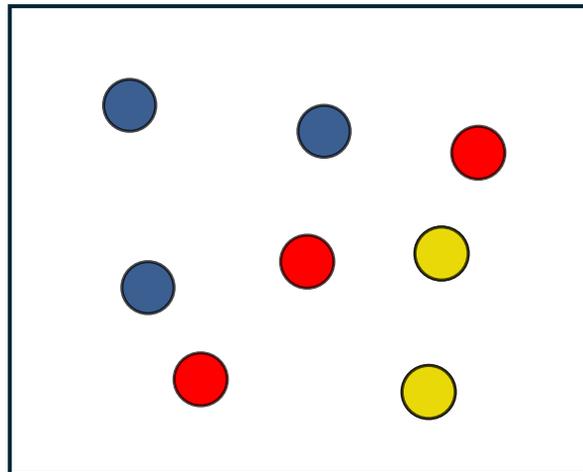
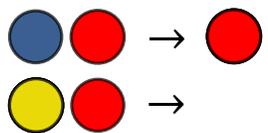
Reachability

- Given initial configuration I and target configuration D , can D ever be reached from I ?

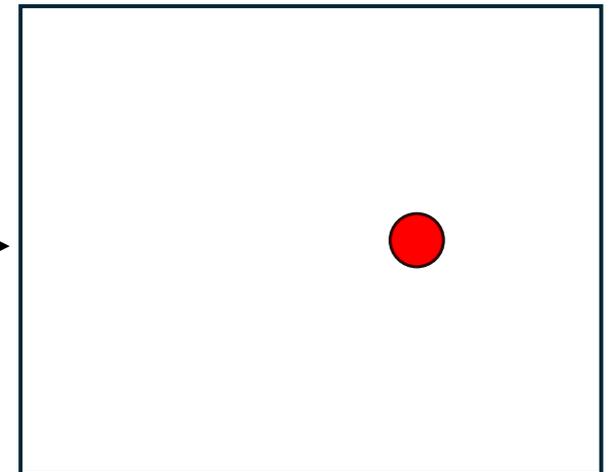
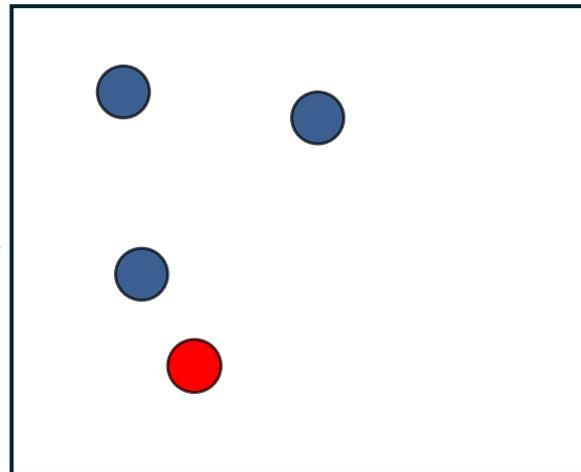
Species:



Rules:



Configuration I :
[3, 3, 2]



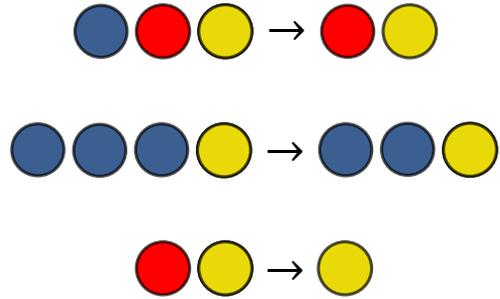
Configuration D :
[0, 1, 0]

Our Contributions

	Basic CRNs (1-step)	
Void Rules	Complexity	Ref.
$(2, 1)$	NL	Thm. 11
$(k, k - 1)^+$	$O(\Lambda ^2 \Gamma)$	Thm. 21
$(2, 0)$	$O(\Lambda ^2 \Gamma \log(\Lambda))$	[1]
$(2, 0), (2, 1)$	$O(\Lambda ^2 \Gamma \log(\Lambda))$	Thm. 18
$(k \geq 3, g \leq k - 2)$	NPC	Cor. 24

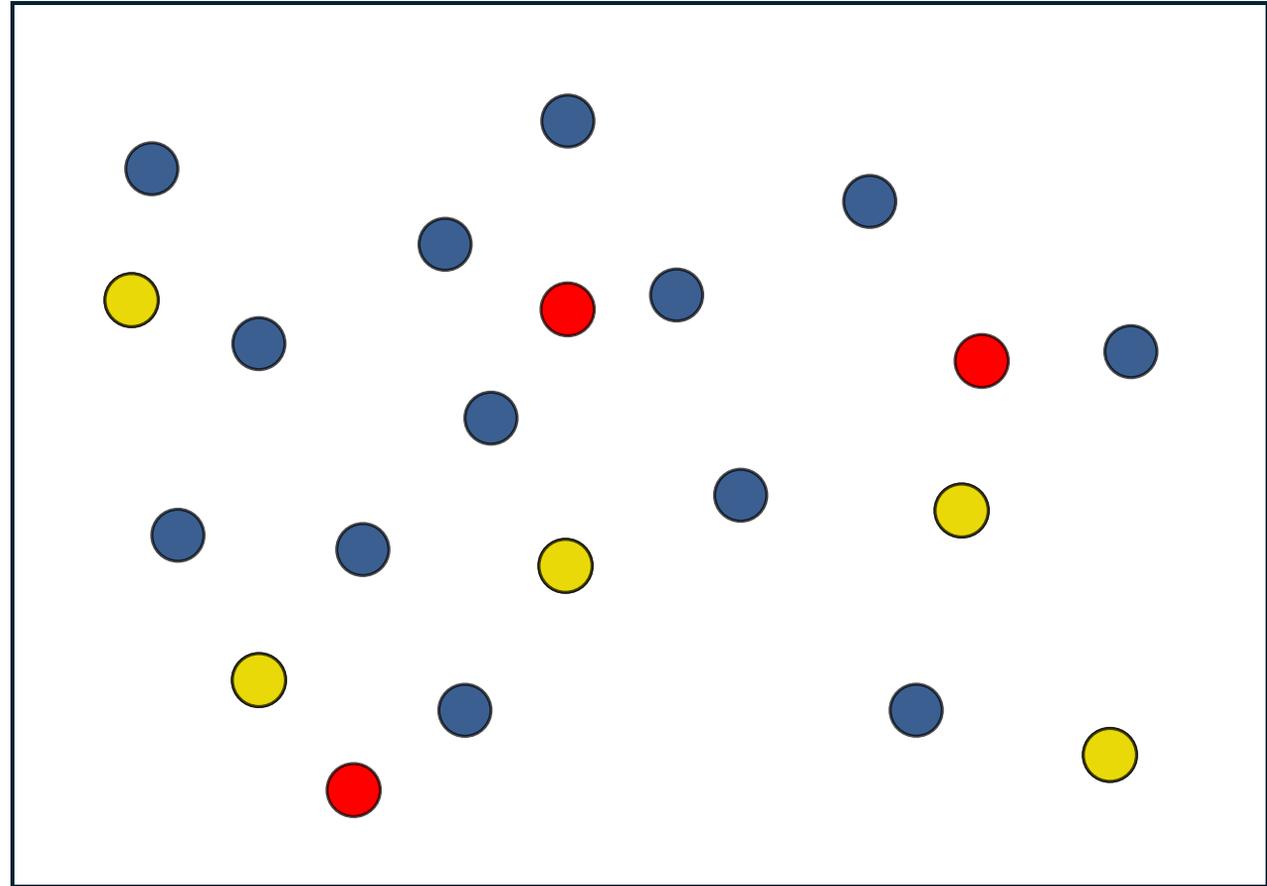
Bin Fu, Timothy Gomez, Ryan Knobel, Austin Luchsinger, Aiden Massie, Marco Rodriguez, Adrian Salinas, Robert Schweller, and Tim Wylie. In 31th International Conference on DNA Computing and Molecular Programming (DNA 25).

High Level Idea

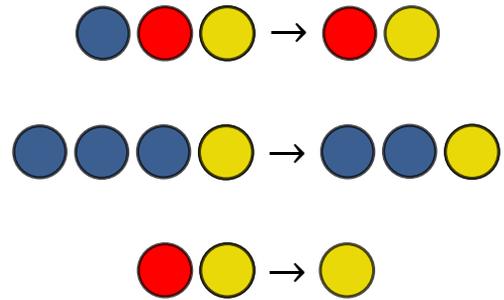


Final Counts:

-  1
-  0
-  5

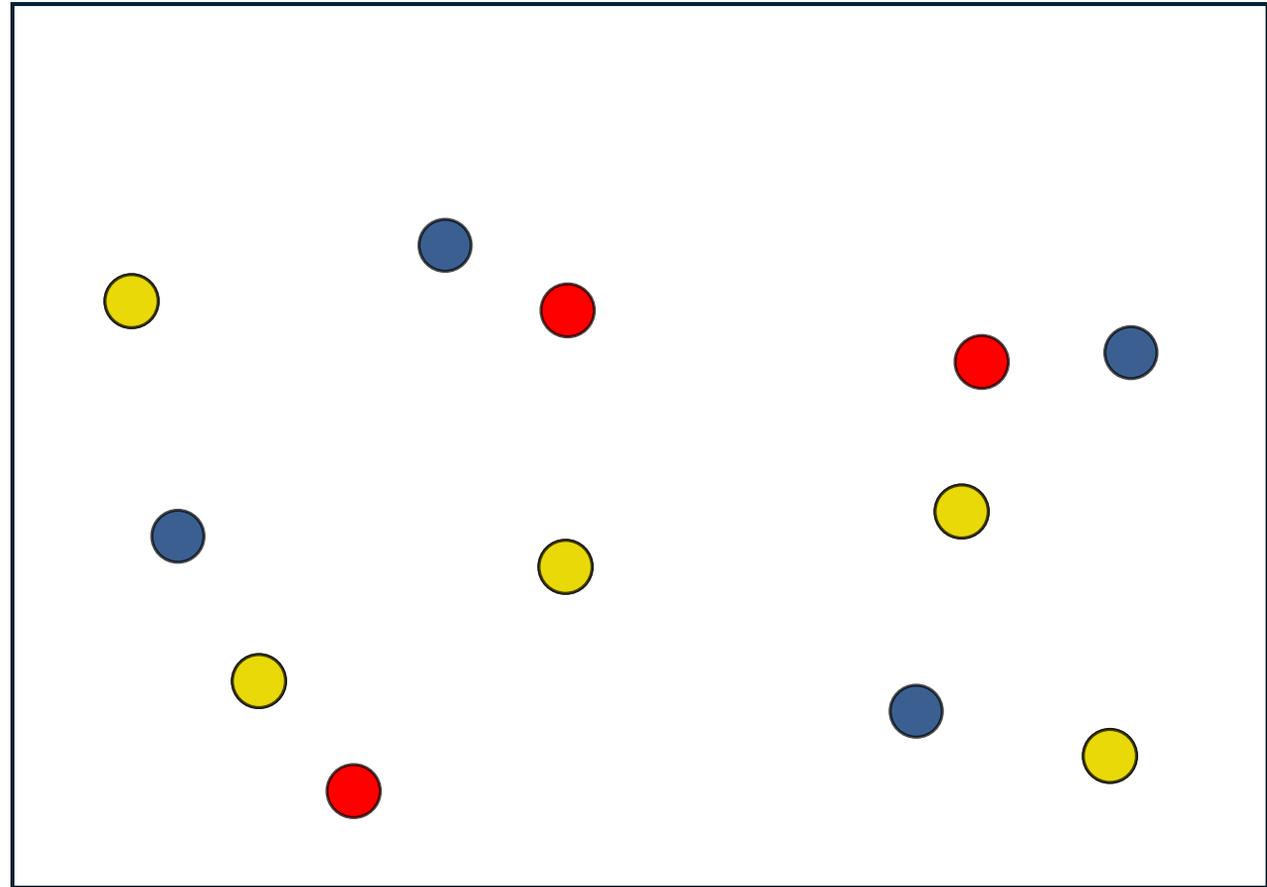


High Level Idea

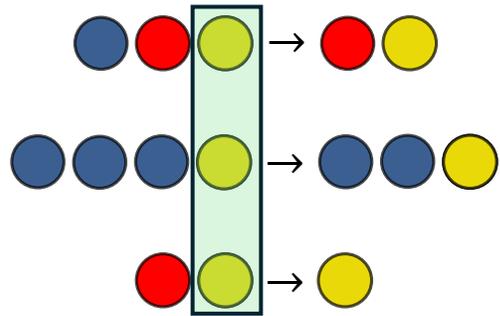


Final Counts:

-  1
-  0
-  5



High Level Idea

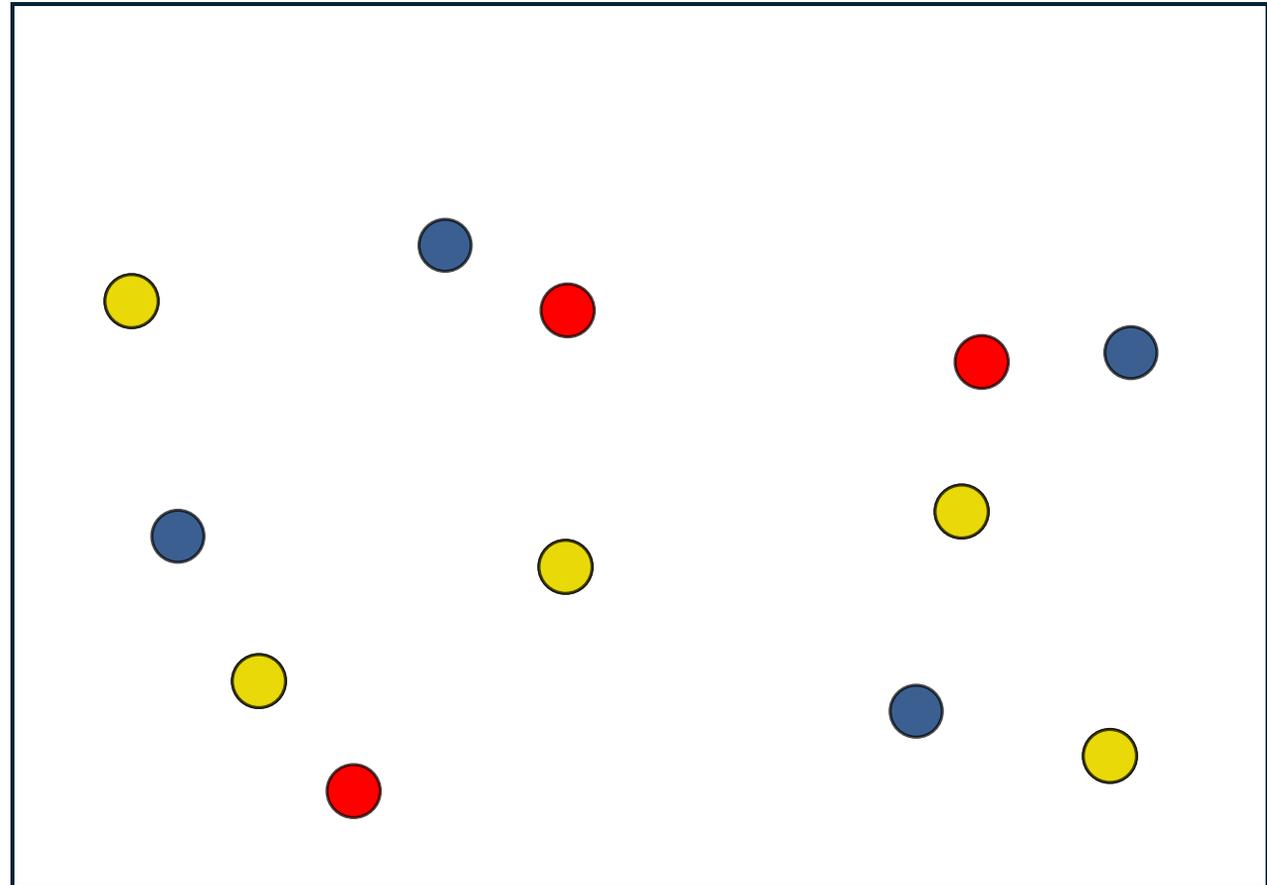


Final Counts:

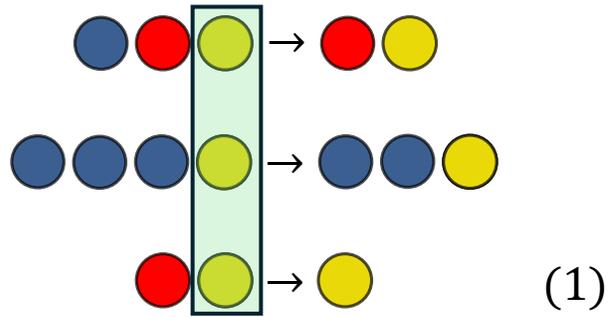
● 1

● 0

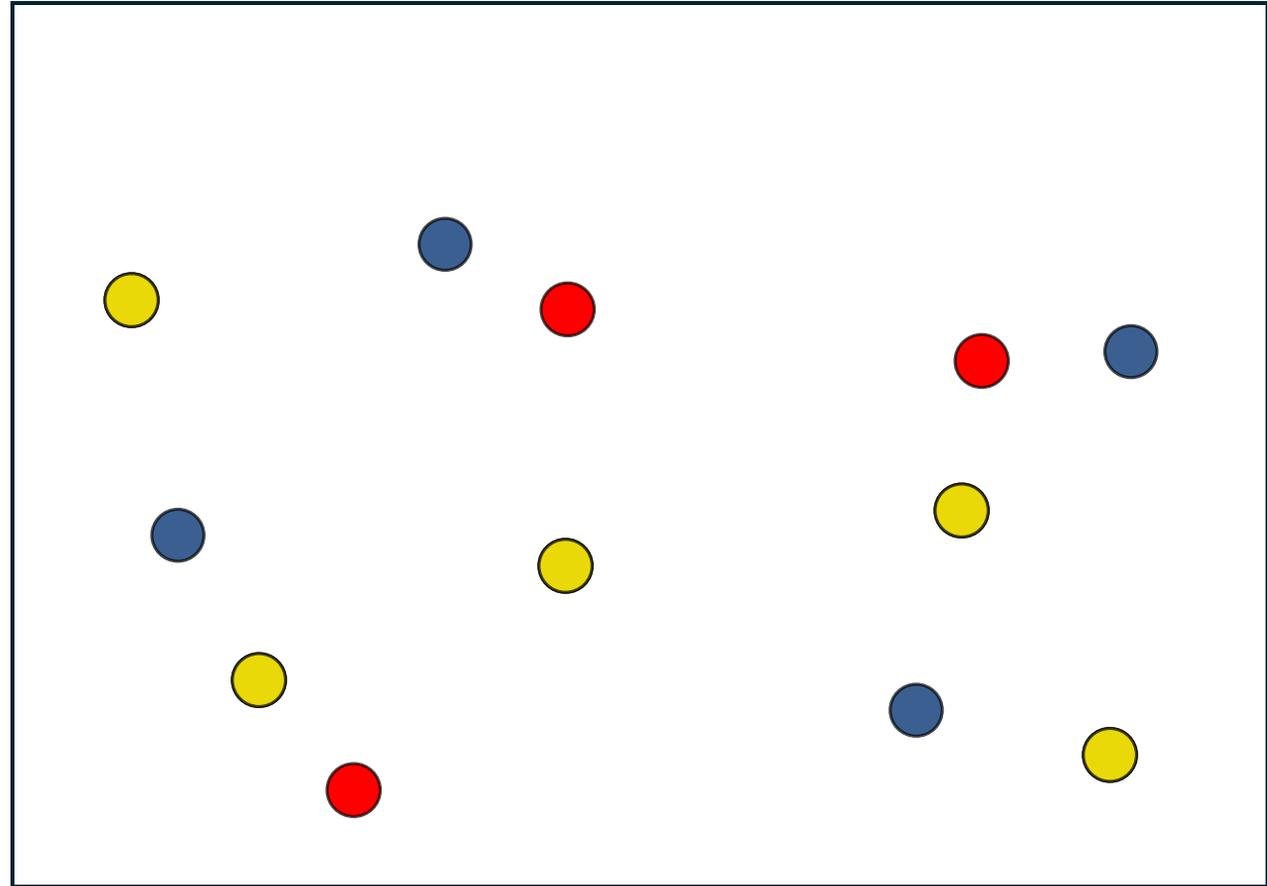
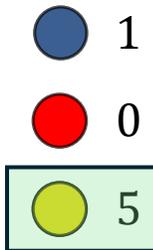
● 5



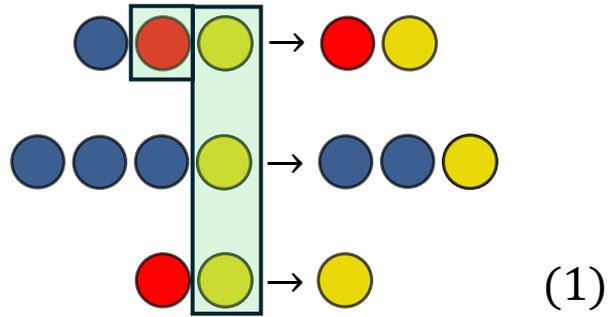
High Level Idea



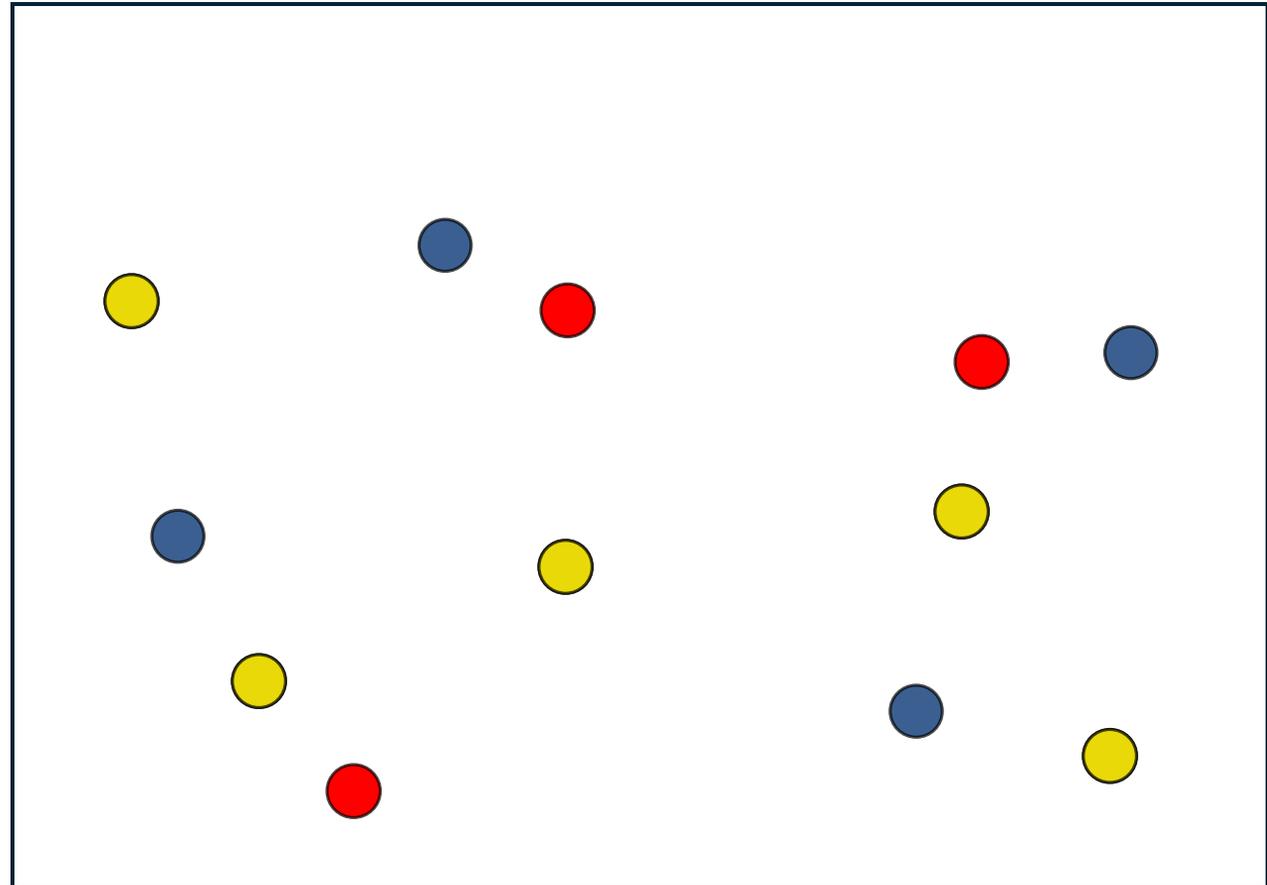
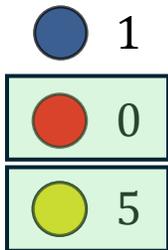
Final Counts:



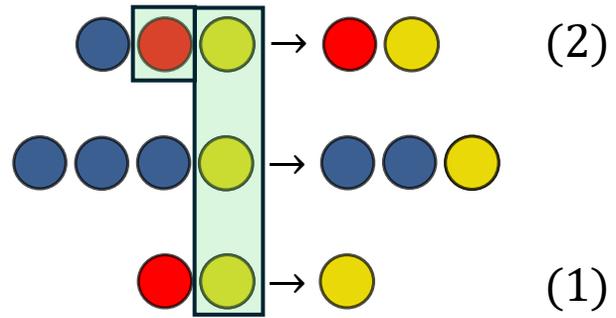
High Level Idea



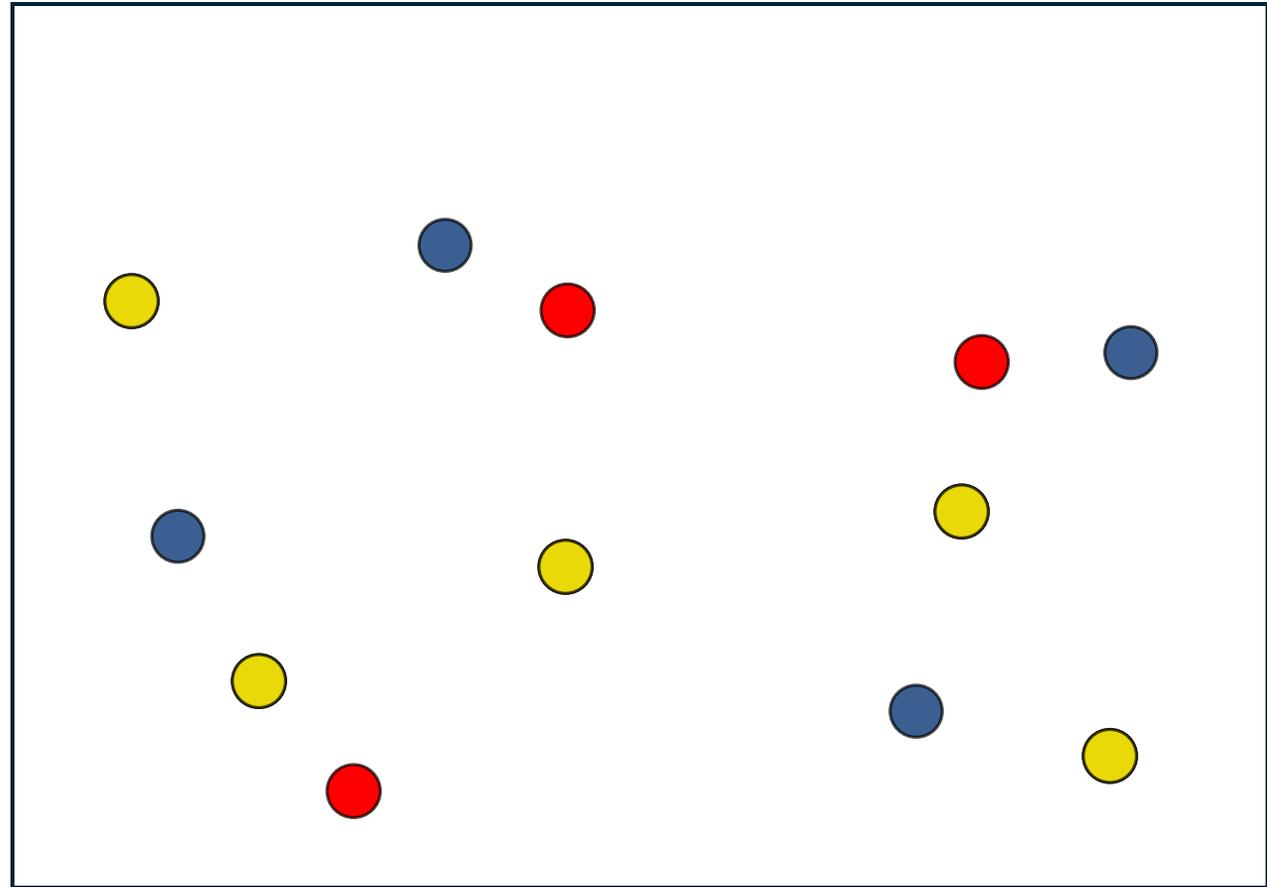
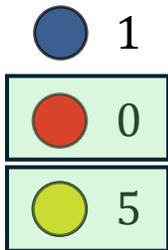
Final Counts:



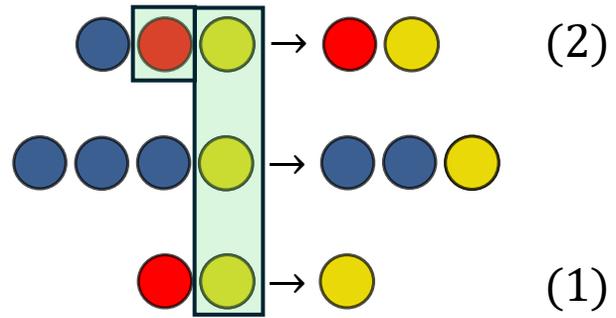
High Level Idea



Final Counts:

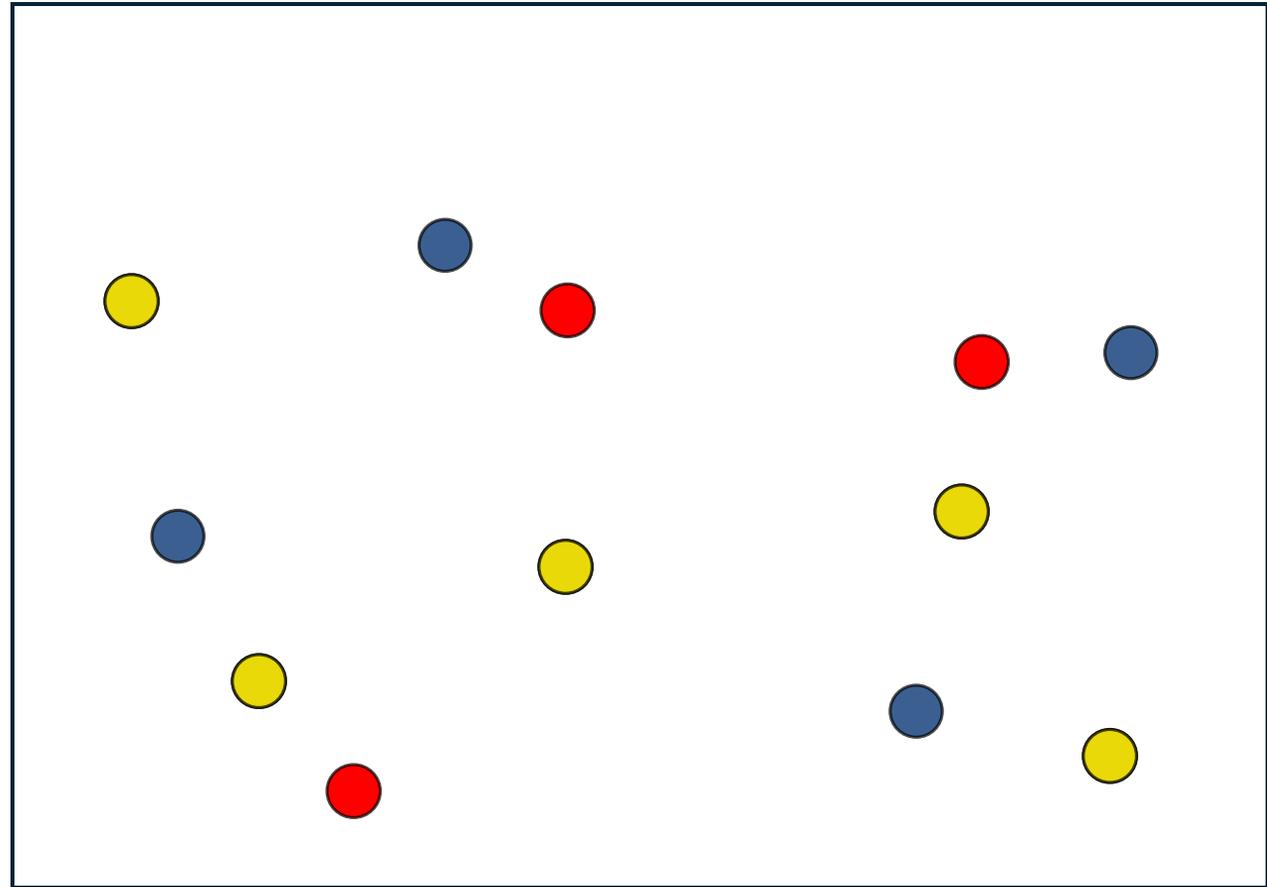


High Level Idea

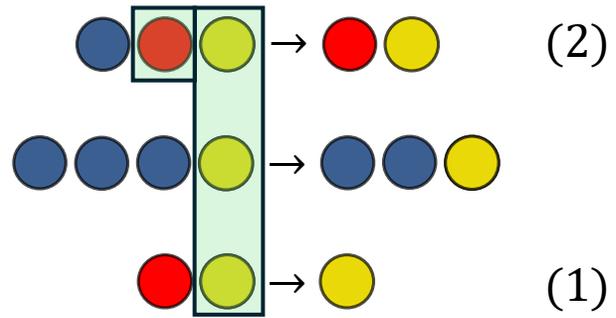


Final Counts:

	1
	0
	5

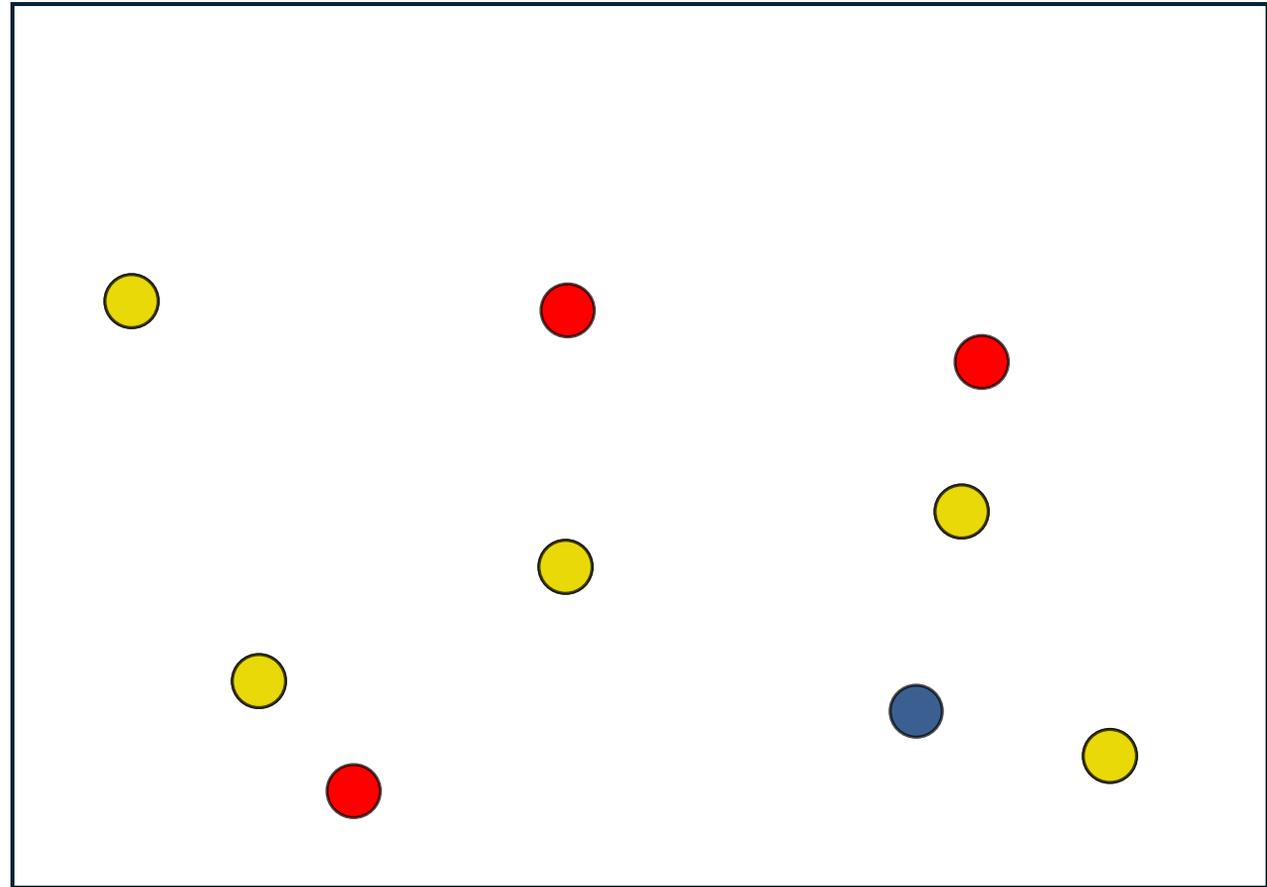


High Level Idea

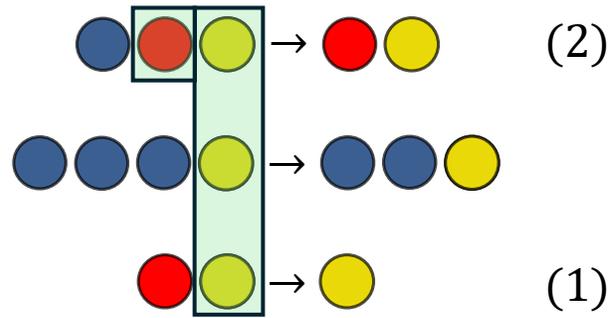


Final Counts:

	1
	0
	5

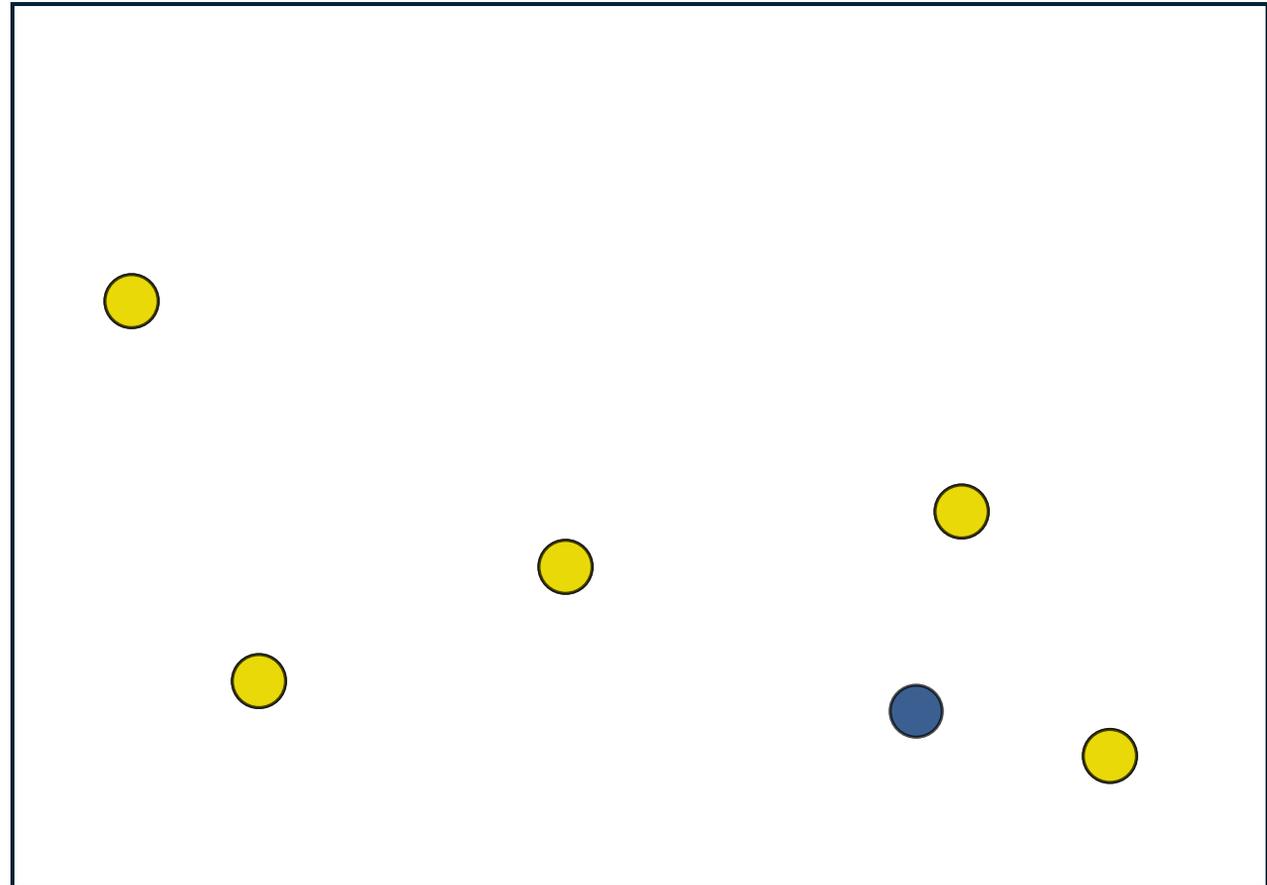


High Level Idea



Final Counts:

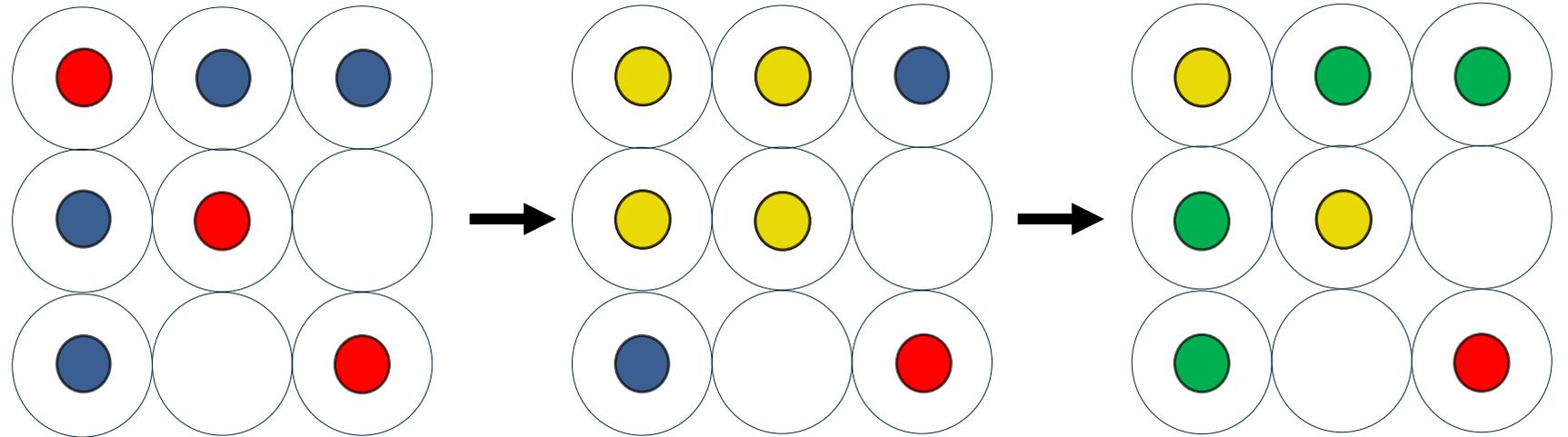
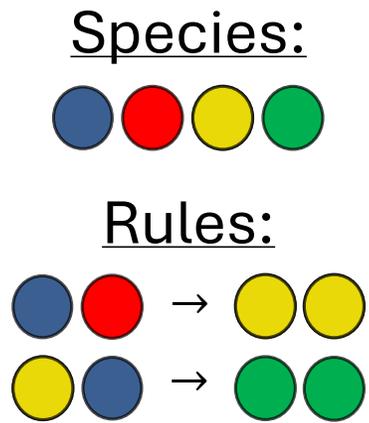
	1
	0
	5



Surface Chemical Reaction Networks

- Ordered pair (Λ, Γ)
 - Λ = Set of input species
 - Γ = Set of rules
- Surface
 - Undirected graph
- Configuration
 - Mapping of input species to vertices on the surface
 - Each vertex has no more than 1 species at a time

Example sCRN System



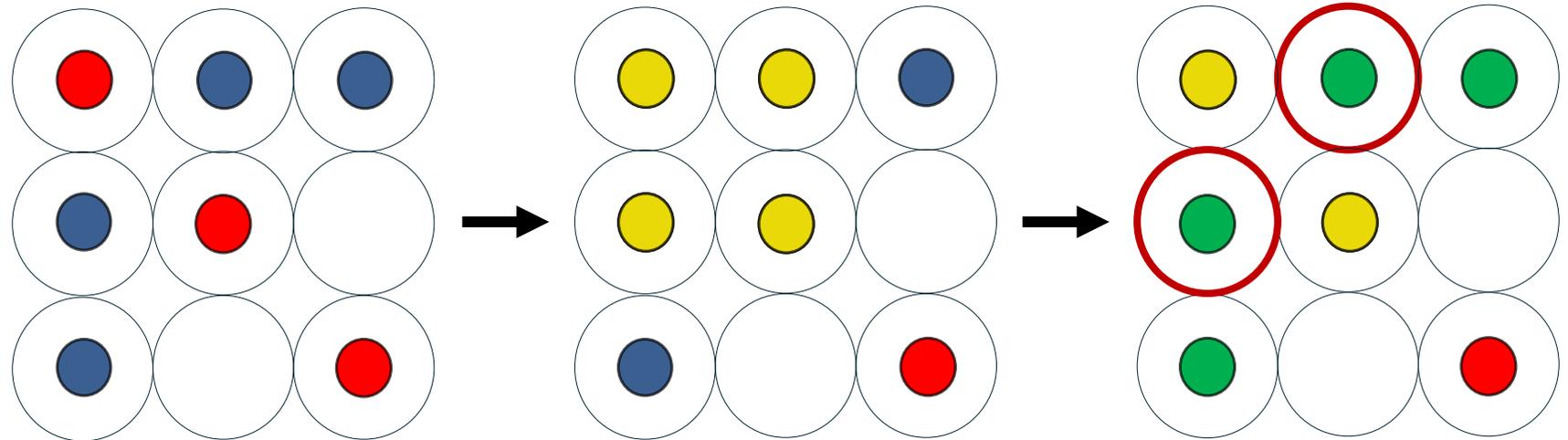
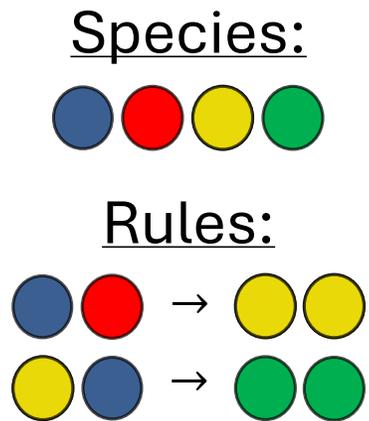
Configuration

/

Surface Chemical Reaction Networks

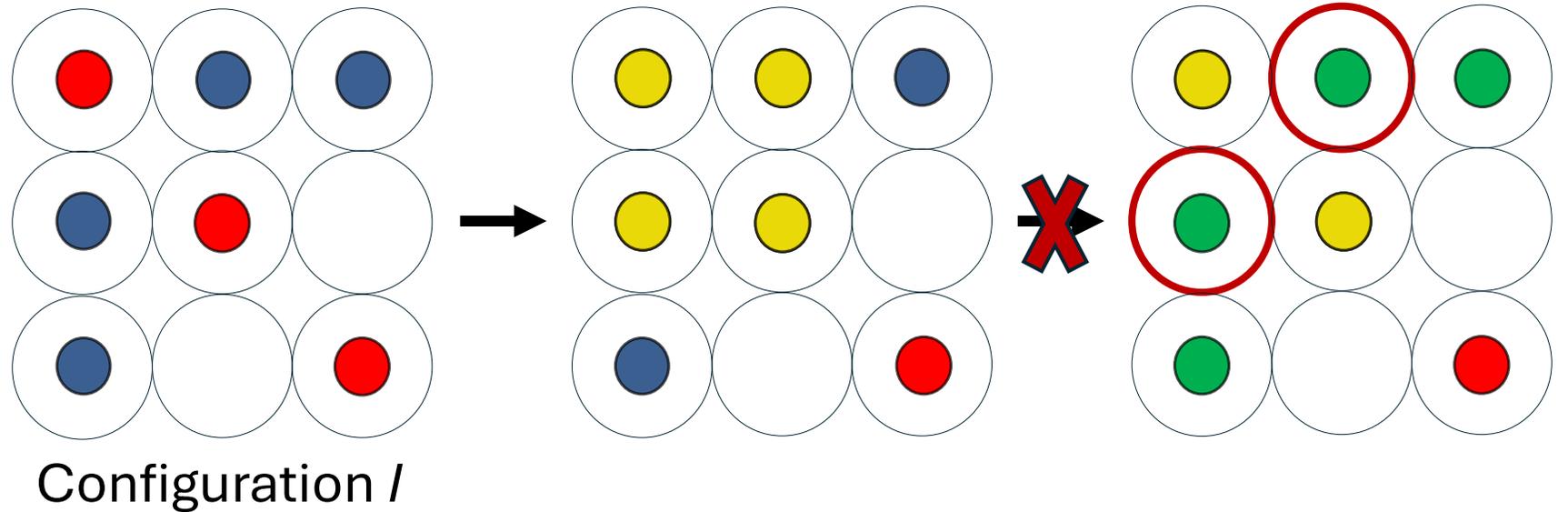
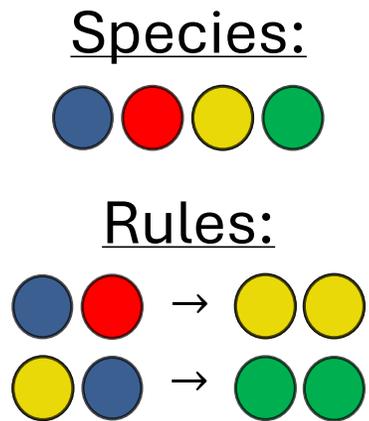
- Ordered pair (Λ, Γ)
 - Λ = Set of input species
 - Γ = Set of rules
- Surface
 - Undirected graph
- Configuration
 - Mapping of input species to vertices on the surface
 - Each vertex has no more than 1 species at a time
- Burnout
 - Limit to how many times a vertex can change states

Example sCRN System: 2 burnout

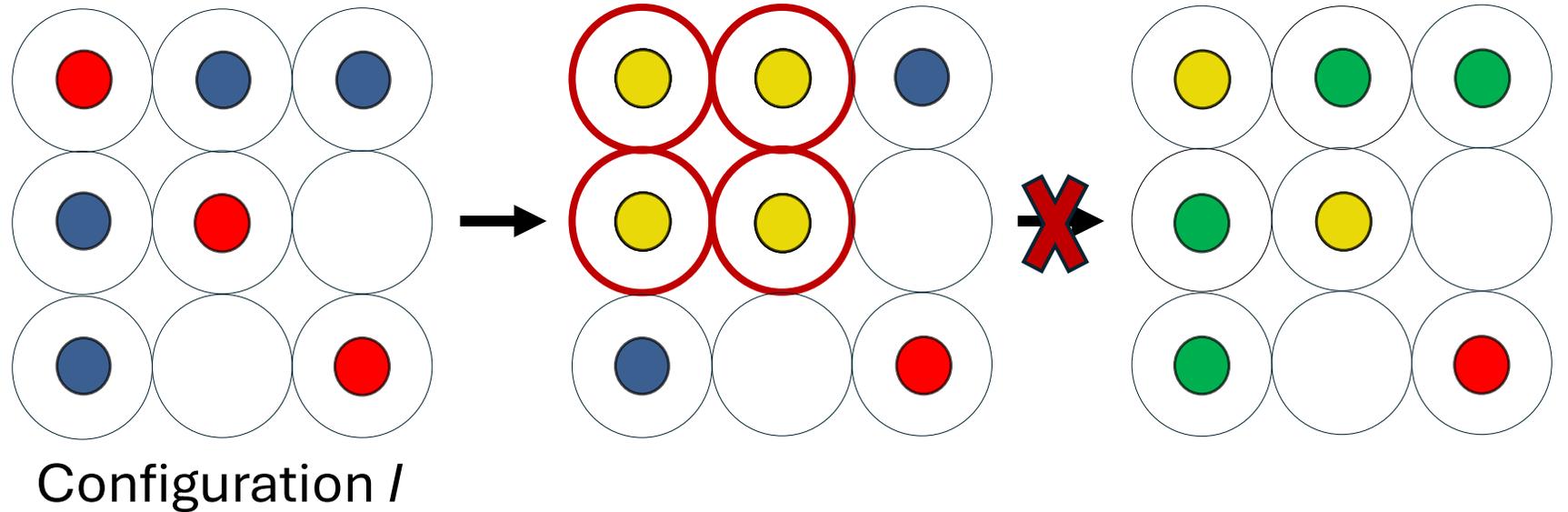
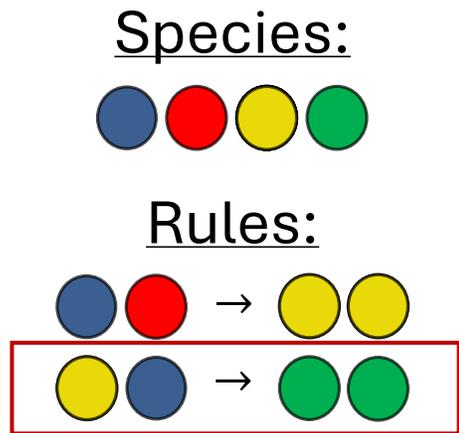


Configuration 1

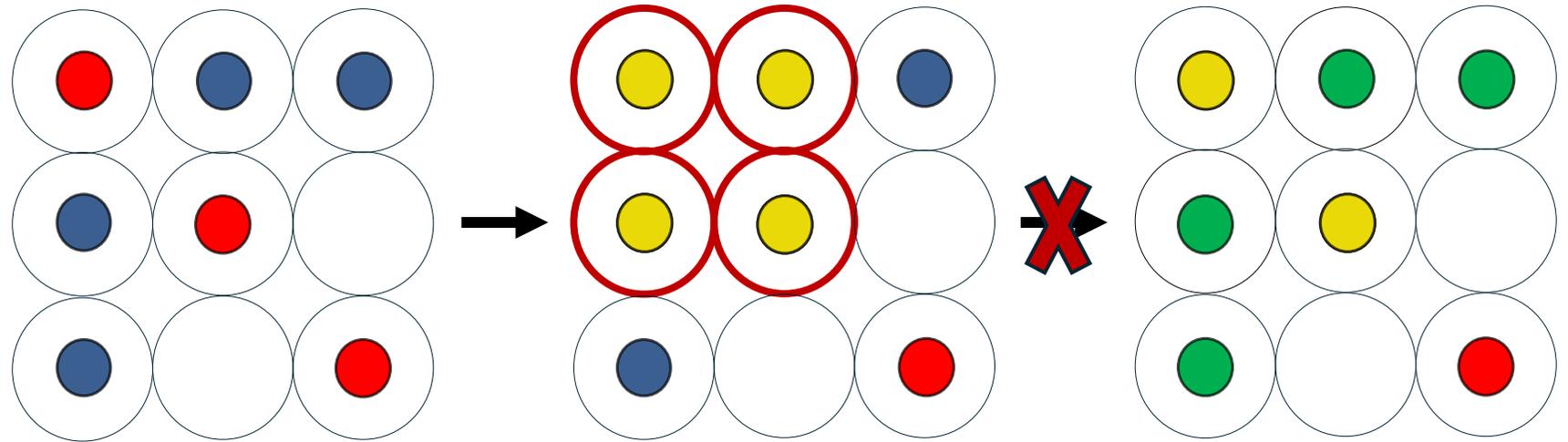
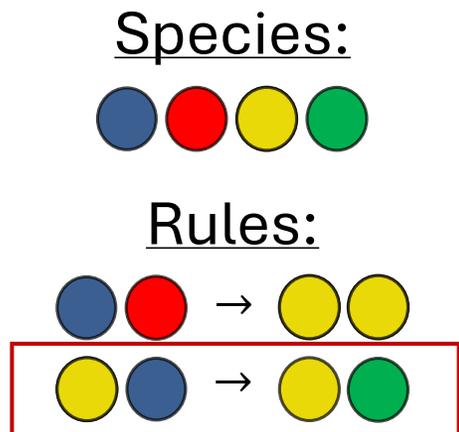
Example sCRN System: 1 burnout



Example sCRN System: 1 burnout

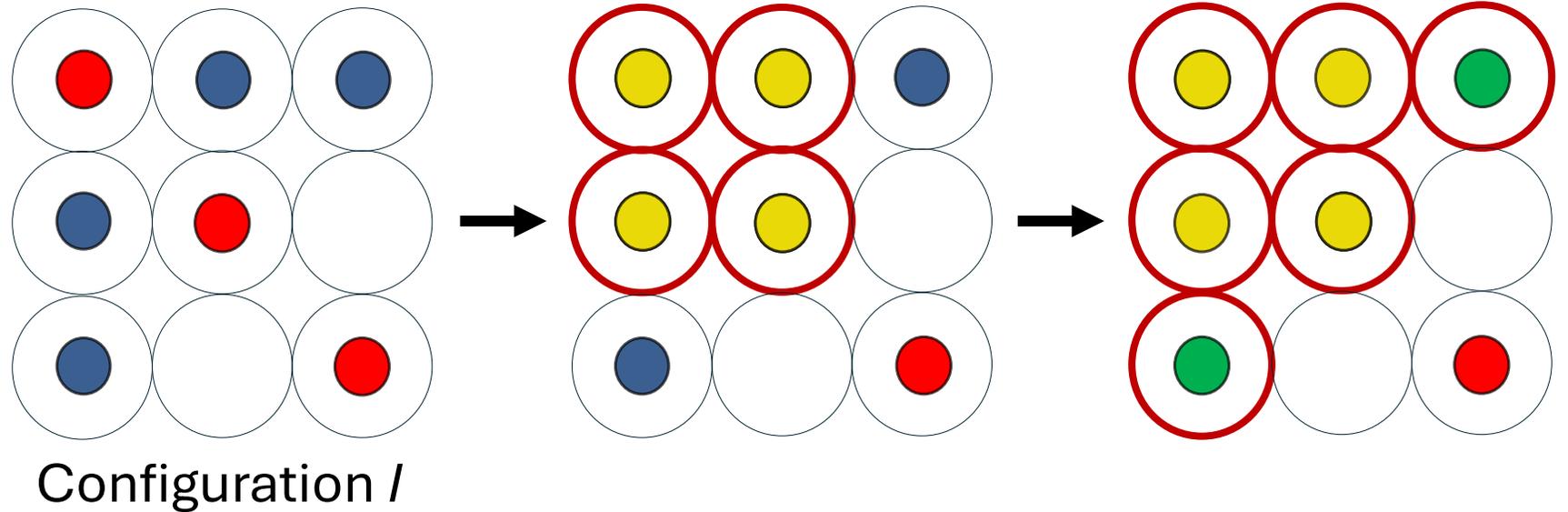
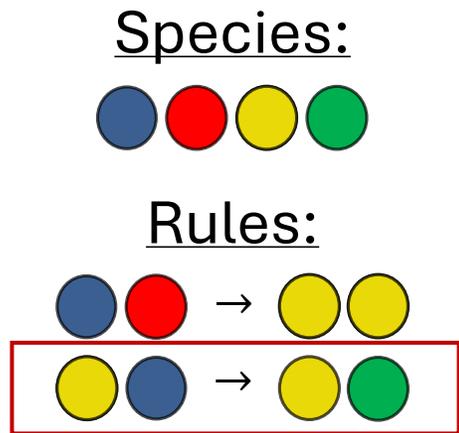


Example sCRN System: 1 burnout



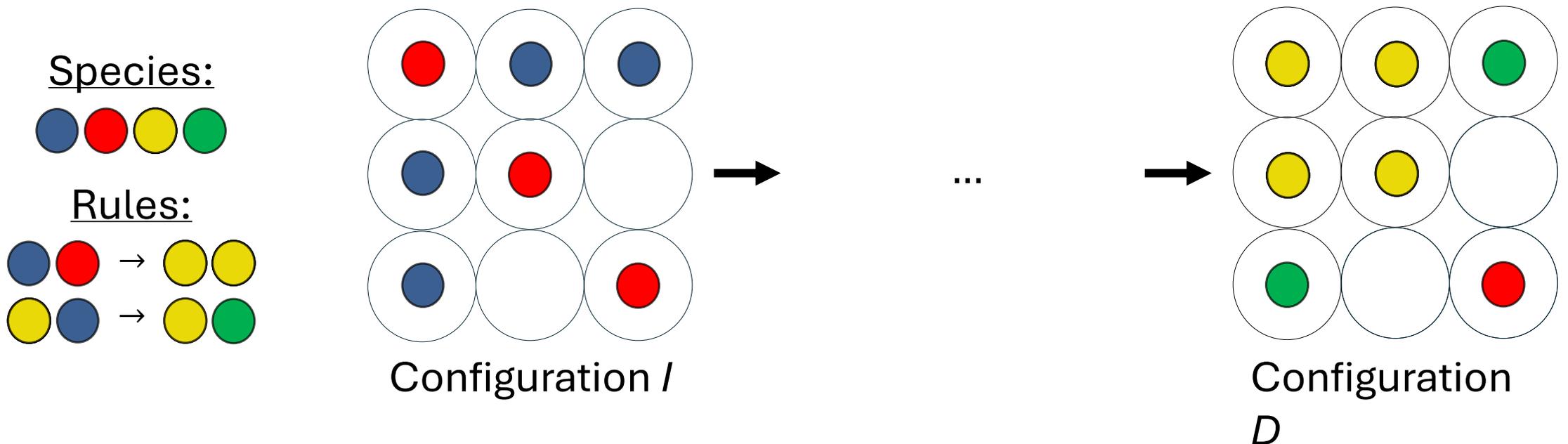
Configuration 1

Example sCRN System: 1 burnout



Reconfiguration

- Given initial configuration I and target configuration D , can D ever be reached from I ?

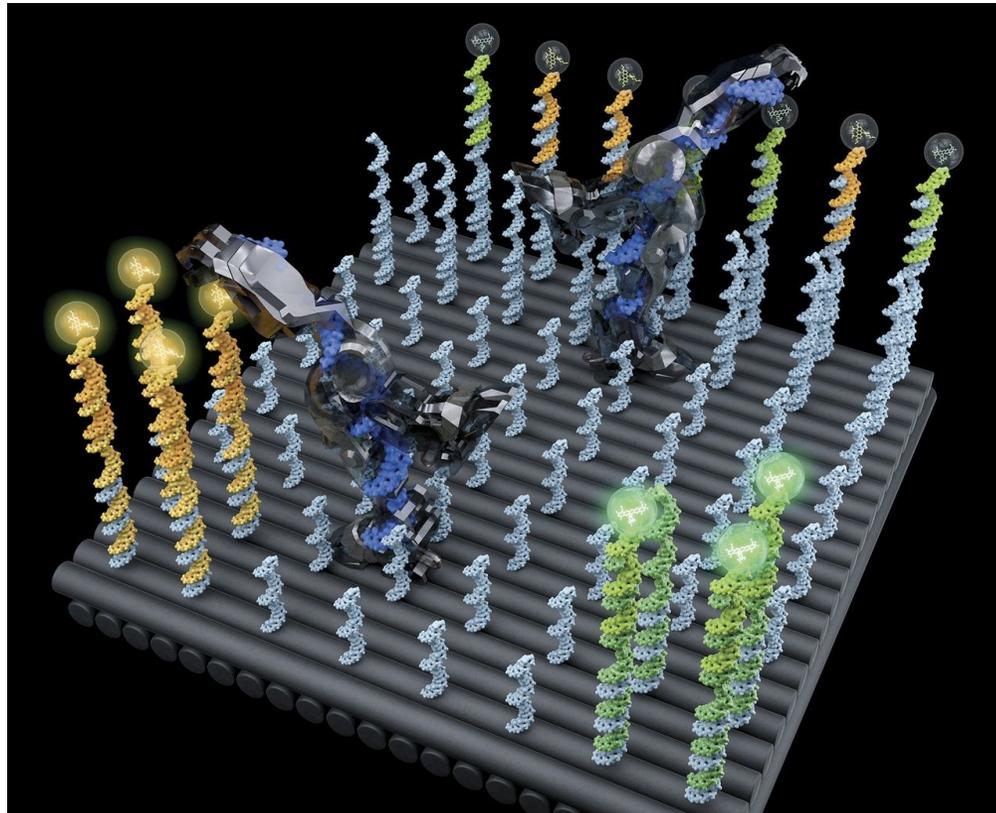


Motivation

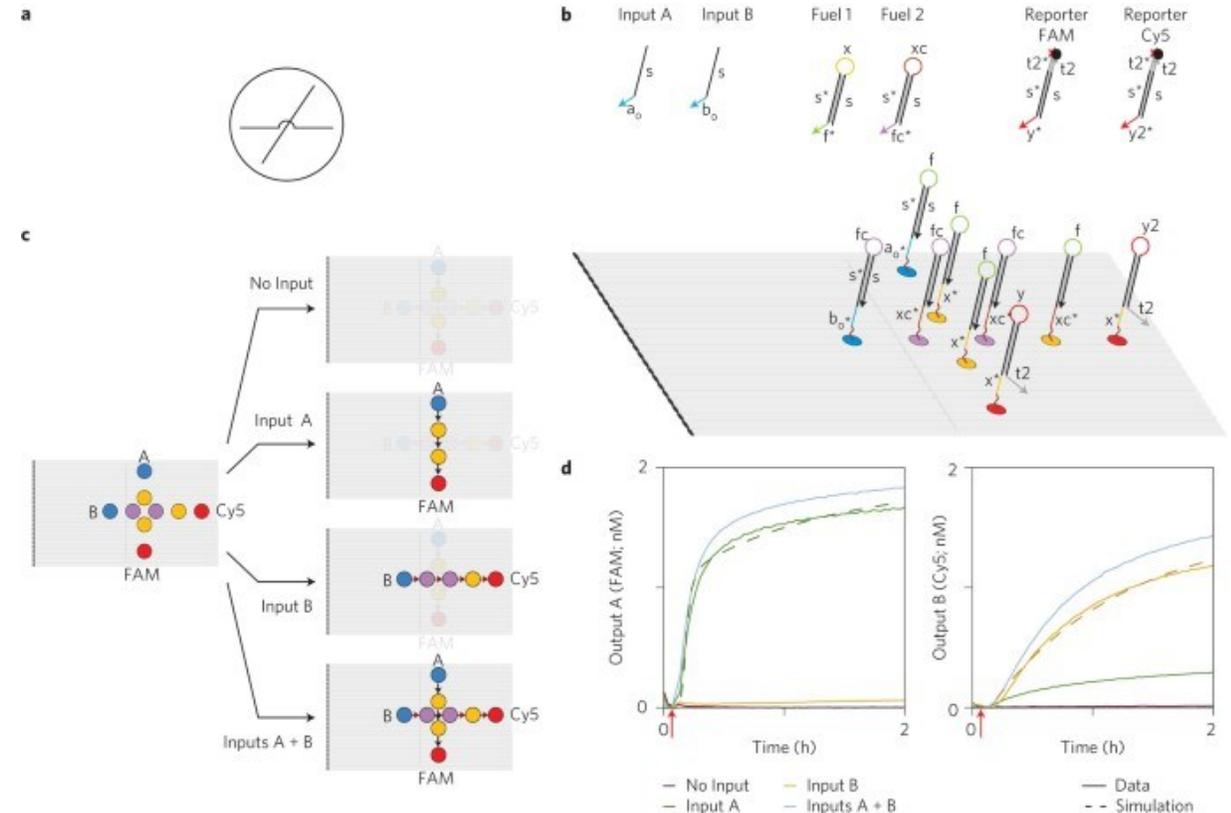
Motivation

- CRNs are practical but limited in computational power
 - Deterministically compute semi-linear functions
- sCRNs help overcome some of these limitations
 - Some geometry
- Burnout reflects how molecules may interact
 - Molecules with limited lifetimes
 - Reactions that consume large quantities of energy

Motivation



A. J. Thubagere, W. Li, R. F. Johnson, Z. Chen, S. Doroudi, Y. L. Lee, G. Izatt, S. Wittman, N. Srinivas, D. Woods, et al. **A cargo-sorting DNA robot.** *Science*, 357(6356):eaan6558, 2017.



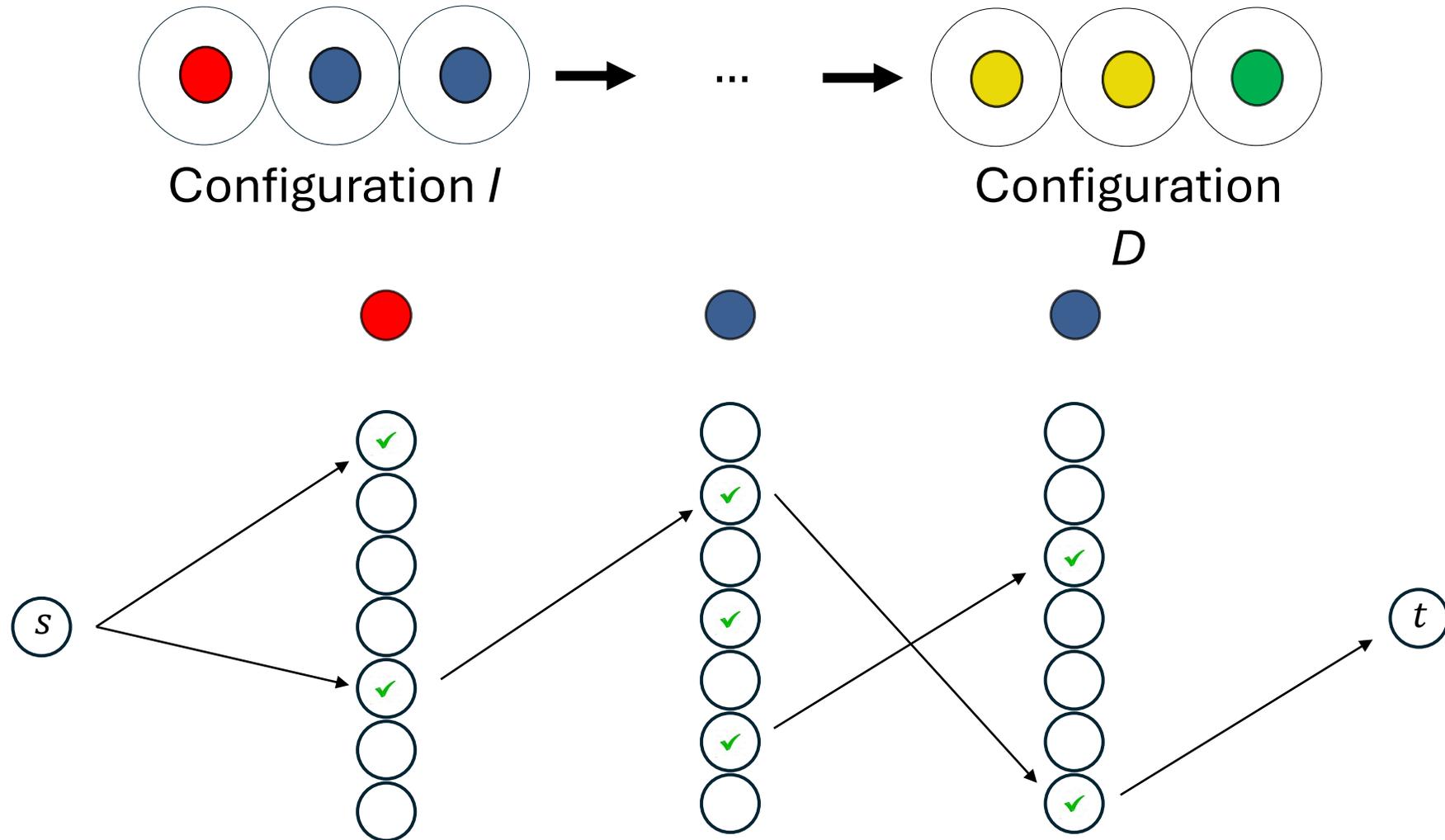
G. Chatterjee, N. Dalchau, R. A. Muscat, A. Phillips, and G. Seelig. **A spatially localized architecture for fast and modular DNA computing.** *Nature nanotechnology*, 12(9):920–927, 2017.

Linear Surfaces

Problem	Burnout	Result
Reconfiguration	1	$O(n + R)$
Reconfiguration	2	$O(n \cdot S ^2 \cdot R ^4)$
Reconfiguration	$O(1)$	P
Reconfiguration	k (unary)	NP – Complete
Reconfiguration	None	PSPACE – Complete

Robert Alaniz, Michael Coulombe, Erik Demaine, Bin Fu, Tim Gomez, Elise Grizzell, Ryan Knobel, Andrew Rodriguez, Robert Schweller, Tim Wylie. Proc. of the 35th Canadian Conf. on Computational Geometry (CCCG 23).

1-burnout



Conclusion

Known + New Results

Linear Surfaces

Problem	Burnout	Result
Reconfiguration	1	$O(n + R)$
Reconfiguration	2	$O(n \cdot S ^2 \cdot R ^4)$
Reconfiguration	$O(1)$	P
Reconfiguration	k (unary)	<i>NP – Complete</i>
Reconfiguration	None	<i>PSPACE – Complete</i>

General Surfaces

Problem	Burnout	Result
Reconfiguration	1	$O(V^{1.5} + R)^*$
Reconfiguration	1	<i>NP – Complete</i>
Reconfiguration	2	<i>NP – Complete</i>

* Non-catalytic reactions

Grid Surfaces

Problem	Burnout	Result
1- Reconfiguration	1	$O(n \cdot (S R)^{2m} \cdot f(m))$
1- Reconfiguration	1	<i>NP – Complete</i>

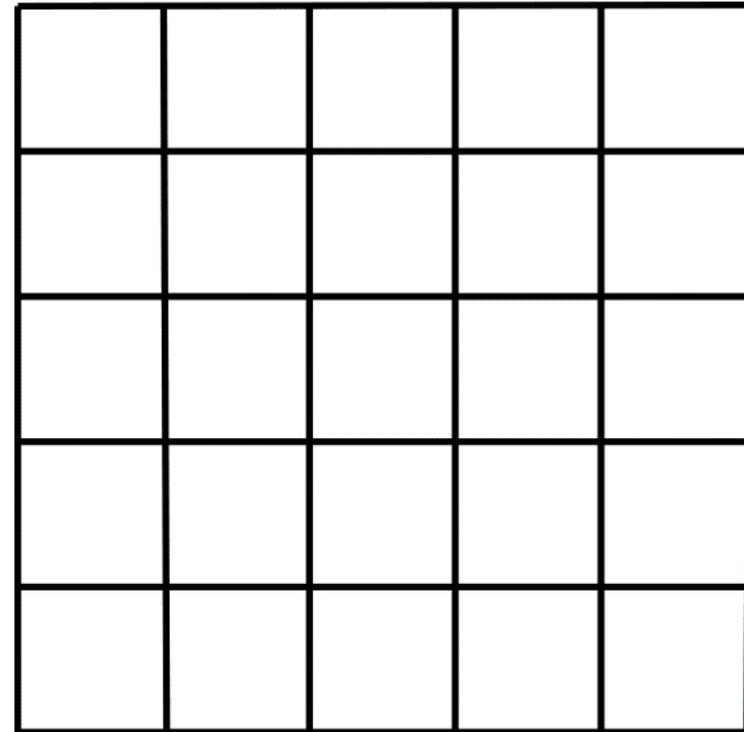
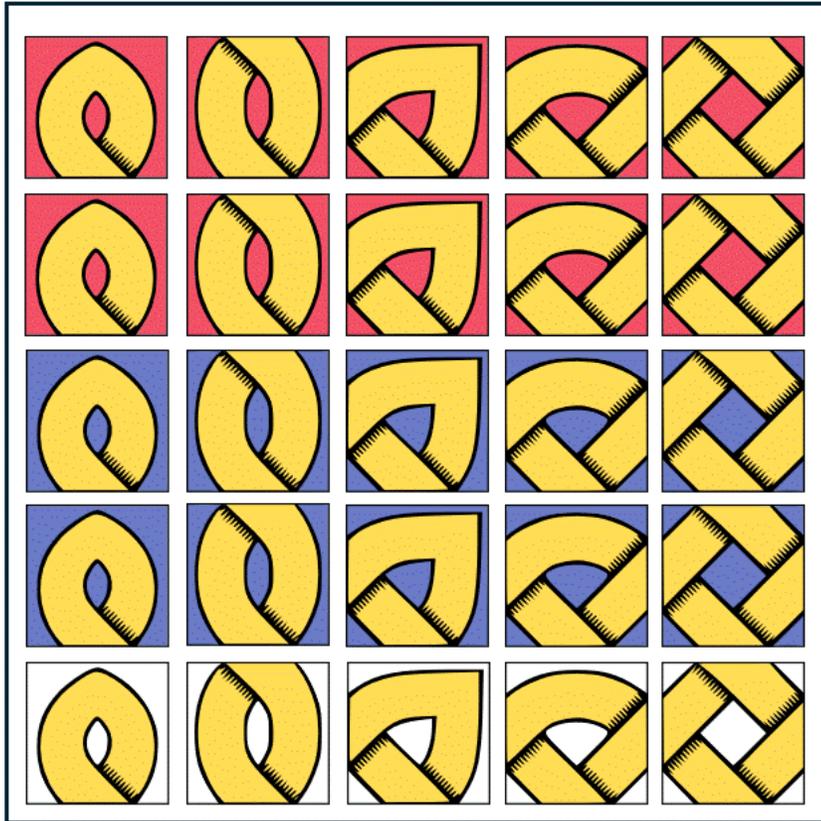
Open Problems

- Lower bounds for k -burnout on linear surfaces
- Other than size of surface, what about:
 - Species, rules and burnout
- Any FPT algorithms for reconfiguration

Game Complexity

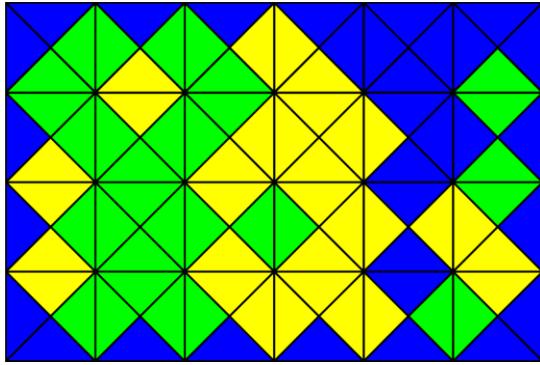


Tile-based Knot Assembly with Celtic!



Authors: Divya Bajaj, **Ryan Knobel**, Juan Manuel Perez, Rene Reyes,
Ramiro Santos, Tim Wylie

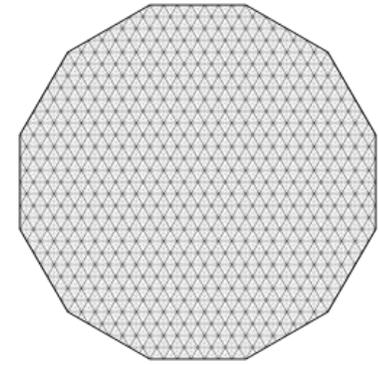
Background



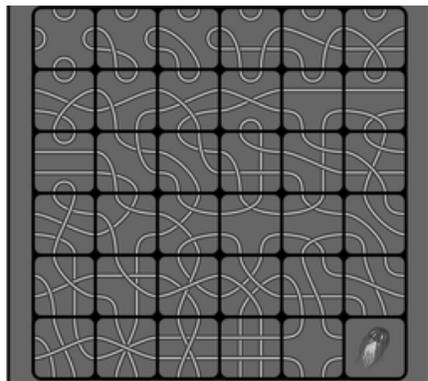
MacMahon Squares



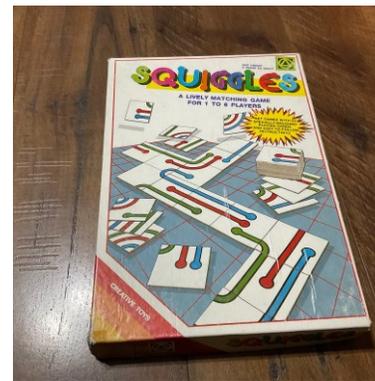
Jigsaw Puzzles



Eternity

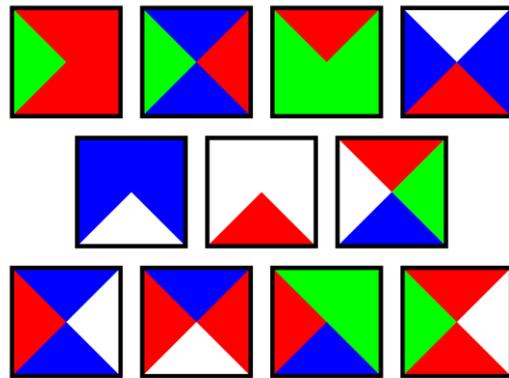
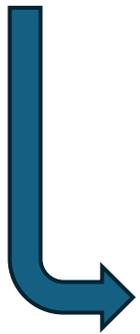
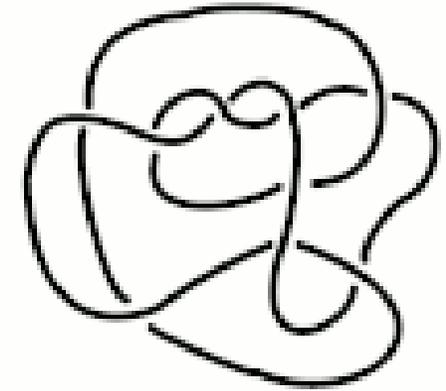
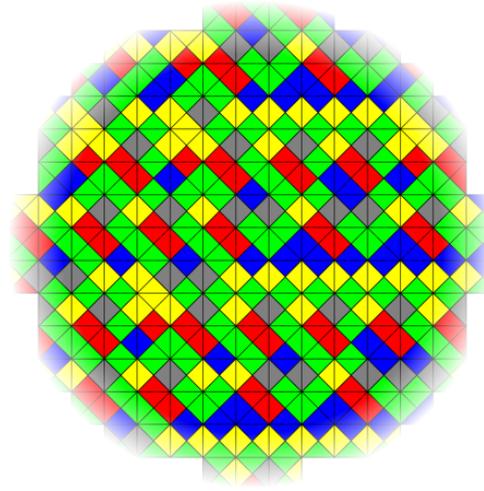
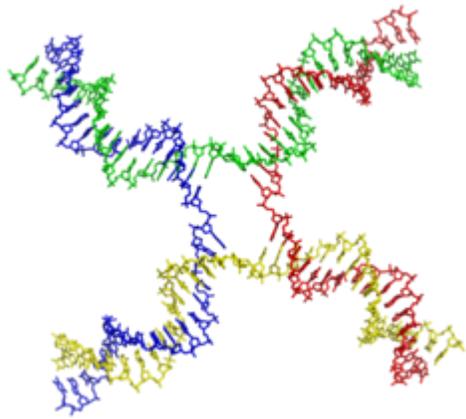


Tsuro



Squiggles

Background

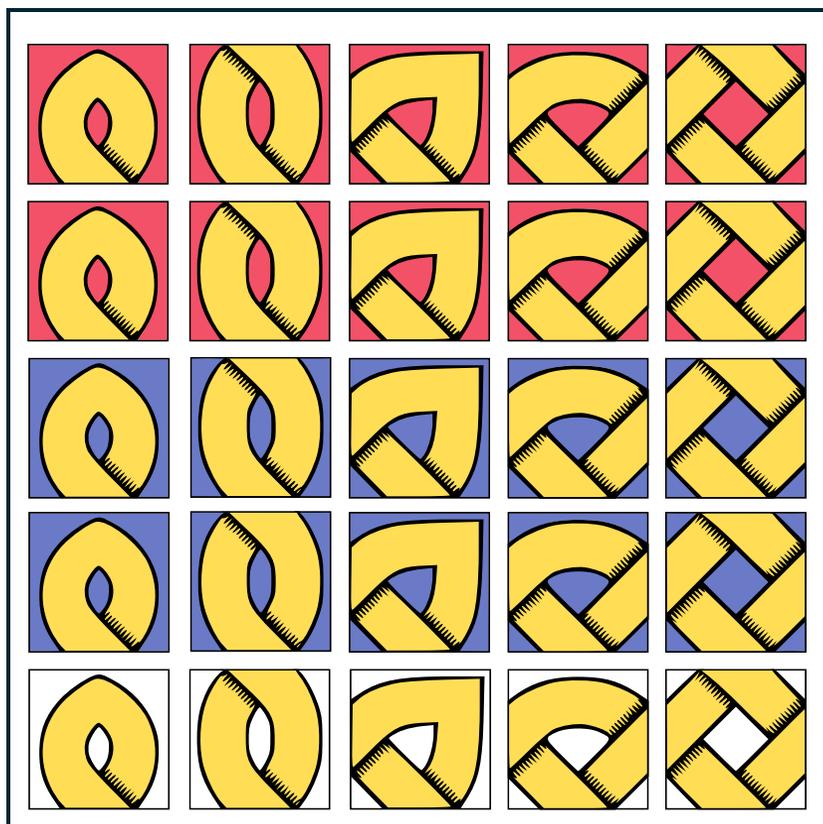


Wang tiles

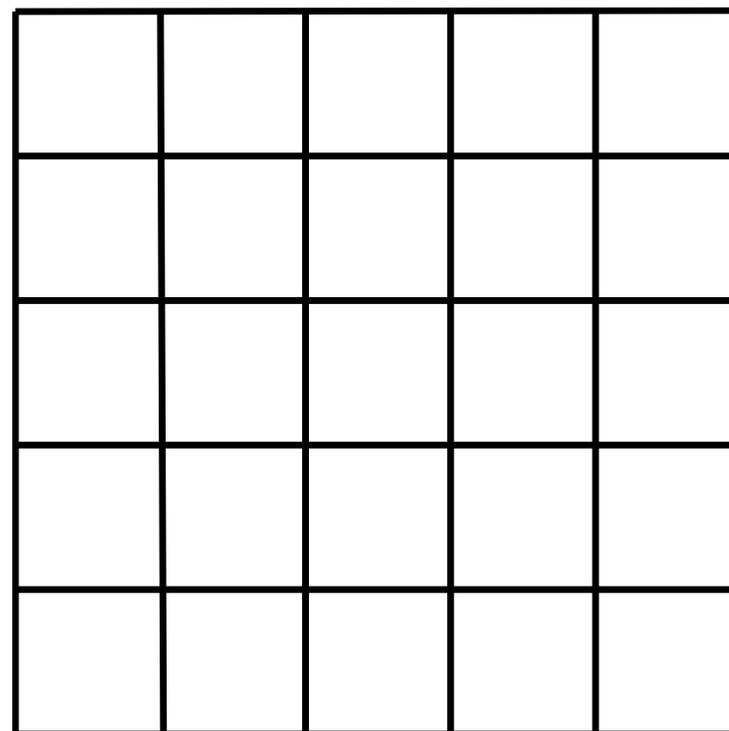


[Knot Theory Wikipedia]

Celtic!

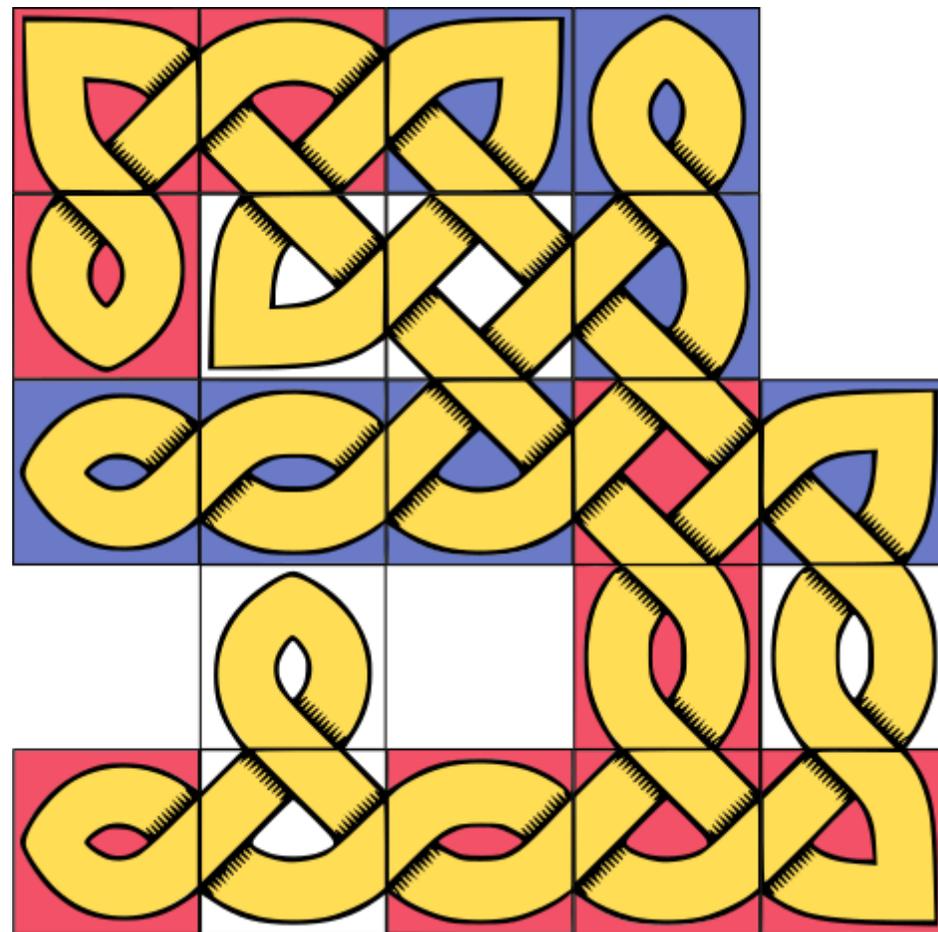


Pieces

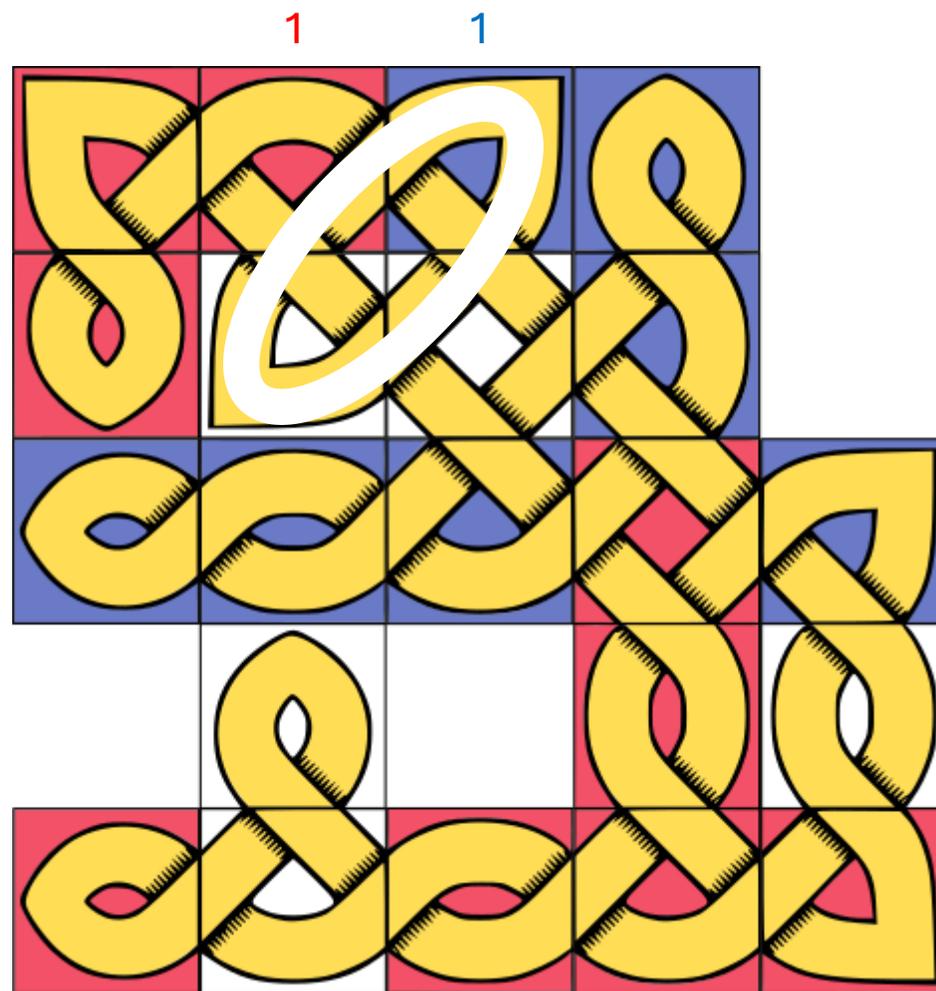


Board

Celtic! - Scoring



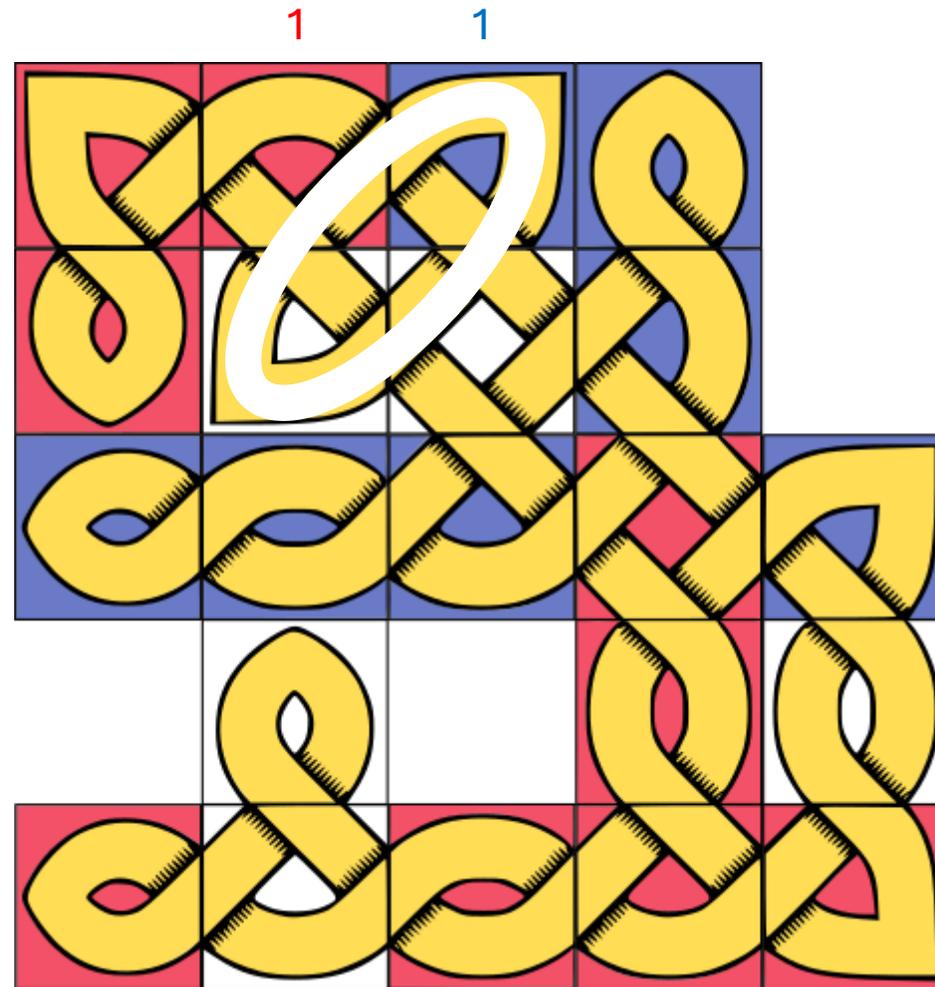
Celtic! - Scoring



Celtic! - Scoring

Score

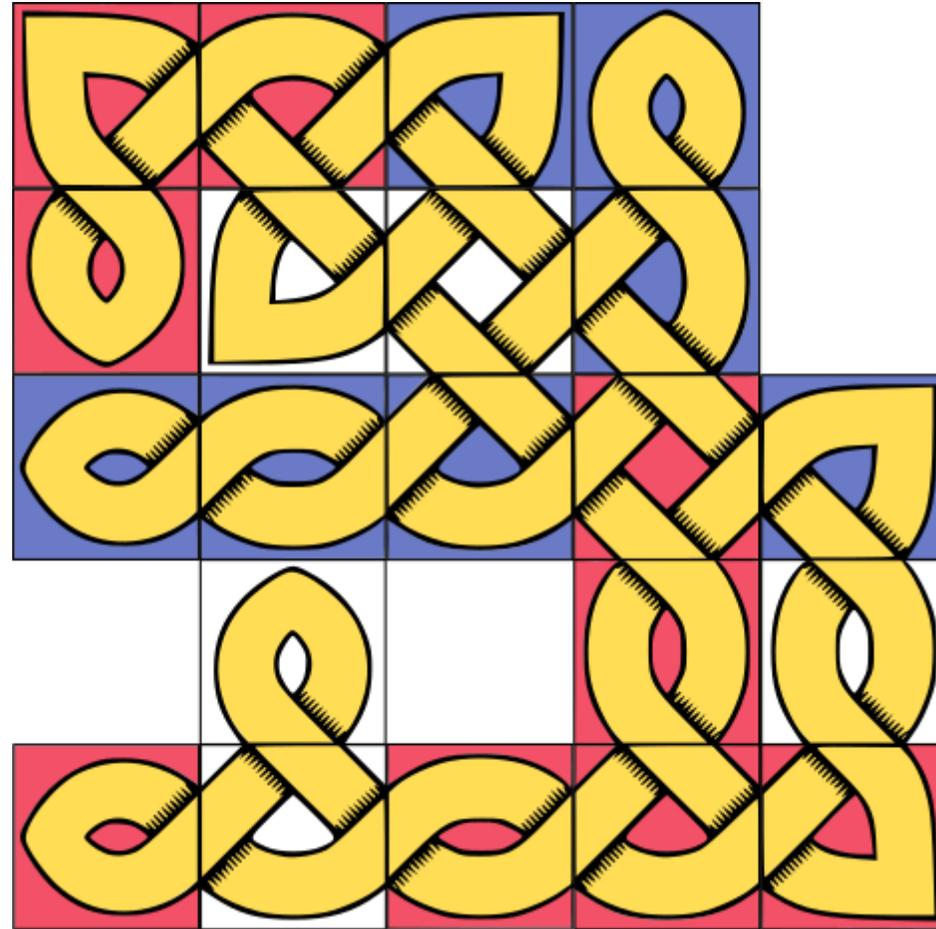
Knot 1: Tie



Celtic! - Scoring

Score

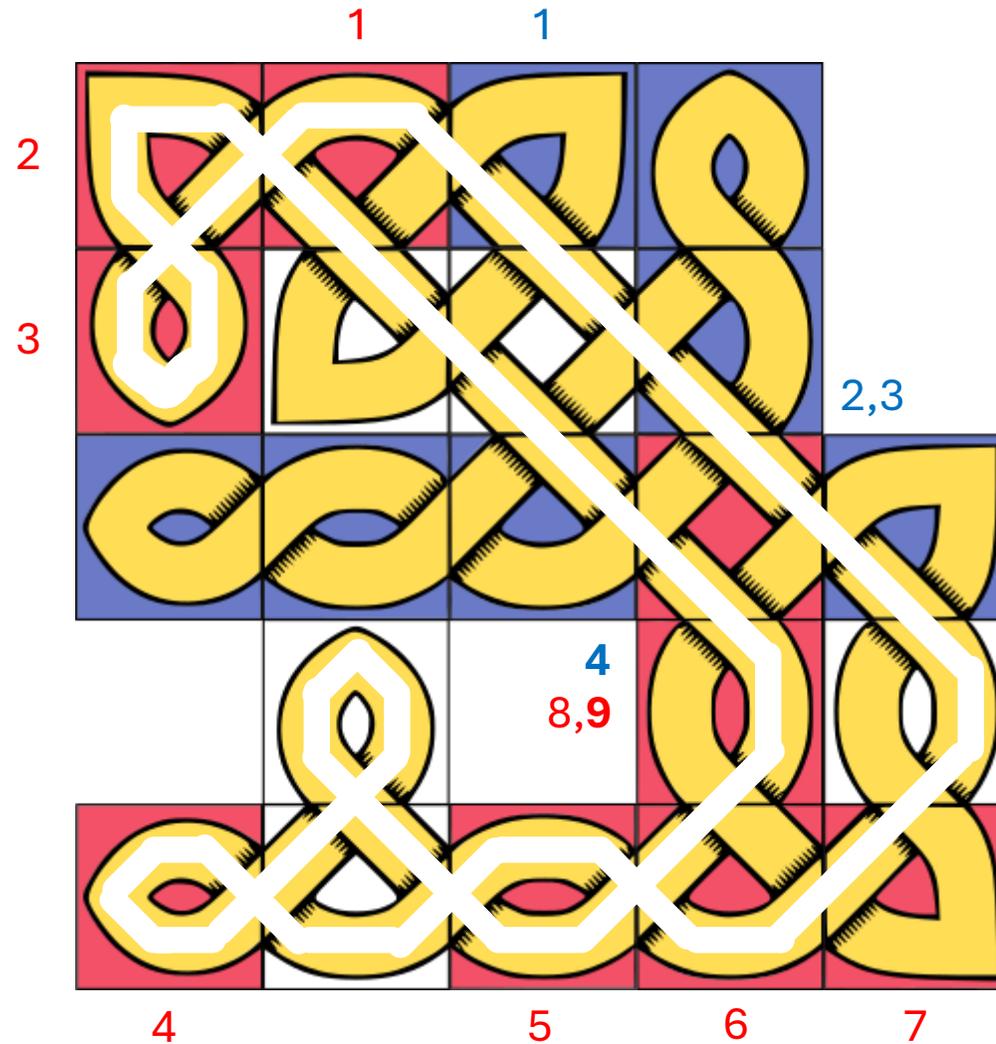
Knot 1: Tie



Celtic! - Scoring

Score

Knot 1: Tie

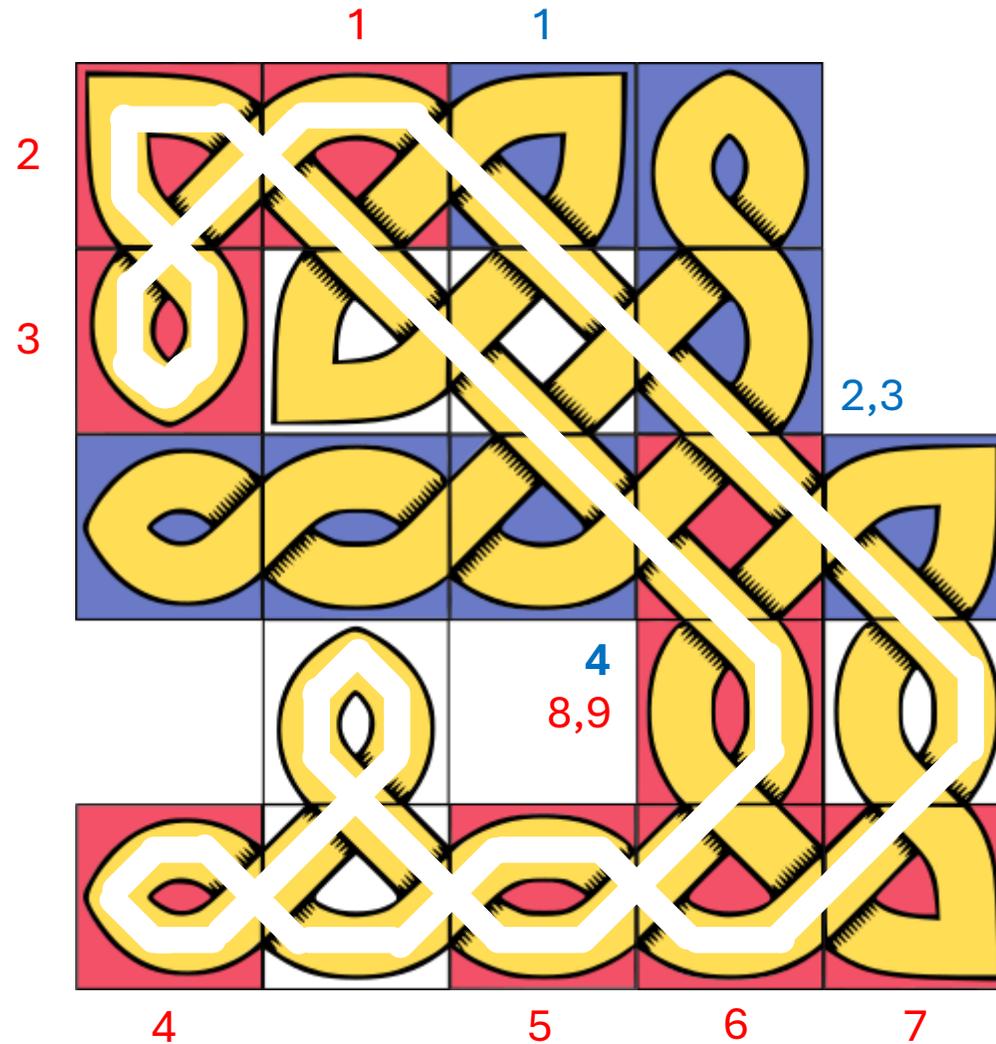


Celtic! - Scoring

Score

Knot 1: Tie

Knot 2: Red (9)

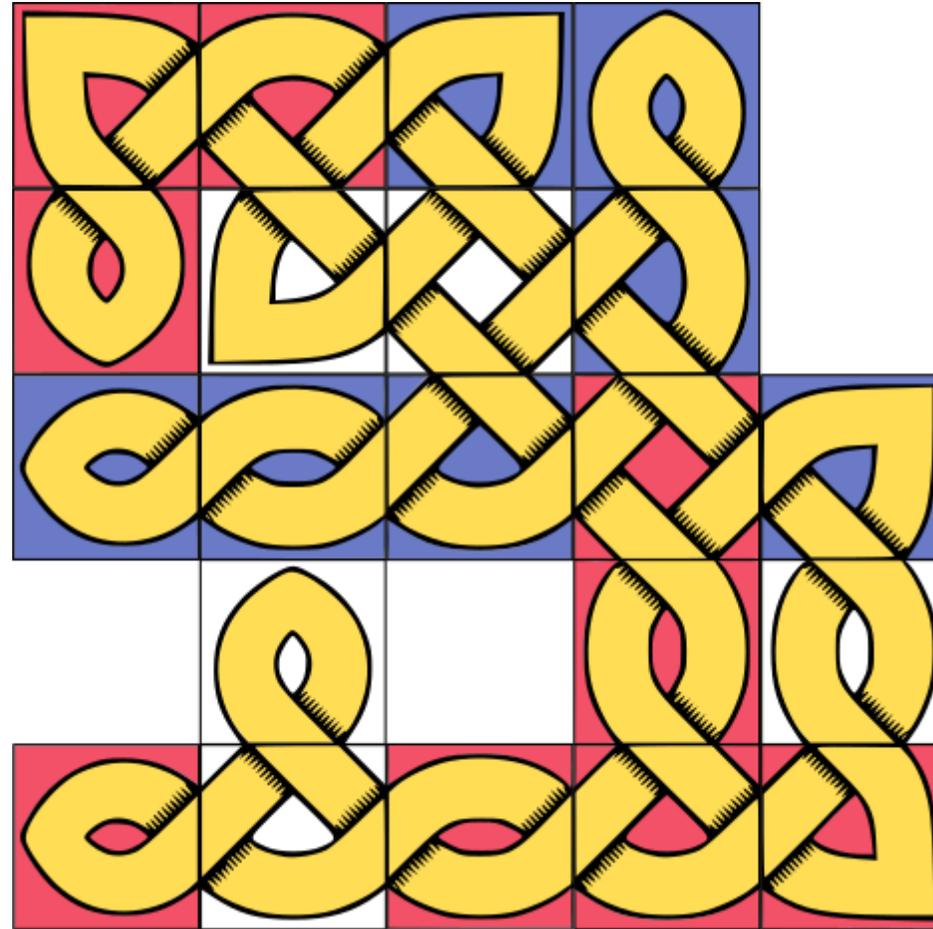


Celtic! - Scoring

Score

Knot 1: Tie

Knot 2: Red (9)



Celtic! - Scoring

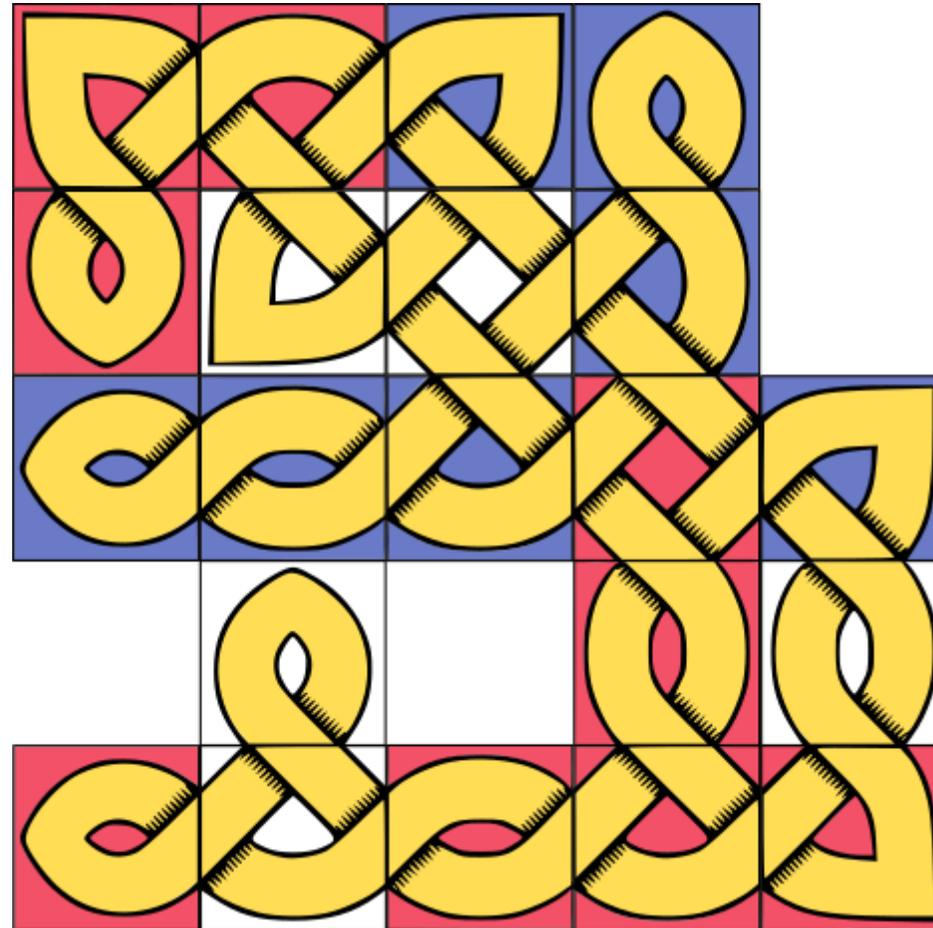
Score

Knot 1: Tie

Knot 2: Red (9)

Knot 3: Blue (5)

Knot 4: Red (4)



Celtic! - Scoring

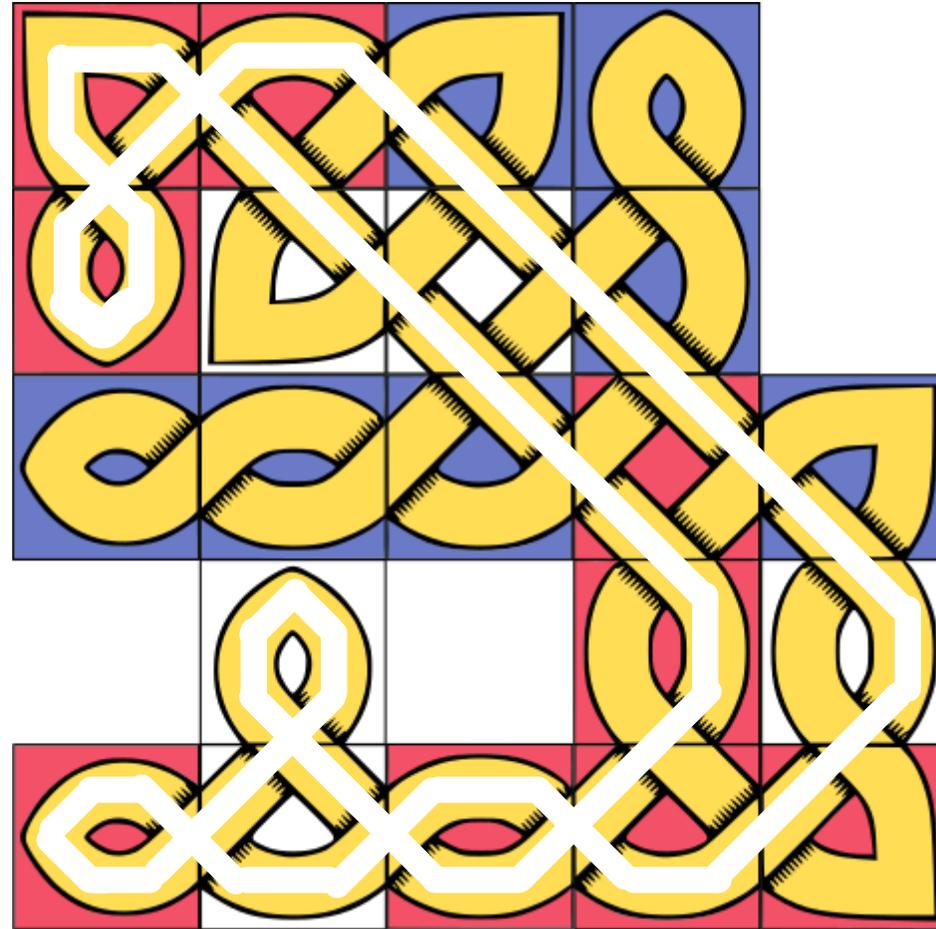
Score

Knot 1: Tie

Knot 2: Red (9)

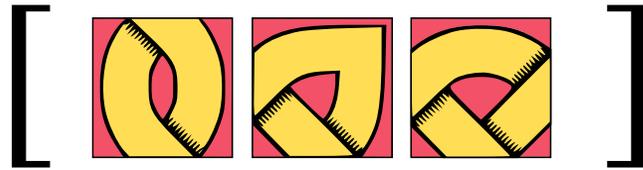
Knot 3: Blue (5)

Knot 4: Red (4)

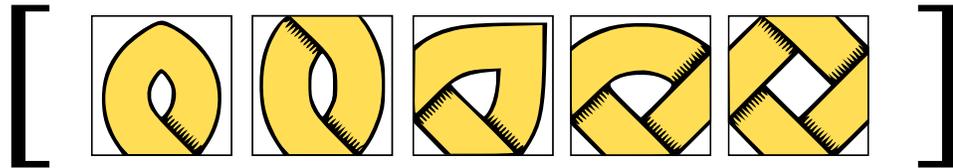


Generalized 1-Player Celtic!

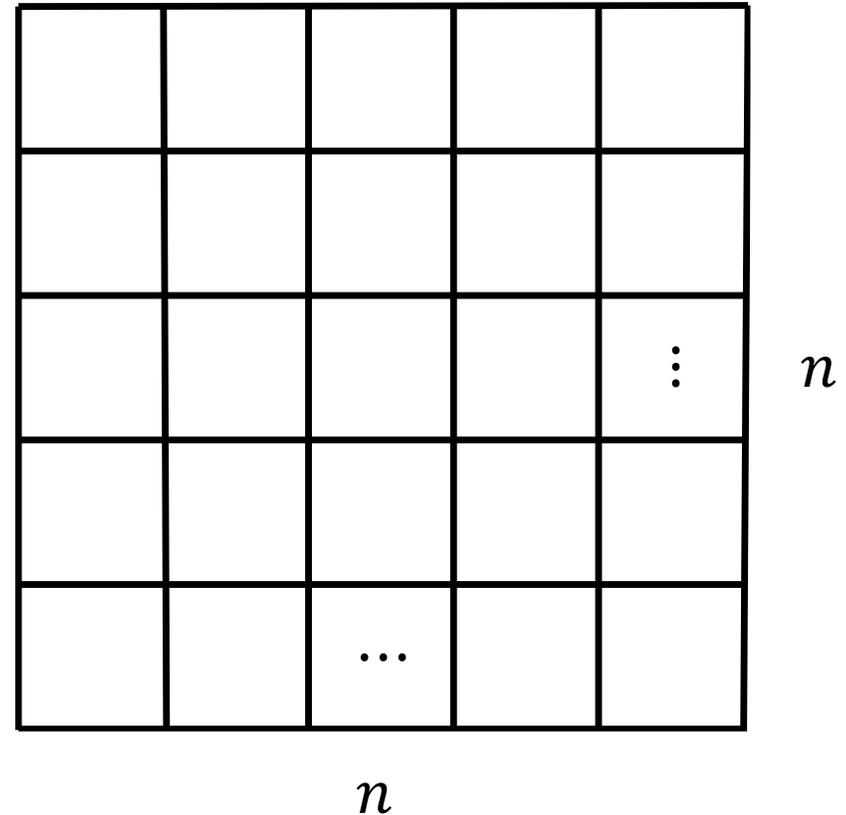
Generalization: 1-Player



Player Pieces

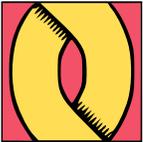
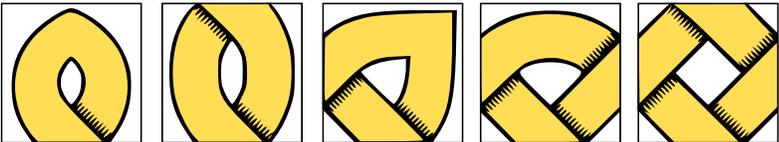


Board Pieces



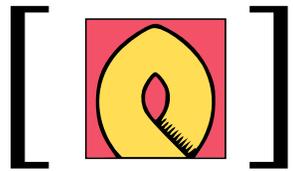
Problem: Can the player build a knot of size $\geq L$ given k pieces?

1-Player Celtic!: The “Easy” problems

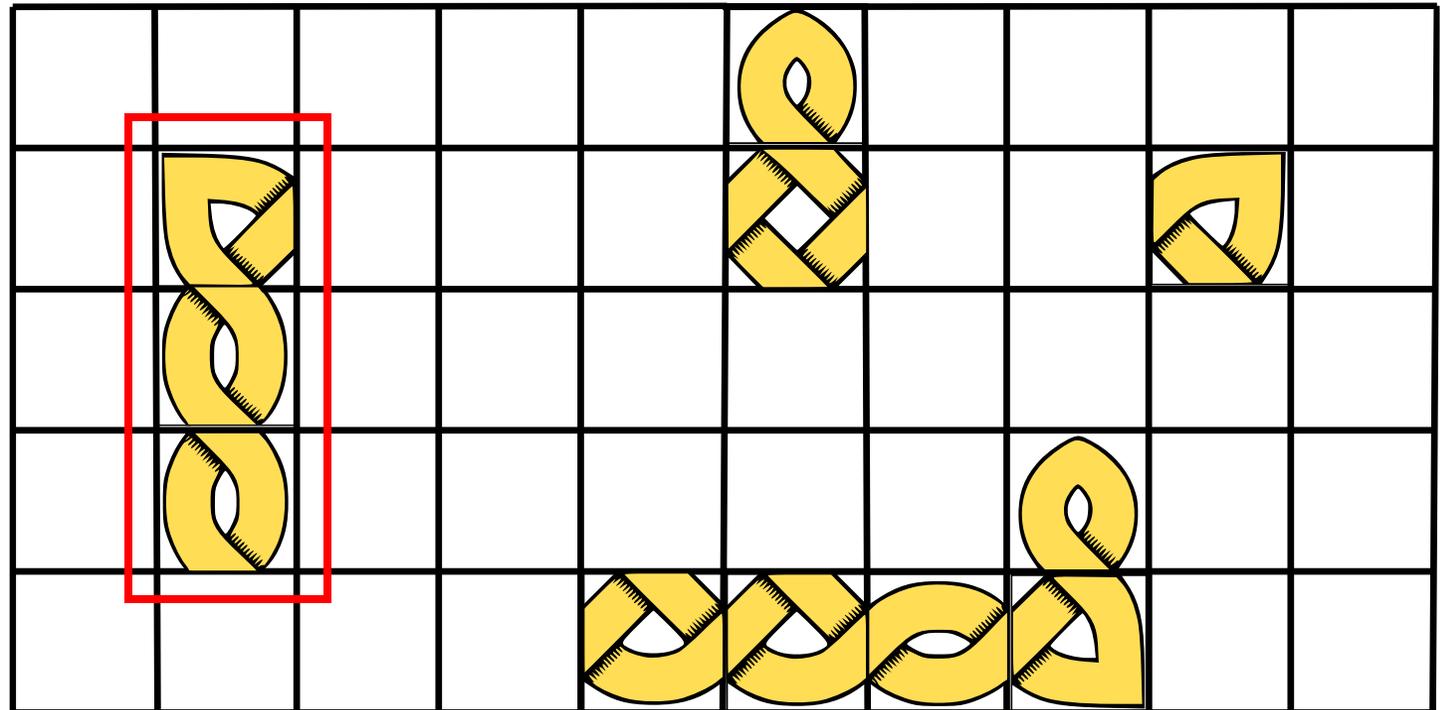
Player Pieces	Board Pieces	Complexity
		
		$O(n^2)$
		

Problem: Can the player build a knot of size $\geq L$ given k pieces?

1-Player Celtic!: The “Easy” problems

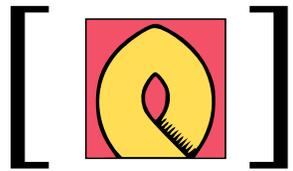


Player Pieces

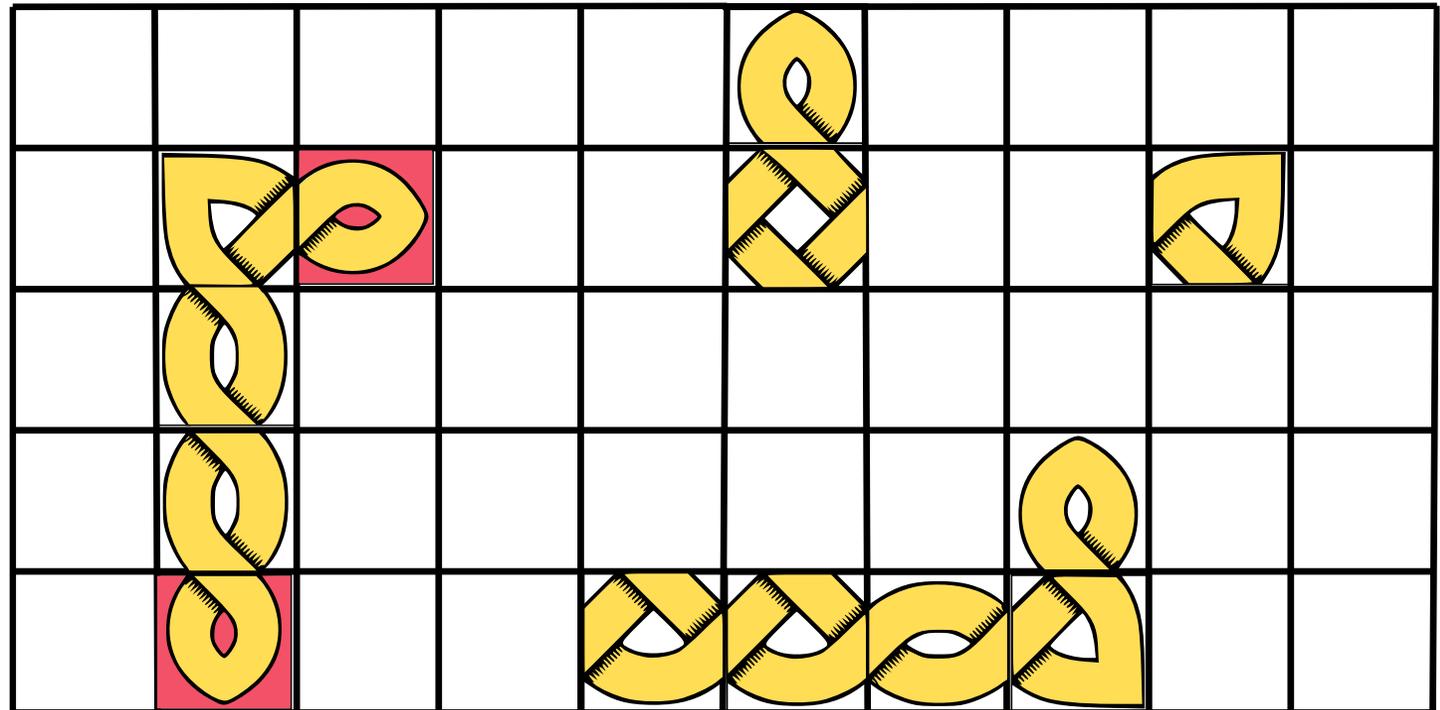


Given: $L = 6, k = 4$

1-Player Celtic!: The “Easy” problems

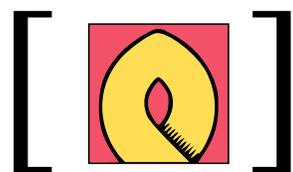


Player Pieces

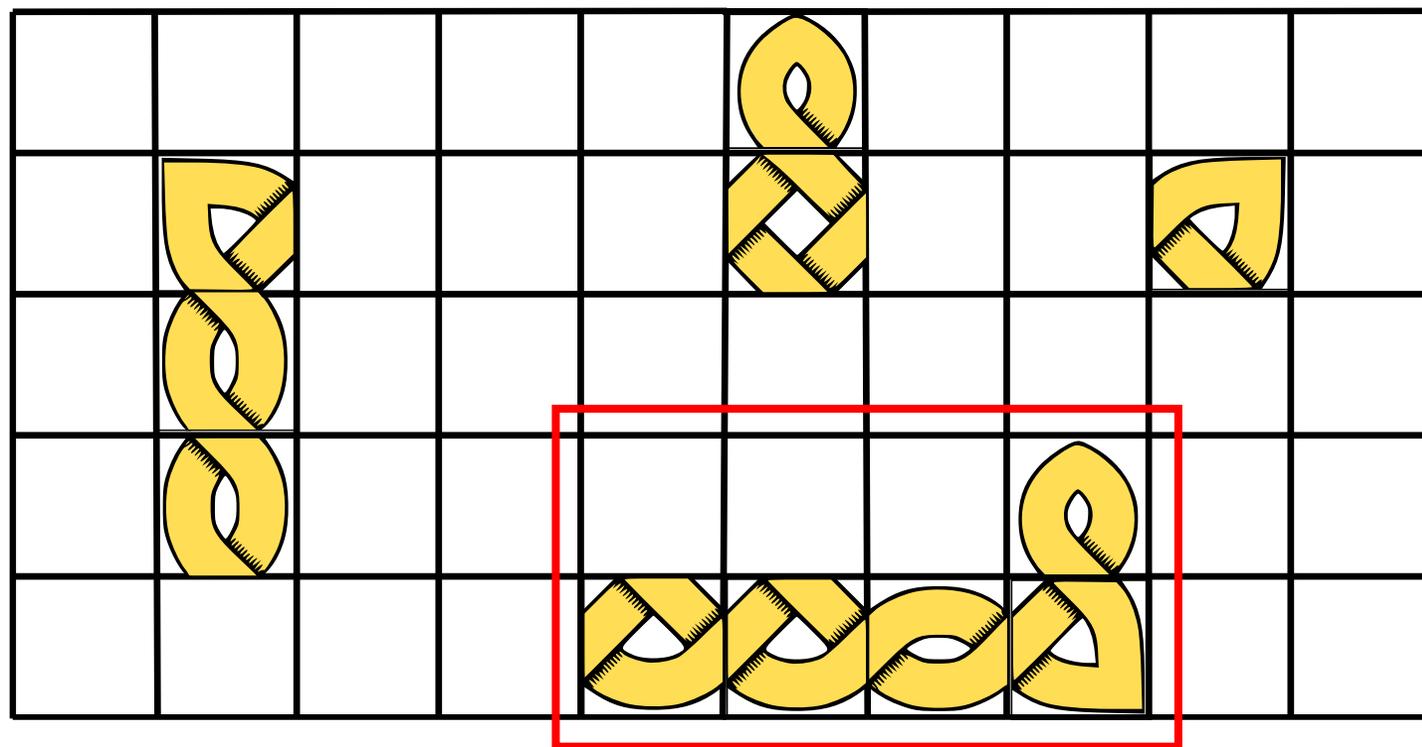


Given: $L = 6, k = 4$

1-Player Celtic!: The “Easy” problems

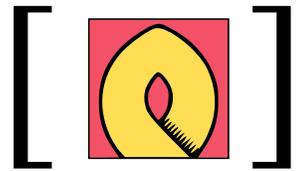


Player Pieces

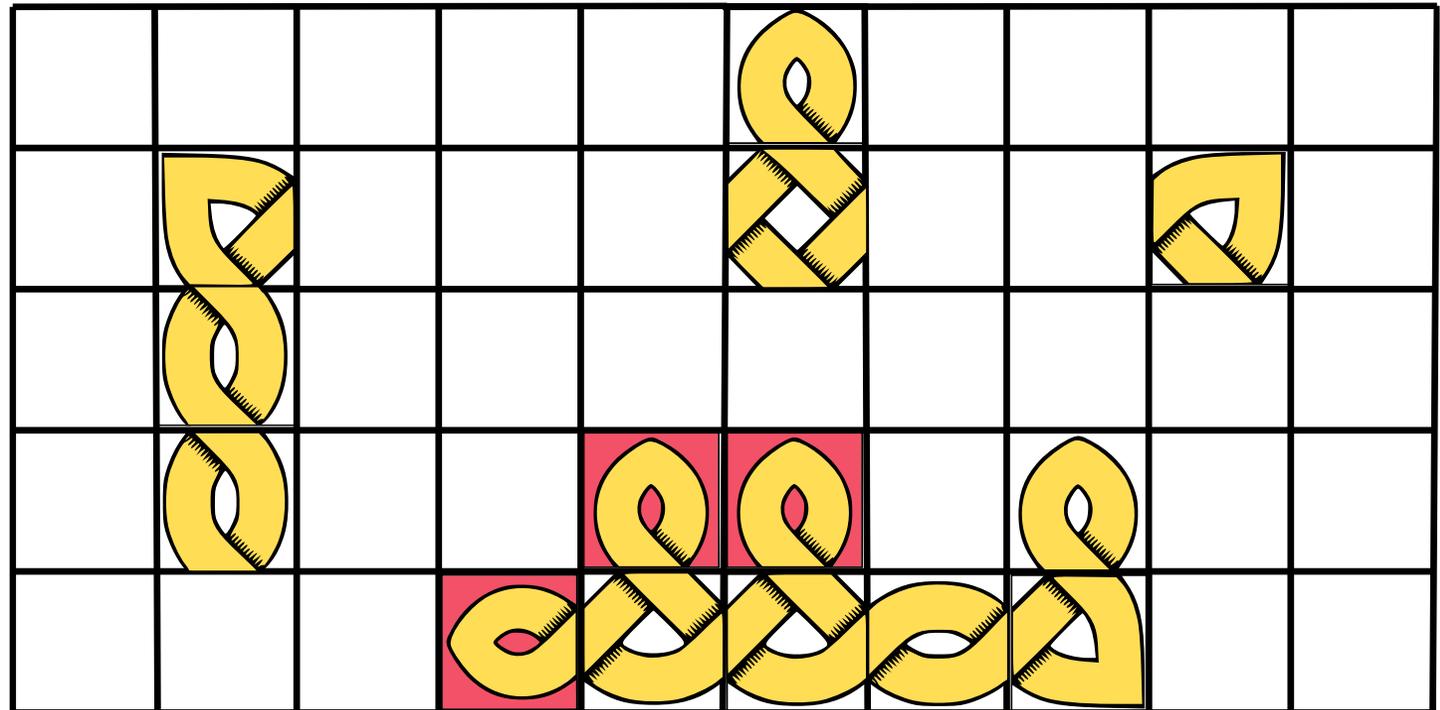


Given: $L = 6, k = 4$

1-Player Celtic!: The “Easy” problems

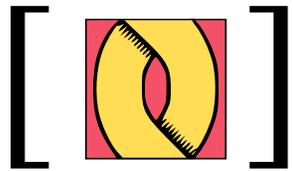


Player Pieces

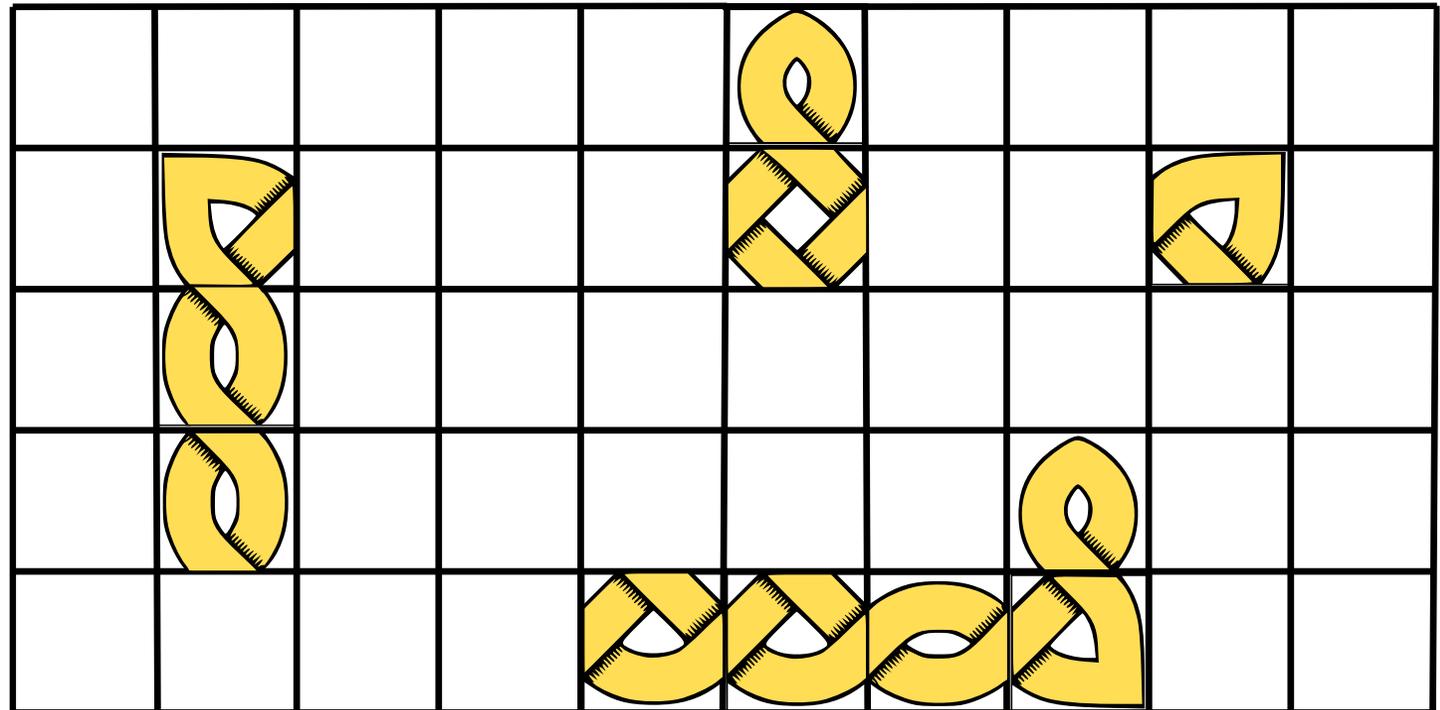


Given: $L = 6$, $k = 4$

1-Player Celtic!: The “Easy” problems

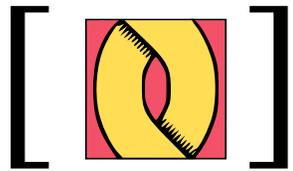


Player Pieces

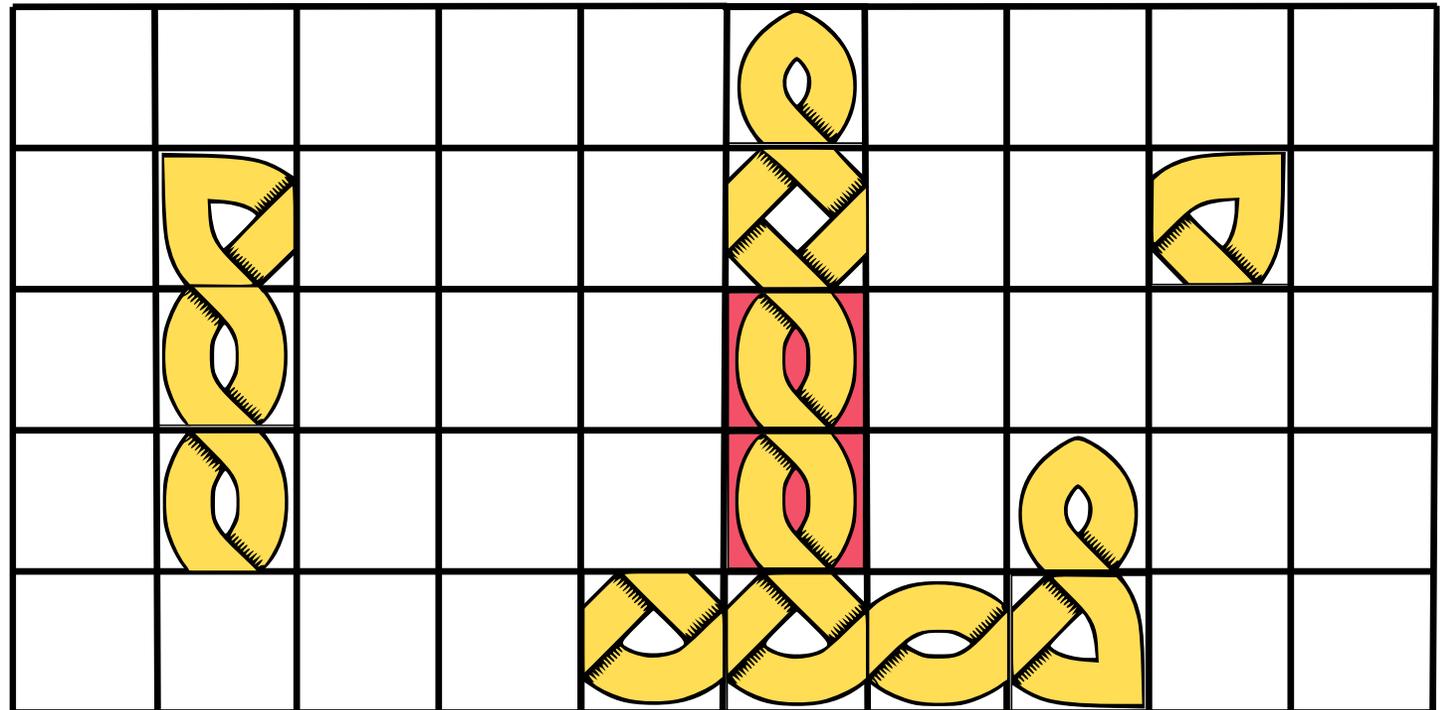


Given: $L = 6$, $k = 4$

1-Player Celtic!: The “Easy” problems

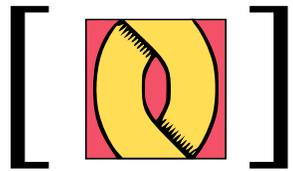


Player Pieces

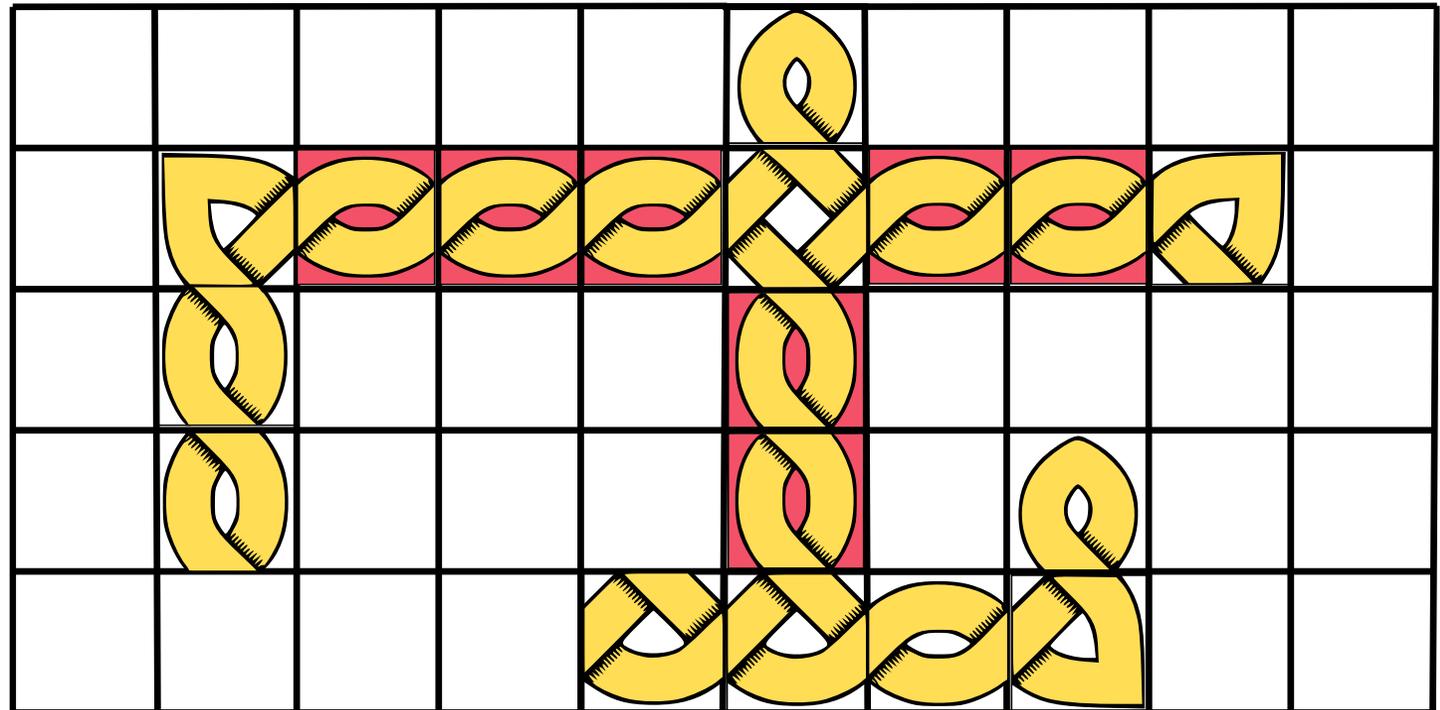


Given: $L = 6, k = 4$

1-Player Celtic!: The “Easy” problems

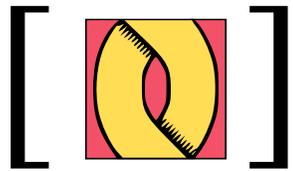


Player Pieces

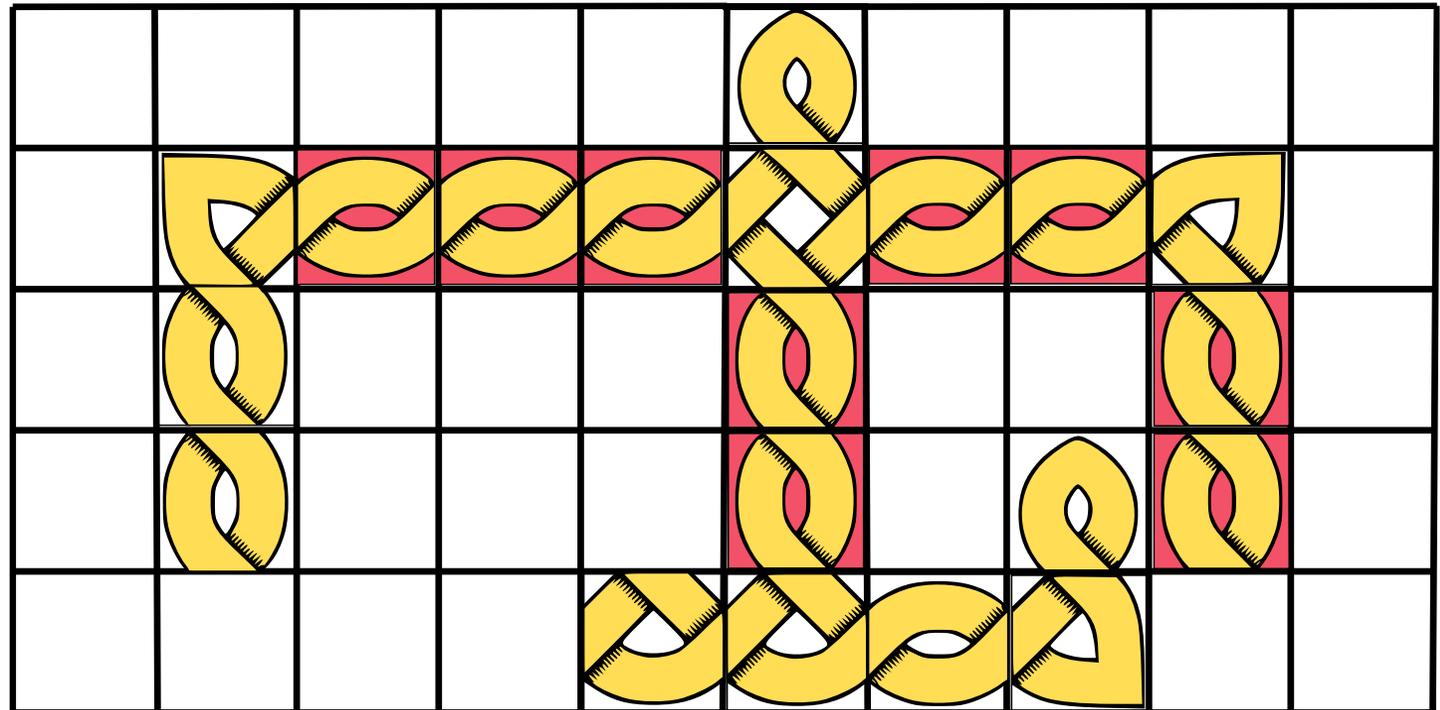


Given: $L = 6$, $k = 4$

1-Player Celtic!: The “Easy” problems

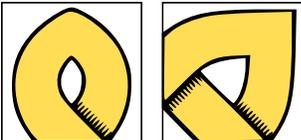
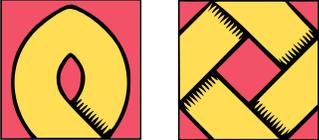
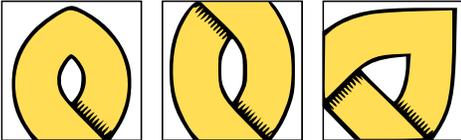


Player Pieces



Given: $L = 6$, $k = 4$

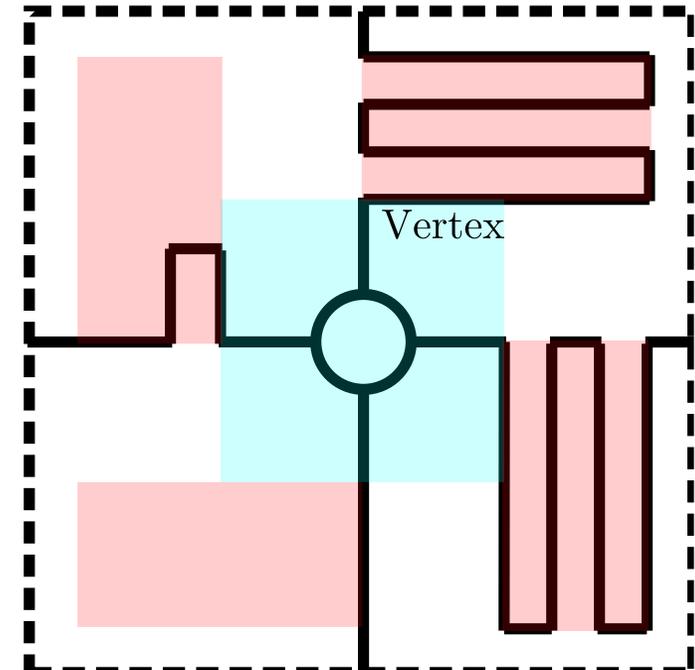
1-Player Celtic!: The “Hard” problems

Player Pieces	Board Pieces	Complexity
		<i>NP-complete</i>
		
		

Problem: Can the player build a knot of size $\geq L$ given k pieces?

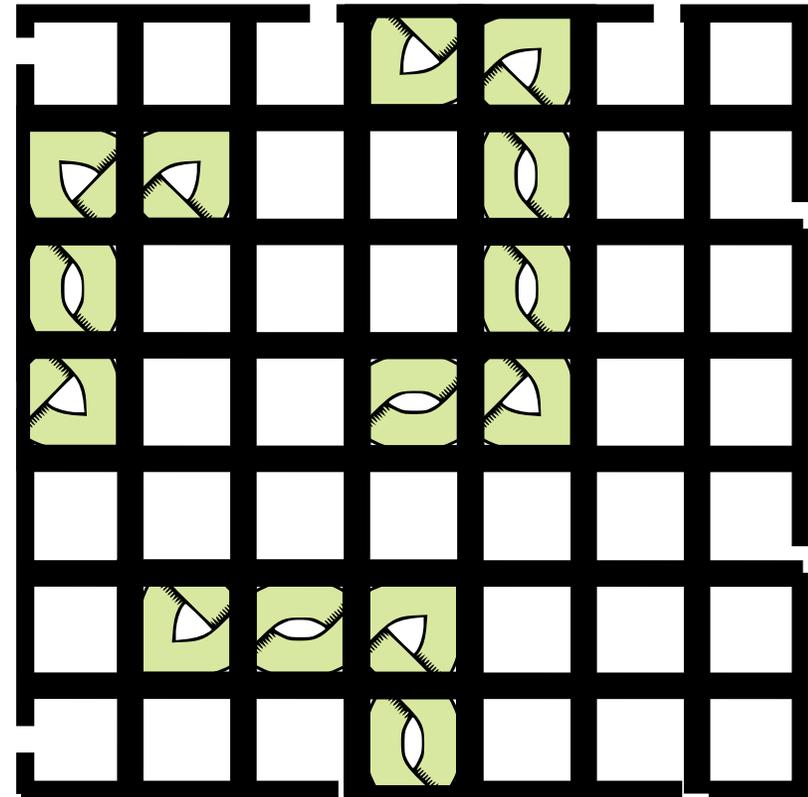
1-Player Celtic!: The “Hard” problems

- Planar, directed Hamiltonian Cycle with max degree 3
- Transform graph into equivalent rectilinear embedding with area $(|V| + 1) \times (|V| + 1)$
- Scale new graph by $O(|V|)$
- Edges are pumped to be roughly the same



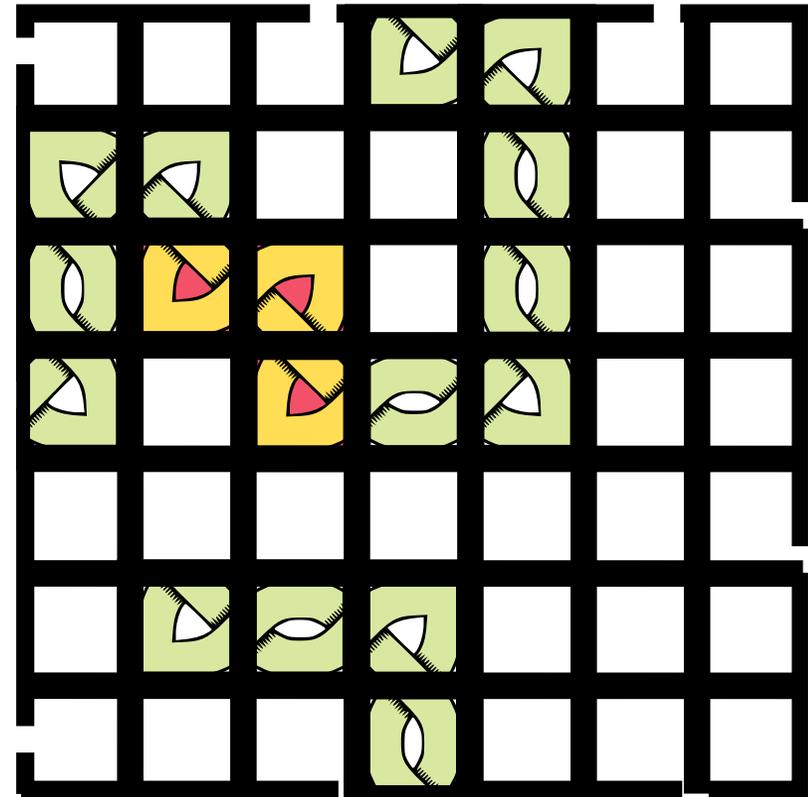
1-Player Celtic!: The “Hard” problems

- Center piece represents the “vertex”
- Incoming edge(s) are moved to one side
- Outgoing edge(s) are moved to the other side
- The “choice” is made by the played pieces

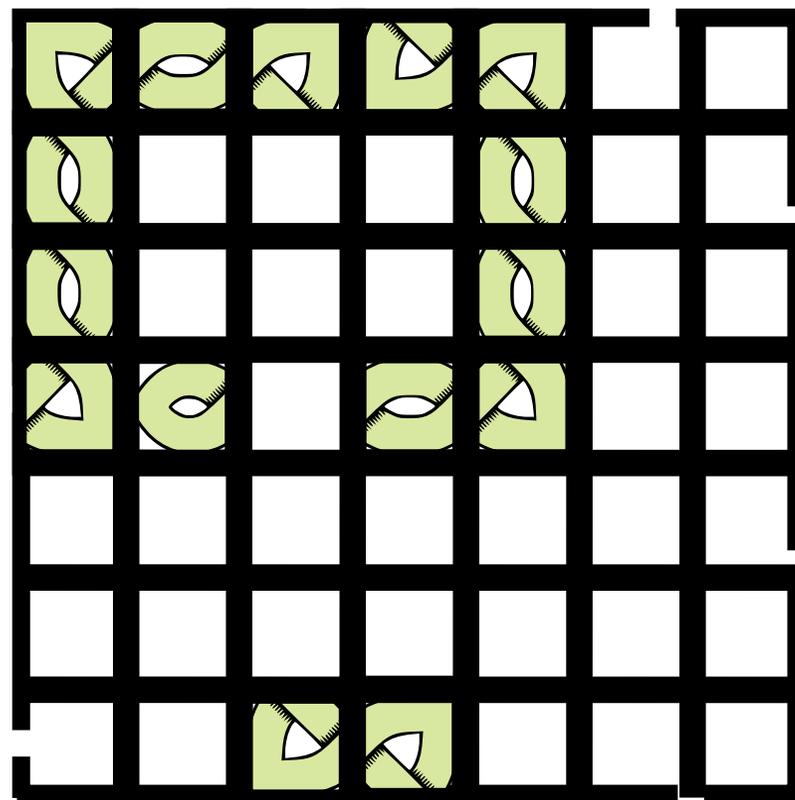
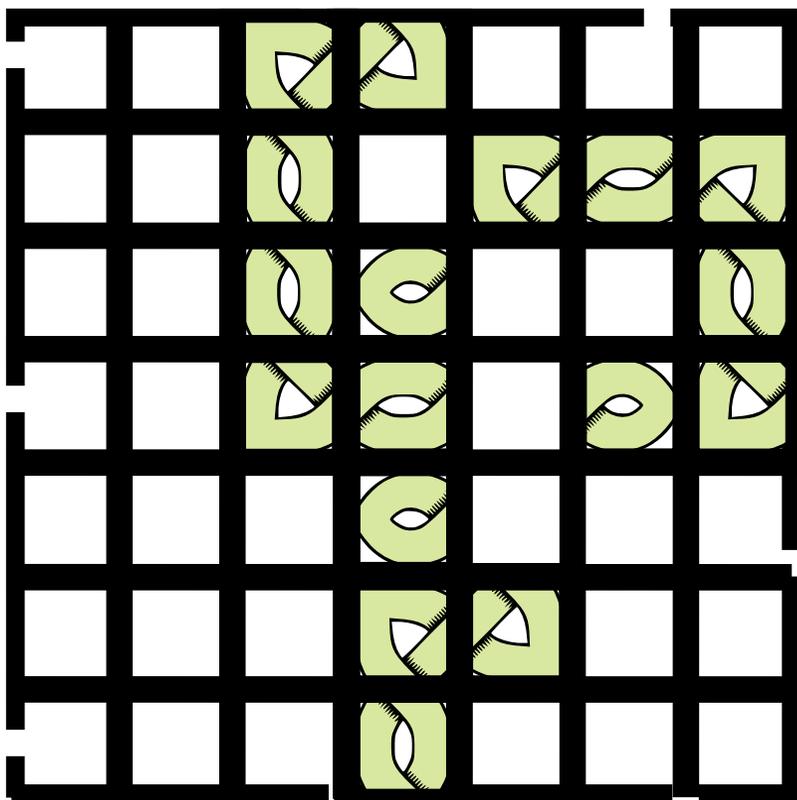


1-Player Celtic!: The “Hard” problems

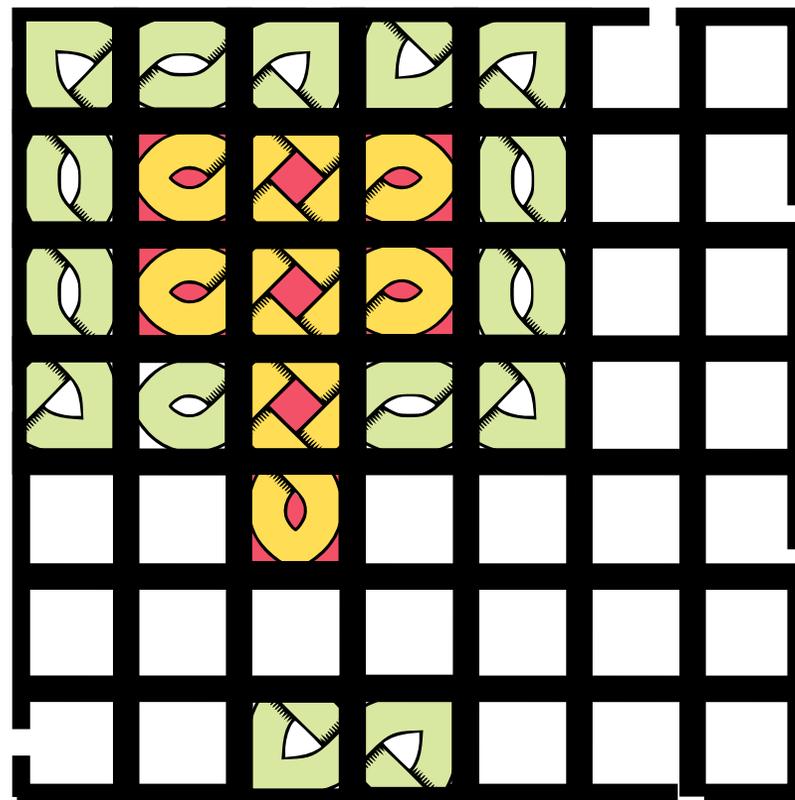
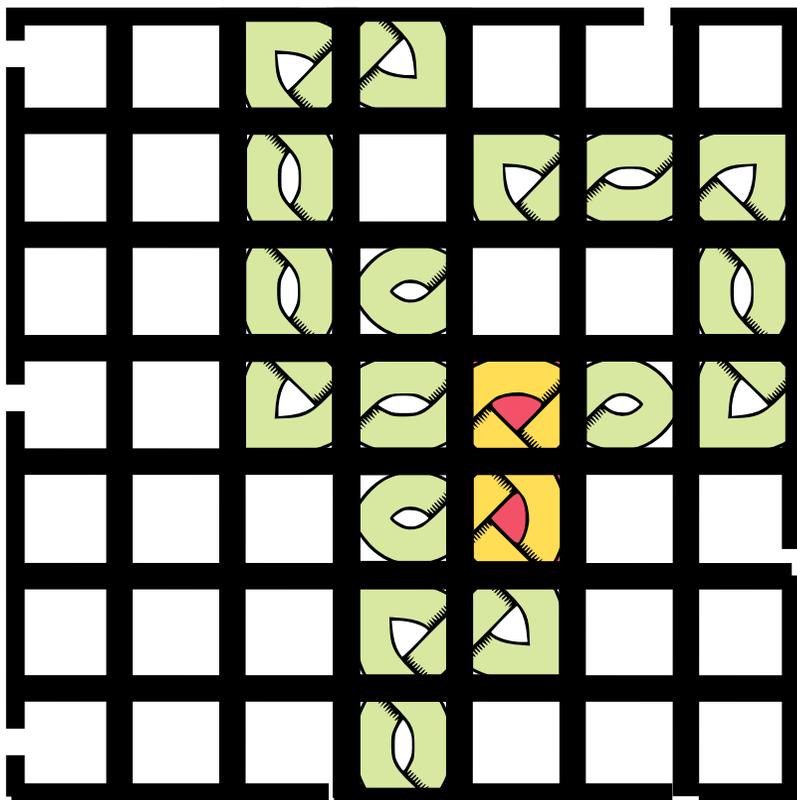
- Center piece represents the “vertex”
- Incoming edge(s) are moved to one side
- Outgoing edge(s) are moved to the other side
- The “choice” is made by the played pieces



1-Player Celtic!: The “Hard” problems



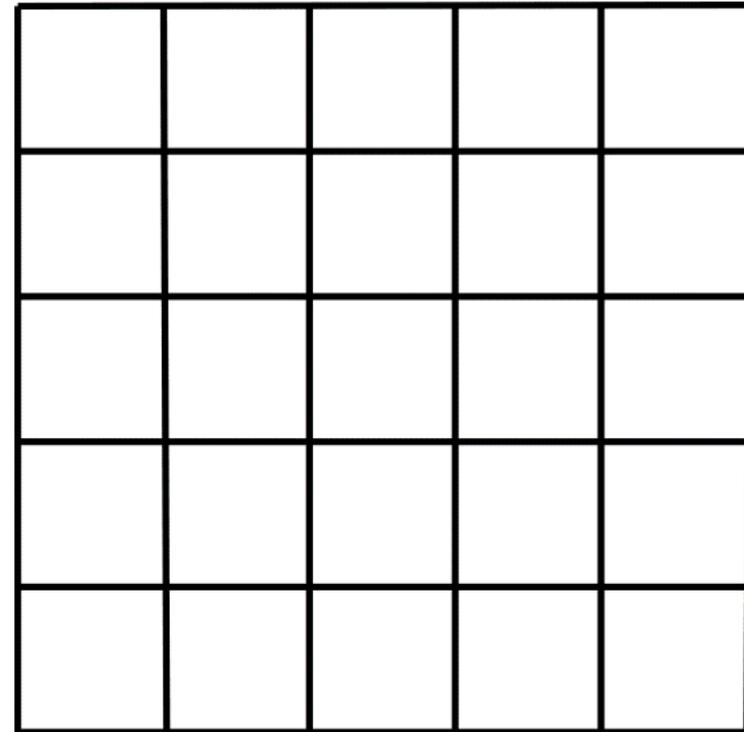
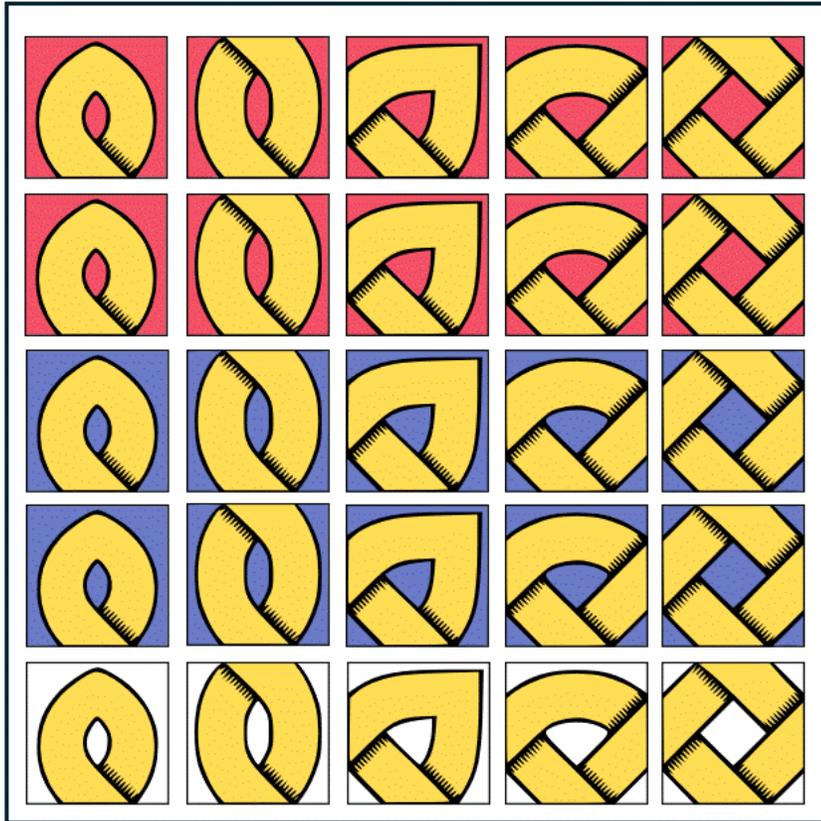
1-Player Celtic!: The “Hard” problems



Conclusion

- Some piece combinations missing for Generalized 1-Player Celtic!
- More balanced pieces for Generalized 2-Player Celtic!
- FPT, approximations for maximally sized knots
- Is Celtic! a 1st player win, 2nd player win, or a draw?
- Pattern based complexity of the knots.
- Consider $>$ genus-1 knot assembly.

Tile-based Knot Assembly with Celtic!



Authors: Divya Bajaj, **Ryan Knobel**, Juan Manuel Perez, Rene Reyes,
Ramiro Santos, Tim Wylie