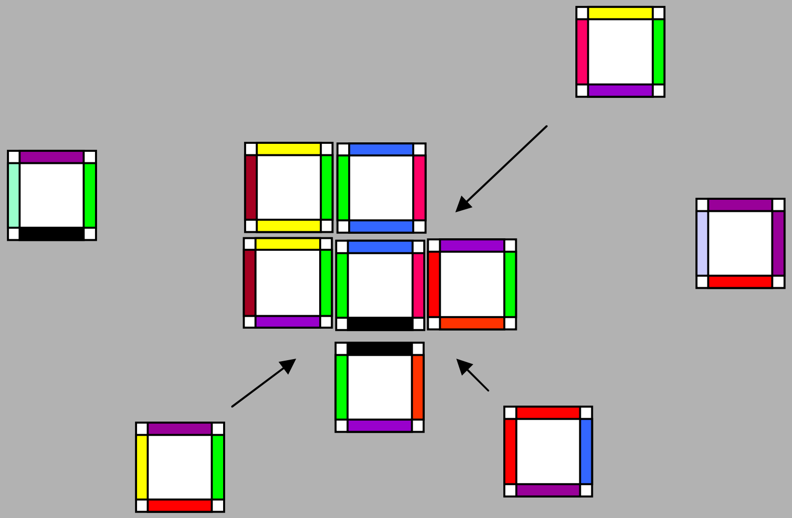
Staged Self-Assembly:
Nanomanufacture of Arbitrary Shapes with O(1) Glues

Thirteenth International Meeting on DNA Computers

June 5, 2007

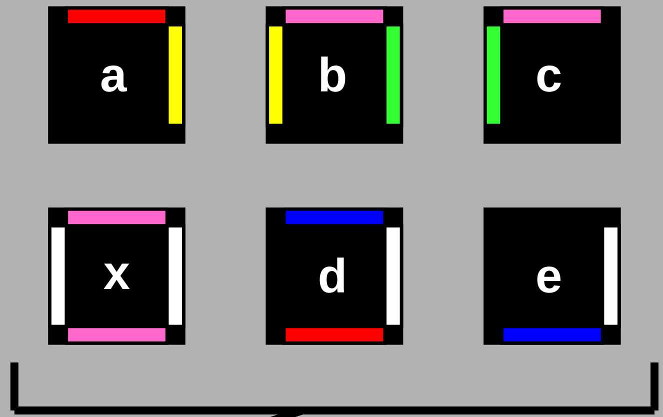


Eric Demaine **Massachusetts Institute of Technology**
Martin Demaine **Massachusetts Institute of Technology**
Sandor Fekete **Technische Universität Braunschweig**
Mashood Ishaque **Tufts University**
Eynat Rafalin **Google**
Robert Schweller **University of Texas Pan American**
Diane Souvaine **Tufts University**

Tile Assembly Model

(Rothemund, Winfree, Adleman)

T =



Tile Set:

Glue Function:

G(y) = 2
G(g) = 2
G(r) = 2
G(b) = 2
G(p) = 1
G(w) = 1

Temperature: t = 2

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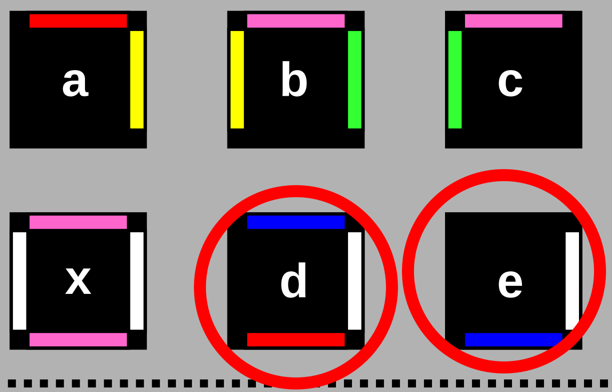
T = 

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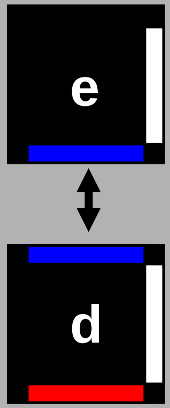

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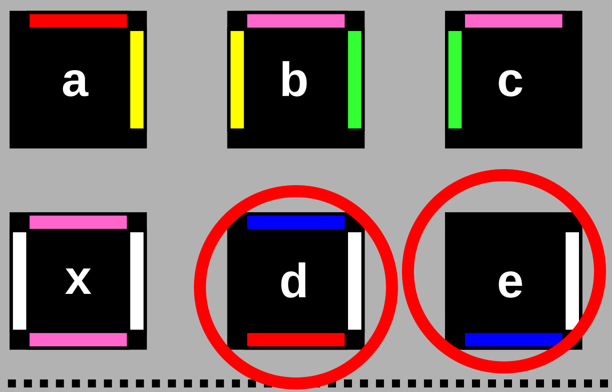

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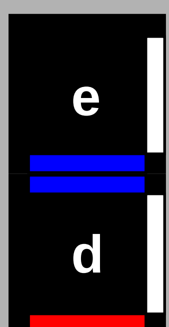

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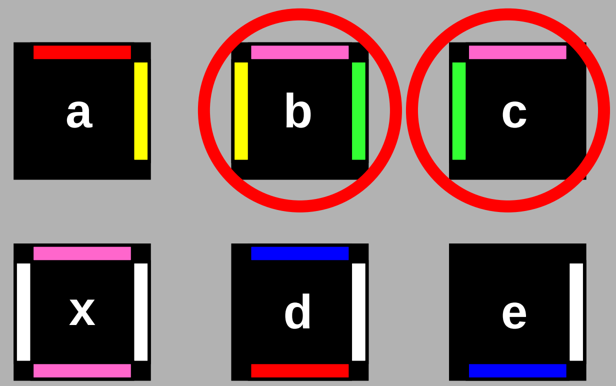

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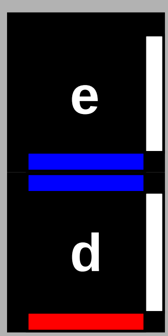
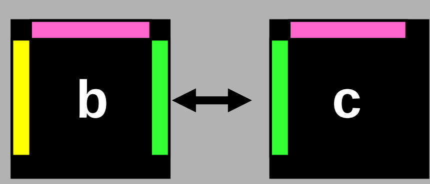


$t = 2$



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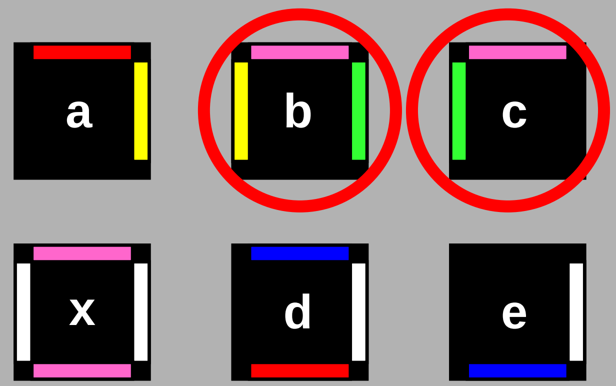

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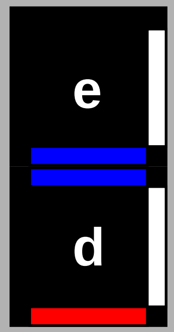

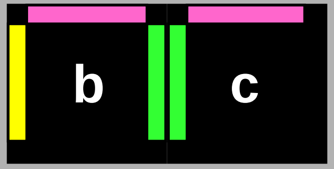

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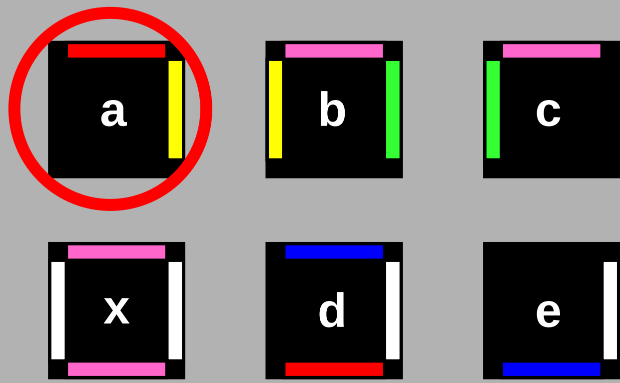

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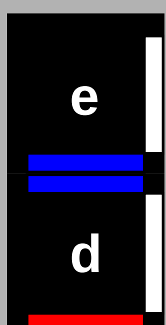

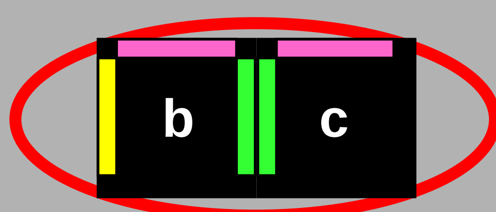

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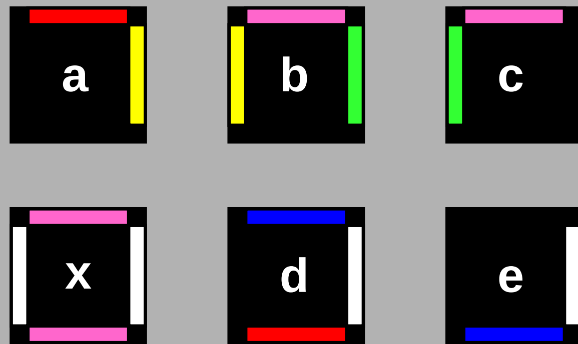

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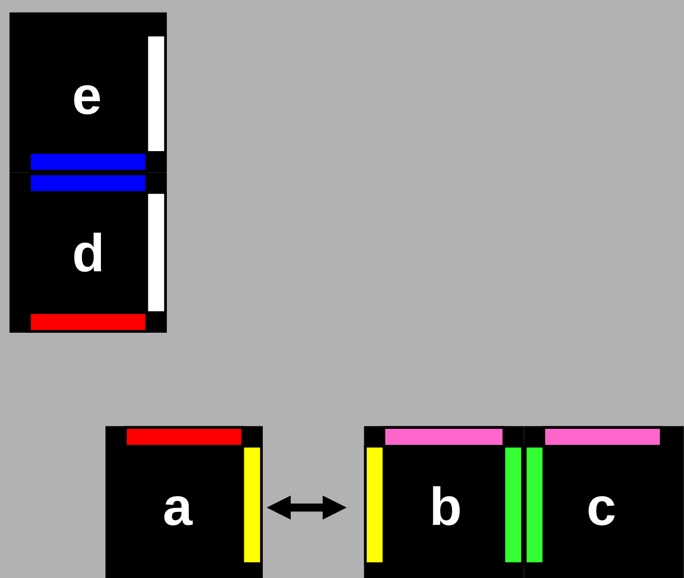

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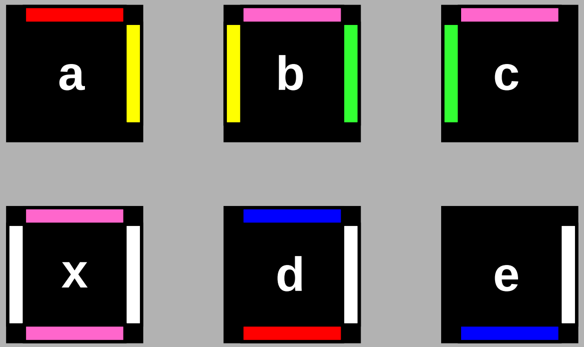

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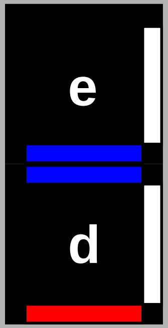

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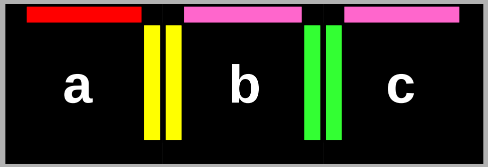

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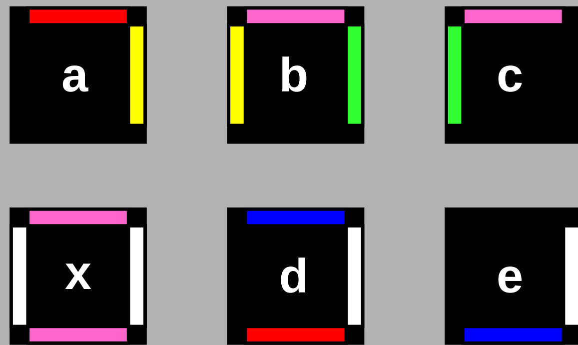

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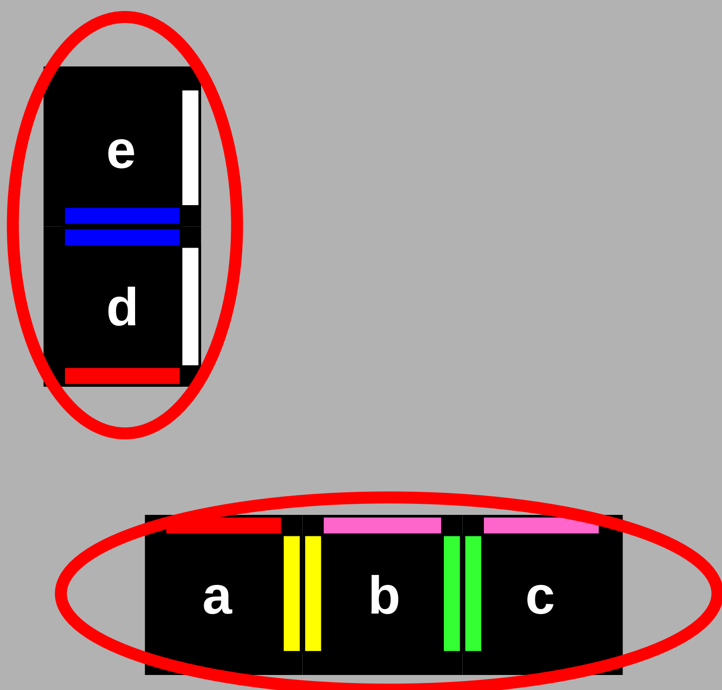

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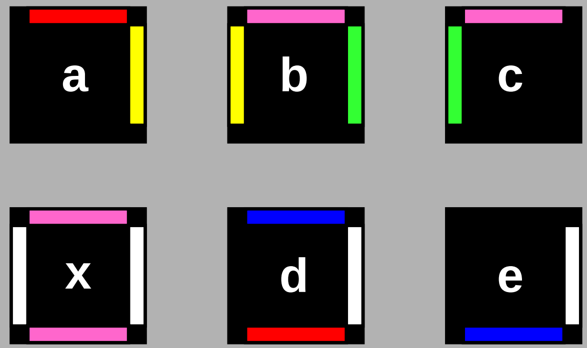

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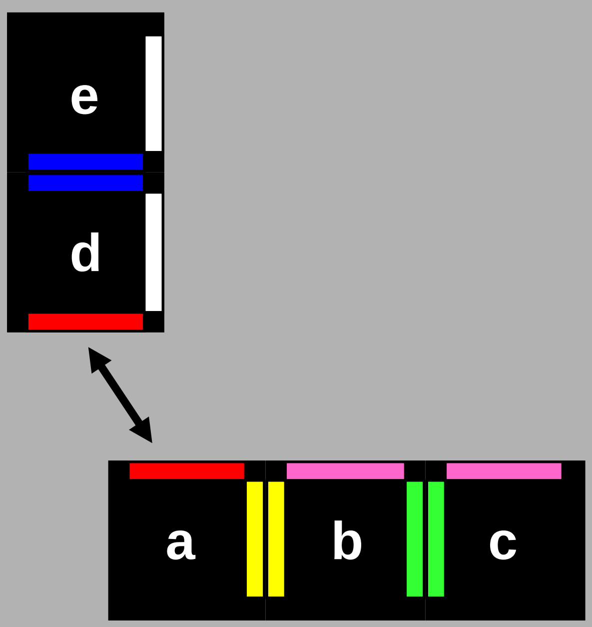

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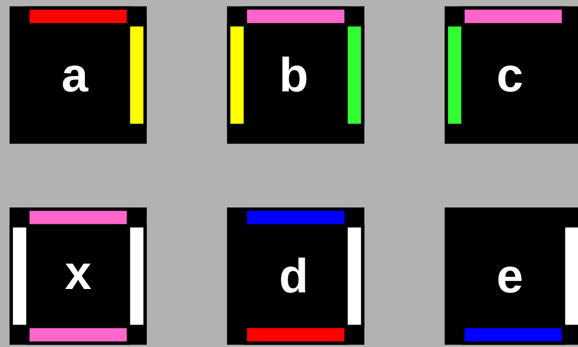

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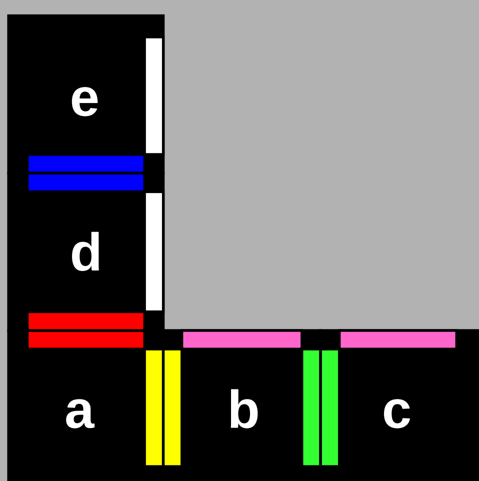

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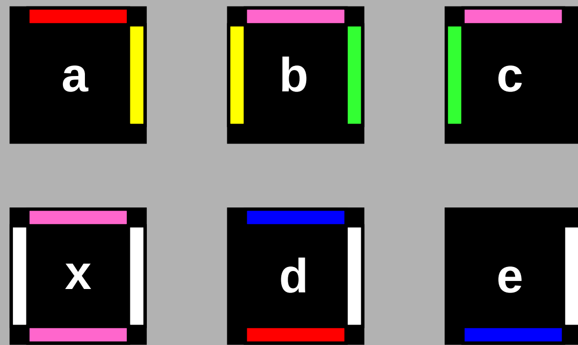

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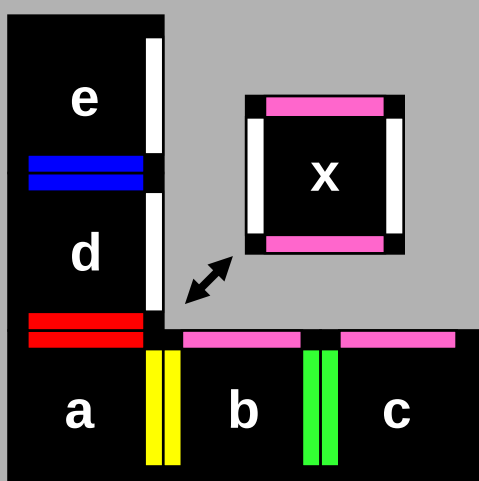

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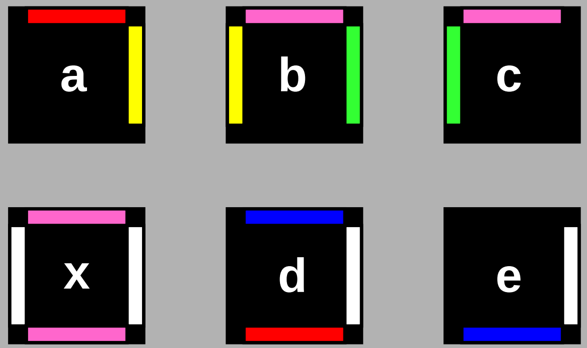
T = 

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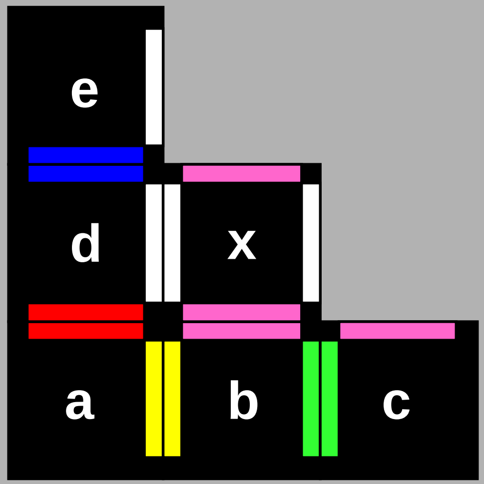

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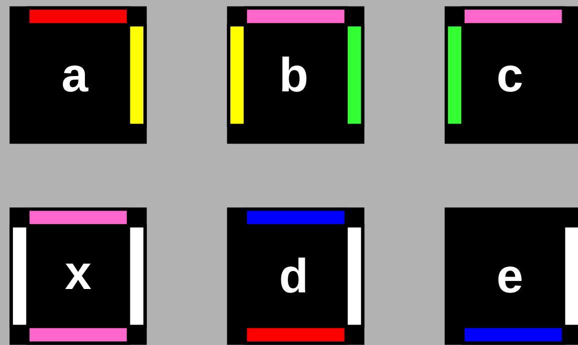

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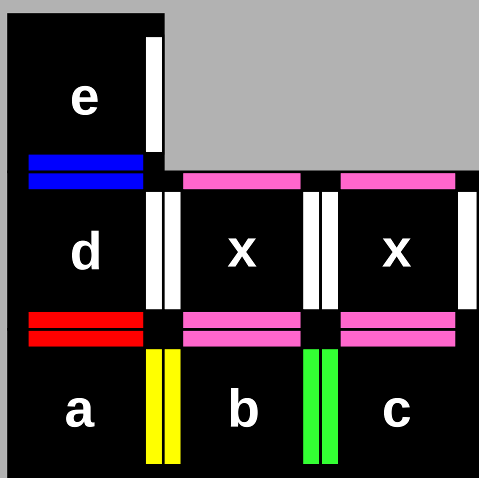

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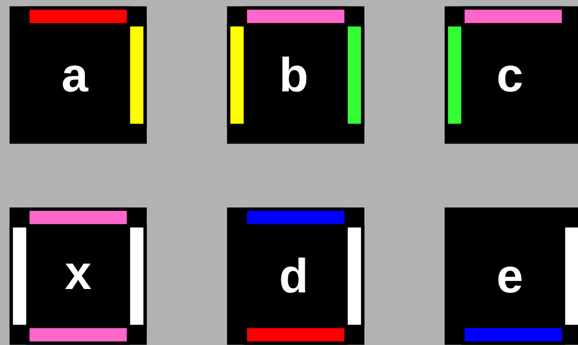

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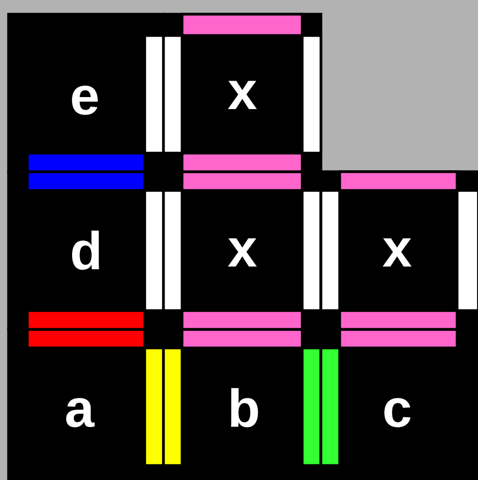

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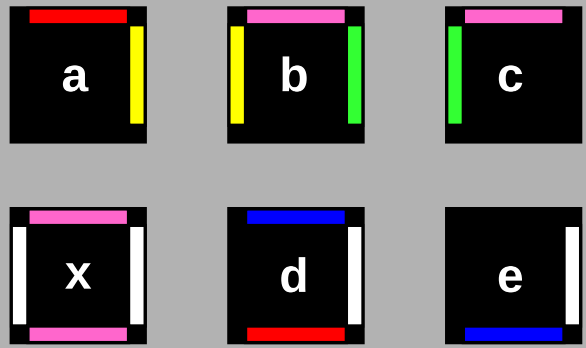
T = 

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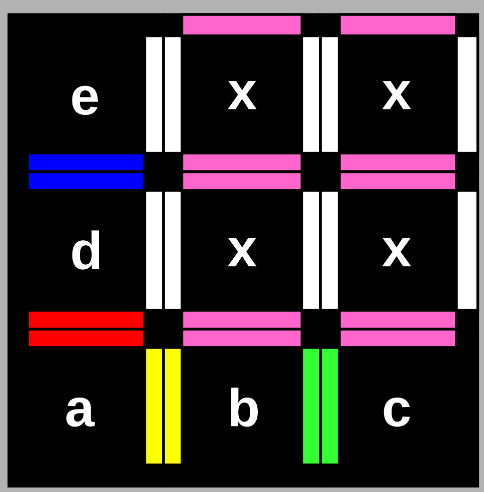

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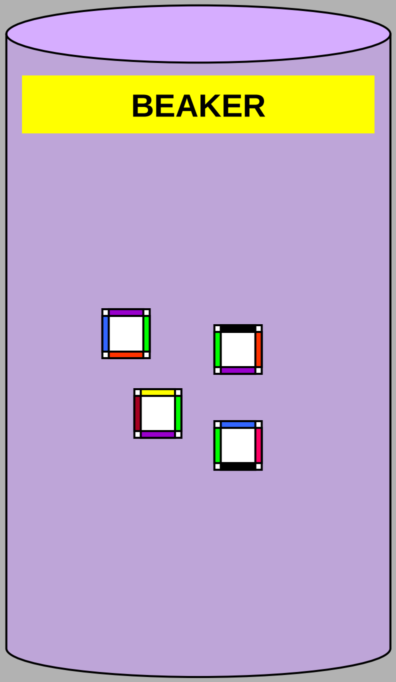
Non-Staged Assembly

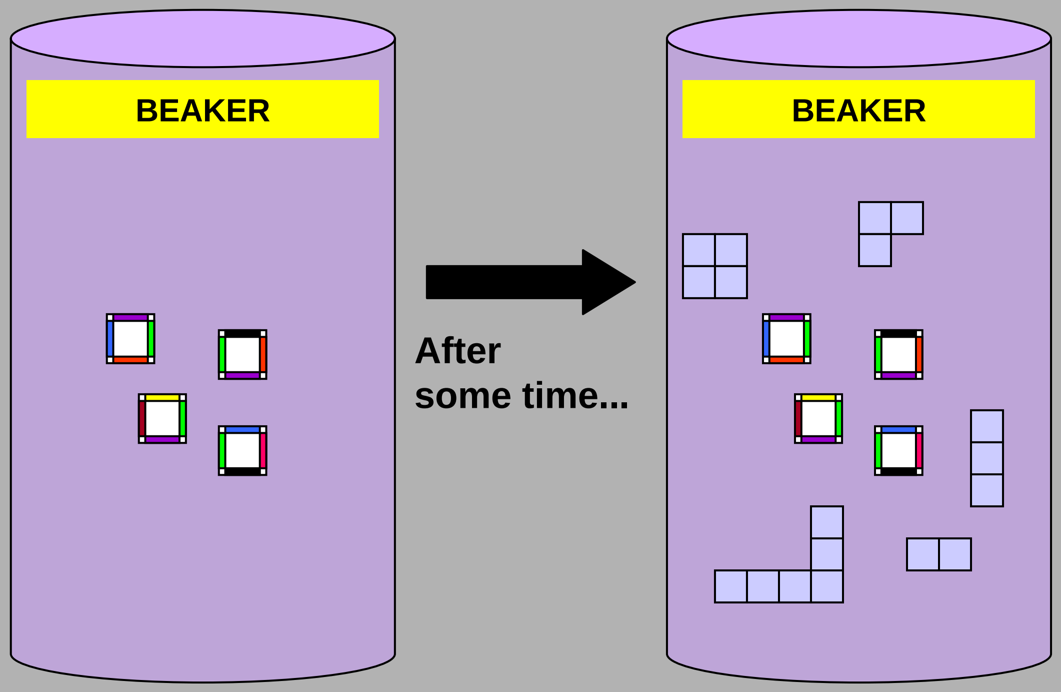


Start with initial Tileset

-Assembly occurs within 1 single container

- Assembly occurs within 1 single stage

Non-Staged Assembly



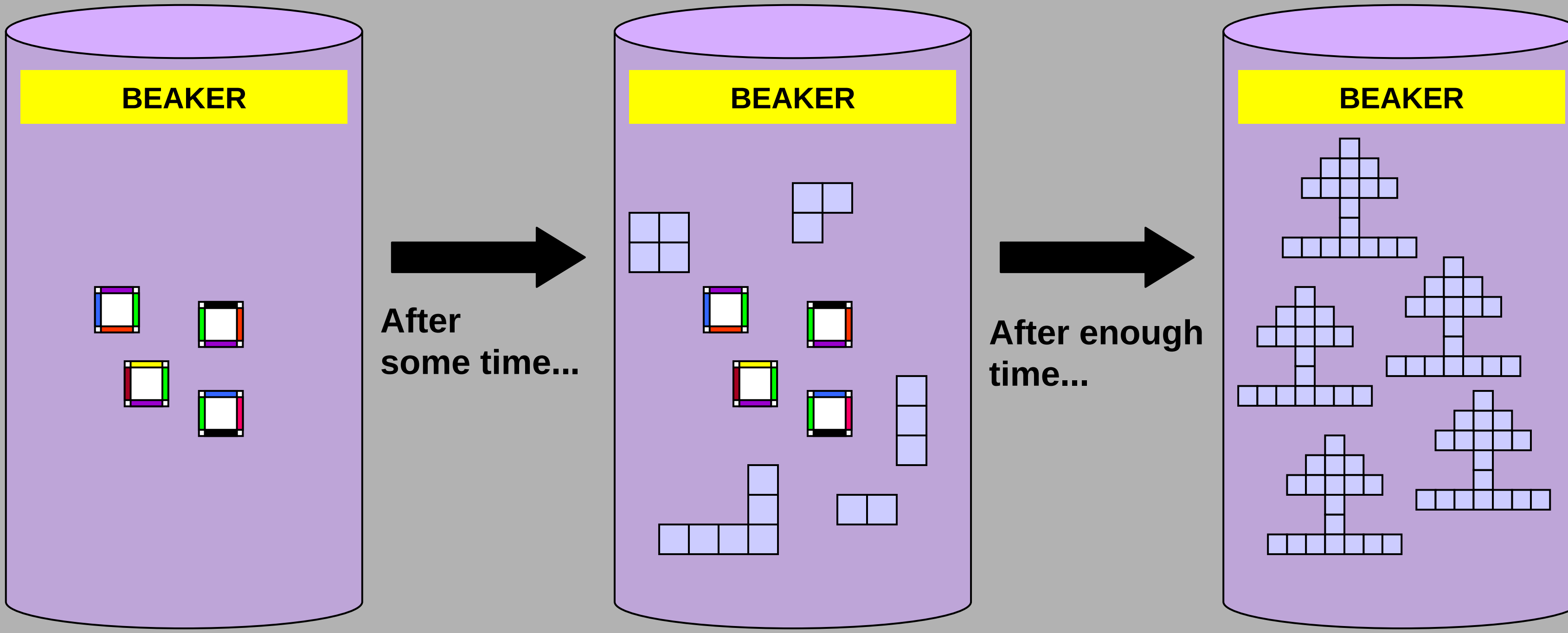
Start with initial Tileset

Various Producible Supertiles exist in solution

-Assembly occurs within 1 single container

- Assembly occurs within 1 single stage

Non-Staged Assembly



Start with initial **Tileset**

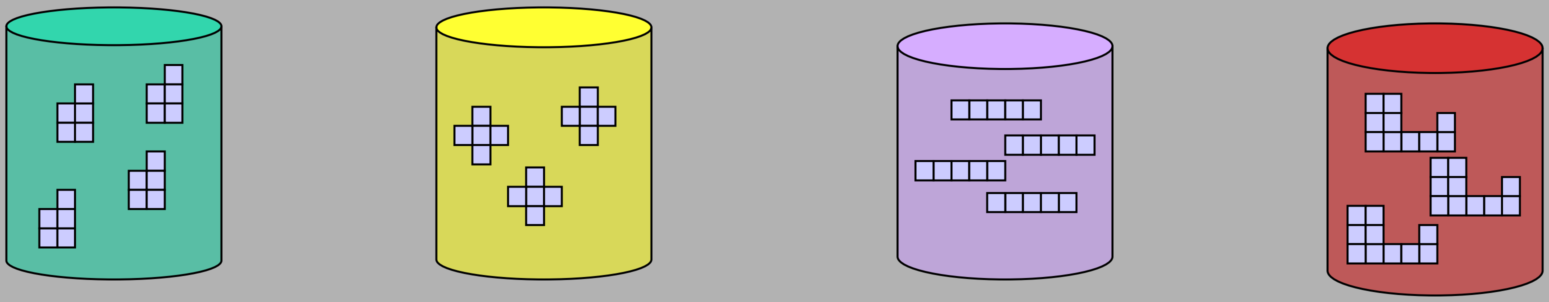
Various **Producible Supertiles** exist in solution

Only **Terminally Produced** assemblies remain

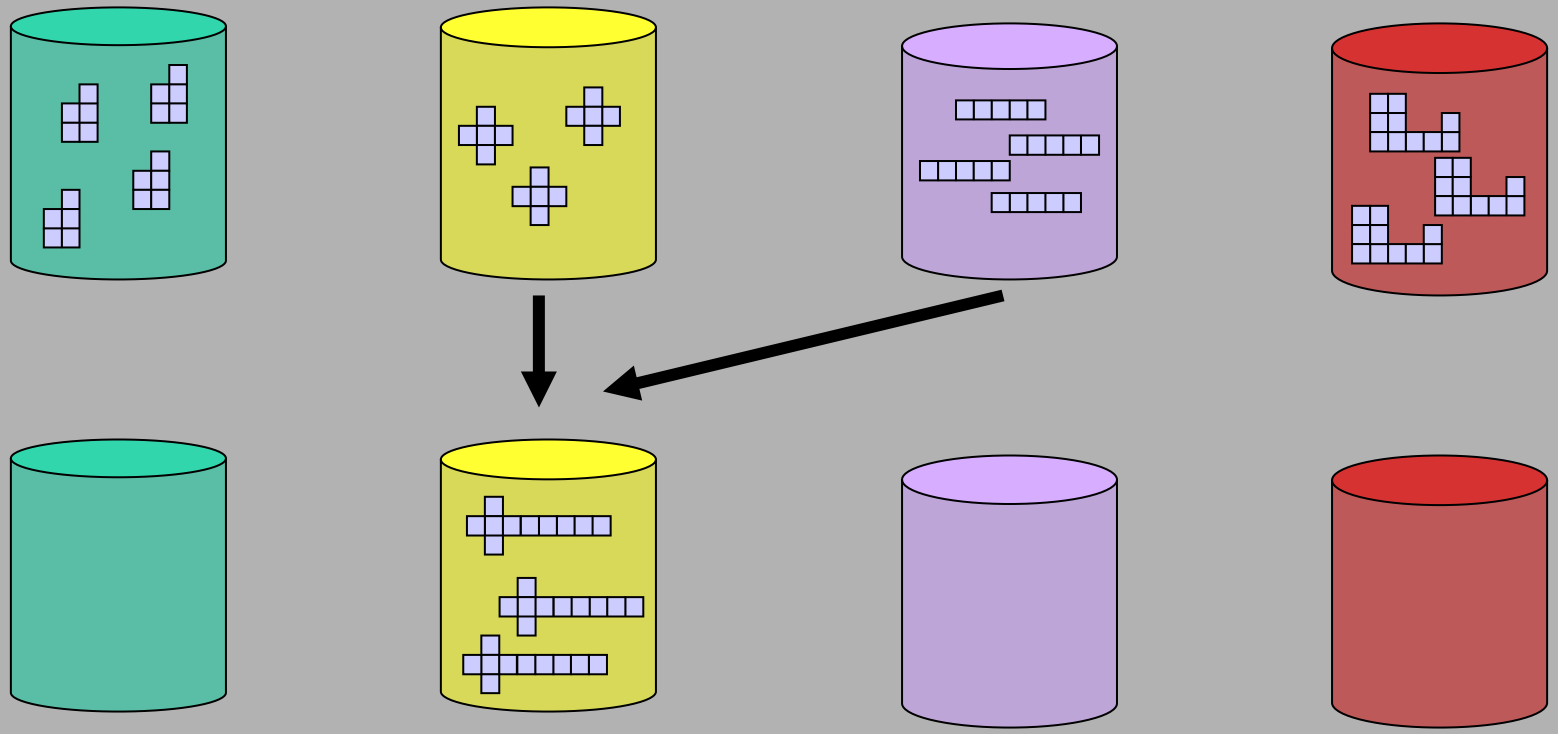
- Assembly occurs within 1 single container

- Assembly occurs within 1 single stage

Staged Assembly

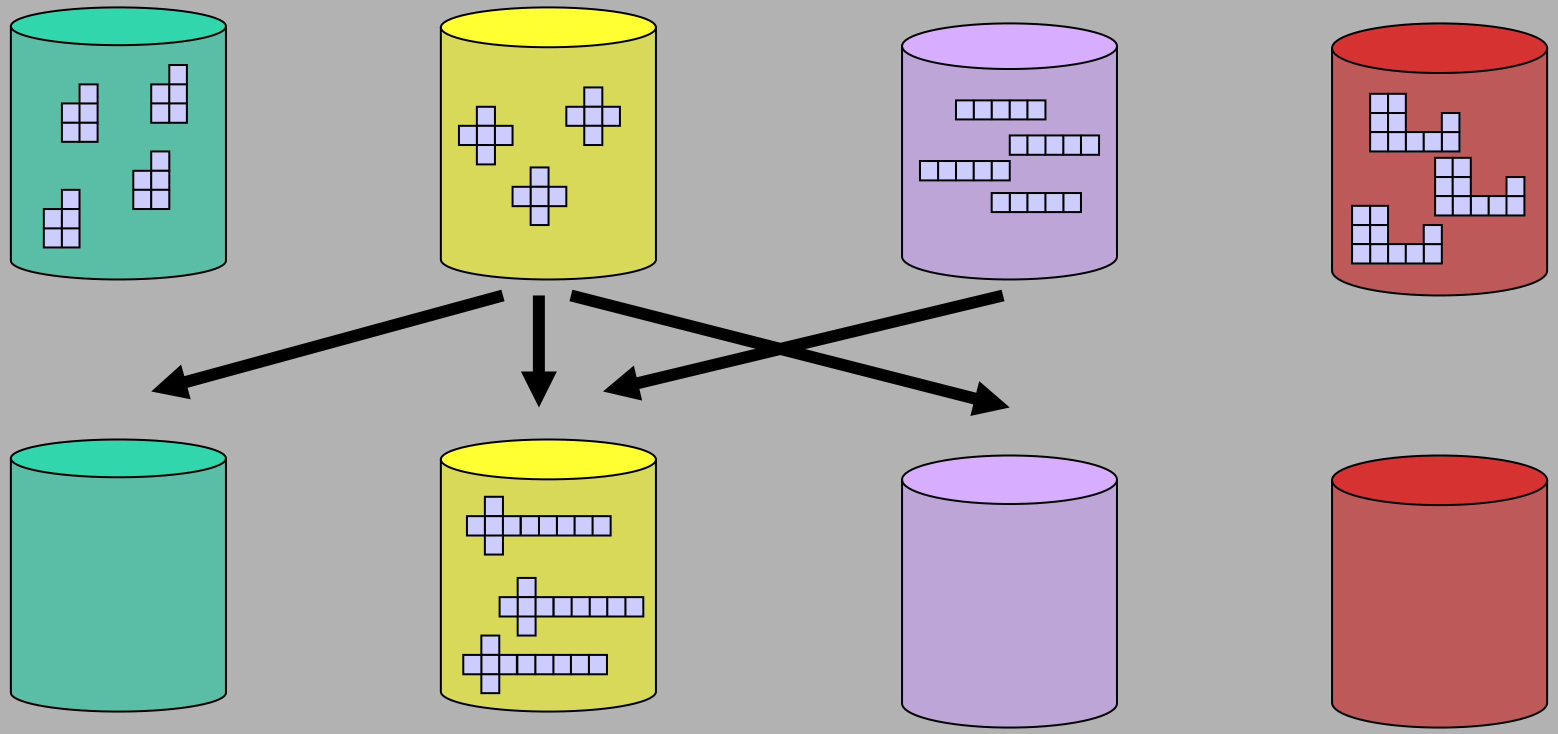


Staged Assembly



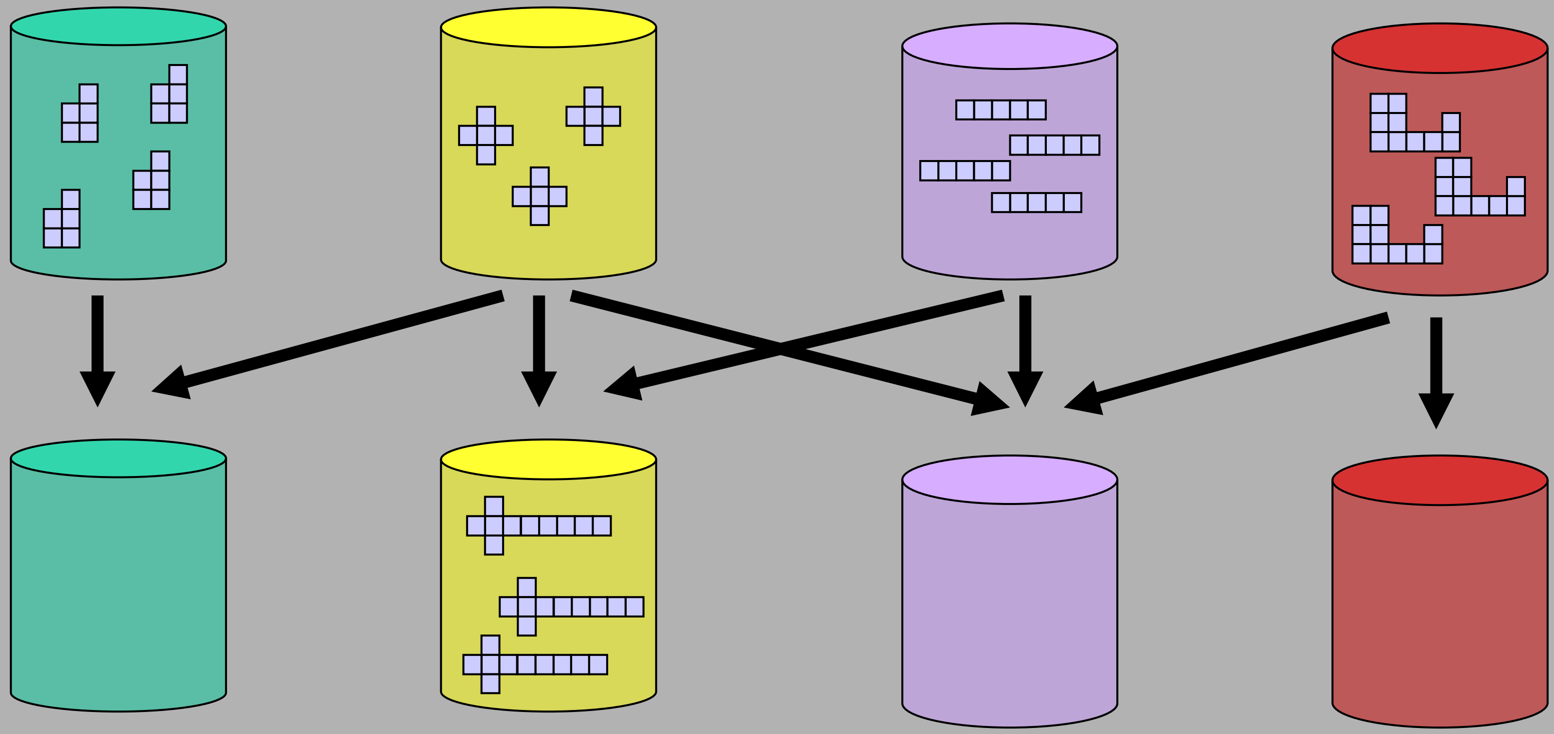
-Pour multiple bins into a single bin

Staged Assembly



-Pour multiple bins into a single bin
-Split contents of any given bin among multiple new bins

Staged Assembly



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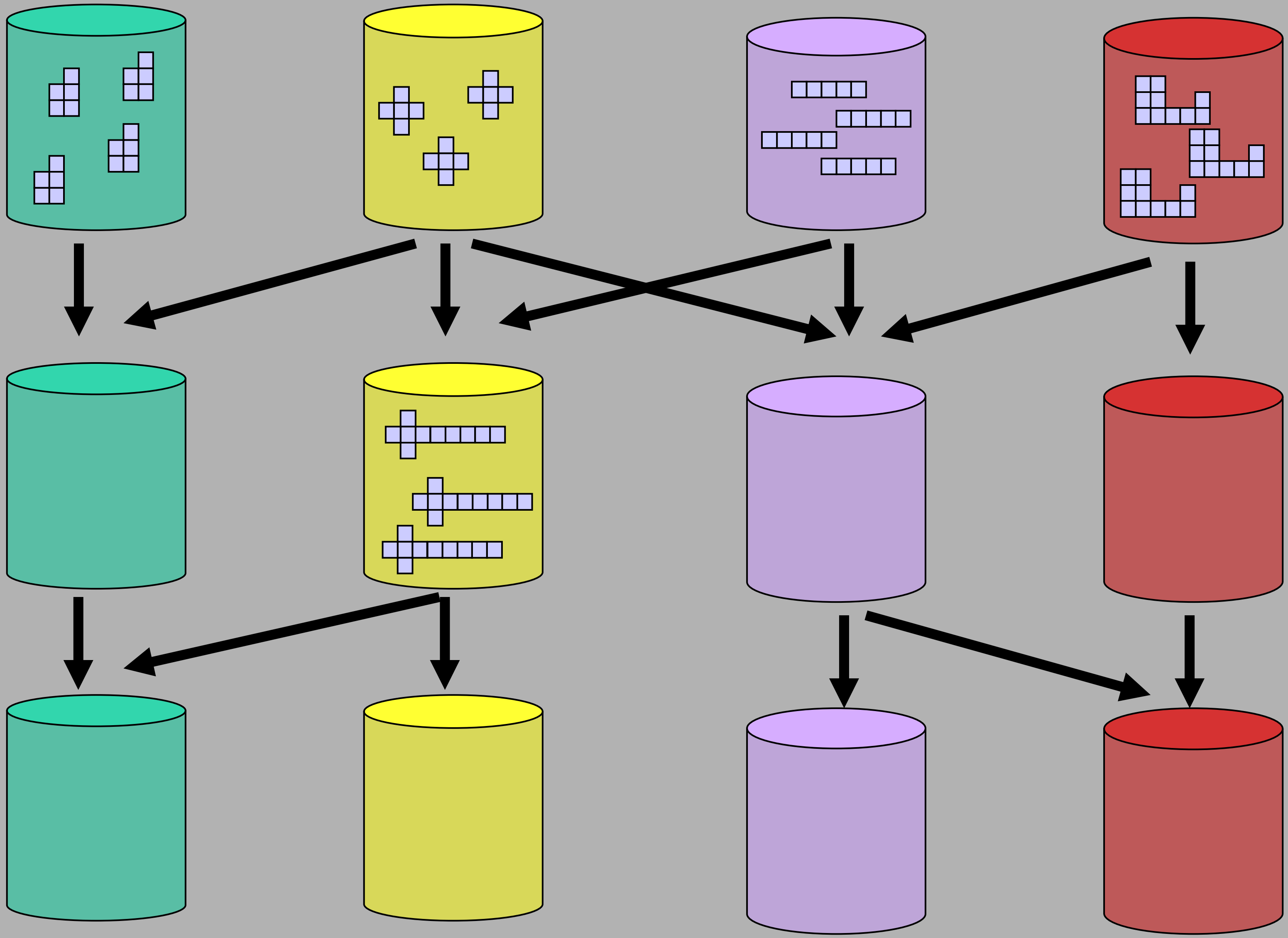
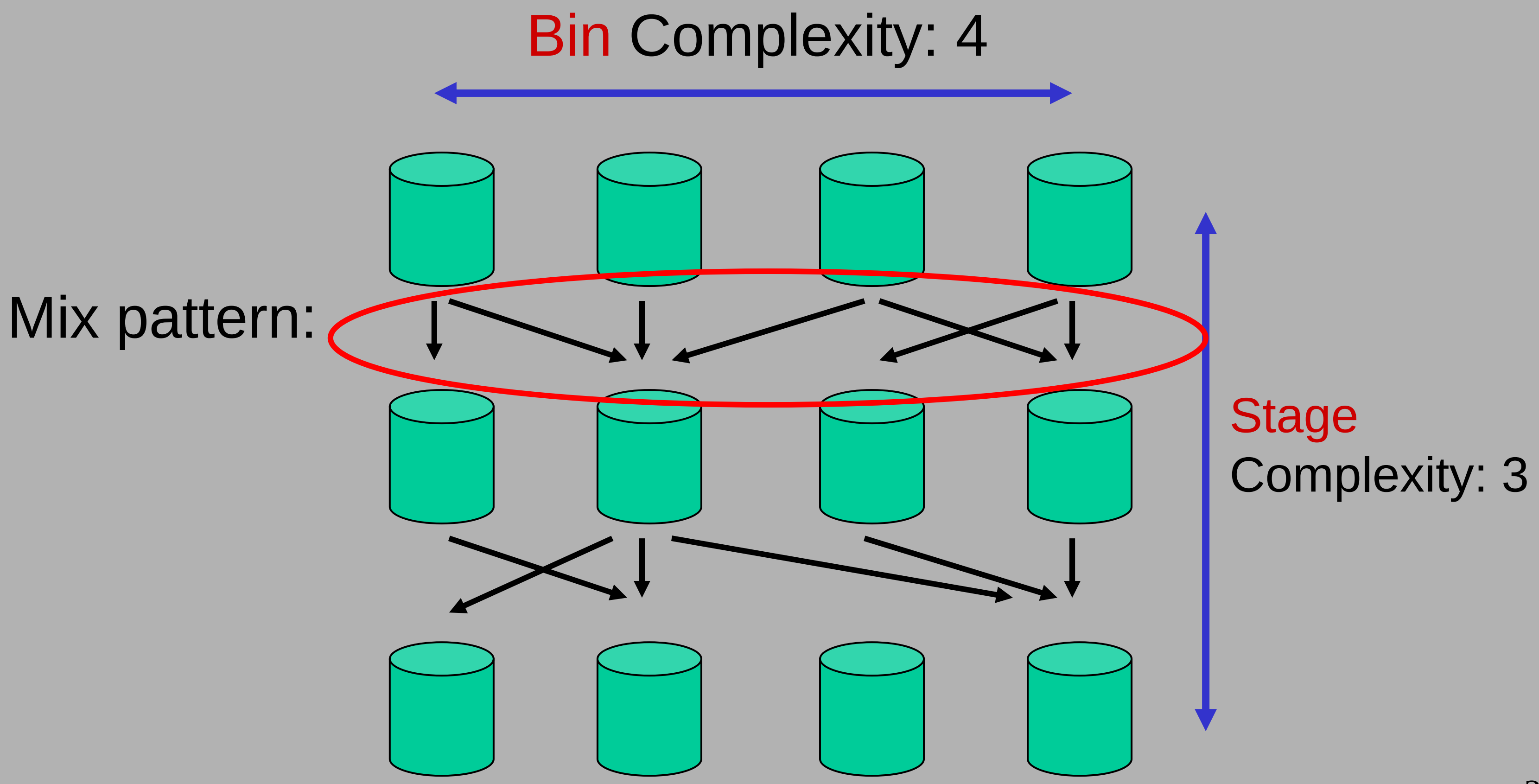


Staged Assembly

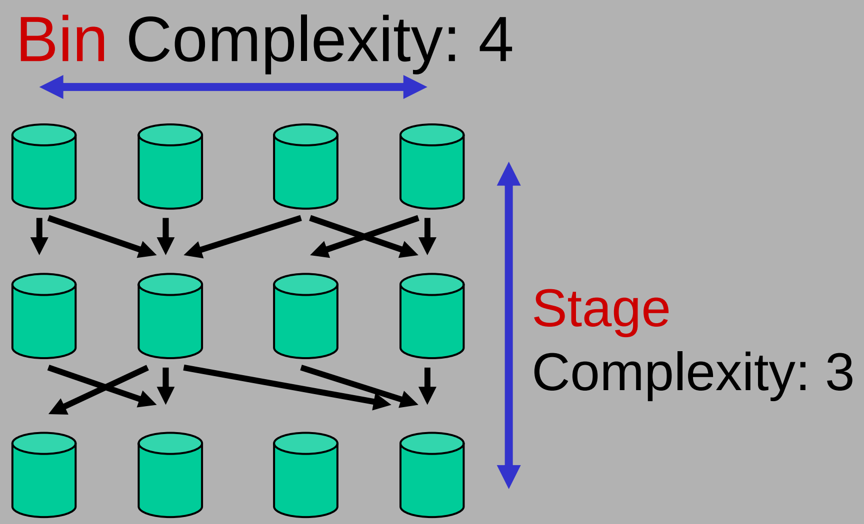
- Assembly occurs in a sequence of stages, and assemblies can be separated into separate bins



Staged Assembly

- Assembly occurs in a sequence of stages, and assemblies can be separated into separate bins

Bins = Space Complexity
Stages = Time Complexity

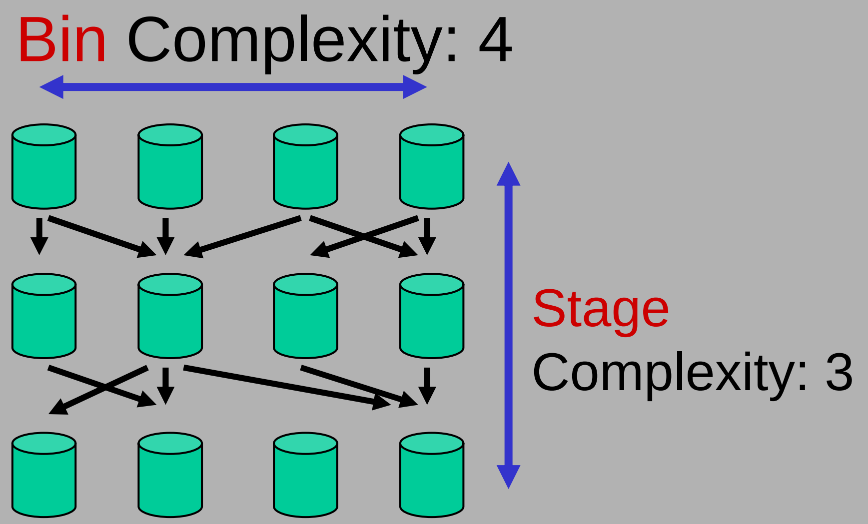


Staged Assembly

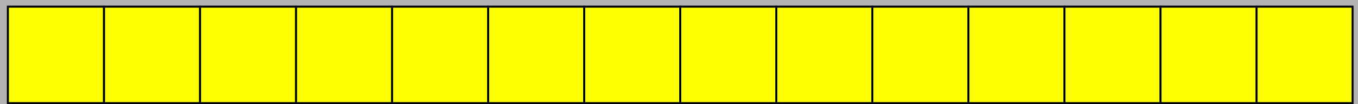
- Assembly occurs in a sequence of stages, and assemblies can be separated into separate bins

- Our Goal:

  Given a target shape, design *mixing algorithms* that:
  - Use only O(1) tiles/glues to build target shape.
  - Are efficient in terms of:
    - Bin complexity
    - Stage complexity.



Simple Example: 1 x n line



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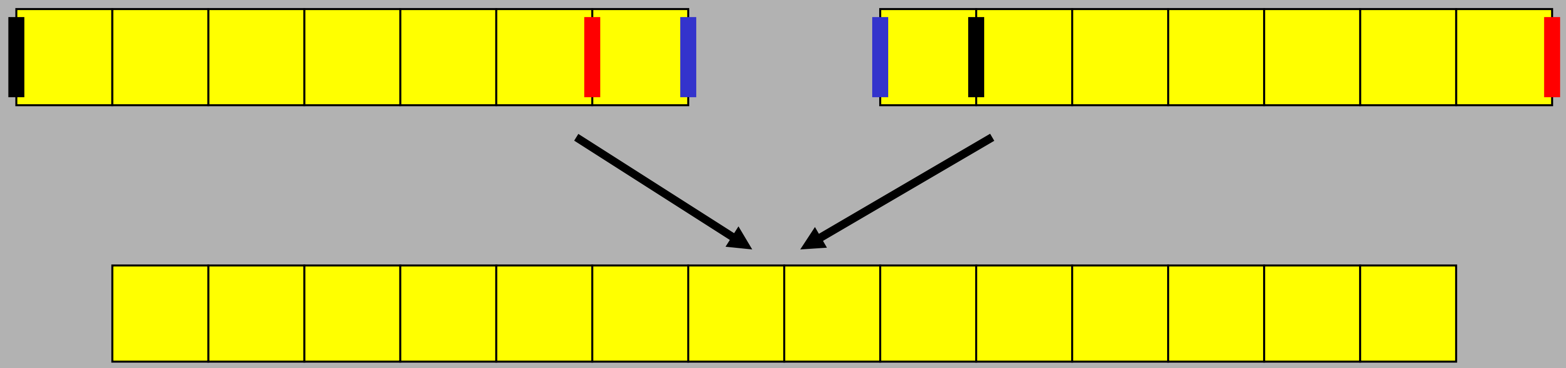

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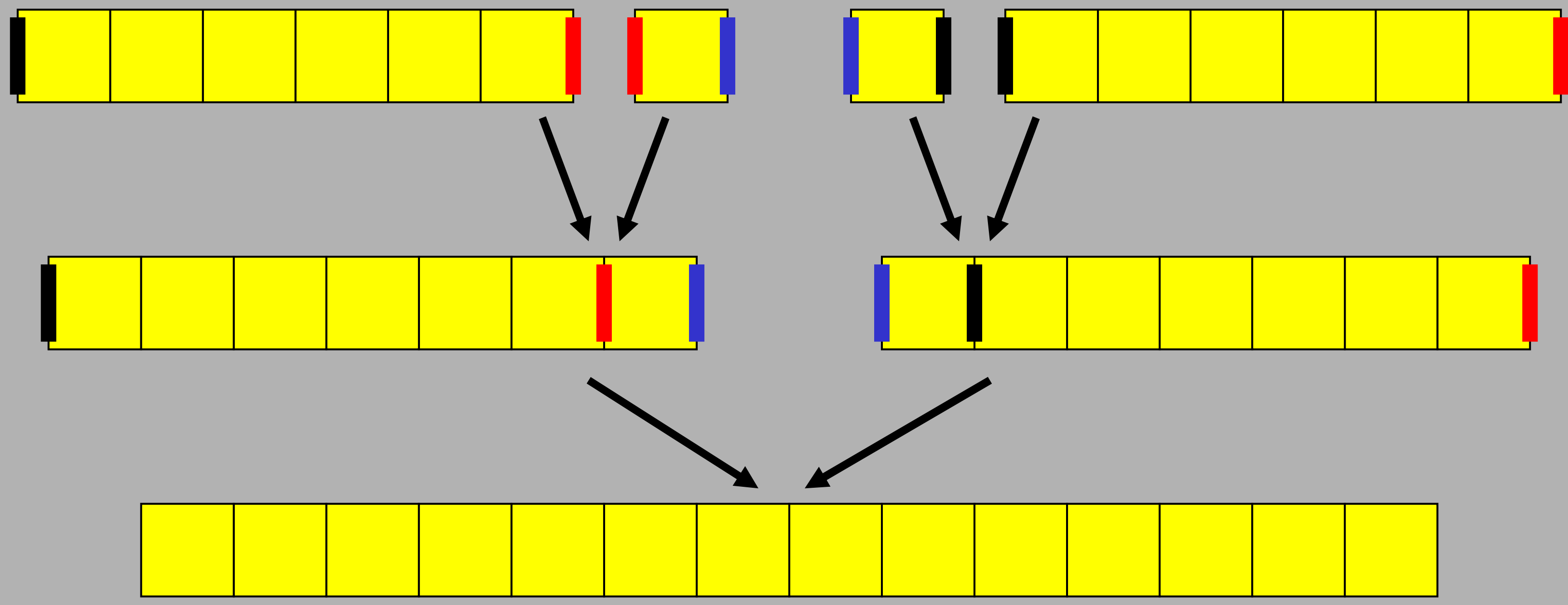

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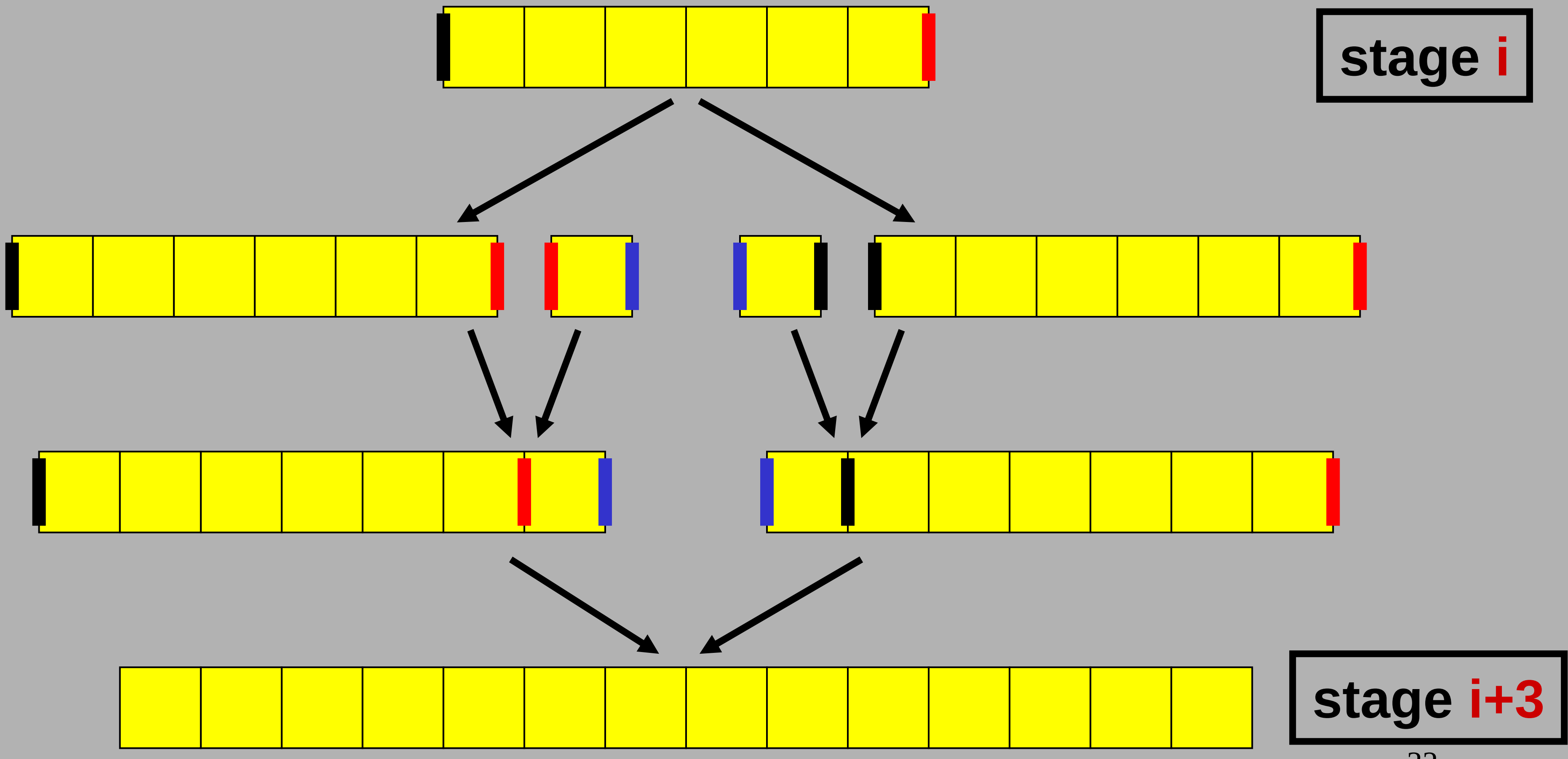
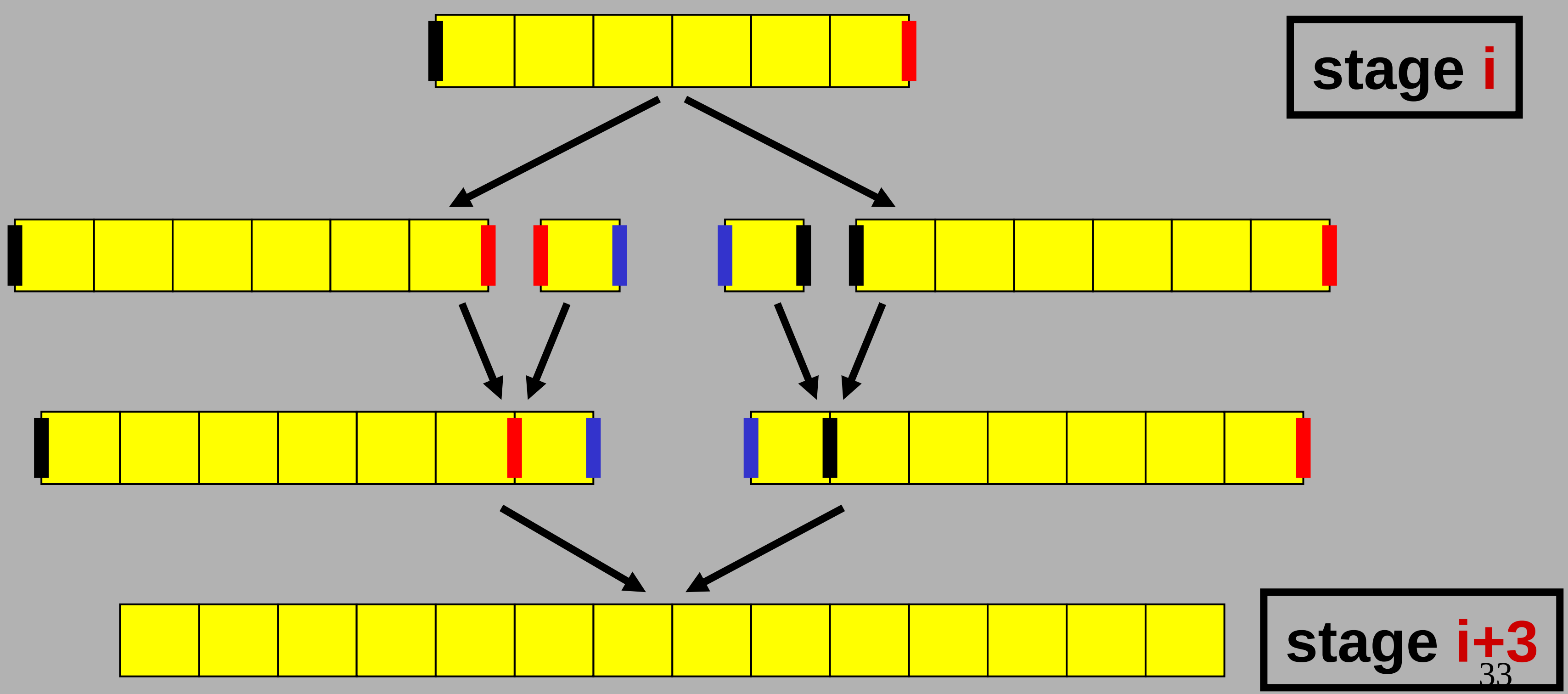


Simple Example: 1 x n line

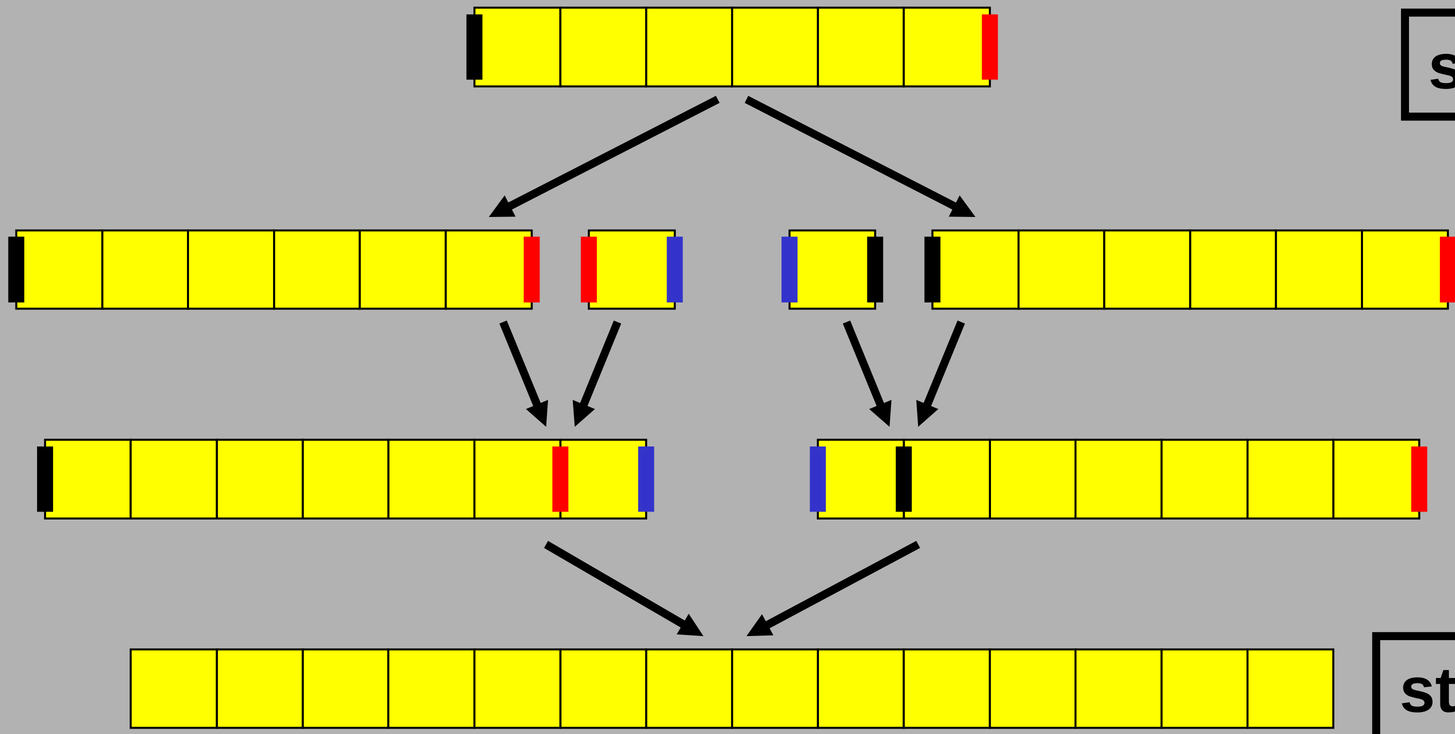
Staged Assembly 1 x n line	
tiles / glues	O(1) = 3
Bins	O(1)
Stages	O(log n)



Simple Example: 1 x n line

Staged Assembly 1 x n line	
tiles / glues	O(1) = 3
Bins	O(1)
Stages	O(log n)

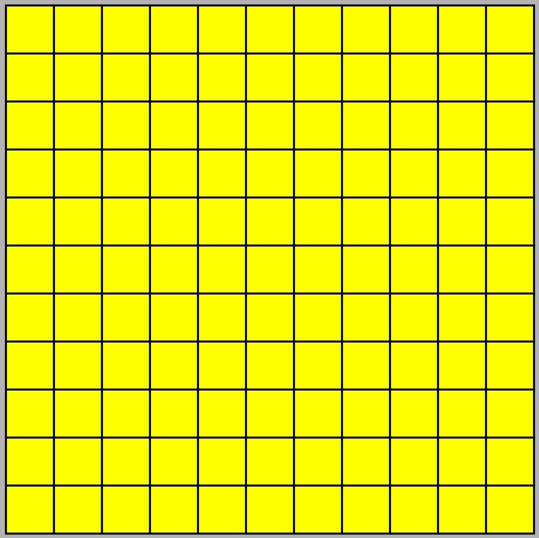
Non-Staged Model 1 x n line	
tiles / glues	Ω(n)
Bins	1
Stages	1



stage i

stage i+3

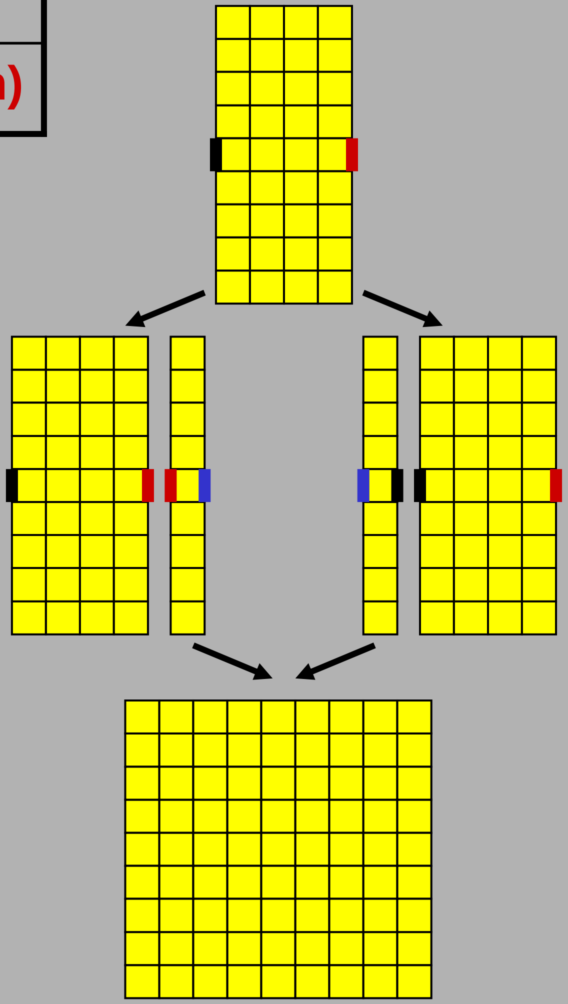
n x n Square



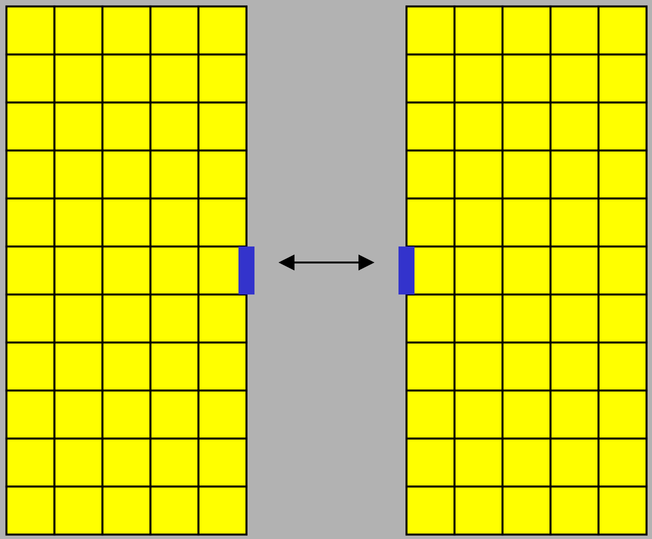
n x n Square

Staged Assembly n x n square	
tiles / glues	O(1)
Bins	O(1)
Stages	O(log n)

Base Case
1 x n line:
Use line algorithm



n x n Square: unstable?



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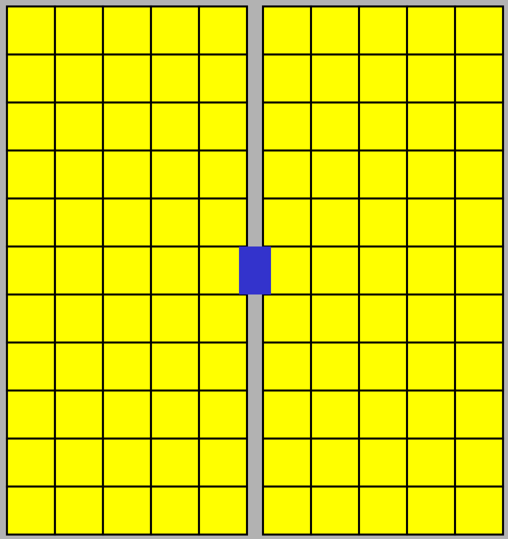

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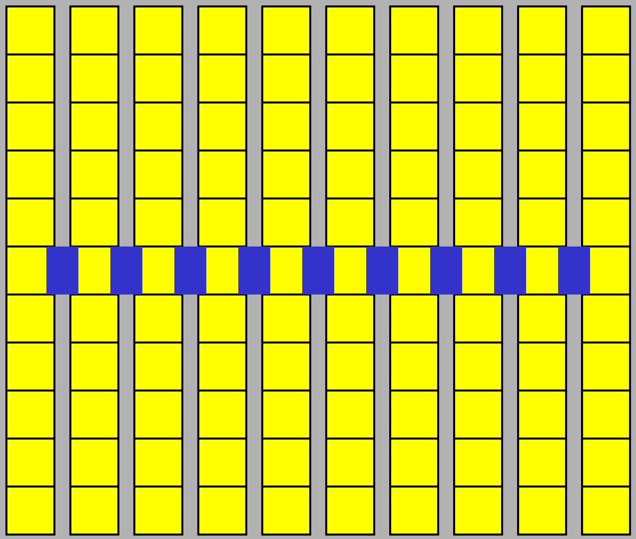
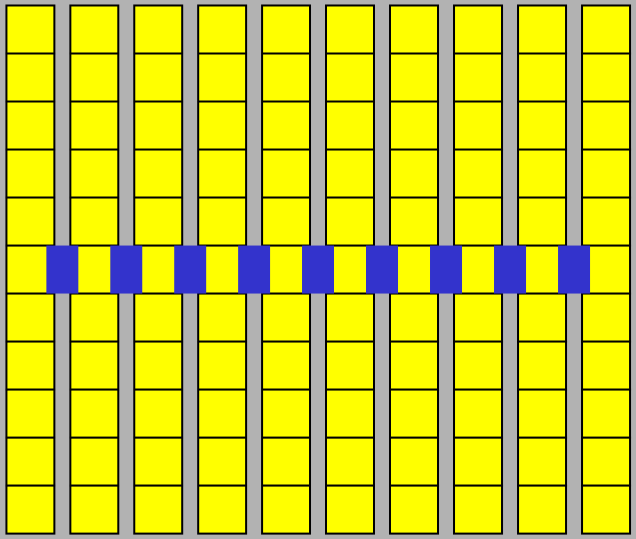


n x n Square: Full Connectivity

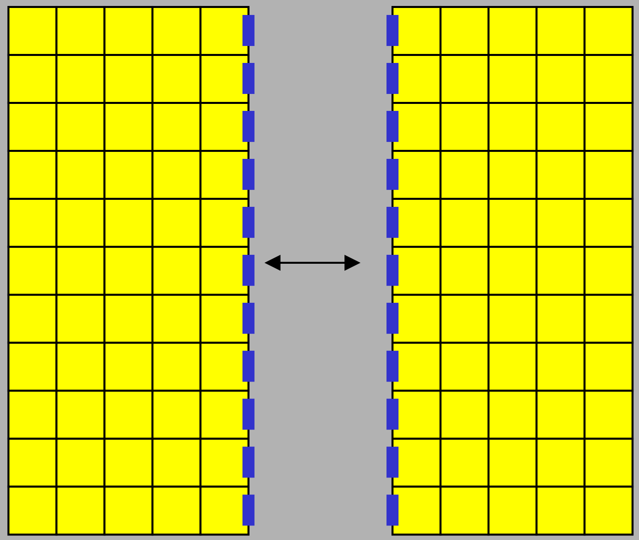
[Rothemund, Winfree STOC 2000]

Full Connectivity Constraint: All adjacent tiles in assembled shape must share a full strength bond



n x n Square: Full Connectivity

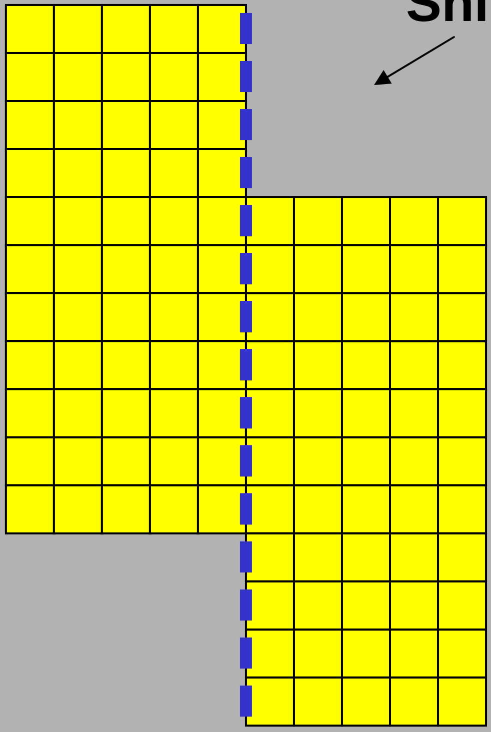
Full Connectivity Constraint: **All adjacent tiles in assembled shape must share a full strength bond**



n x n Square: Full Connectivity

Full Connectivity Constraint: All adjacent tiles in assembled shape must share a full strength bond

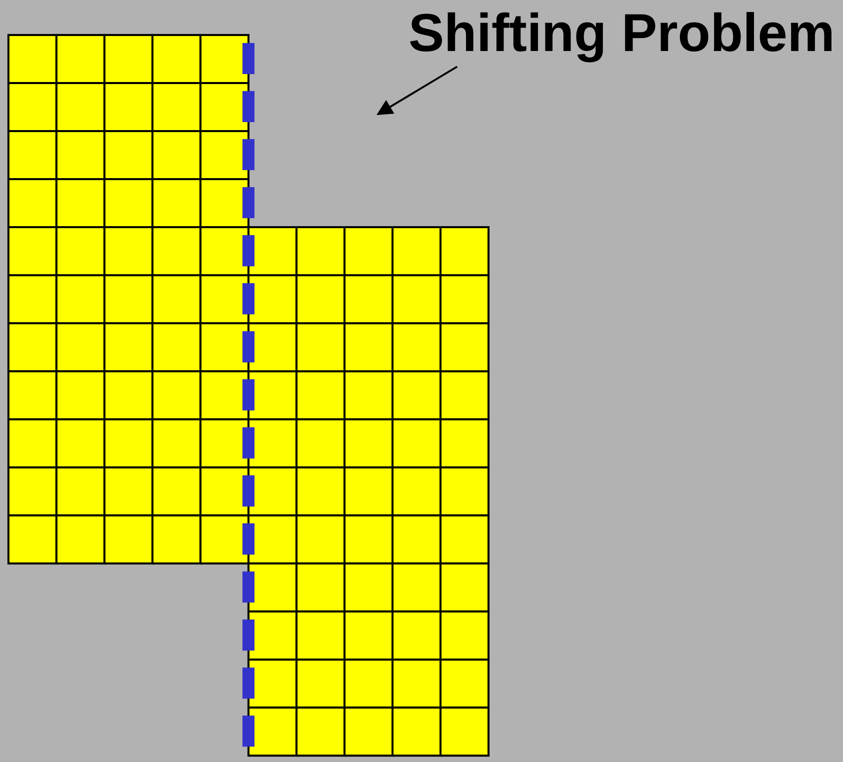
Shifting Problem



n x n Square: Full Connectivity

Full Connectivity Constraint: **All adjacent tiles in assembled shape must share a full strength bond**

Jigsaw Technique:
Use Geometry to enforce proper binding.



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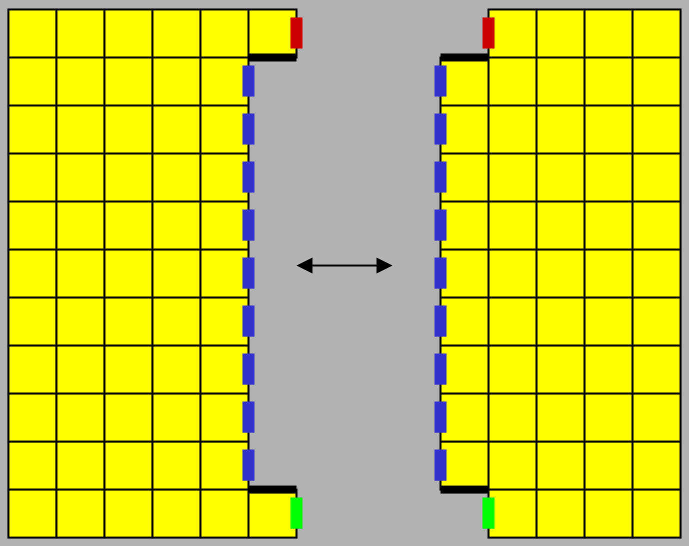

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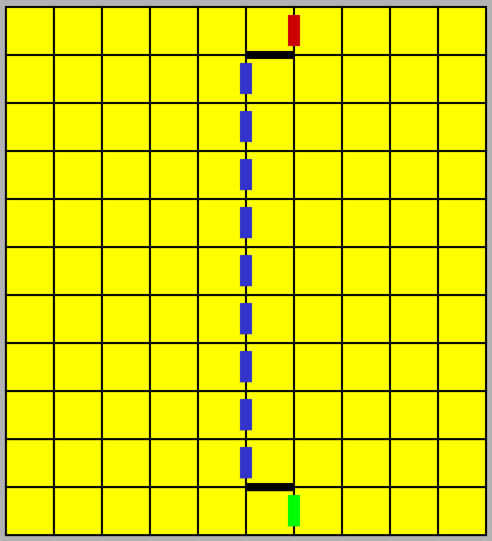
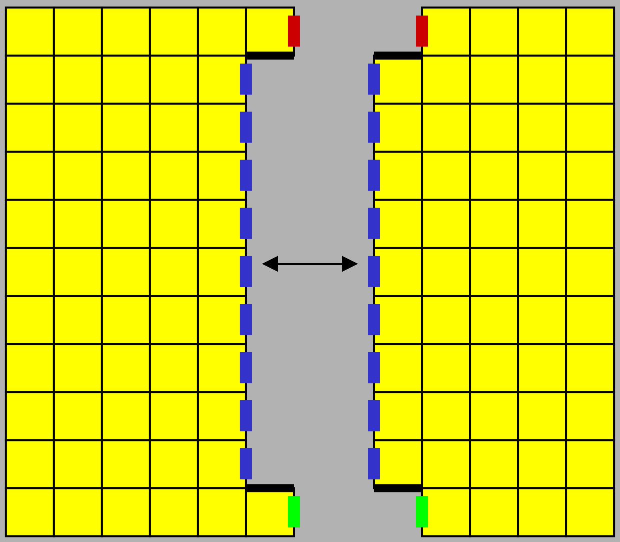


n x n Square: Full Connectivity

Staged Assembly Fully Connected n x n square	
tiles / glues	O(1)
Bins	O(1)
Stages	O(log n)
Temperature	1

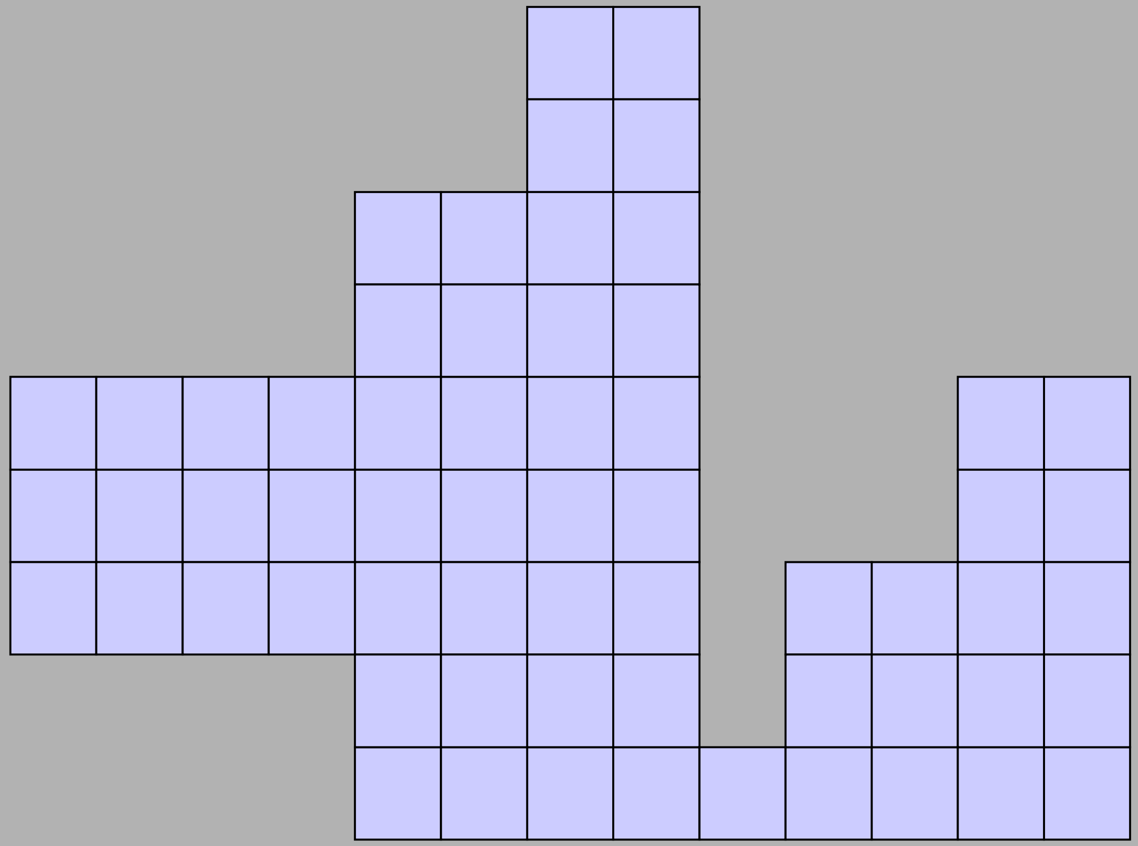
Non-Staged Model Fully Connected n x n square	
tiles / glues	Θ(log n / log log n)
Bins	1
Stages	1
Temperature	2

[adleman, cheng, goel, huang STOC 2001]

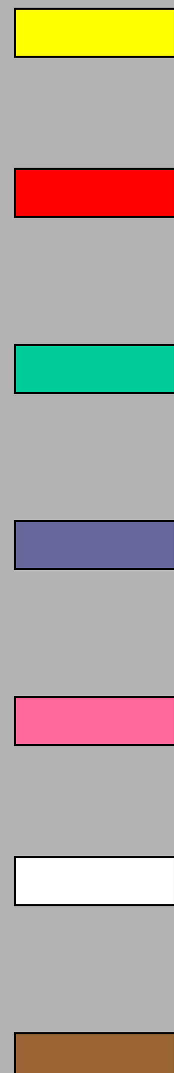


Arbitrary Shapes

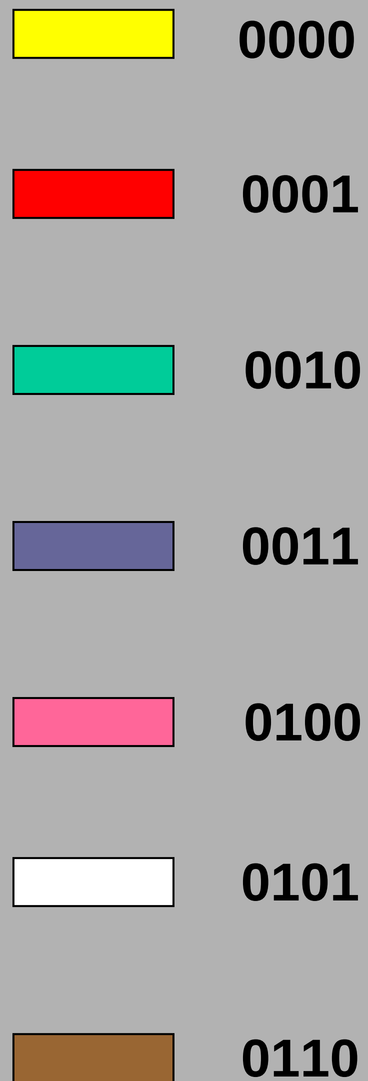
- Spanning Tree Method
- Jigsaw Method for non-hole Shapes
- Simulation Method



Simulate Large Tilesets



Simulate Large Tilesets



Simulate Large Tilesets

0000

0001

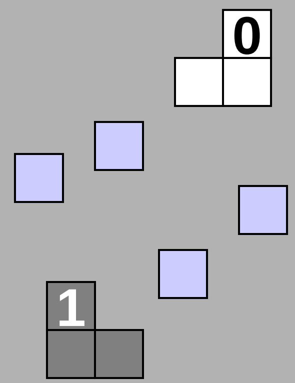
0010

0011

0100

0101

0110



Simulate Large Tilesets

Simulate Large Tilesets

0000

0001

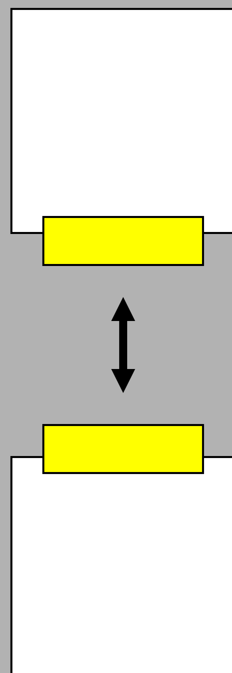
0010

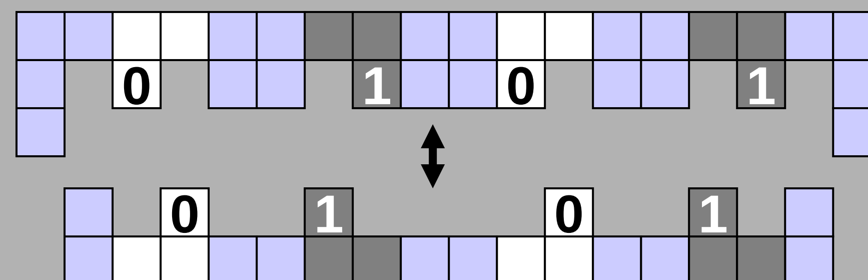
0011

0100

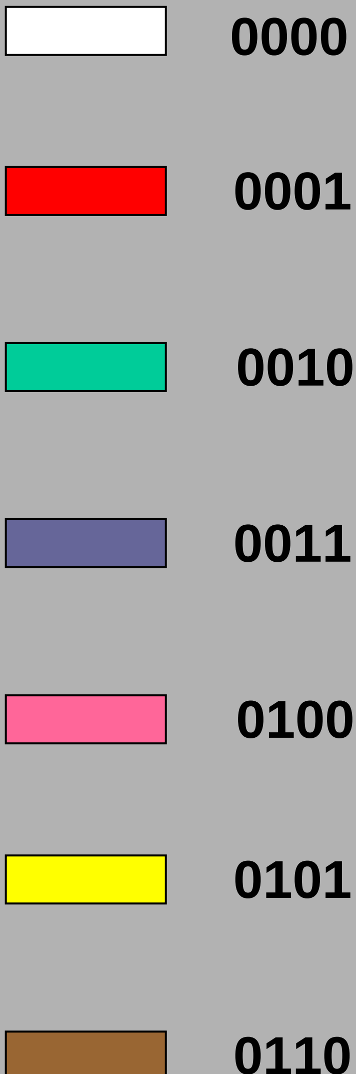
0101

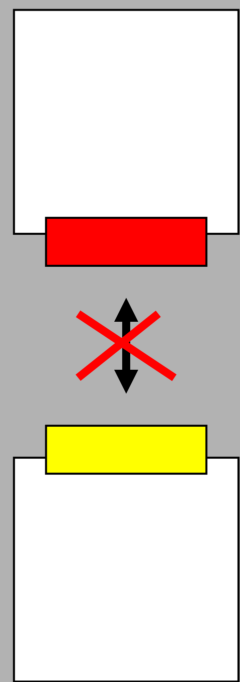
0110

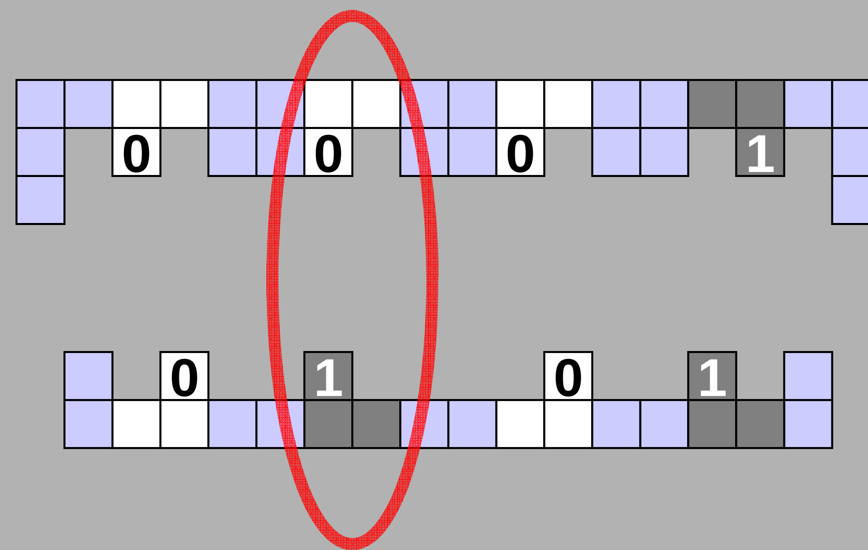




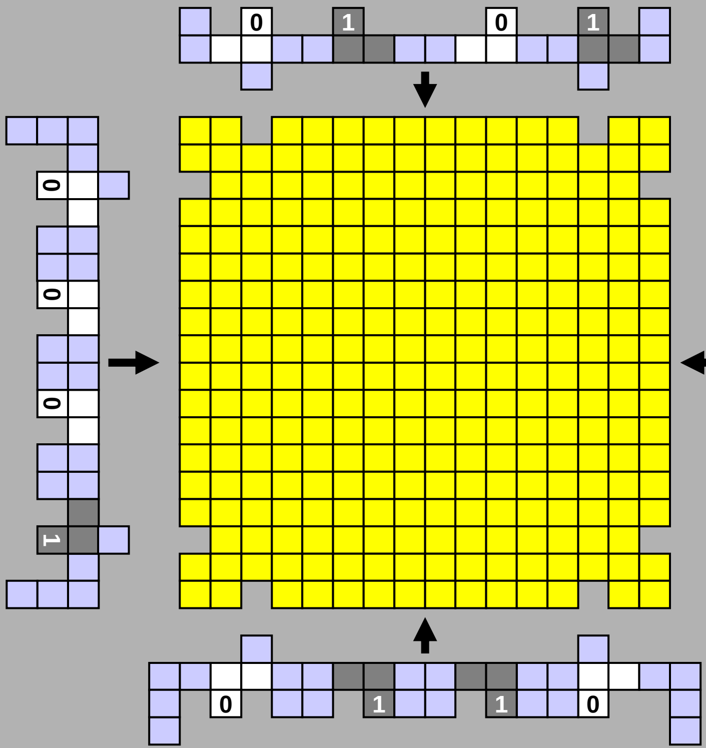
Simulate Large Tilesets

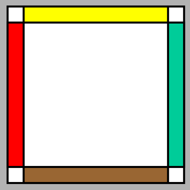




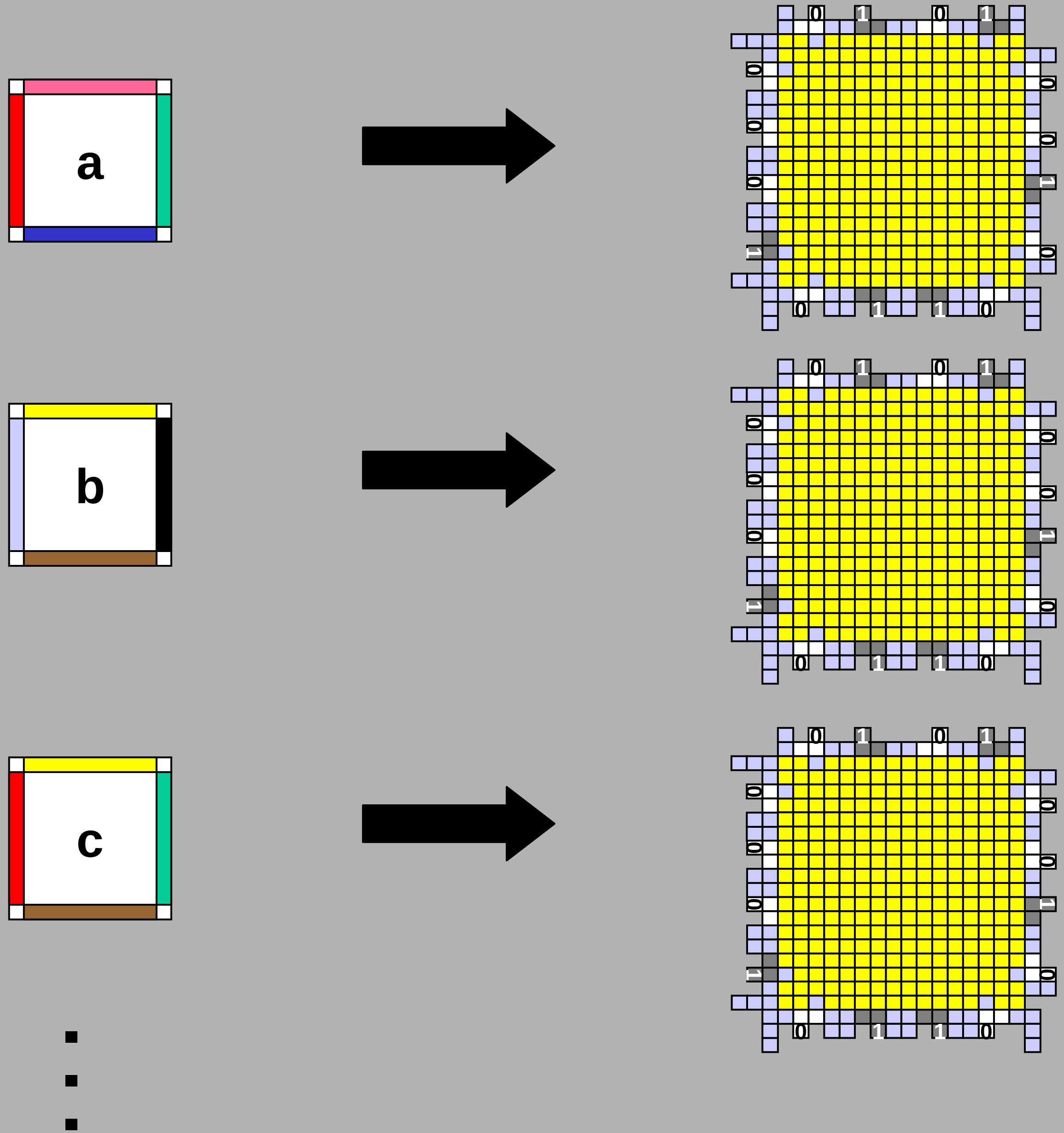


Simulate Large Tilesets

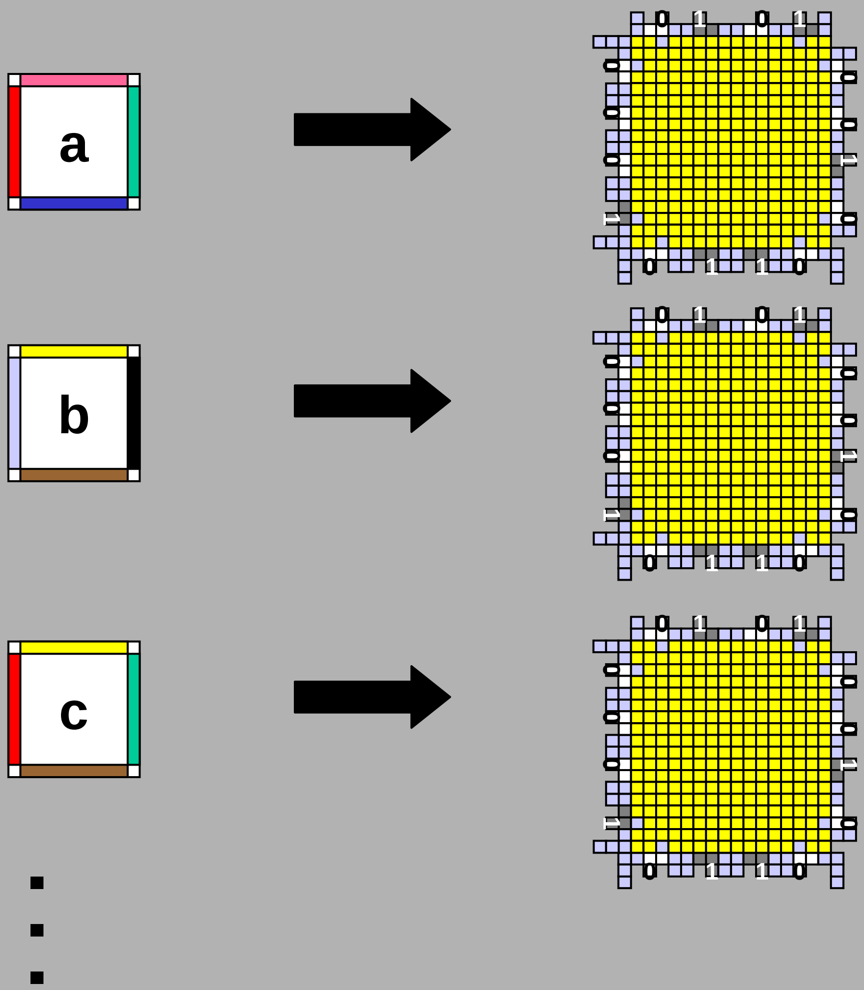




Simulate Large Tilesets



Simulate Large Tilesets



Simulate temp=1 tileset T	
tiles / glues	O(1)
Bins	O(|T|)
Stages	O(log log |T|)

Arbitrary n tile Shape	
tiles / glues	O(1)
Bins	O(n)
Stages	O(log log n)
Scale	O(log n)

Arbitrary Shape Assembly

- Spanning Tree Method
- Jigsaw Method for non-hole Shapes
- Simulation Method

Spanning Tree Method	
tiles / glues	O(1)
Bins	O(log n)
Stages	O(diameter)
Connectivity	Partial
Scale	1
Generality	ALL

Jigsaw Method	
tiles / glues	O(1)
Bins	O(n)
Stages	O(n)
Connectivity	FULL
Scale	2
Generality	Hole Free

Simulation Method	
tiles / glues	O(1)
Bins	O(n)
Stages	O(log log n)
Connectivity	FULL
Scale	O(log n)
Generality	ALL

Near Optimal Tradeoff: Bins versus Stages (Crazy Mixing)

First Result:

Staged Assembly n x n square	
tiles / glues	**O(1)**
Bins	**O(1)**
Stages	**O(log n)**

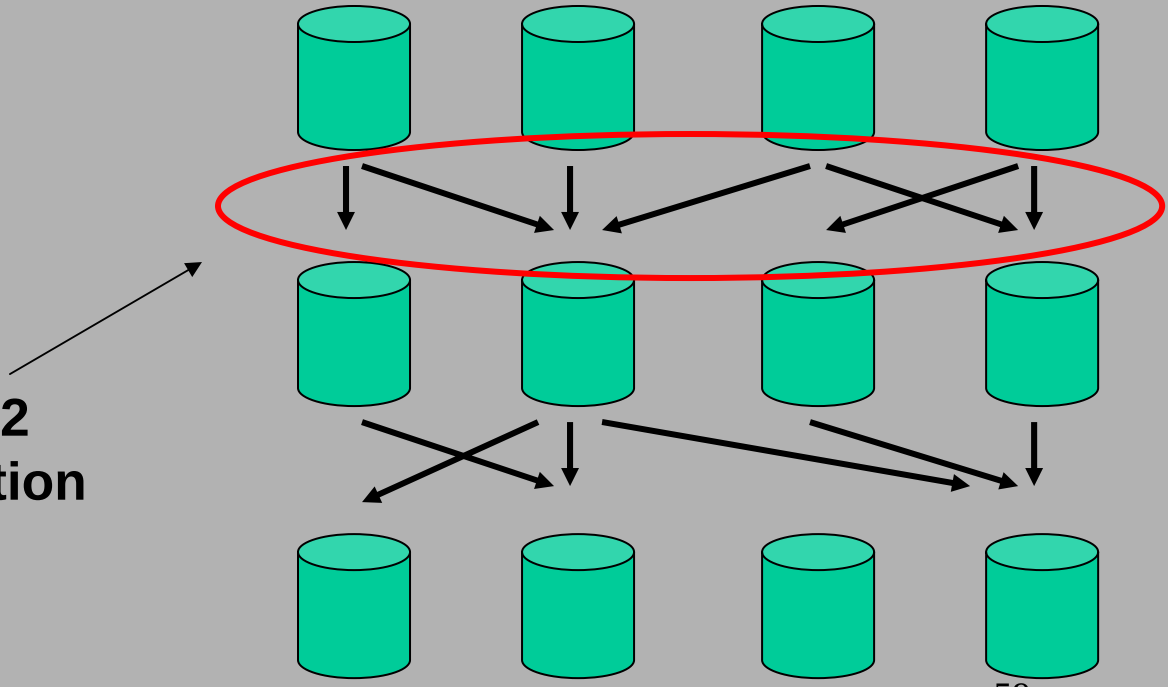
What if we have B bins?

Near Optimal Tradeoff: Bins versus Stages (Crazy Mixing)

First Result:

Staged Assembly n x n square	
tiles / glues	O(1)
Bins	O(1)
Stages	O(log n)

What if we have B bins?



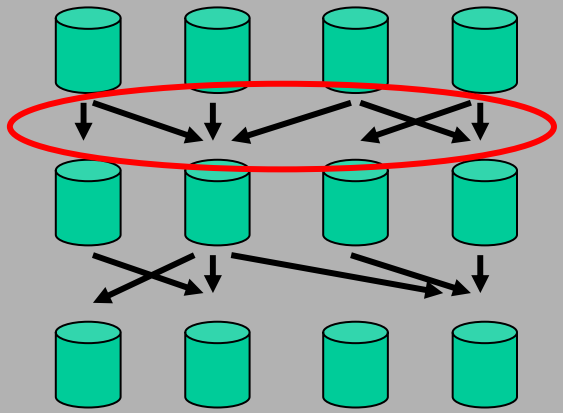
B^2 edges,
Can encode B^2
Bits of information
Per stage.

Near Optimal Tradeoff: Bins versus Stages (Crazy Mixing)

Assembly of n x n squares with B bins:

Lower Bound for almost all n	
tiles / glues	O(1)
Bins	B
Stages	Ω(log n / B^2)

Upper Bound	
tiles / glues	O(1)
Bins	B
Stages	O(log n / B^2 + log B)



Upper bound technique:

-Encode B^2 bits describing target square at each stage

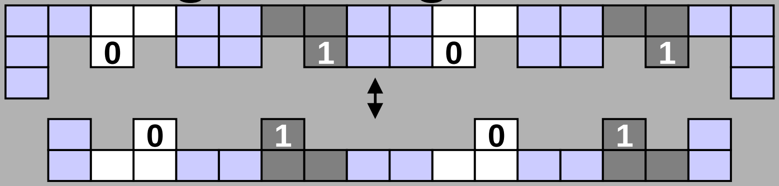
-Combine with Simulation macro tiles.

Conclusions

- Staged Assembly permits various techniques for the assembly of arbitrary shapes with O(1) tiles/glues.
- For some shapes (squares) we achieve near optimal tradeoffs in bin versus stage complexity.
- Staged assembly may shed light on natural assembly systems
  - Cells of body perhaps serve as bins
  - Staged assembly emphasizes importance of geometric shape for bonding, perhaps similar to protein shape determining function.

Future Work

- Problems with model?
- Applications in DNA code design using synthetic DNA words?



- Incorporating produced structures as well as terminally produced structures
- Experiments, simulations
- Apply more intense mixing patterns to general shapes
- Tradeoffs between tile complexity and bin/stage complexity.
- Simulation of t=2 systems

Thanks for listening. Questions?