kinetic Tile Assembly Model

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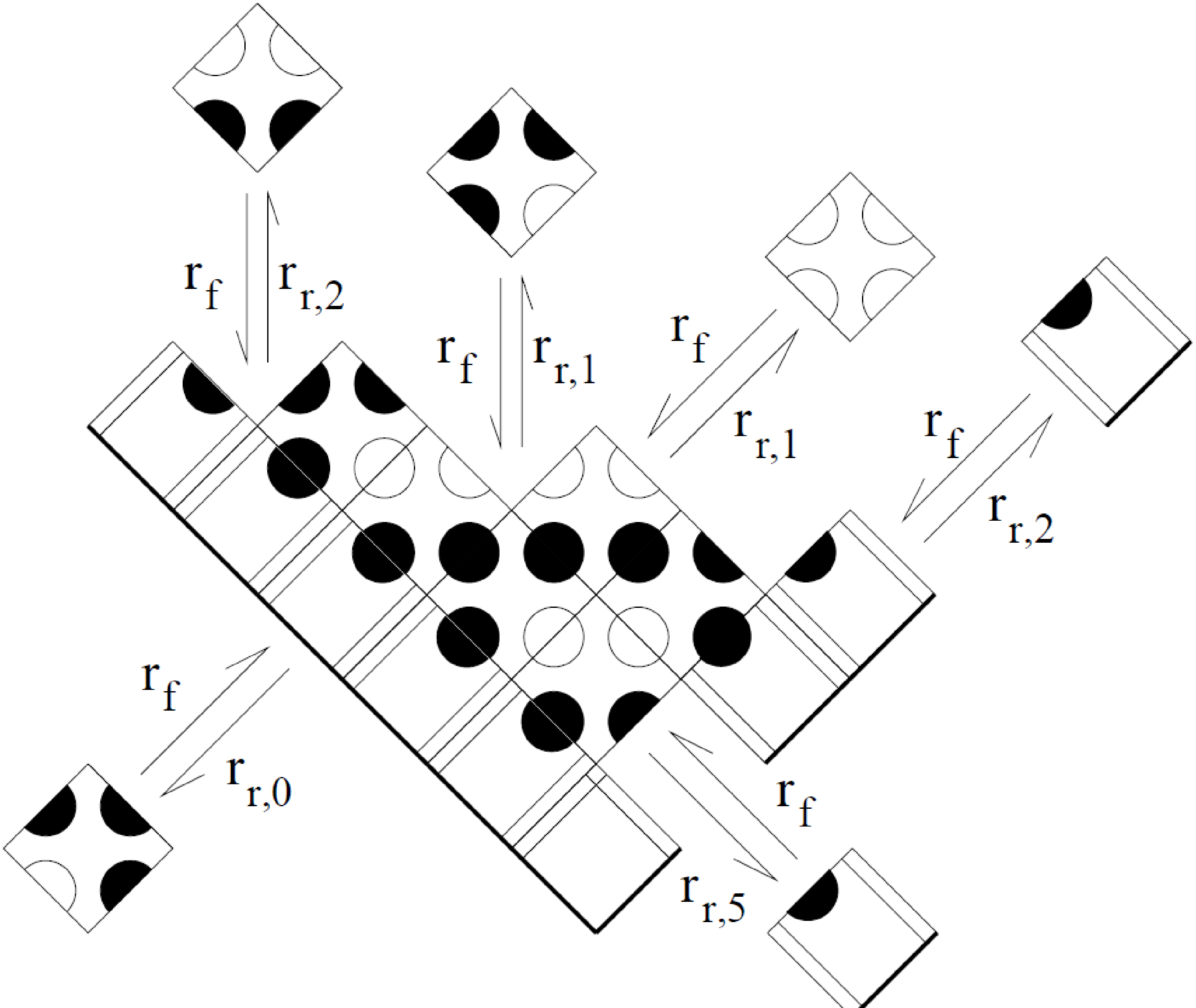
optimal growth when **forward rate just barely larger than reverse rate**, i.e., when

$$G_{mc} \approx 2 \cdot G_{se}$$

kTAM



Proofreading: Error-correction in the kTAM

Definition: error = attachment by single strength 1 glue

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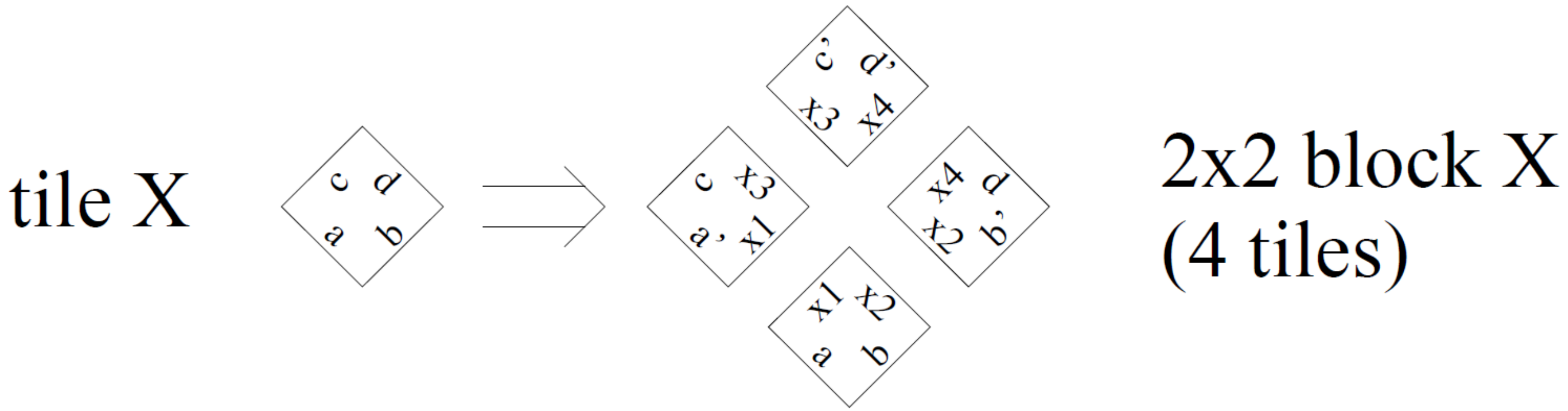

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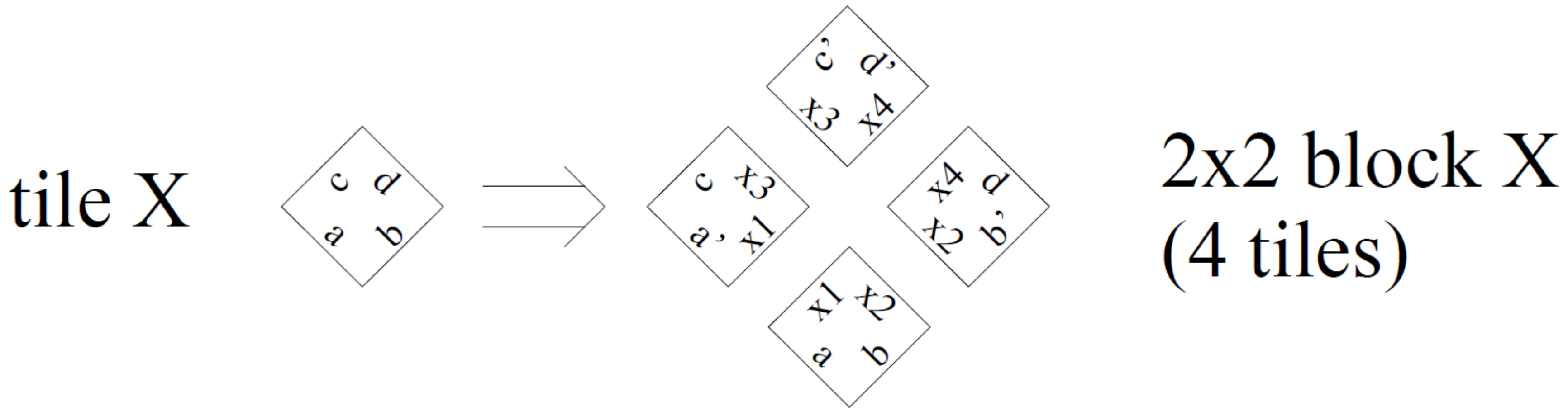

glues internal to block are all unique

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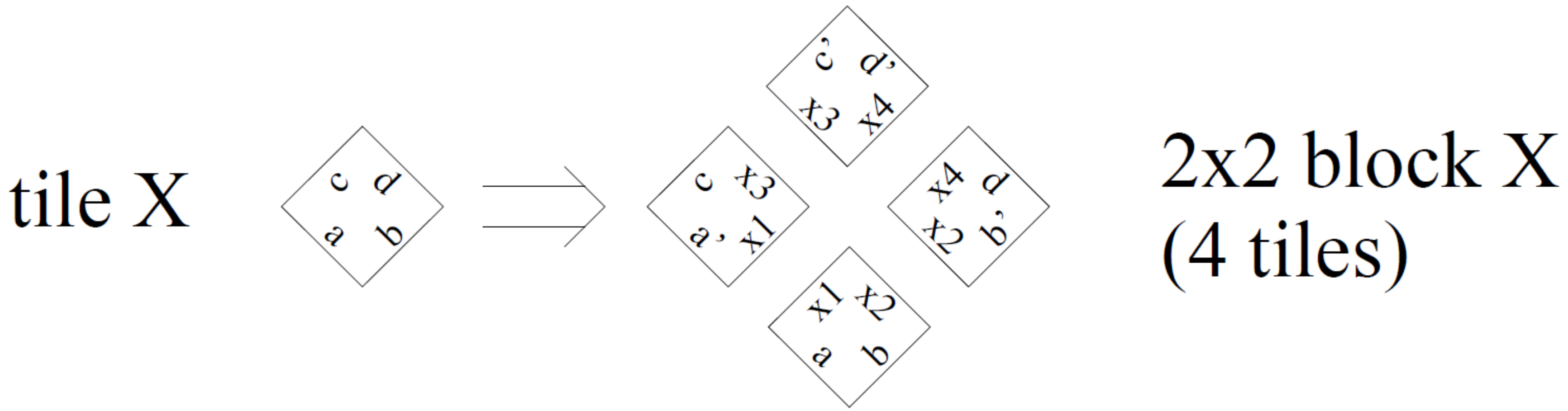

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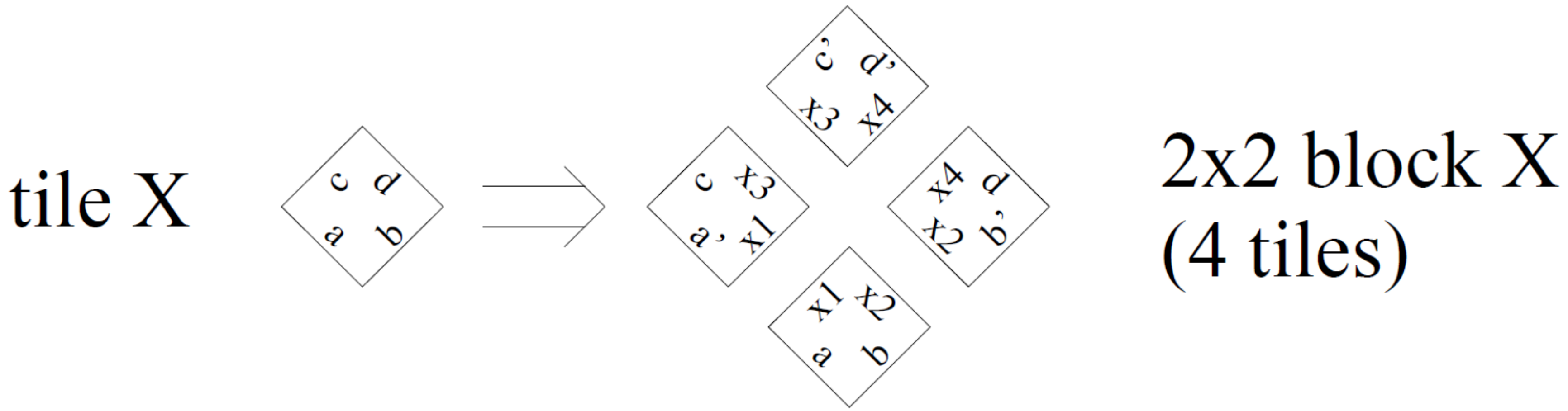

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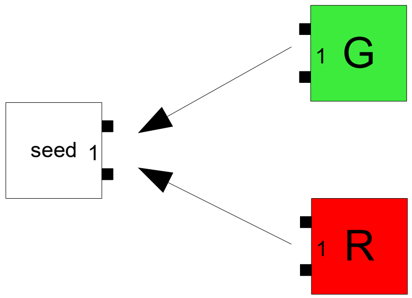
$k \times k$ proofreading roughly turns error rate of ε into ε^k

Concentration programming

Nondeterministic binding



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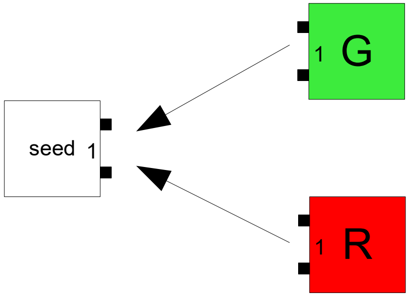

concentration 11

concentration 1

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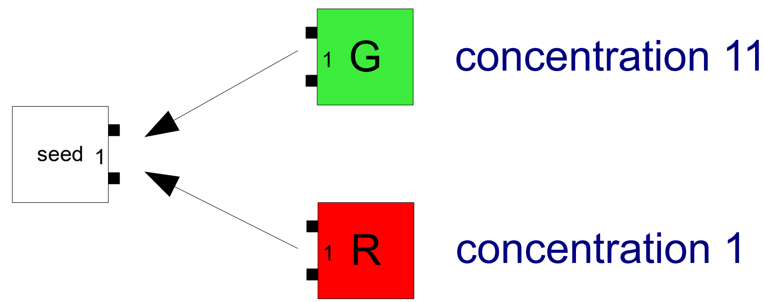
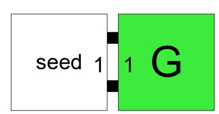
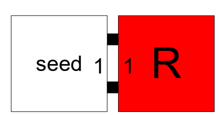


Pr[] = 11/12

Pr[] = 1/12

Concentration programming of universal self-assembling molecules

A **singly-seeded** TAS can assemble *any* finite (scaled) shape (with high probability) by mixing them in the right concentrations.

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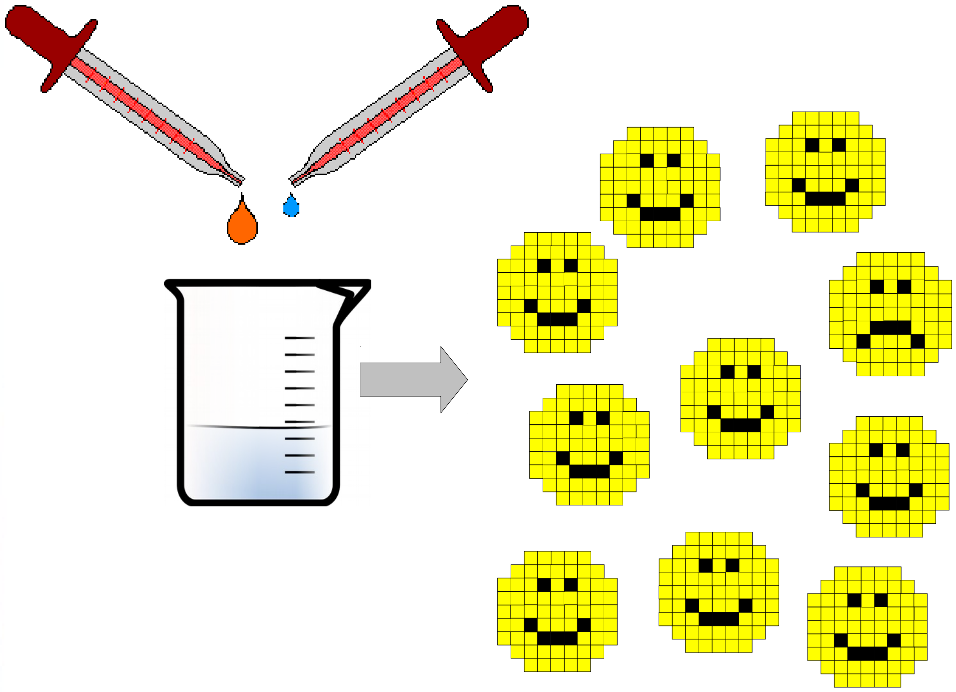

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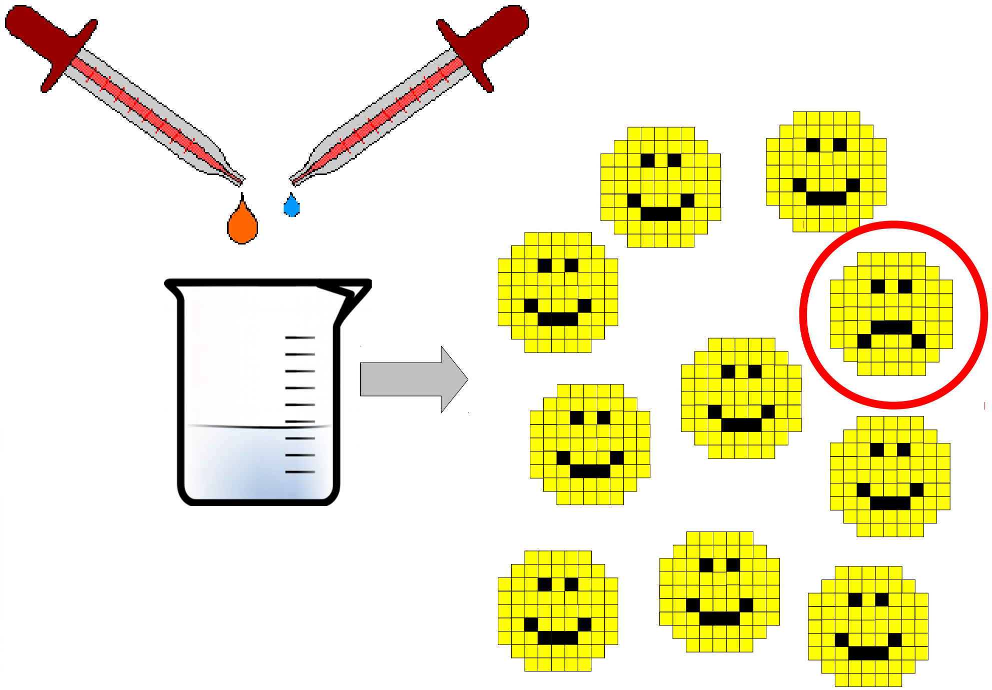

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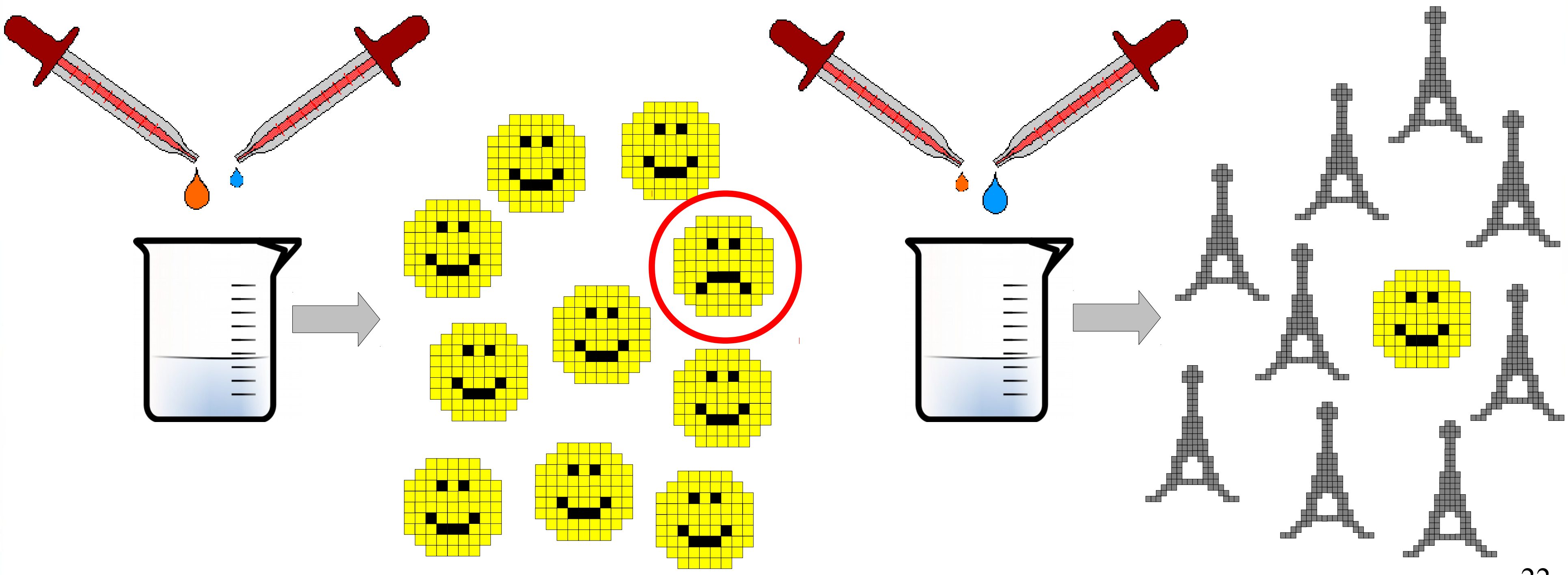
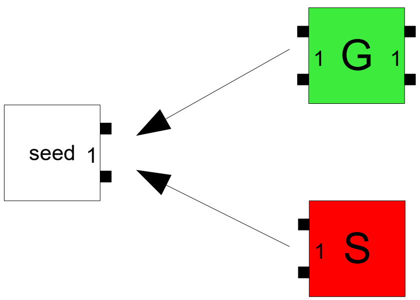


Programming polymer length with concentrations

[Becker, Rapaport, Rémila, *FSTTCS* 2006]



concentration 11

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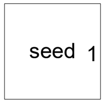

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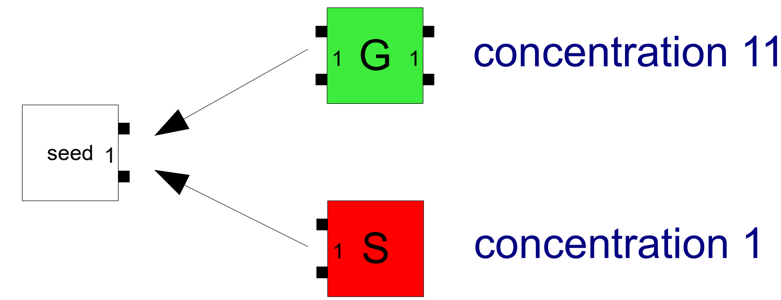

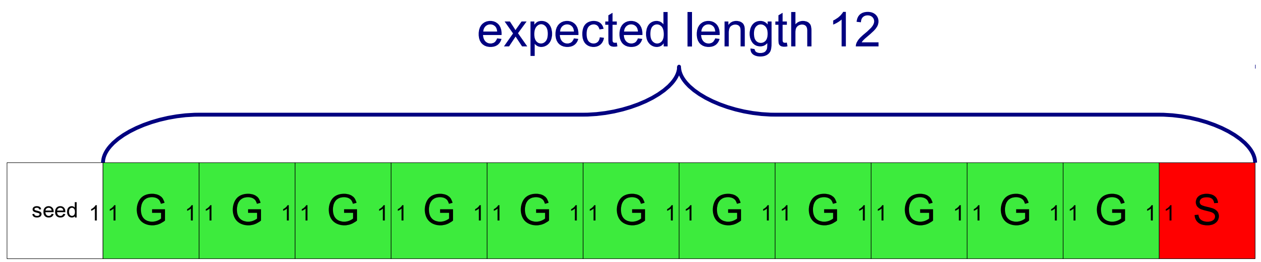

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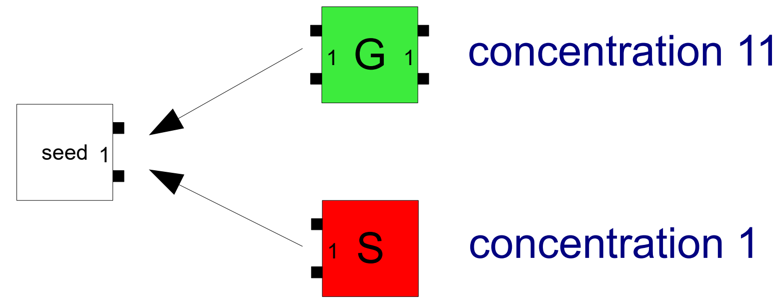
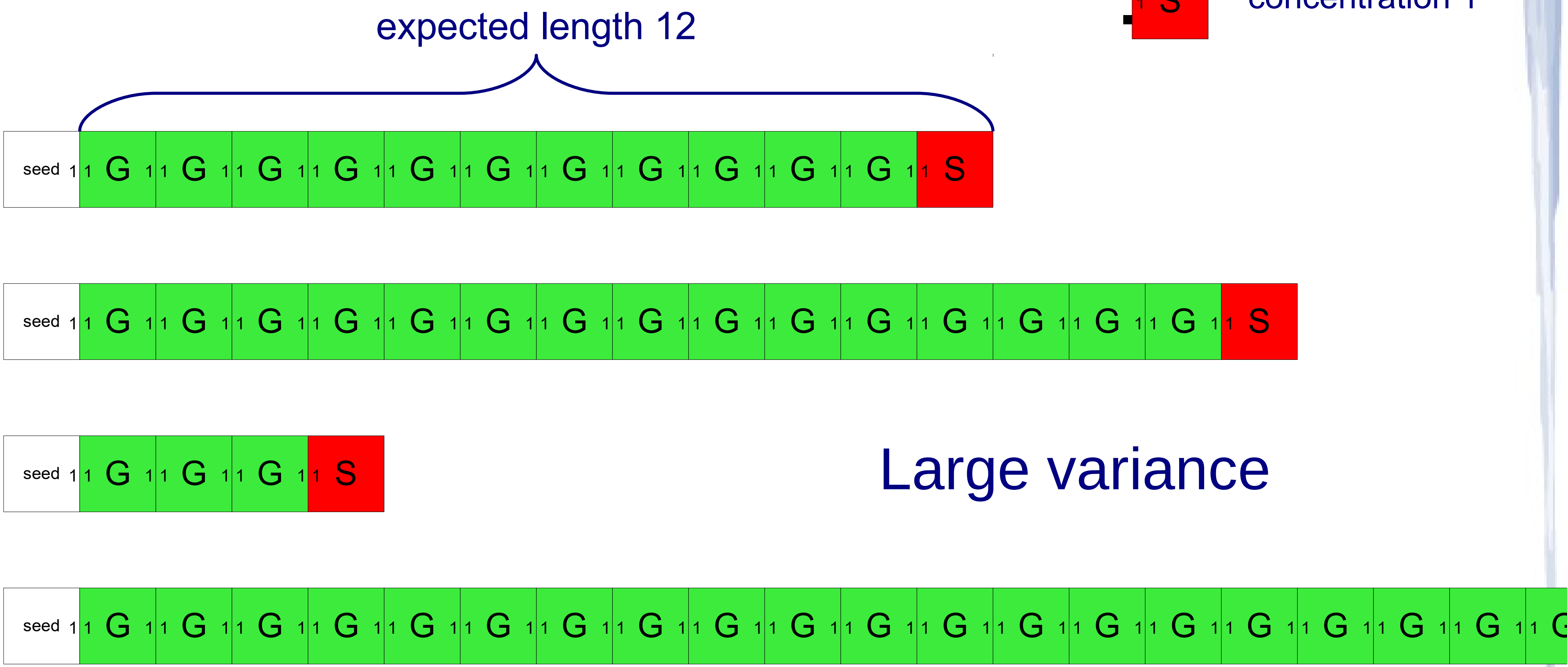
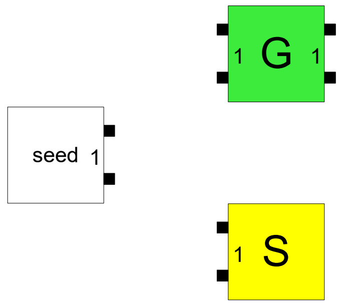




Programming polymer length (improved)



concentration 3

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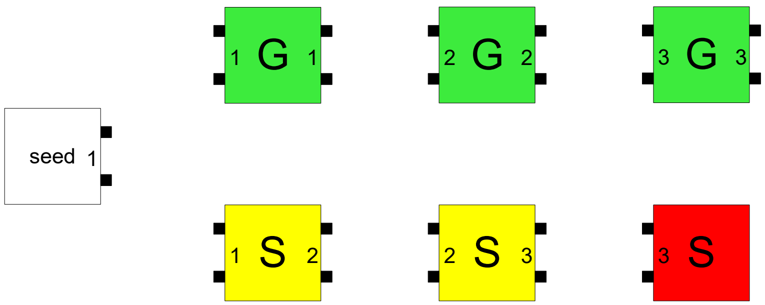

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3 "stages", each of
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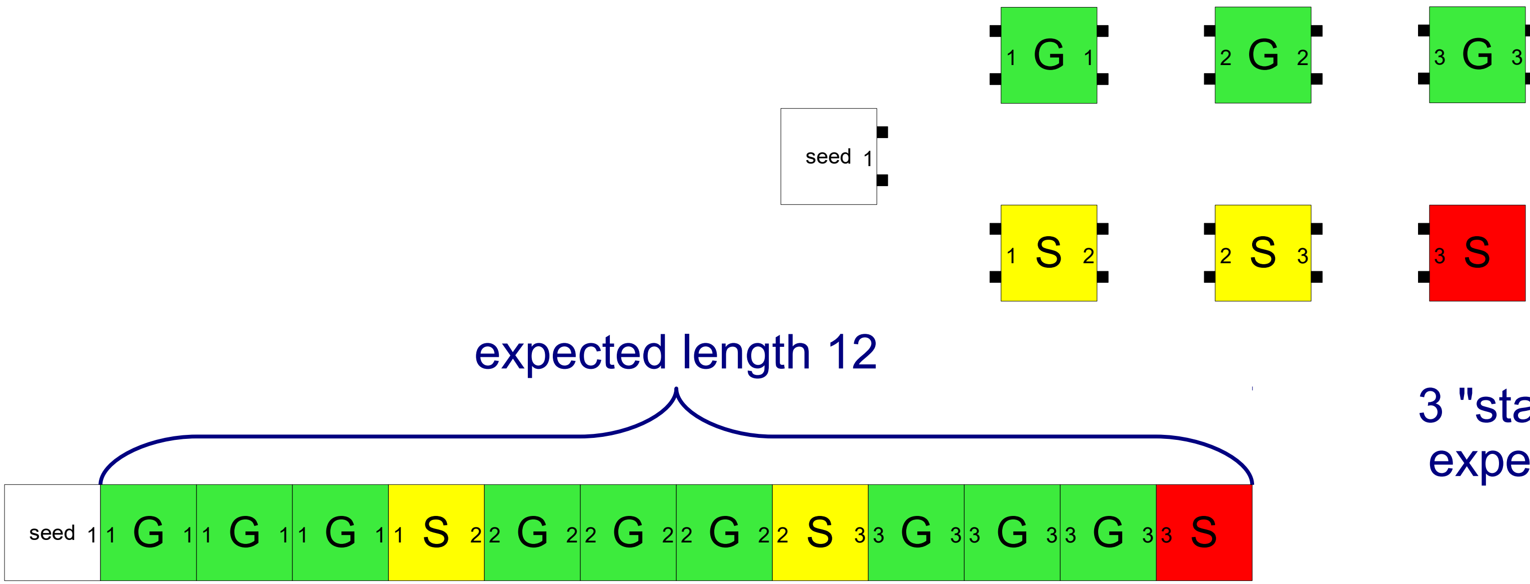

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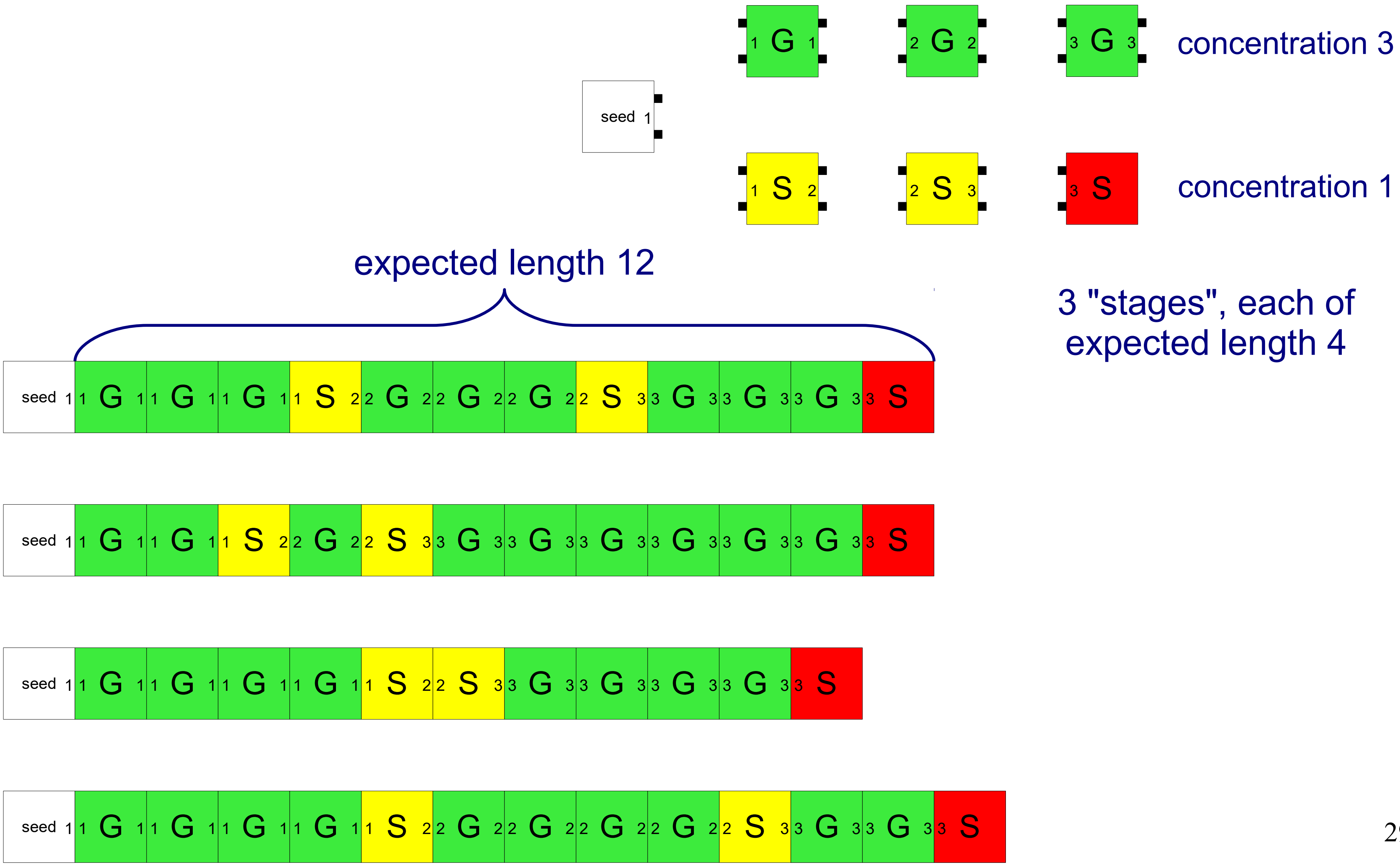

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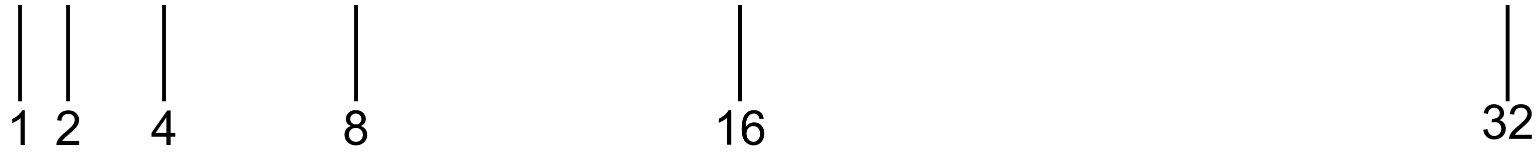
90 stages, expected length midway in $[2^{a-1}, 2^{a})$

→ with probability > 99% **actual** length in $[2^{a-1}, 2^{a})$



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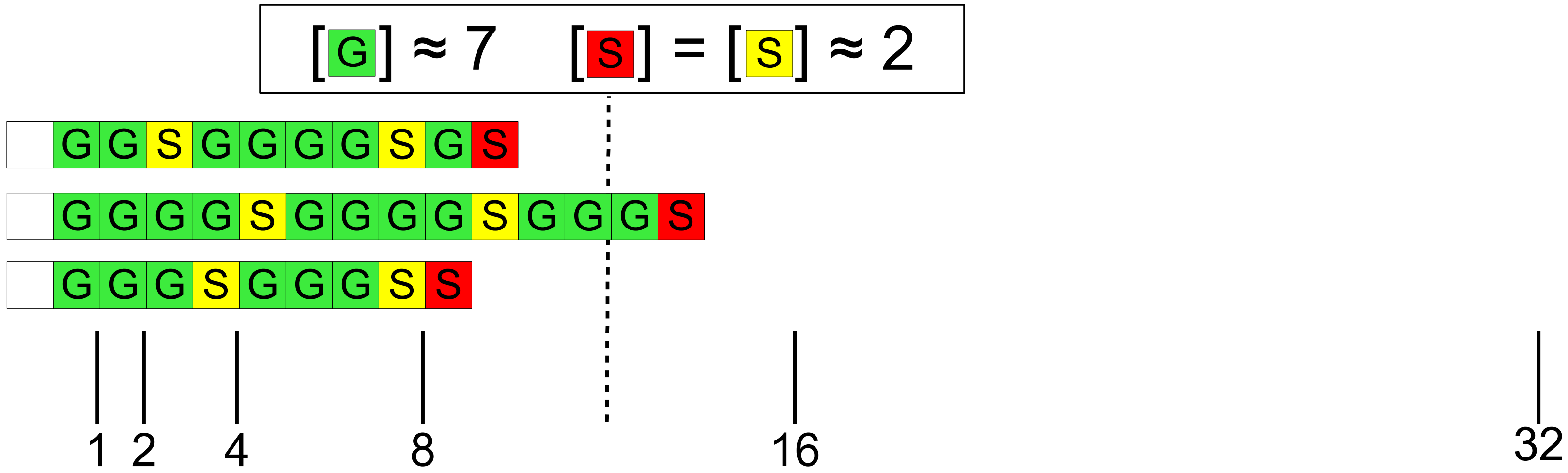

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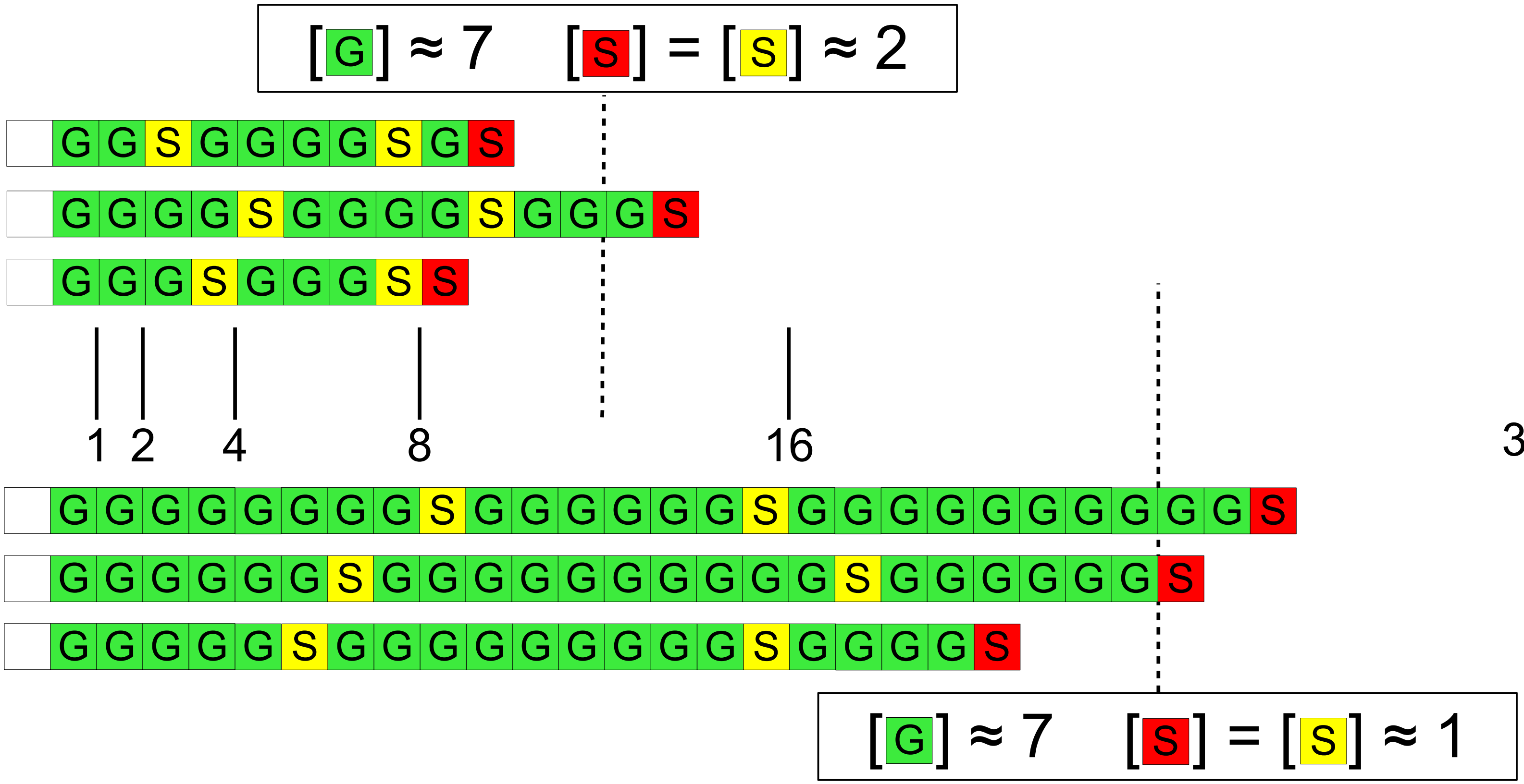
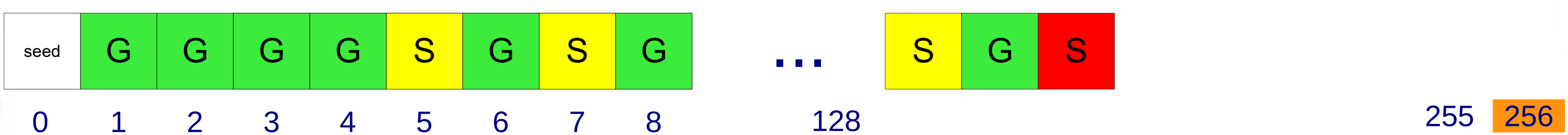


Programming polymer length 2^a precisely

256

Programming polymer length 2^a precisely



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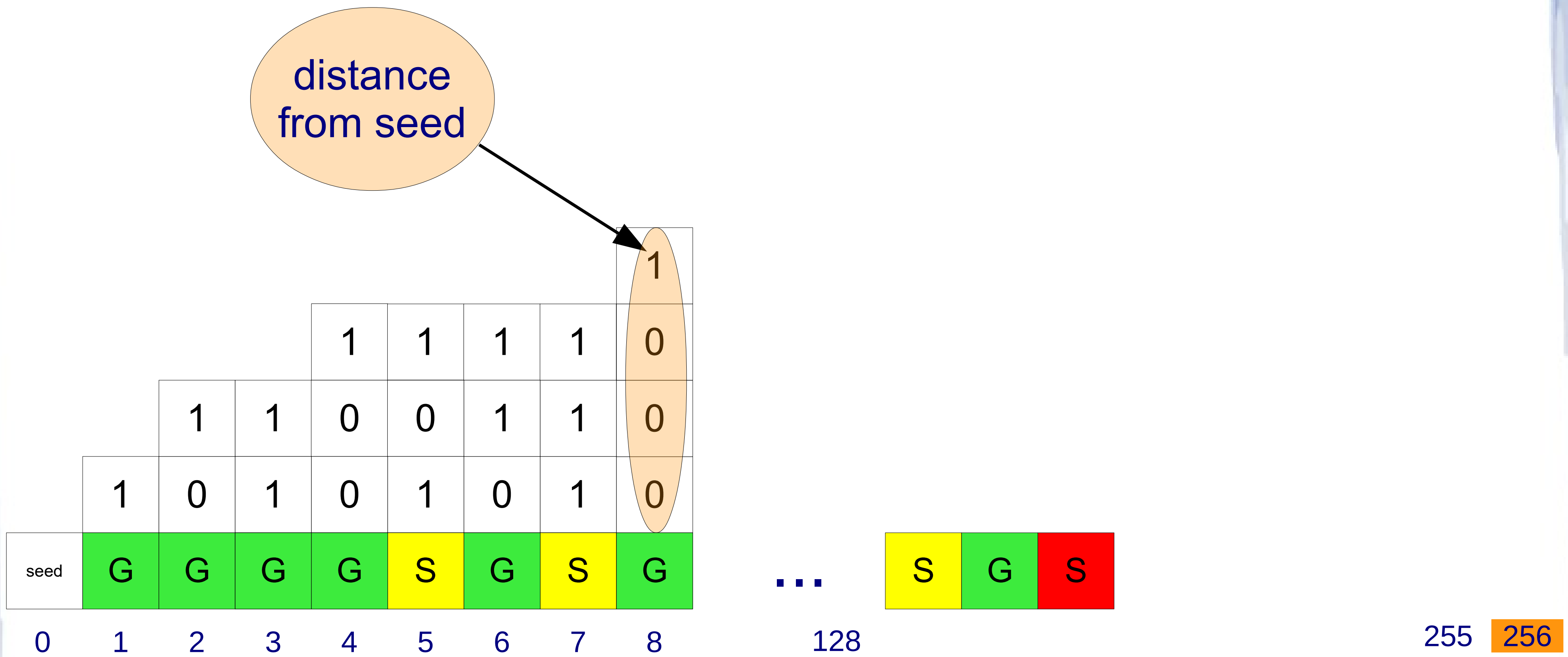

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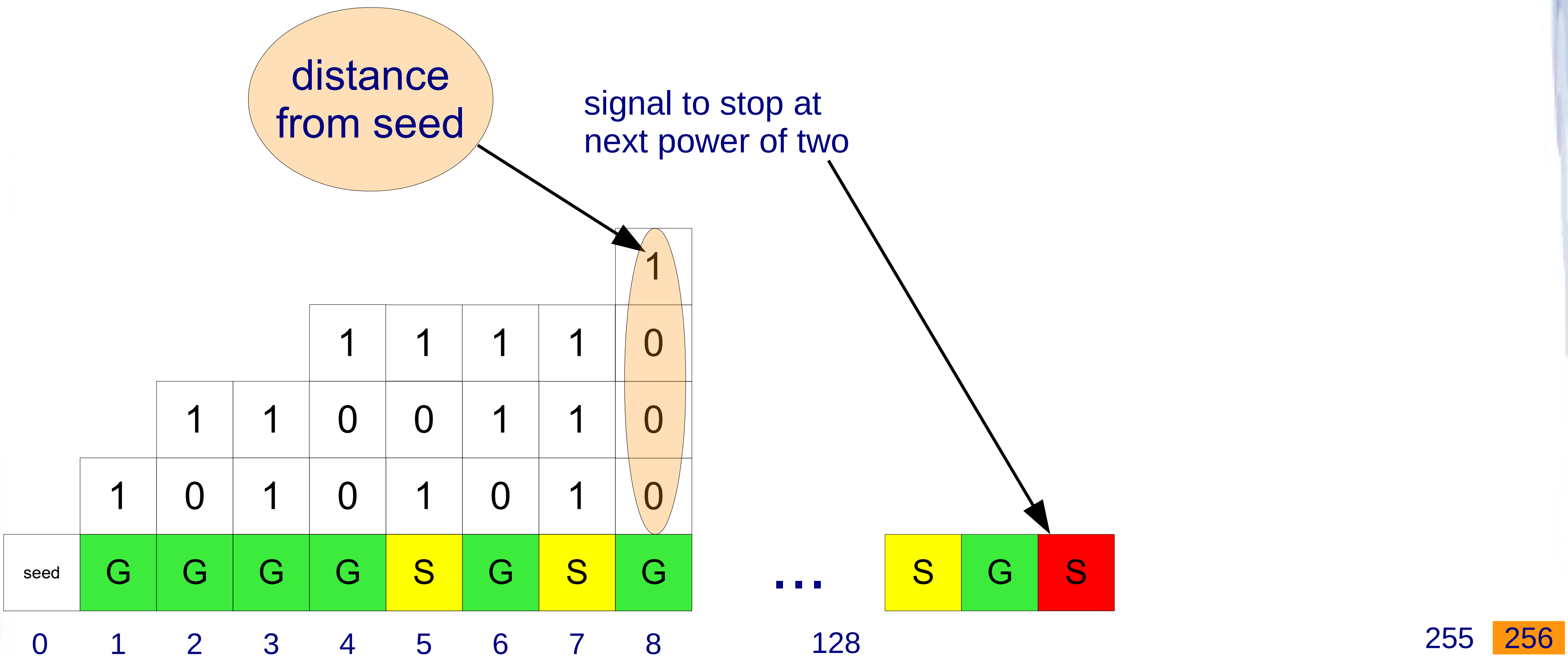

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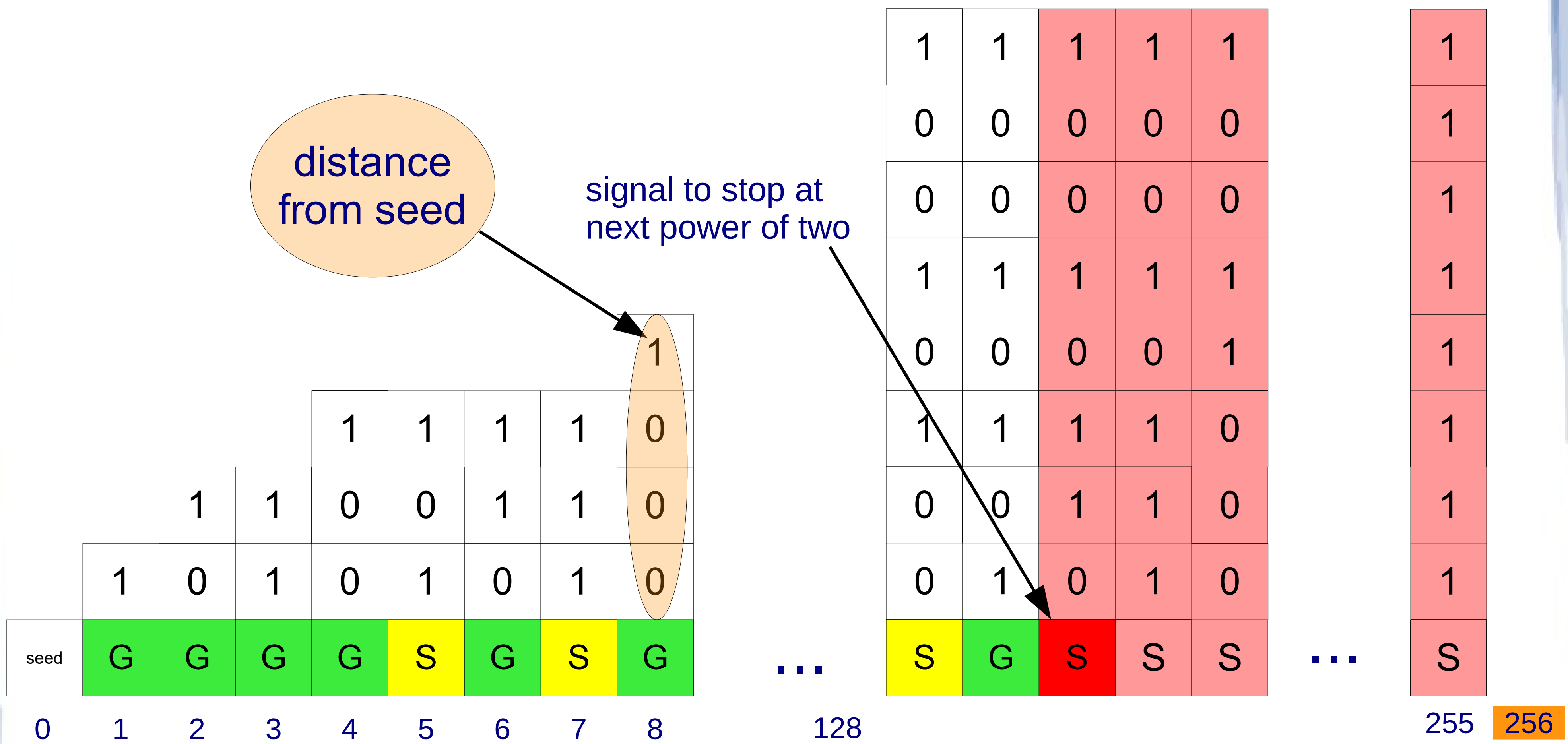

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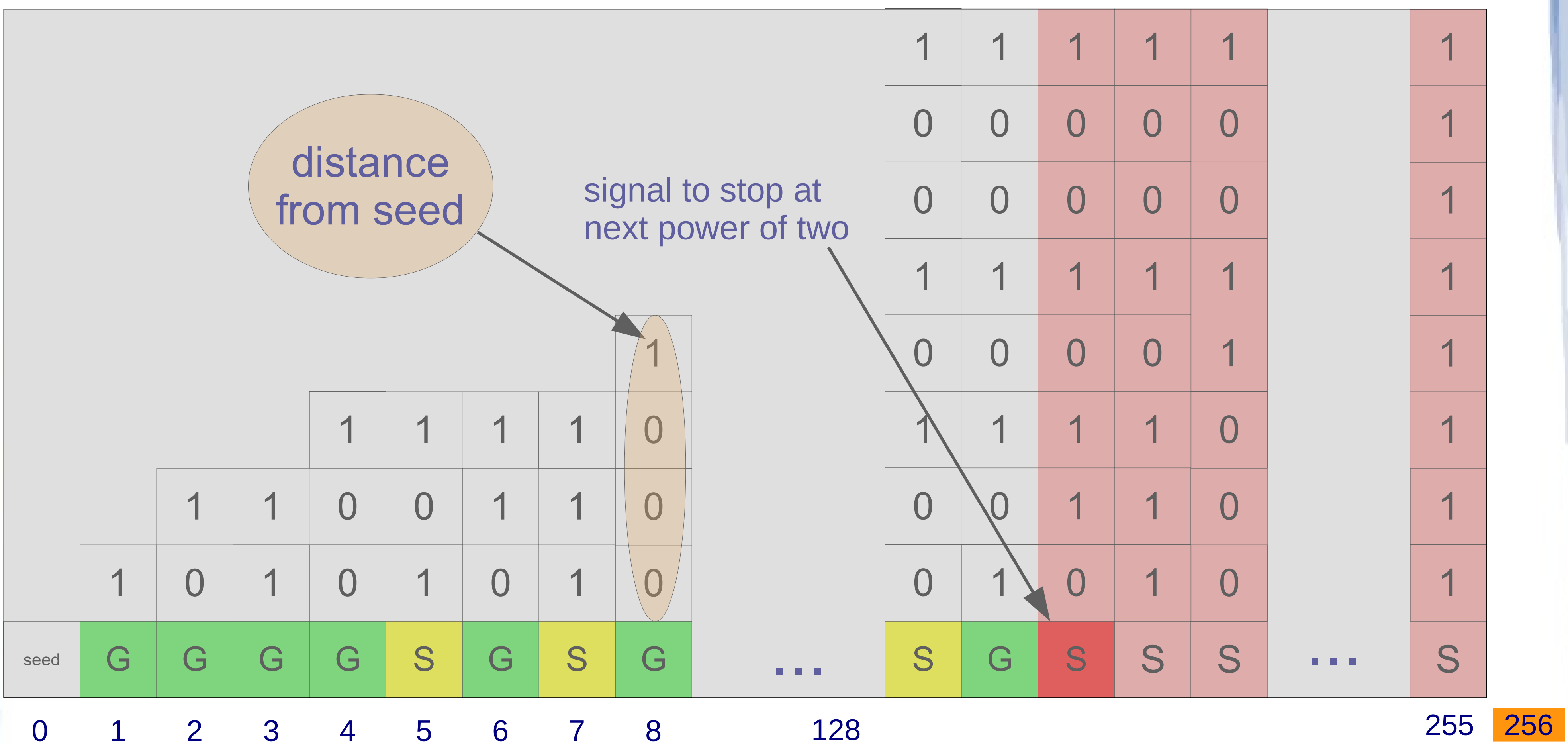
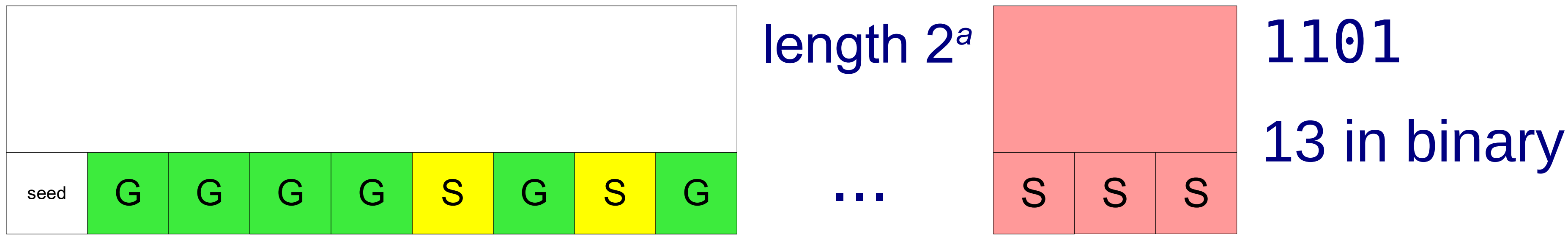


Programming a binary string

`1101`

13 in binary

Programming a binary string



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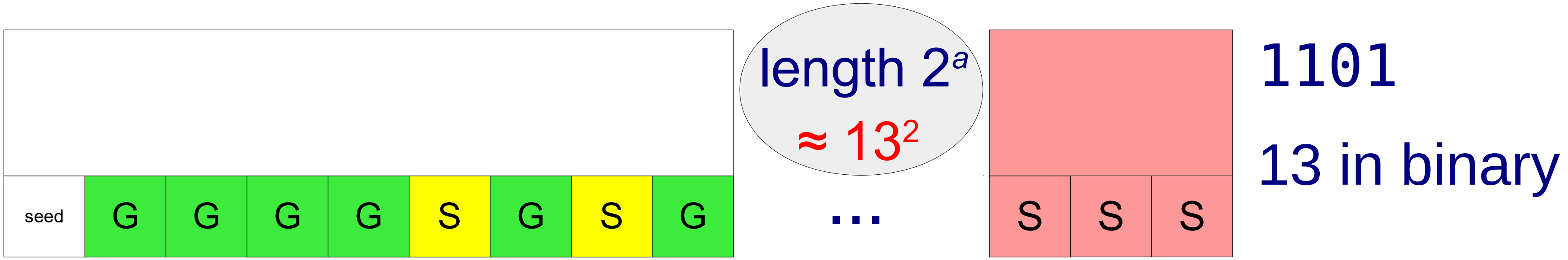

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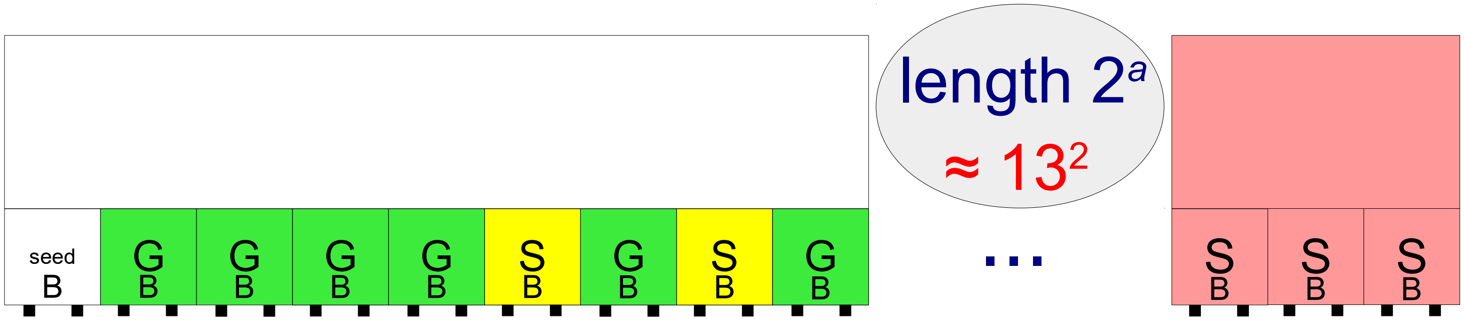

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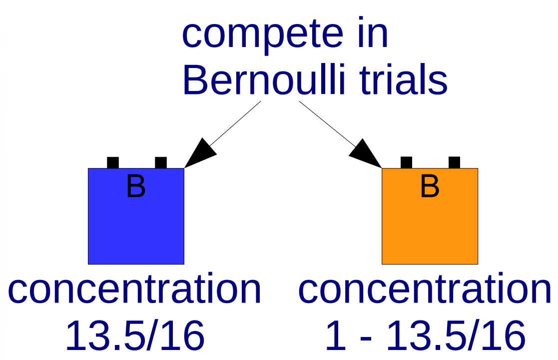

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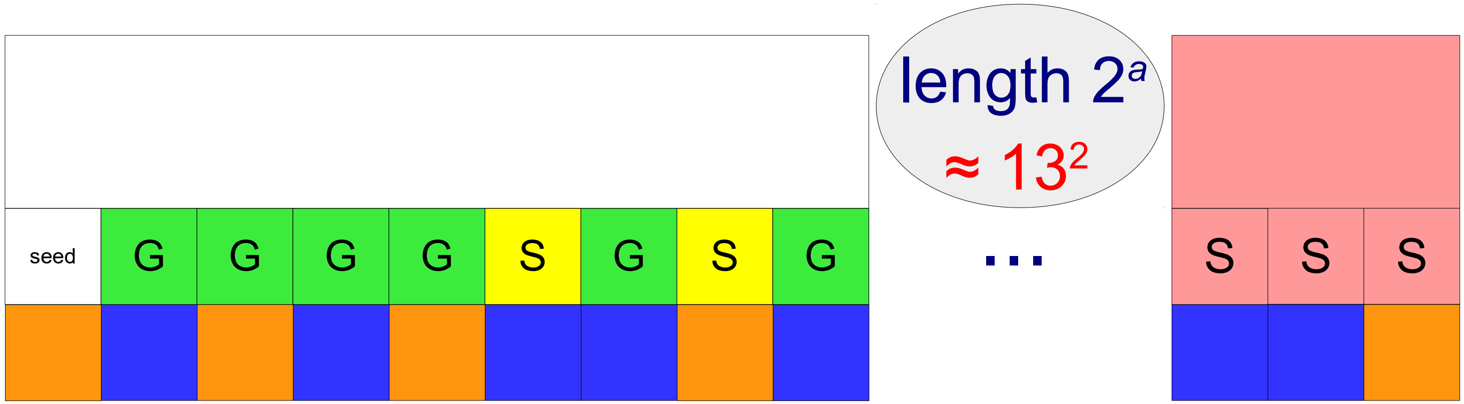
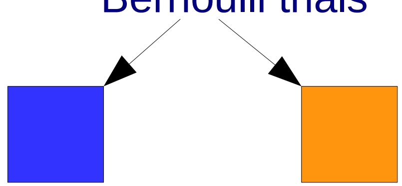


1101

13 in binary

compete in
Bernoulli trials



concentration
13.5/16

concentration
1 - 13.5/16

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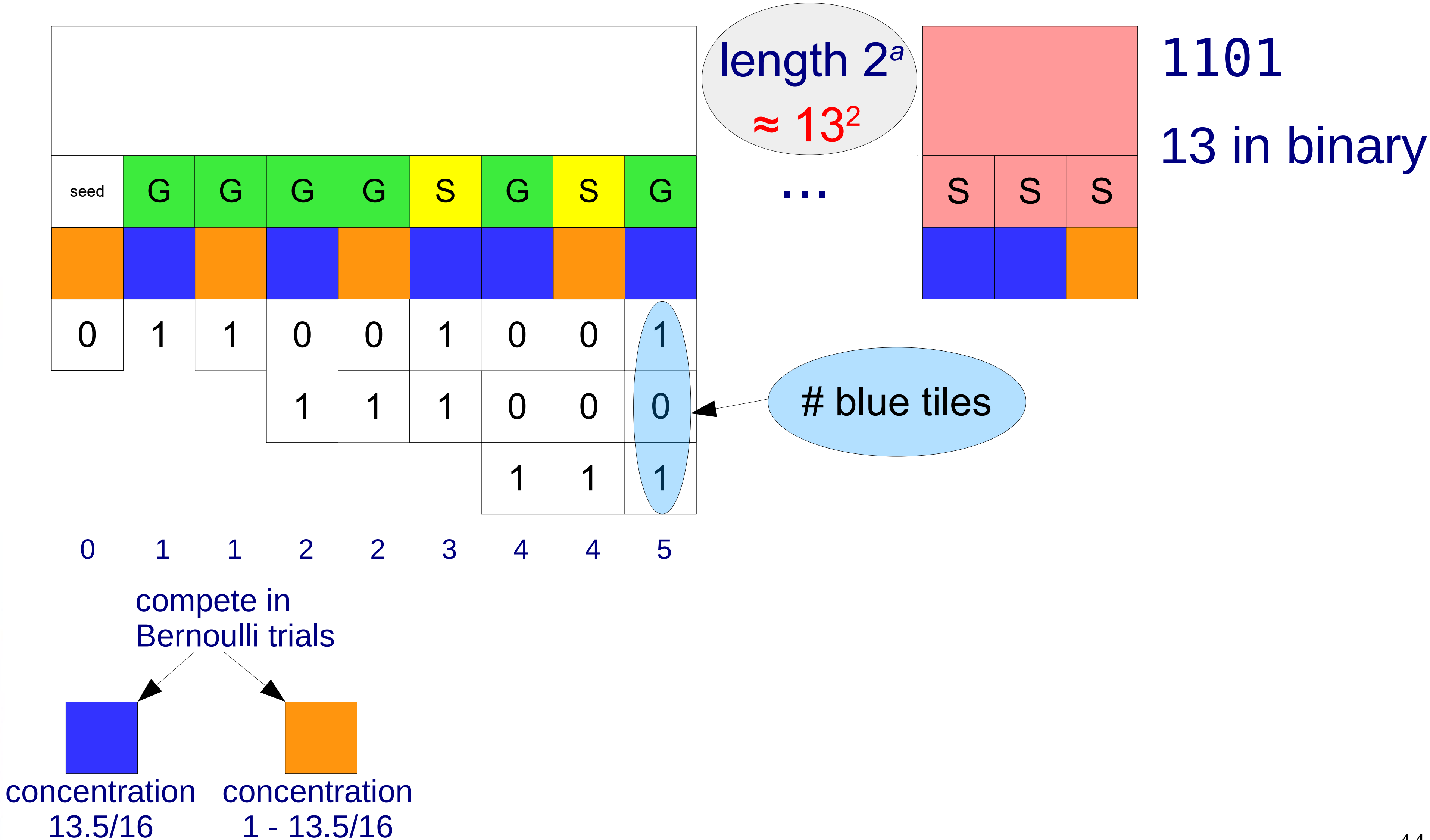

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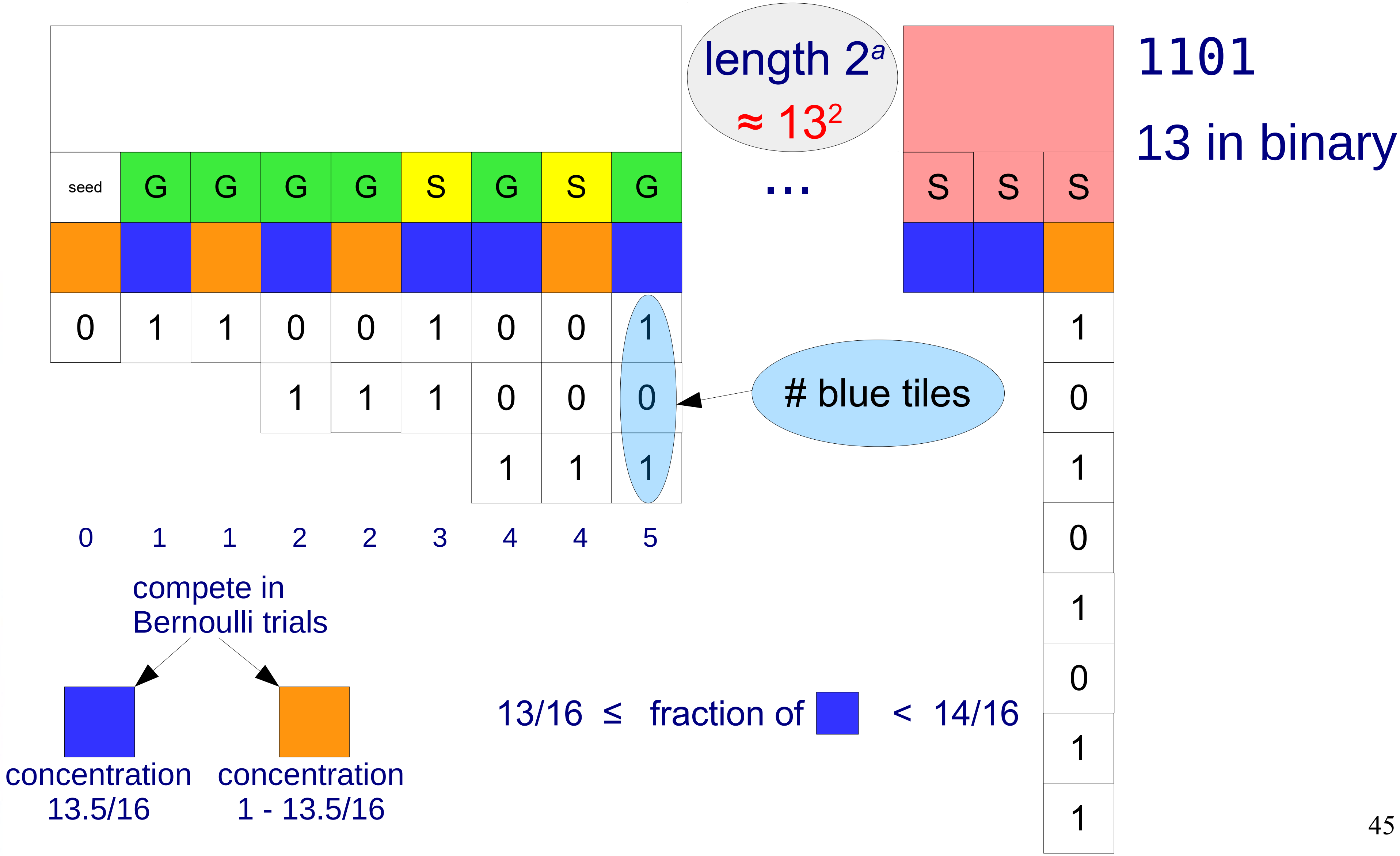

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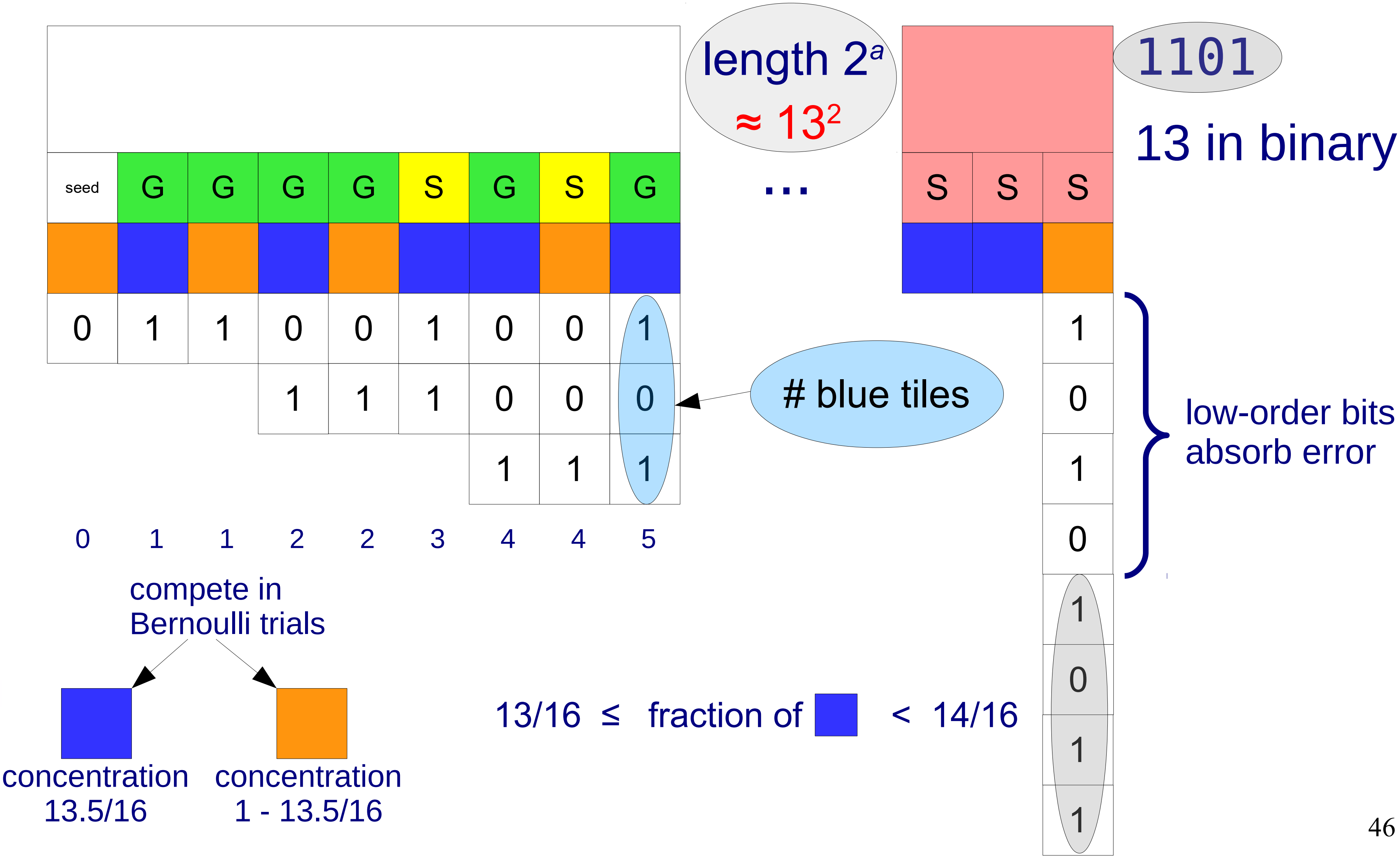
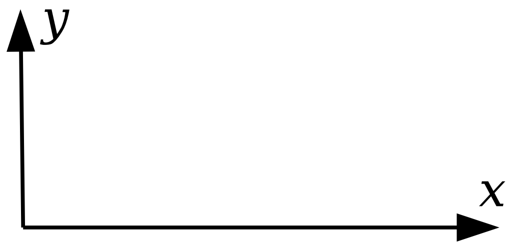


Programming a shape



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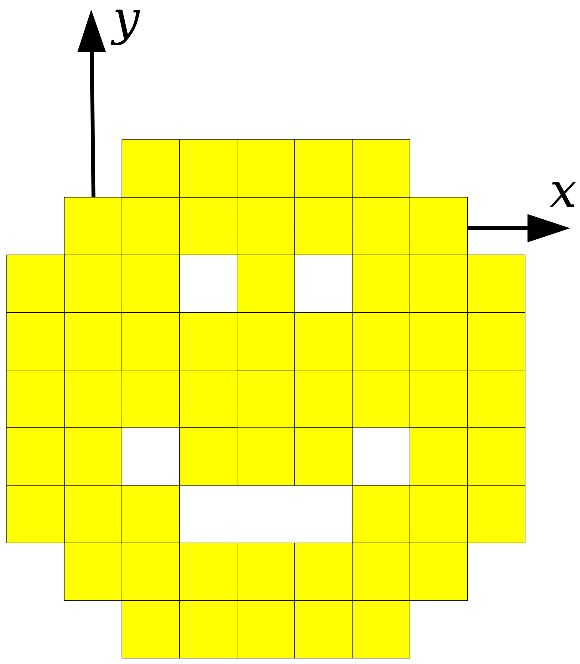

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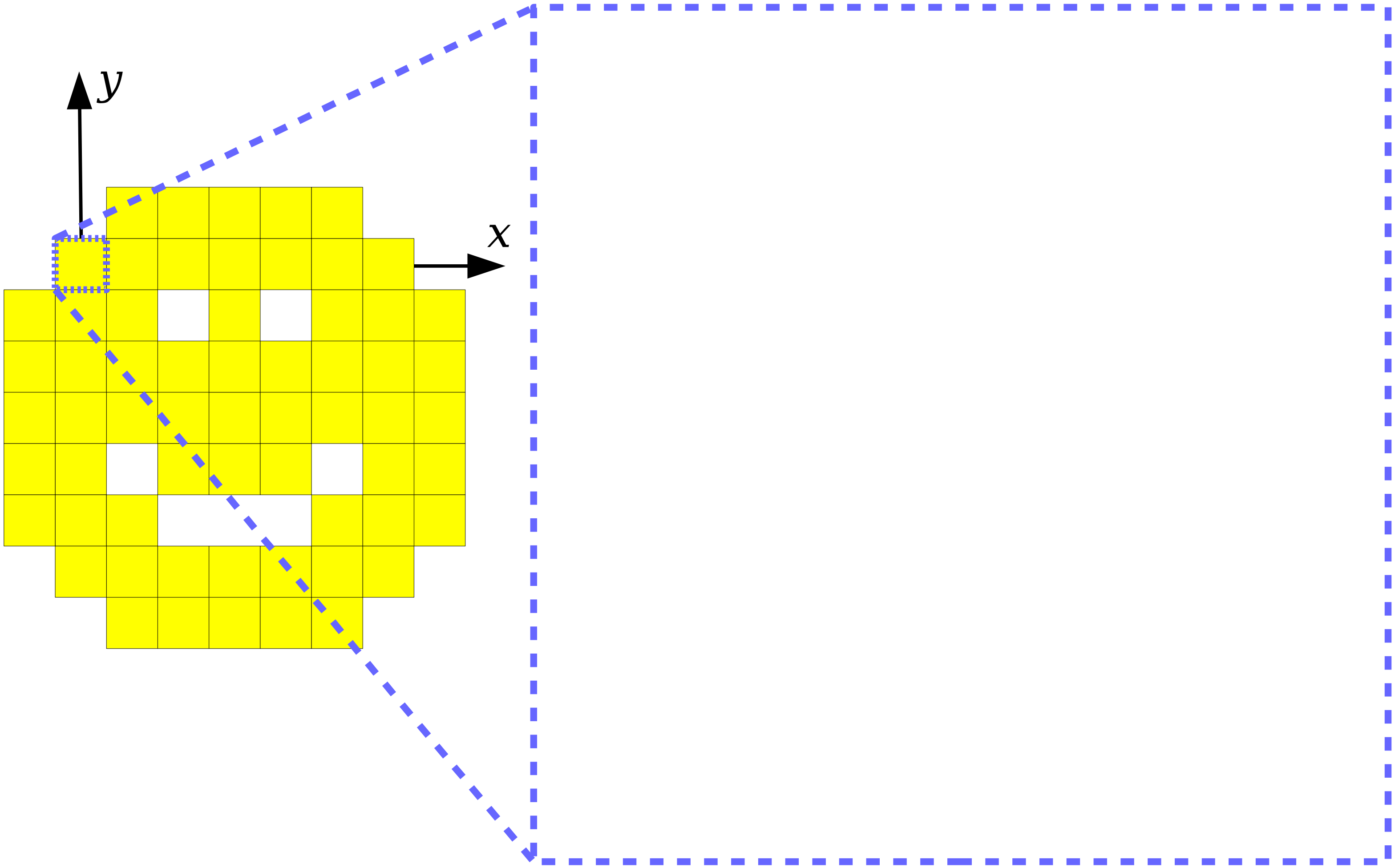

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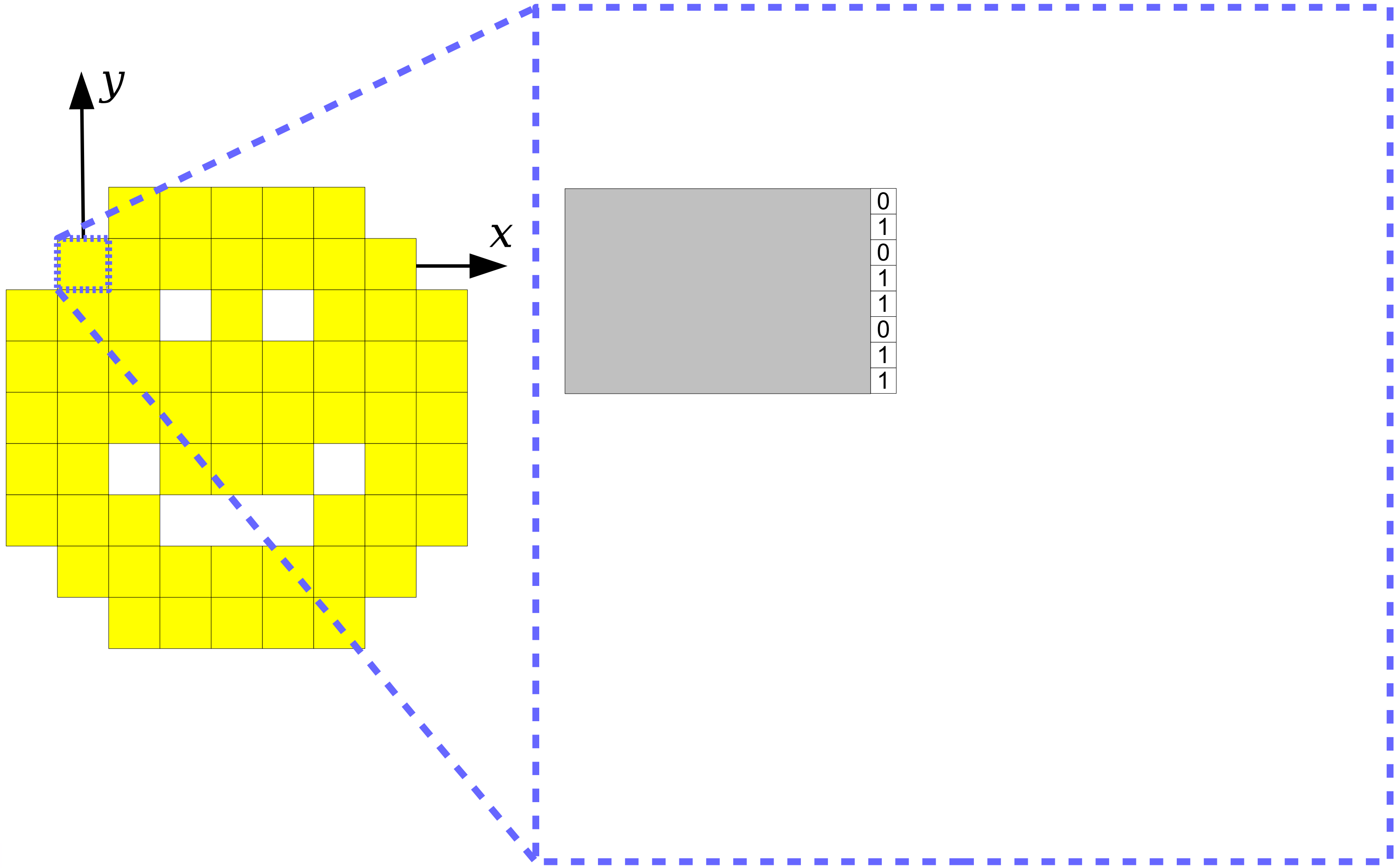

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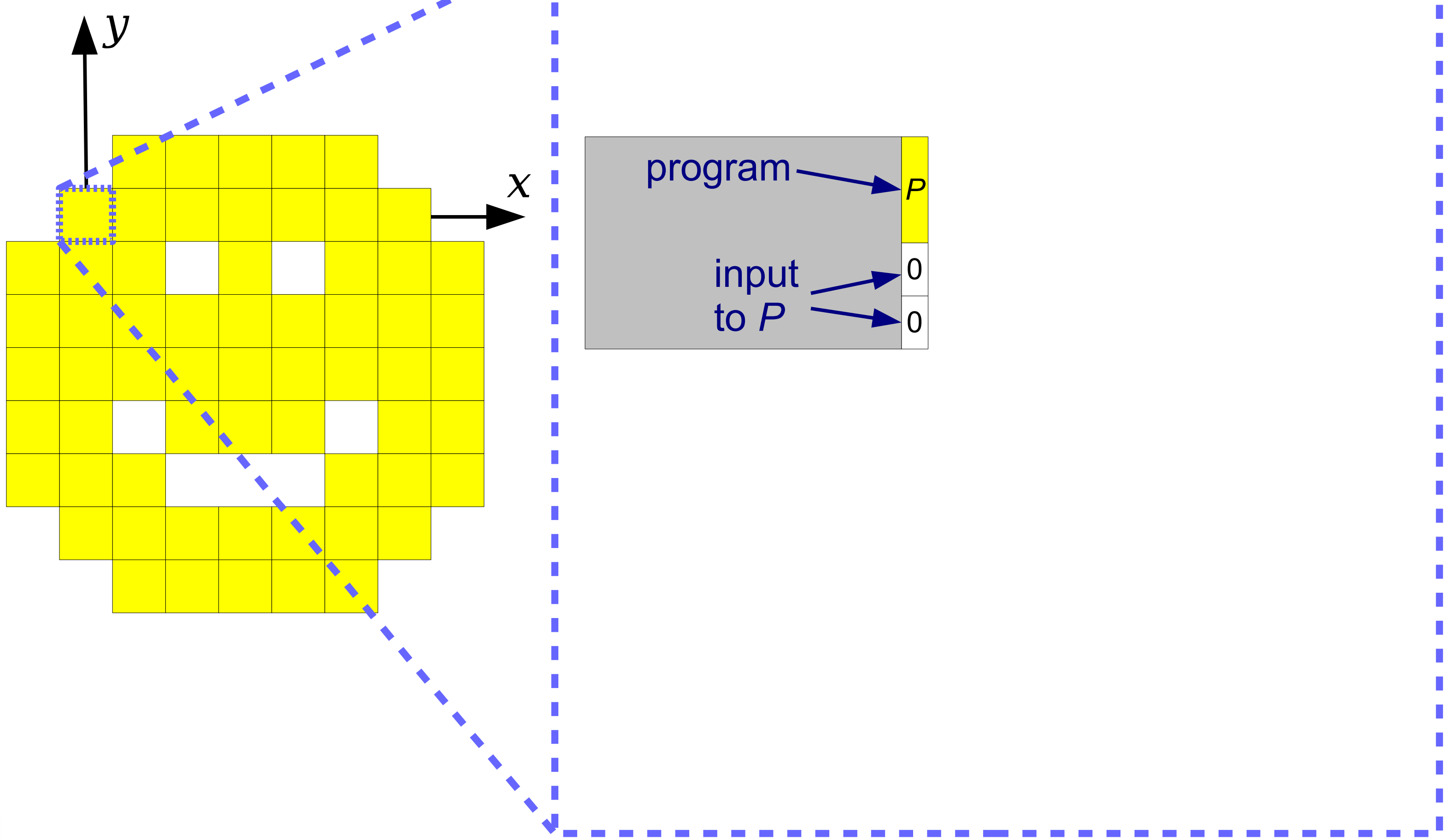

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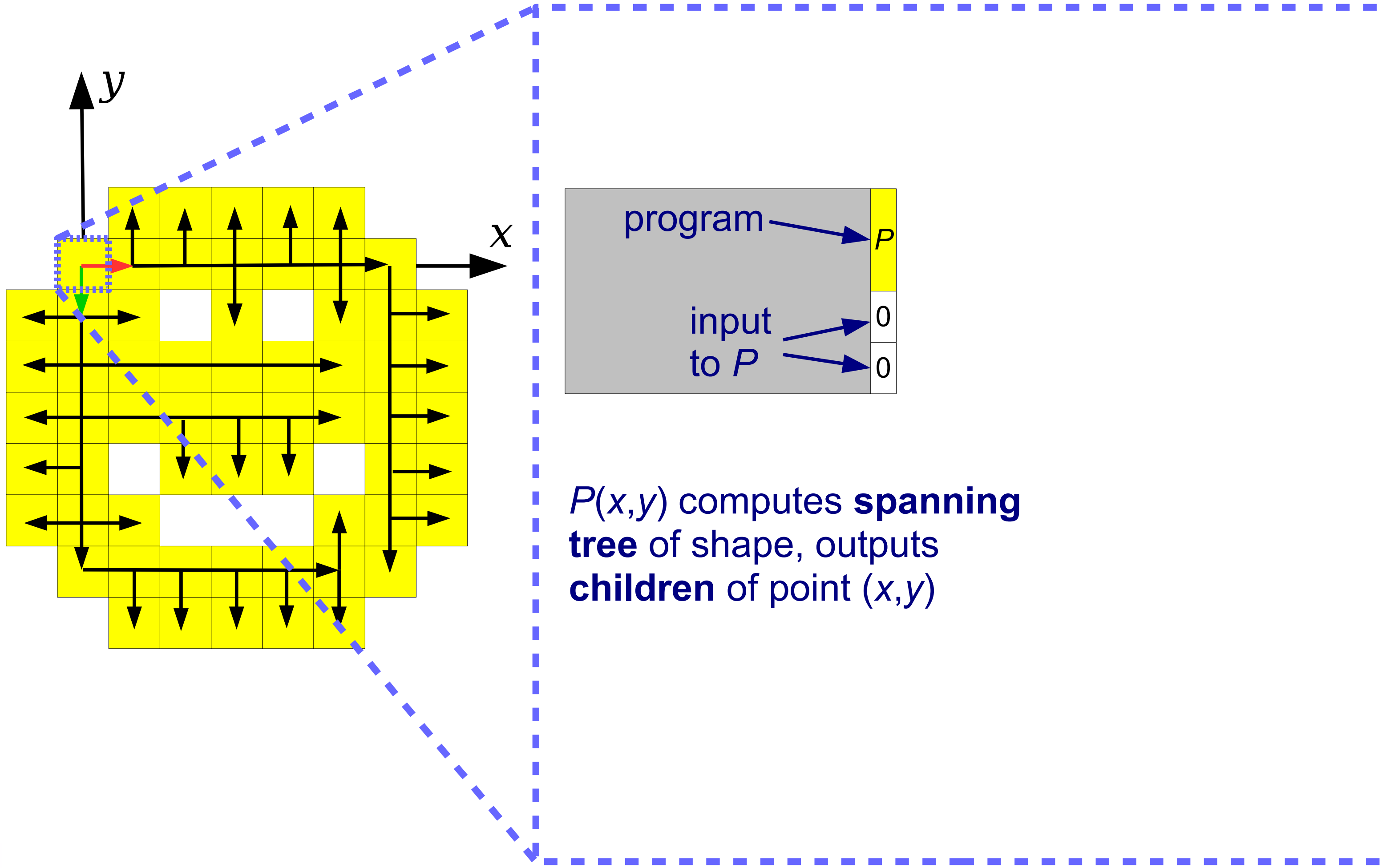
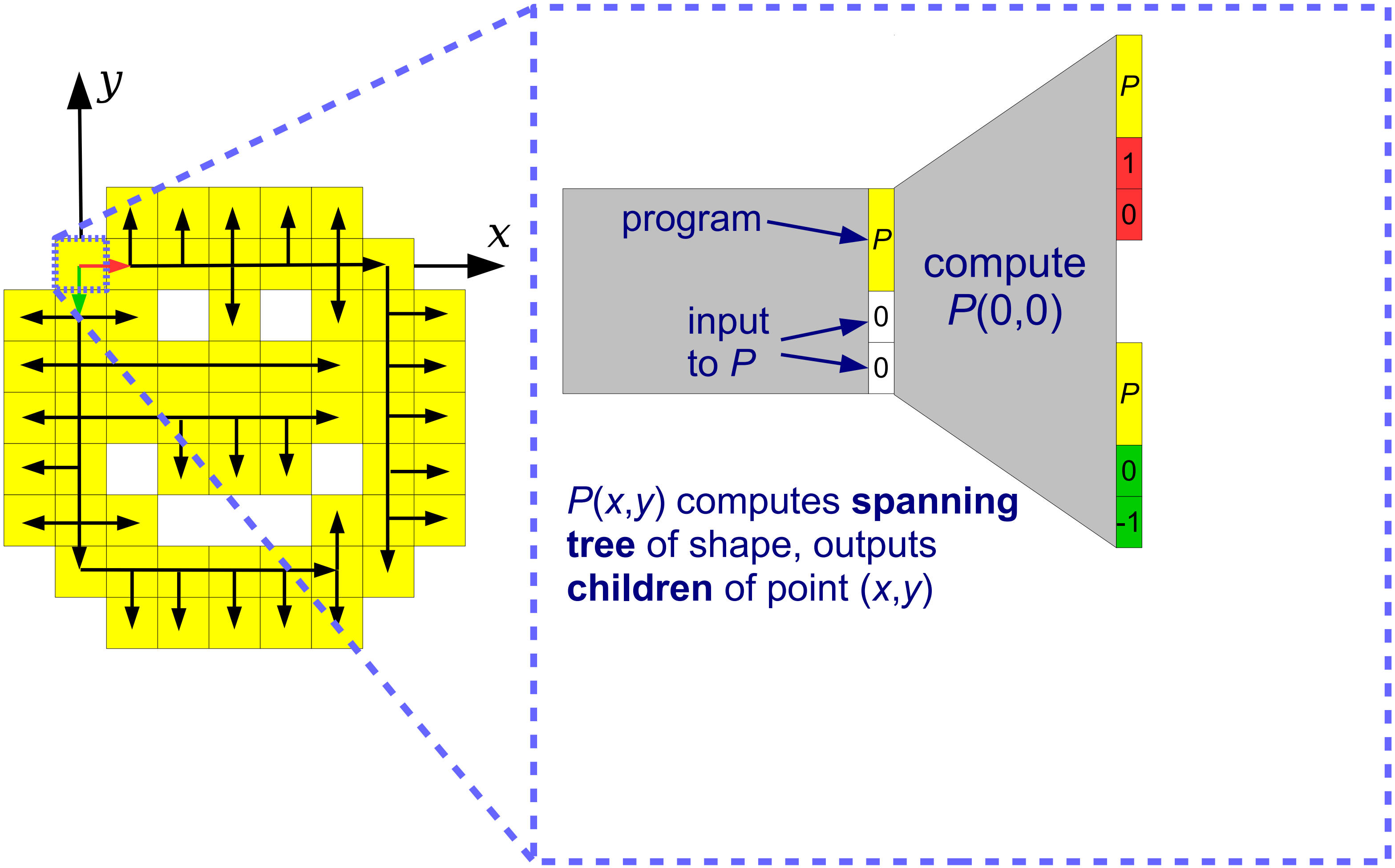


P(*x*,*y*) computes **spanning tree** of shape, outputs **children** of point (*x*,*y*)

Programming a shape



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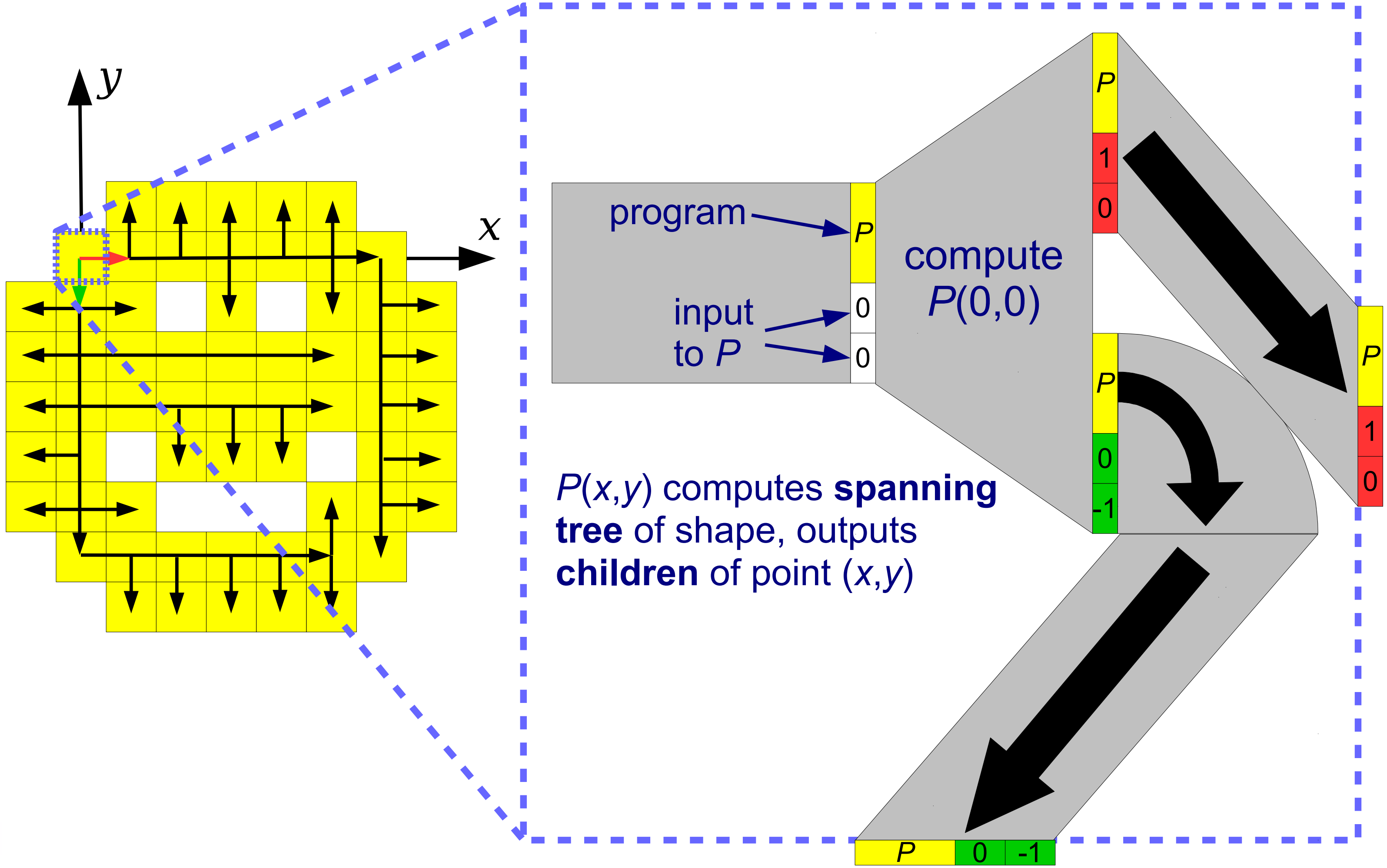

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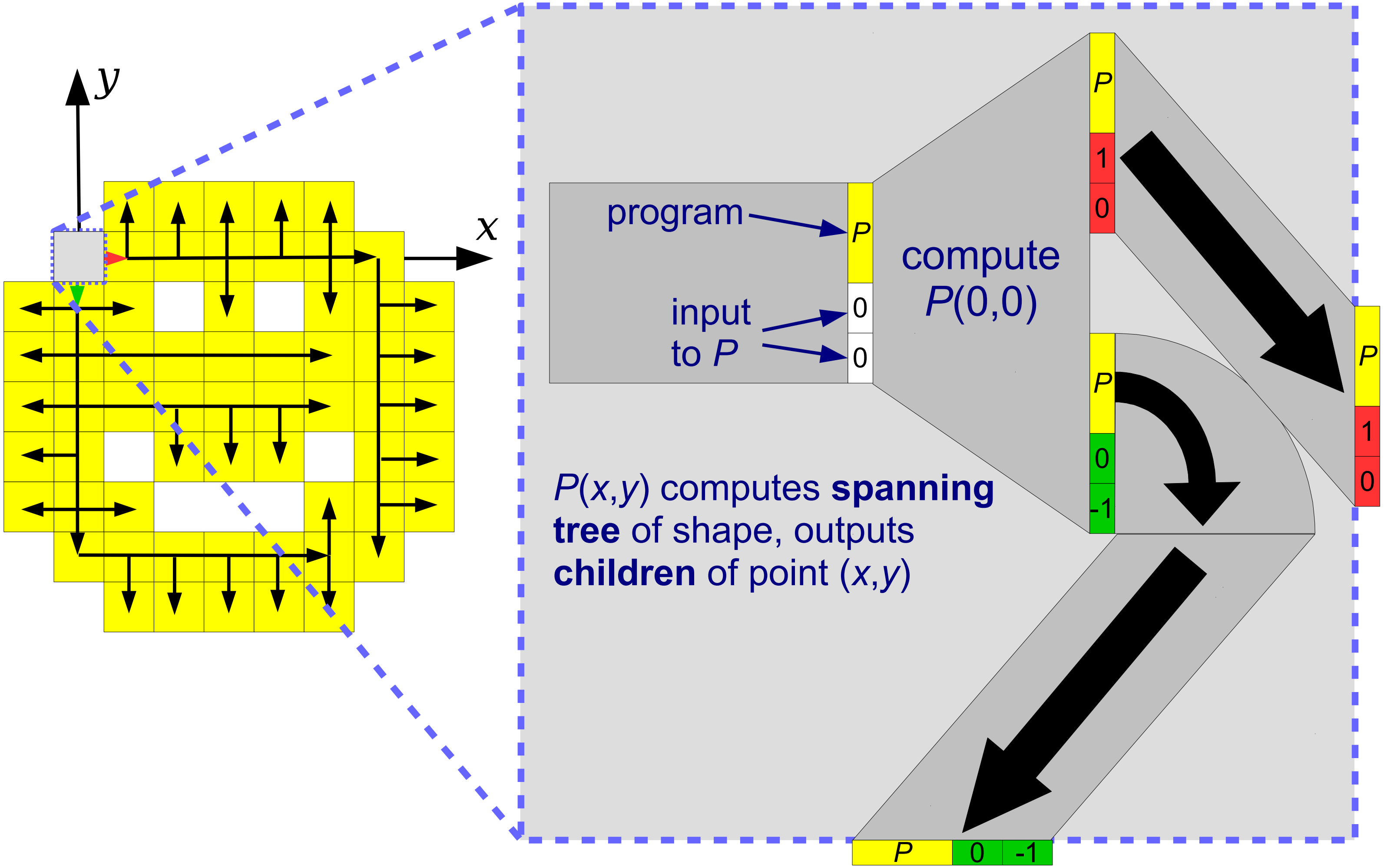

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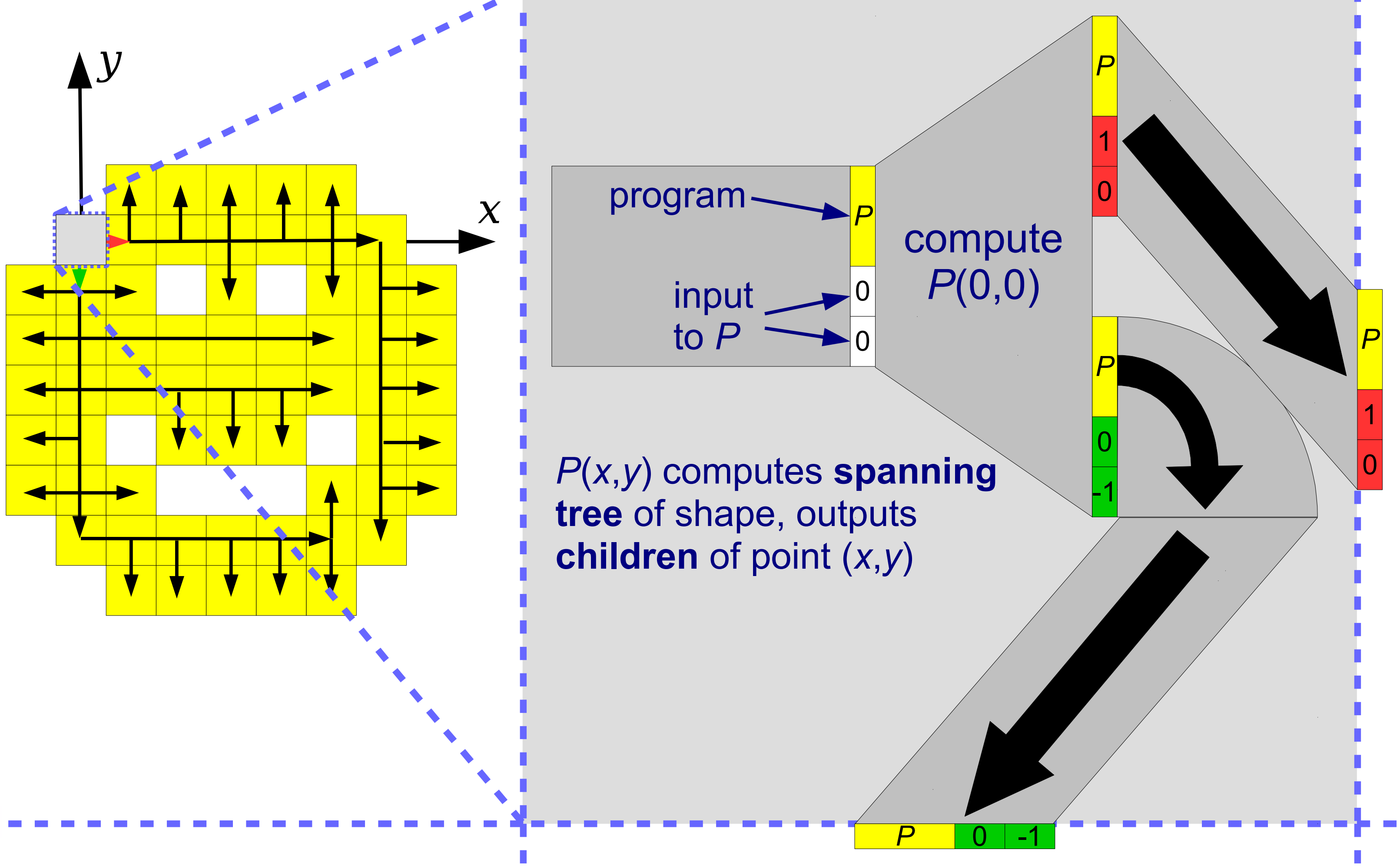

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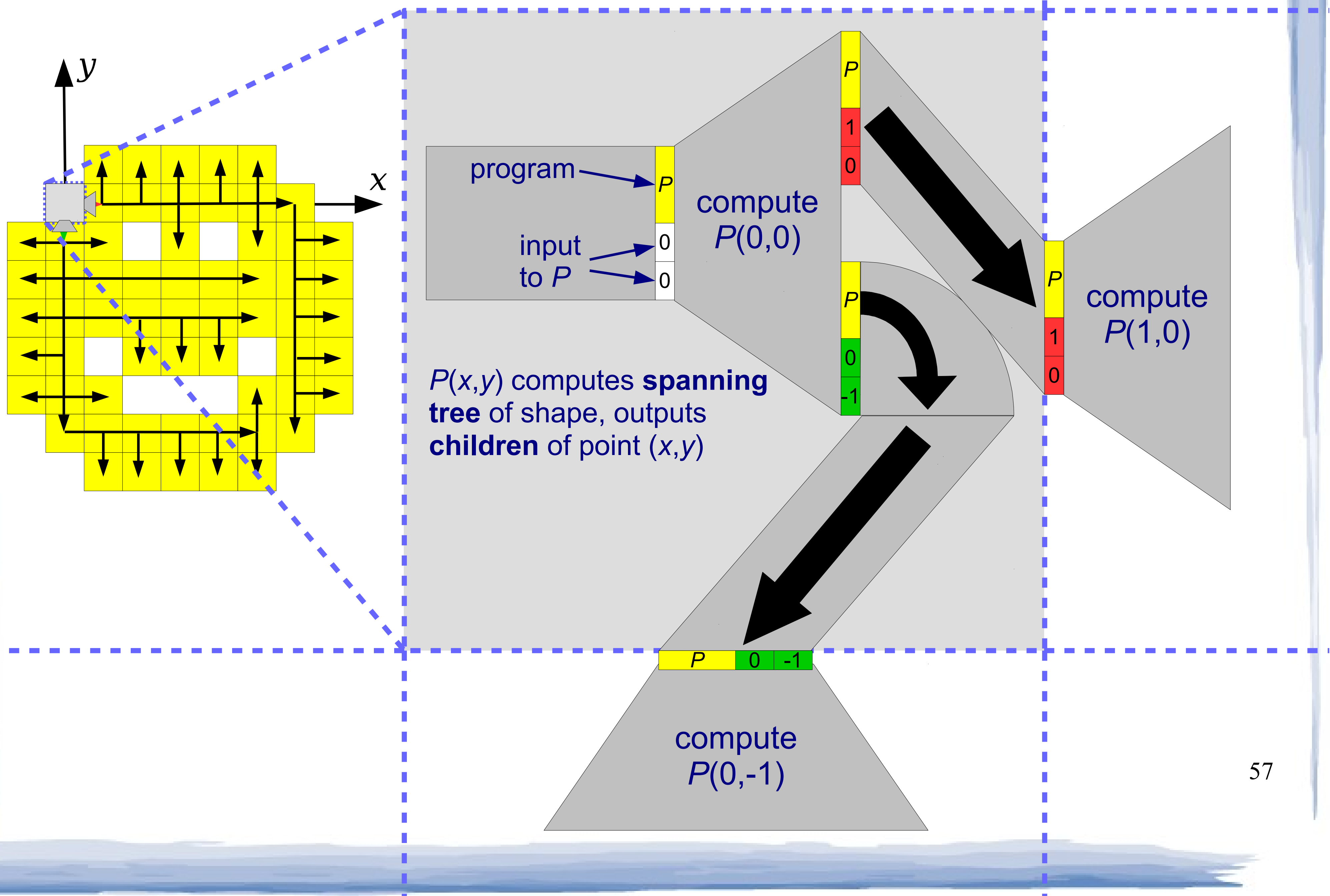

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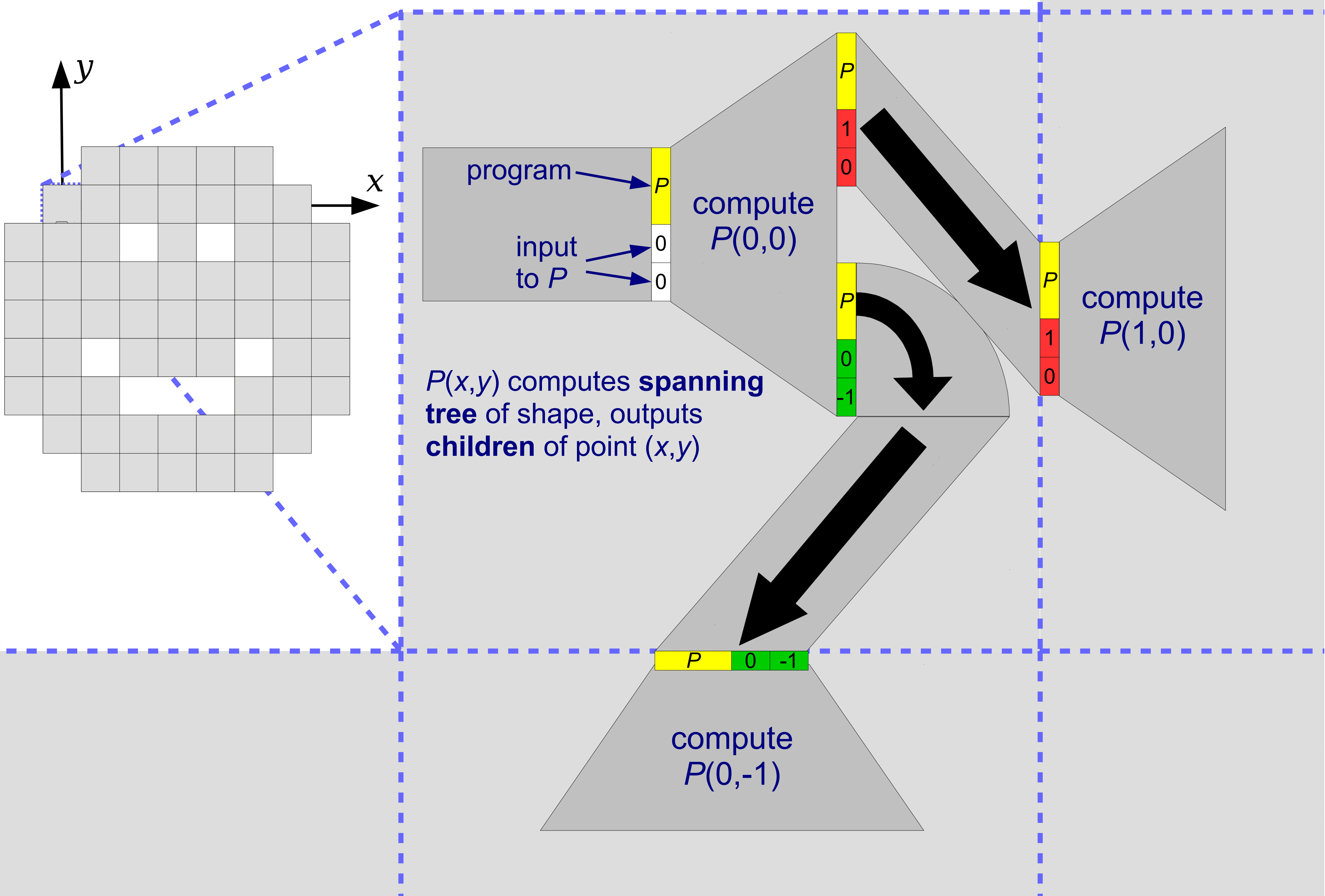
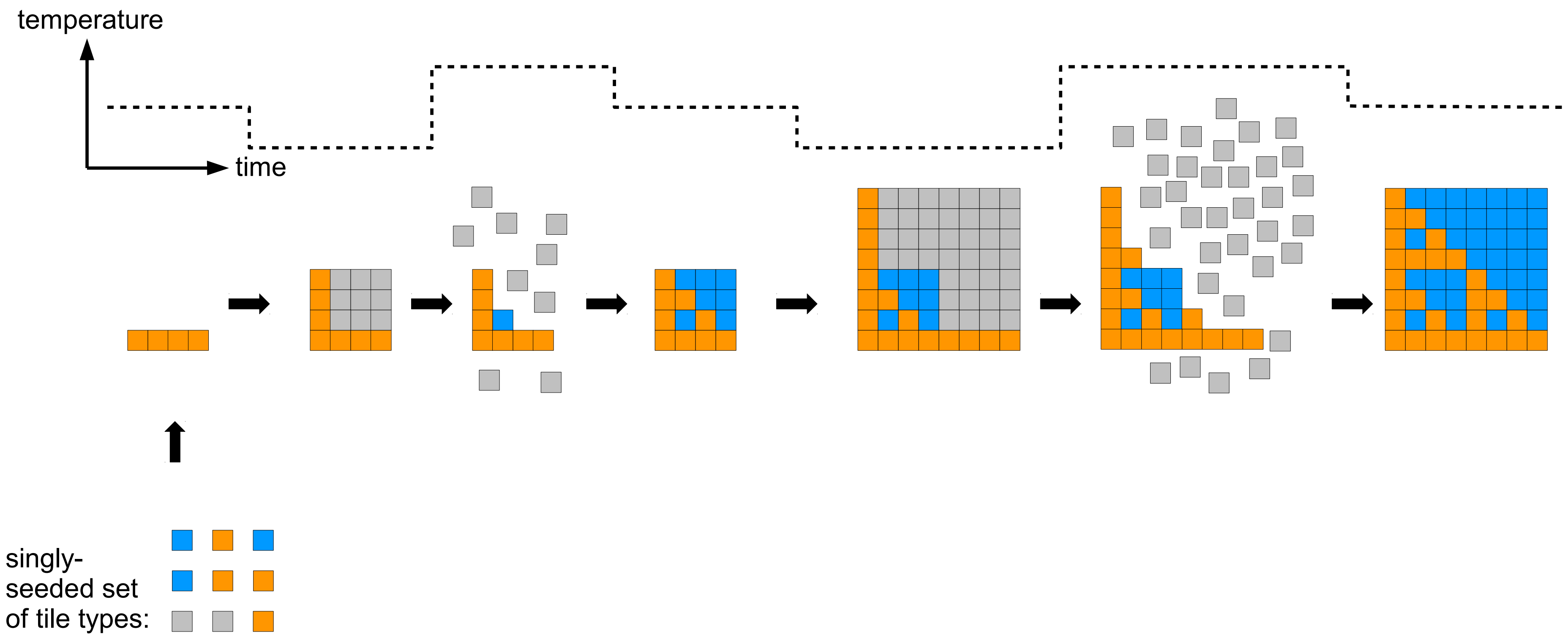


Temperature programming

Temperature programming

(Kao, Schweller, SODA 2006): Vary temperature (binding strength threshold) throughout assembly to control what assembles.



Complexity of Temperature Programming

Scott Summers: A fixed set of (singly-seeded) tile types can assemble any finite scaled shape through temperature programming.

Number of tile types (a self-assembly "resource") is constant (maybe big), no matter the shape.

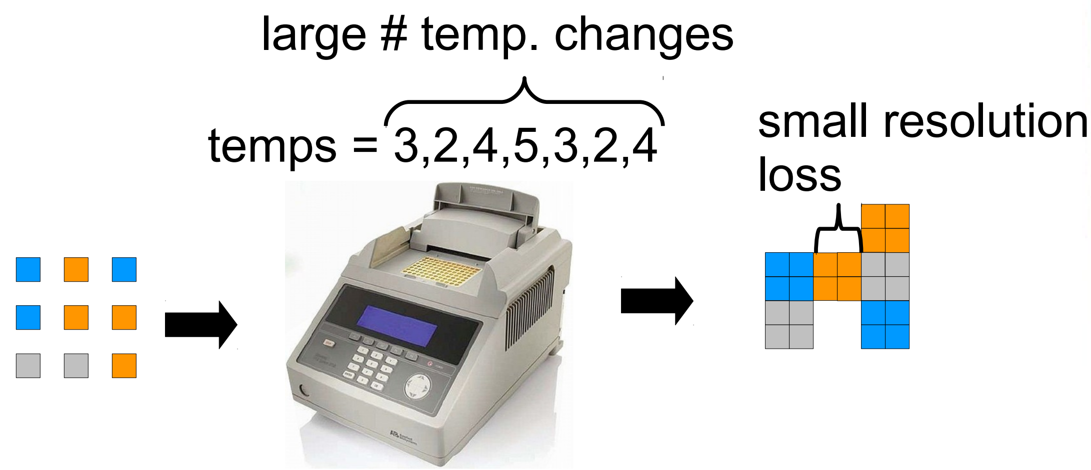
Scott wondered about two other self-assembly resources that might change for each shape:

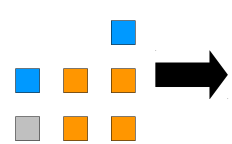
- What **resolution loss** is required?
- What **number of temperature changes** are required?

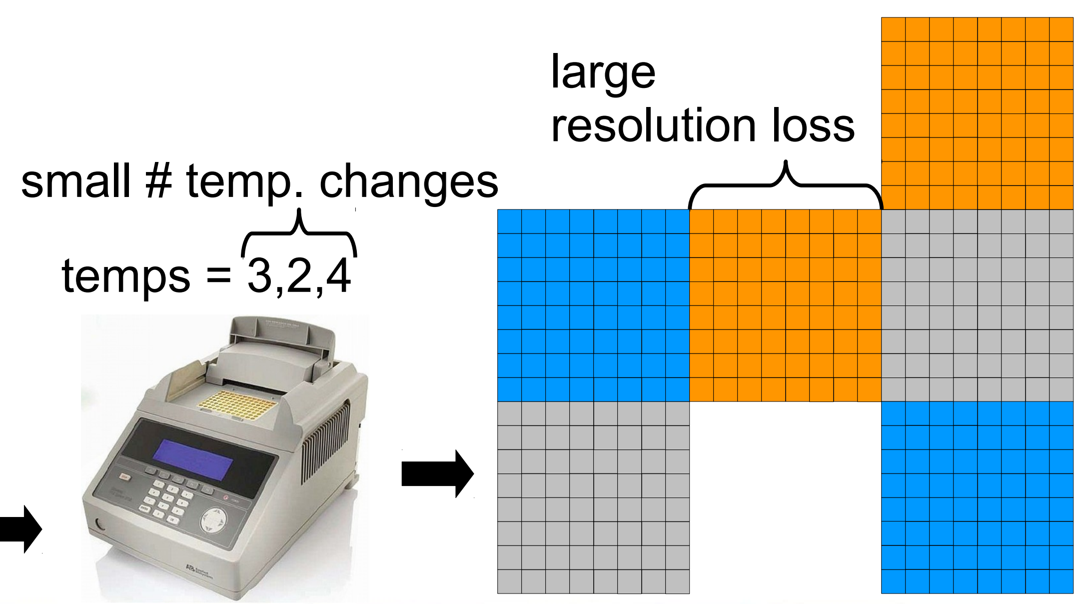
Complexity of Temperature Programming

For shape *S* with *n* points, trade-off between **resolution loss** and **number of temperature changes**:

- With *optimal resolution loss* = constant (22 in Scott's paper although shown smaller in the example), need ≈ *n* temperature changes.
- With *optimal number of temperature changes* = size of smallest program *p* that prints *S*, need resolution loss ≈ *t* = running time of *p*.







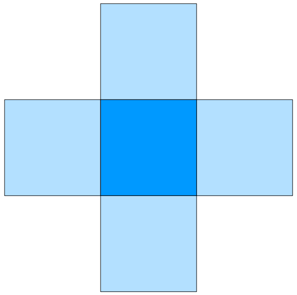
Hierarchical assembly

Parallelism in the Model

potential attachment location

attached tile

time step 0

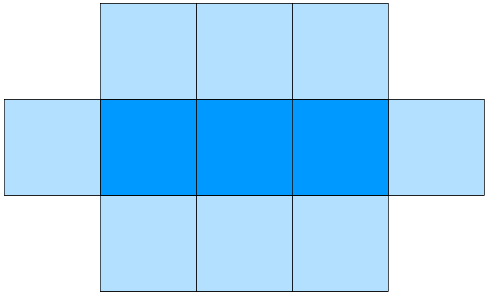


Parallelism in the Model

potential attachment location

attached tile

time step 1

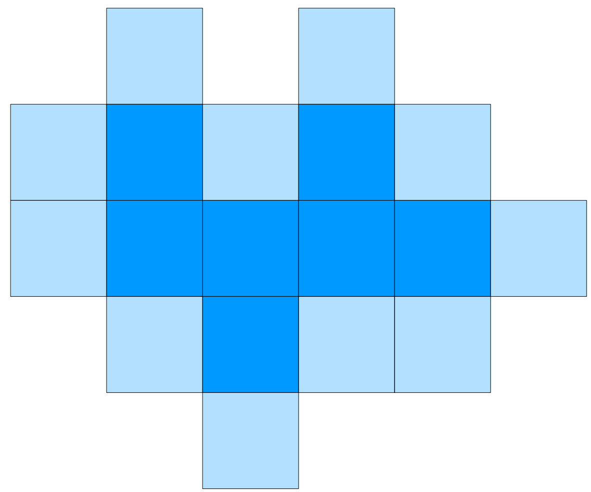


Parallelism in the Model

potential attachment location

attached tile

time step 2

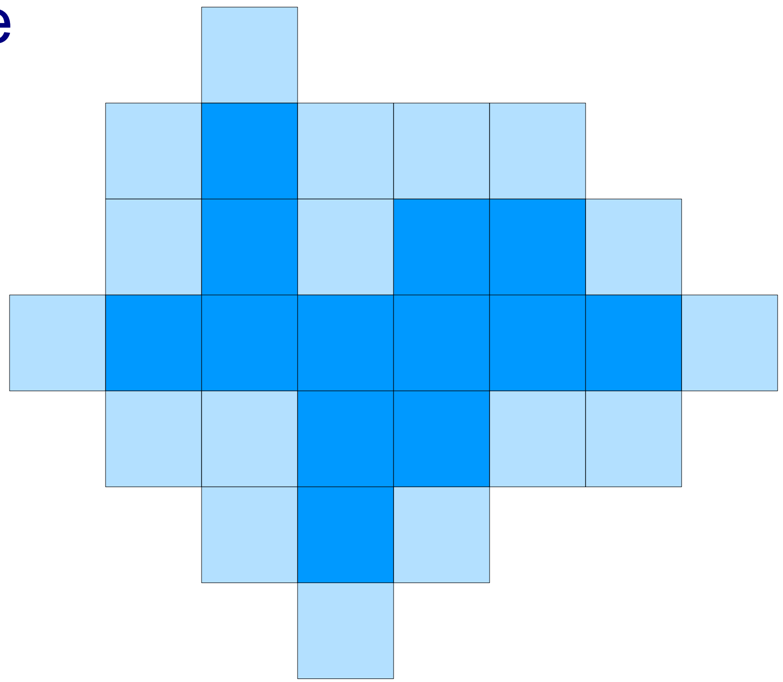


Parallelism in the Model

potential attachment location

attached tile

time step 3



Parallelism in the Model

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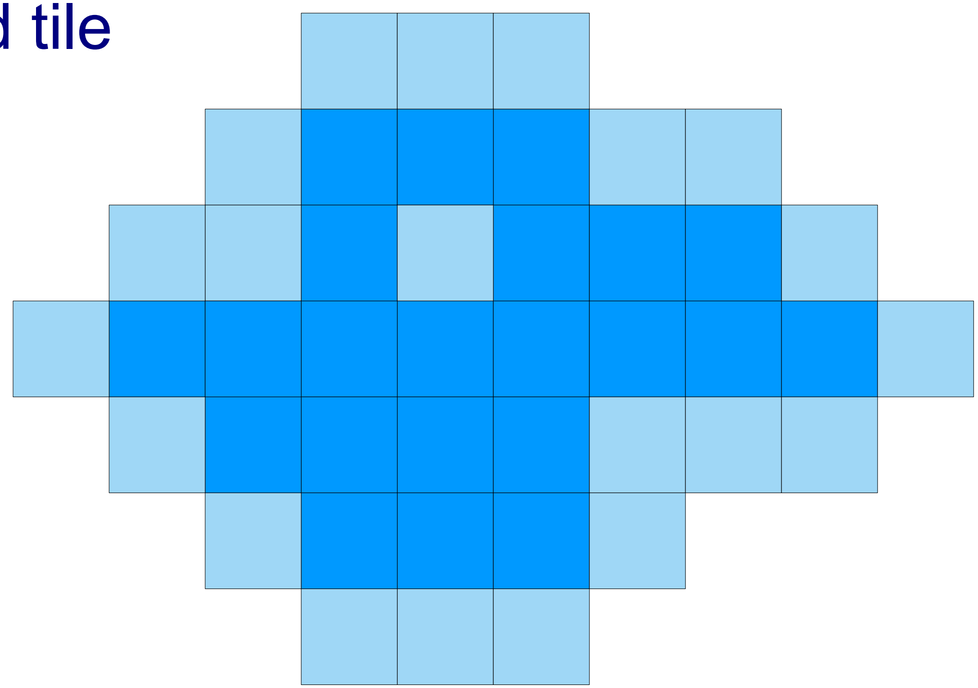
attached tile

time step 4



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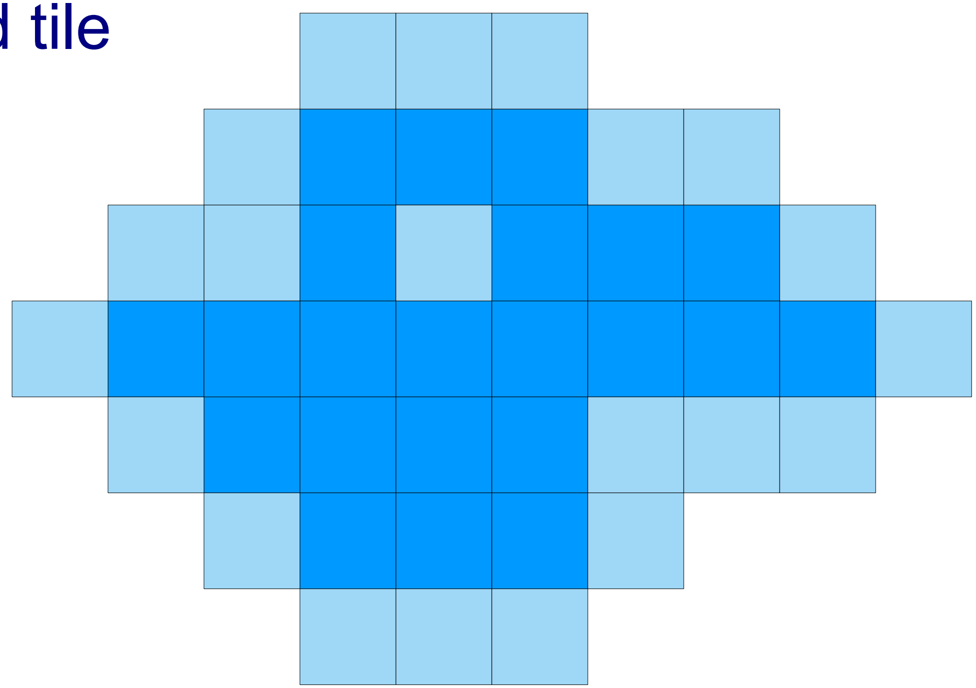

time t: perimeter ≤ $O(t)$ (with high probability)

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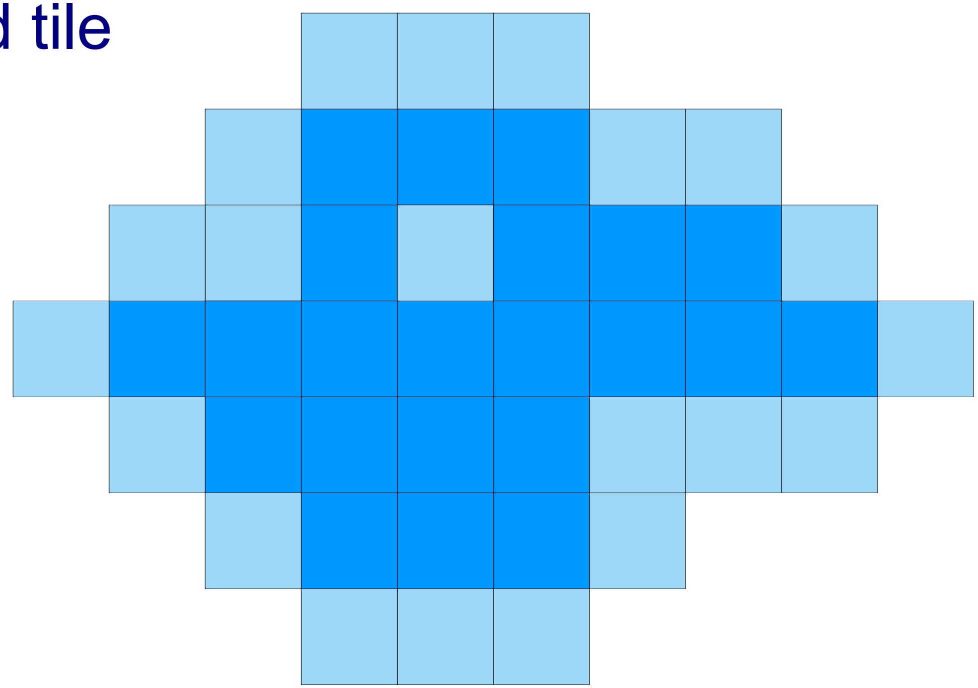

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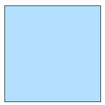
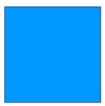
$\rightarrow$ max attachments per time step $\leq O(t)$

Parallelism in the Model

 potential attachment location

 attached tile

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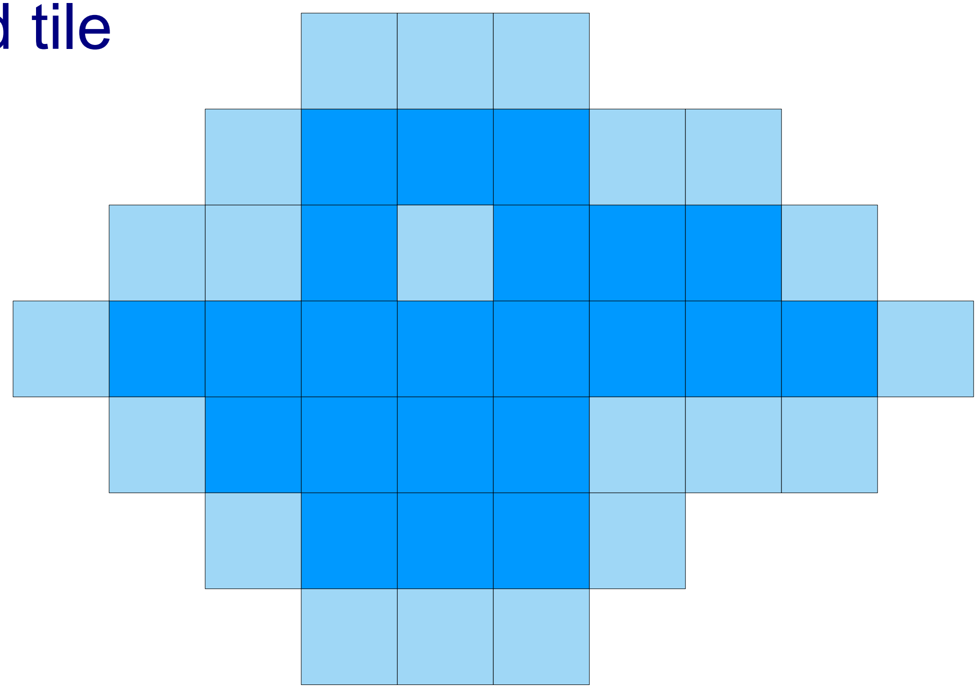

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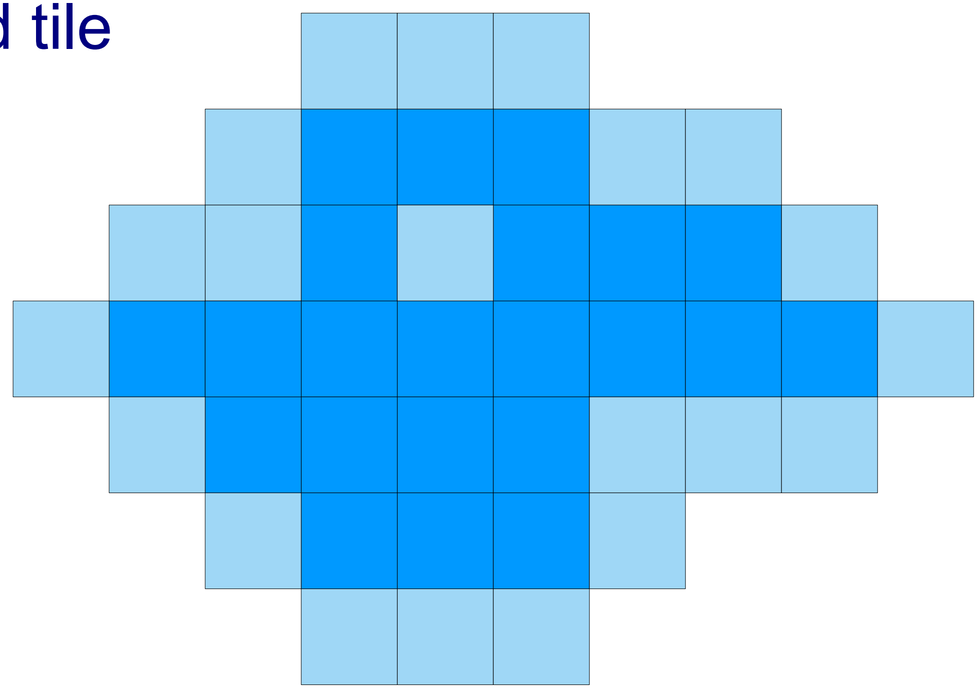

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→ min time to assemble any shape of size $N \geq \Omega(\sqrt{N})$

Parallelism and Time

Can we speed up assembly by allowing large assemblies to form in parallel and then attach to each other in one step?

Hierarchical Tile Assembly Model

- **seeded** model
  - growth nucleates from a single seed tile
  - tiles attach one at a time

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  - growth nucleates from a single seed tile
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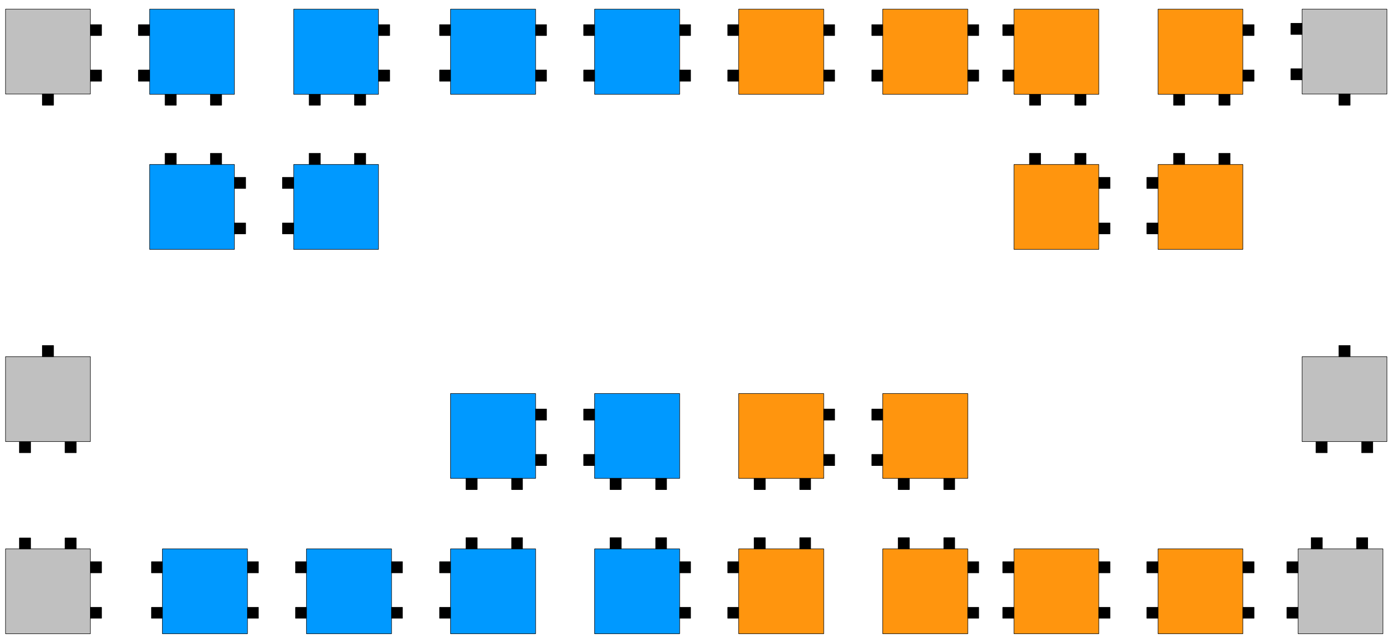
- **hierarchical** model: assembly is producible if
  - base case: it is a single tile, or
  - recursive case: it results from translating two producible assemblies so they *stably attach* without overlap

Hierarchical Tile Assembly Model



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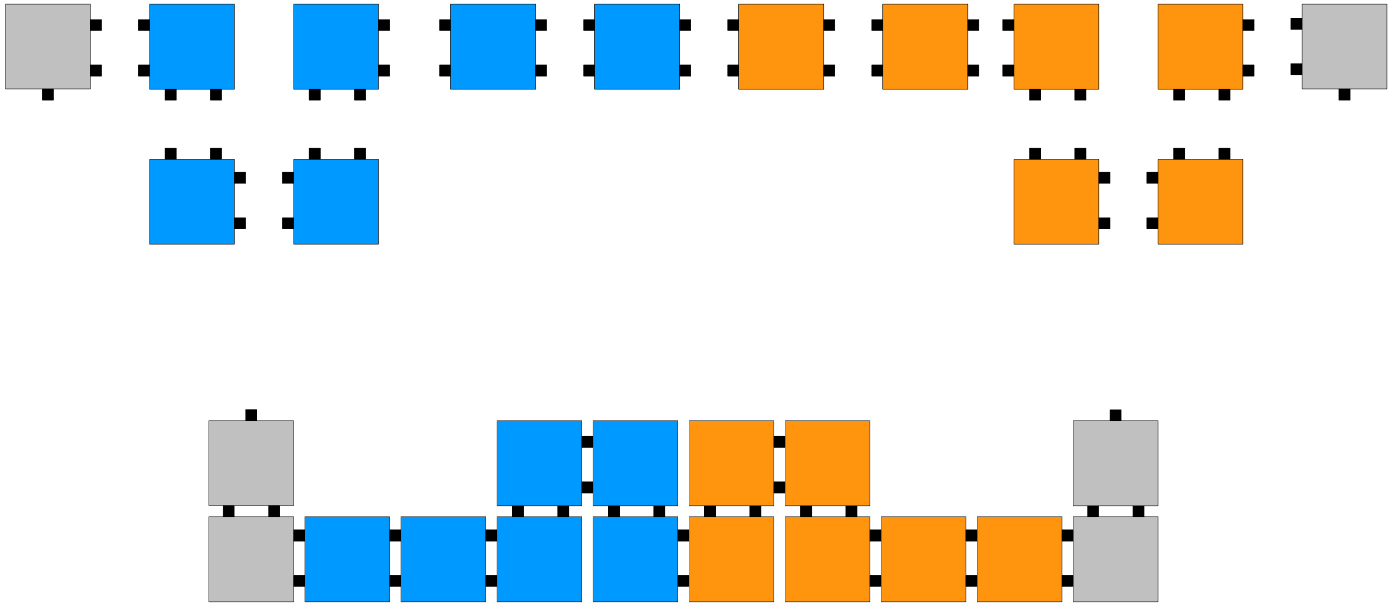

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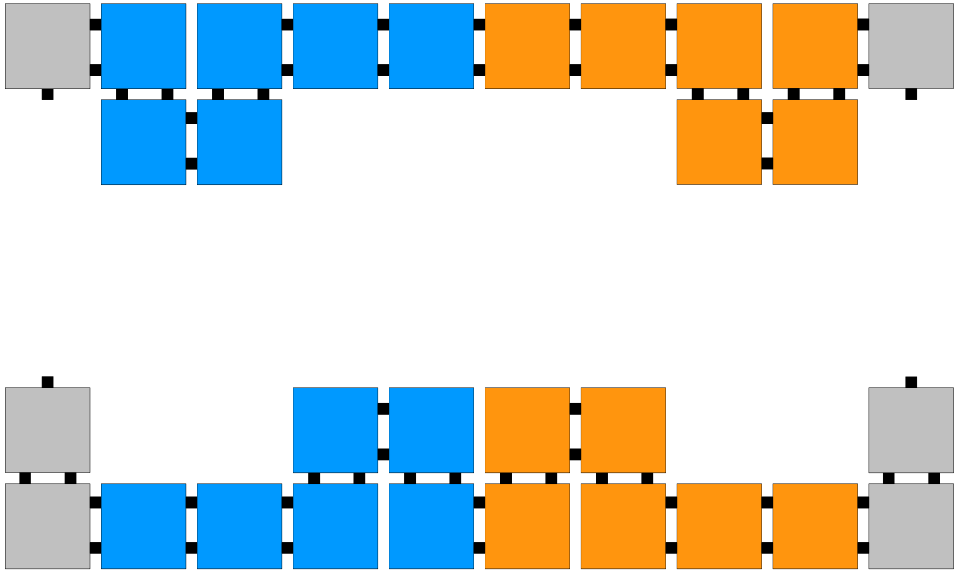

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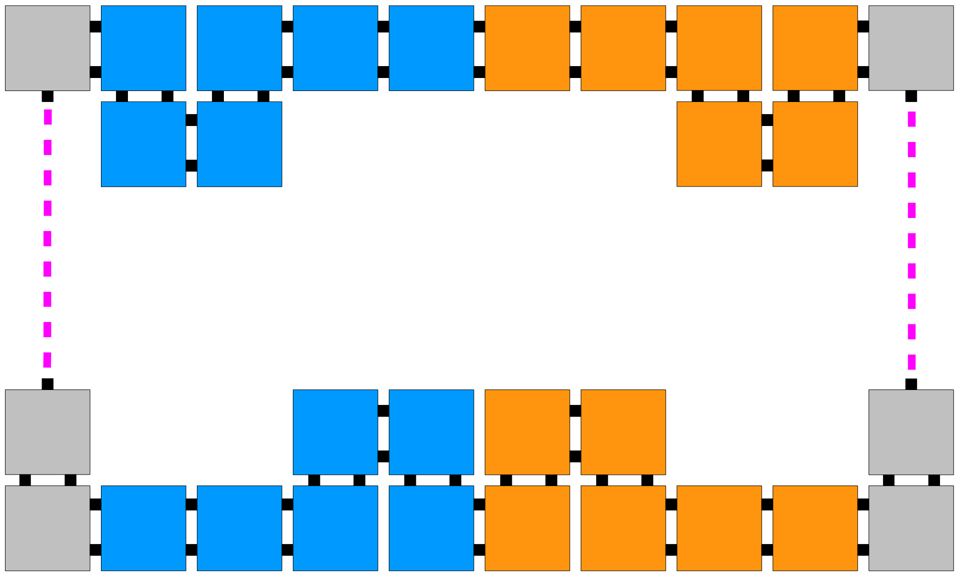

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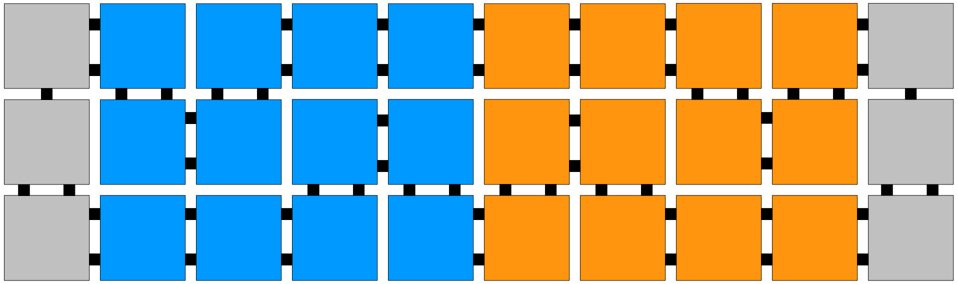
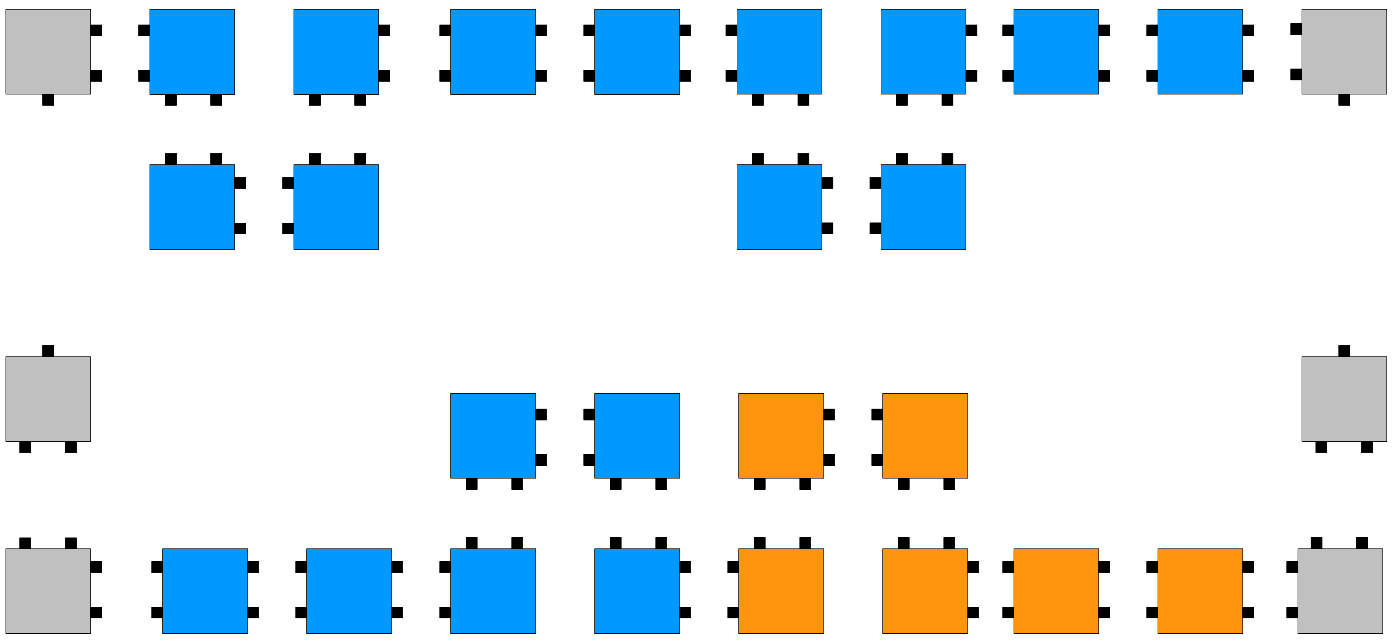


Hierarchical Tile Assembly Model

Overlap disallowed in attachment events ("steric protection")



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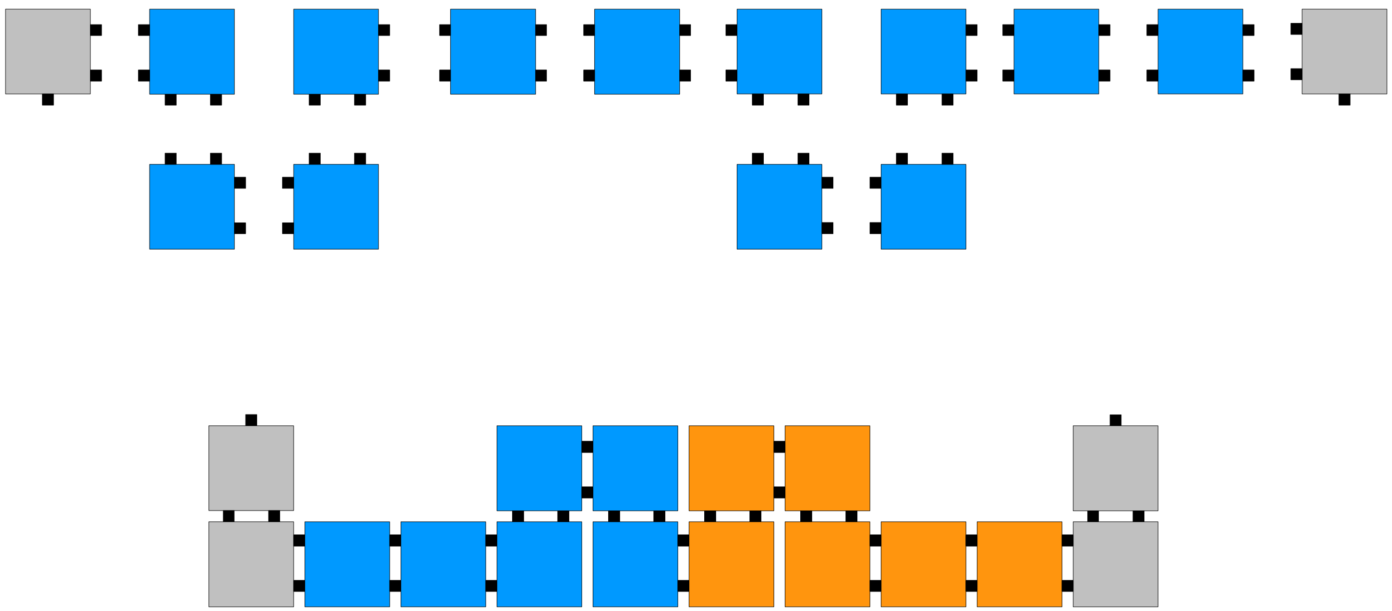

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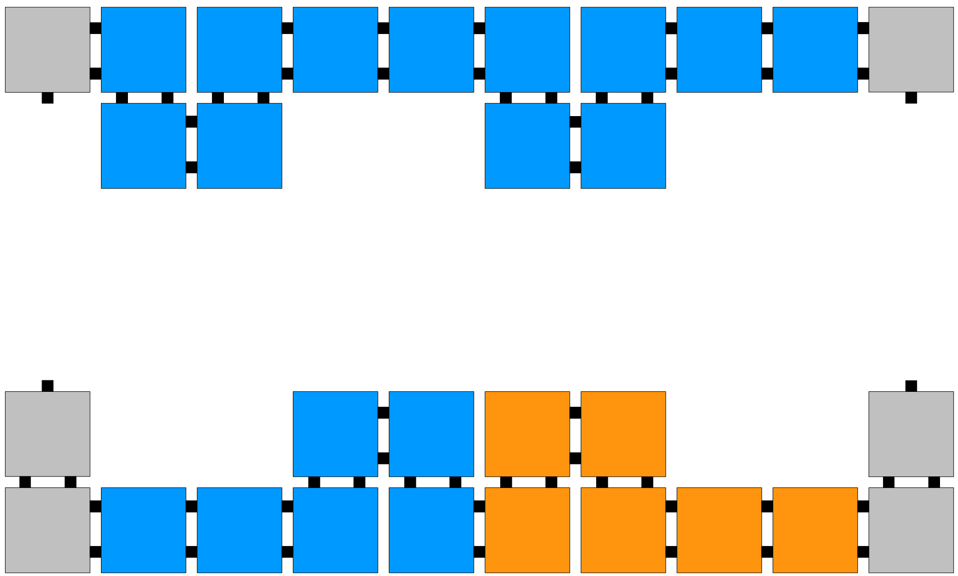

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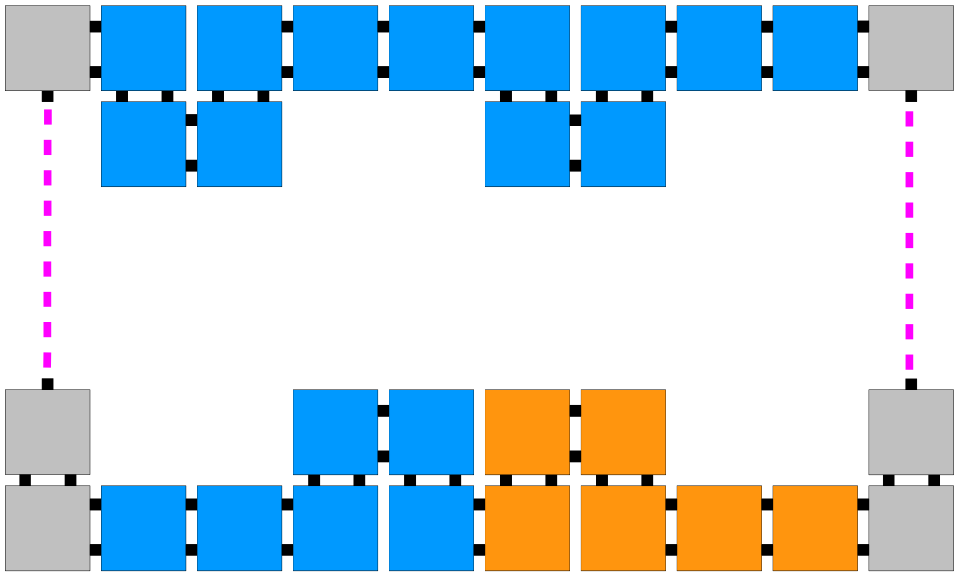

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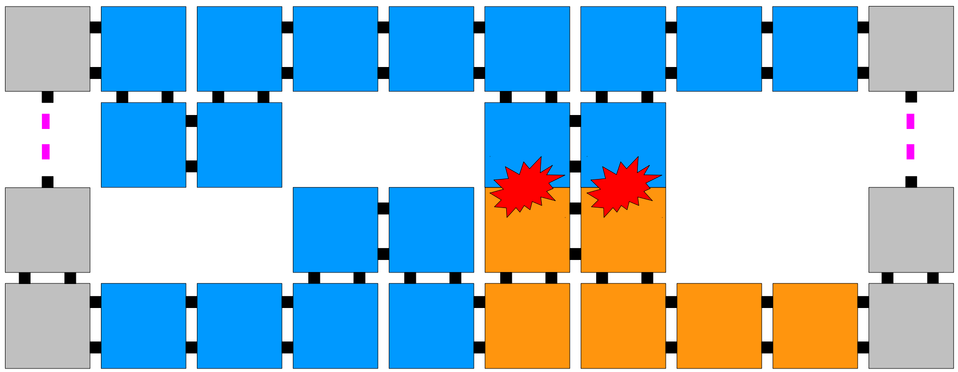

Potentially Unrealistic Aspects of the Hierarchical Assembly Model

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} artificially boost assembly speed

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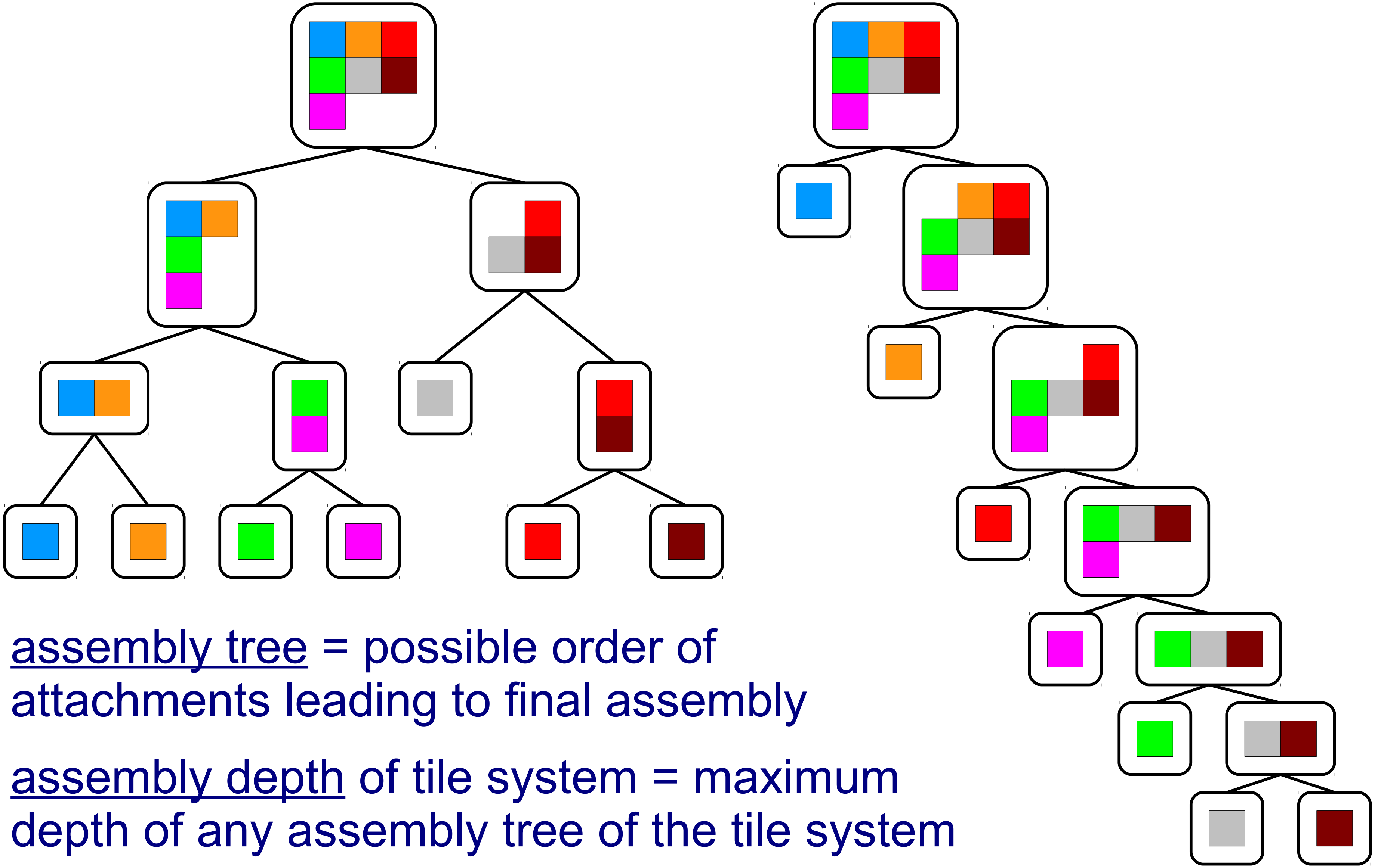
Definition of Hierarchical Parallelism



<u>assembly tree</u> = possible order of attachments leading to final assembly

<u>assembly depth</u> of tile system = maximum depth of any assembly tree of the tile system

Highly Parallel Square Assembly

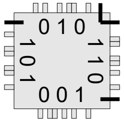
- Best possible assembly depth for any shape with *N* points is log *N*.

Highly Parallel Square Assembly

- Best possible assembly depth for any shape with N points is $\log N$.
- **Theorem:** For every positive integer n, there is a tile system with $O(\log n / \log \log n)$ tile types and assembly depth $O(\log^2 n)$ that assembles an n x n square.

Idea: Blocks of size $O(\log n) \times O(\log n)$, assembled "nonparallelly", randomly guess their (x,y) position in square and bind only to carefully selected neighboring blocks.

$O(\log n)$ x $O(\log n)$
block of tiles



Idea: Blocks of size *O*(log *n*) x *O*(log *n*), assembled “nonparallelly”, randomly guess their (*x*,*y*) position in square and bind only to carefully selected neighboring blocks.

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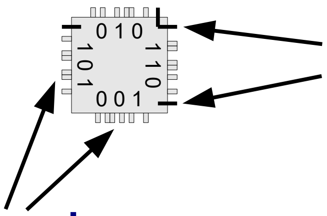
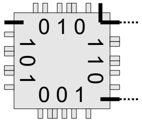
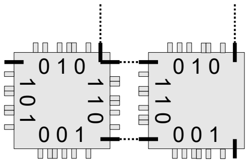


strength 1
glues

bumps encode
(*x*,*y*) address




010
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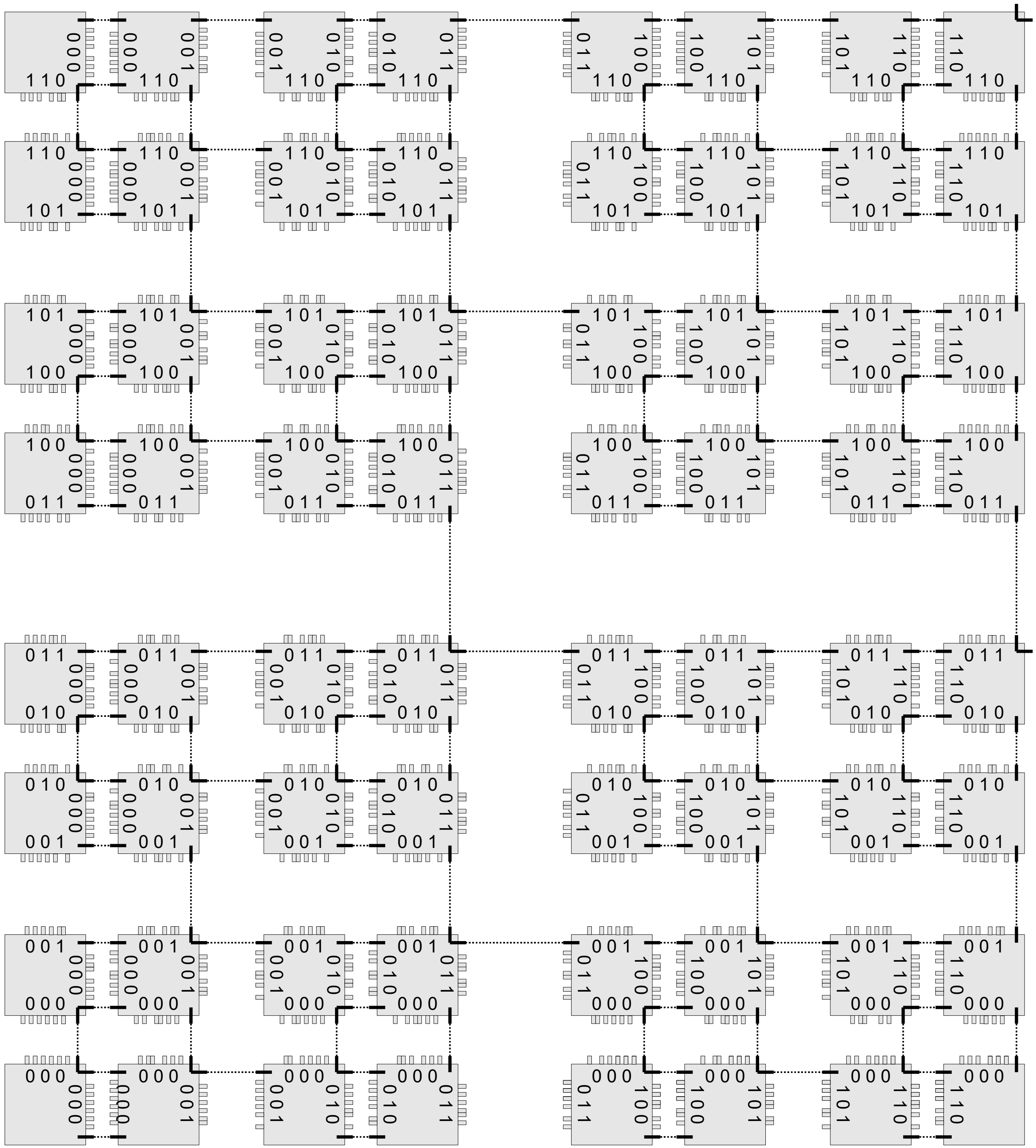
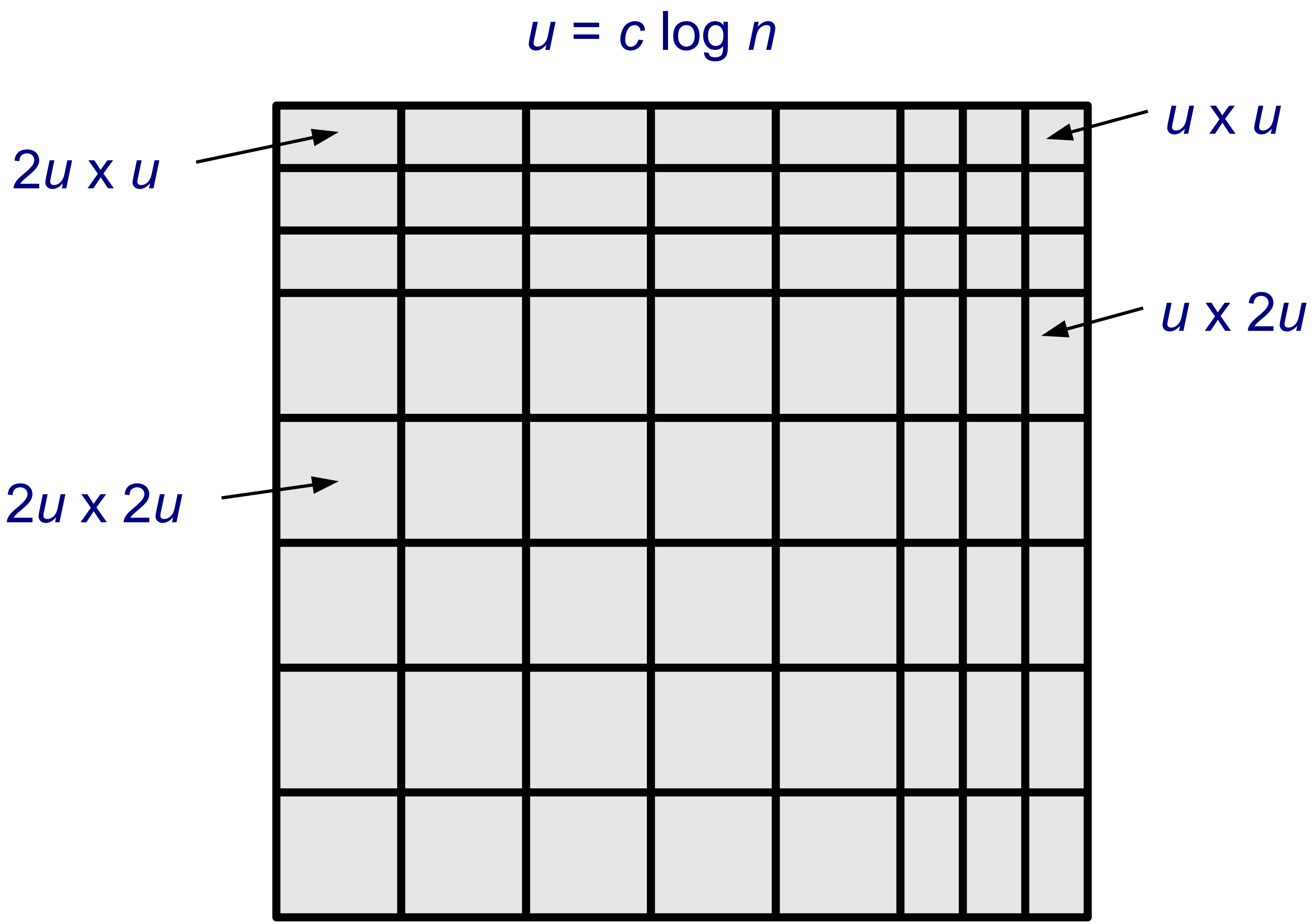
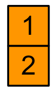


Handling Non-Powers-of-2



Assembly of Each Block

n in base *b* ≈ log n / log log *n*



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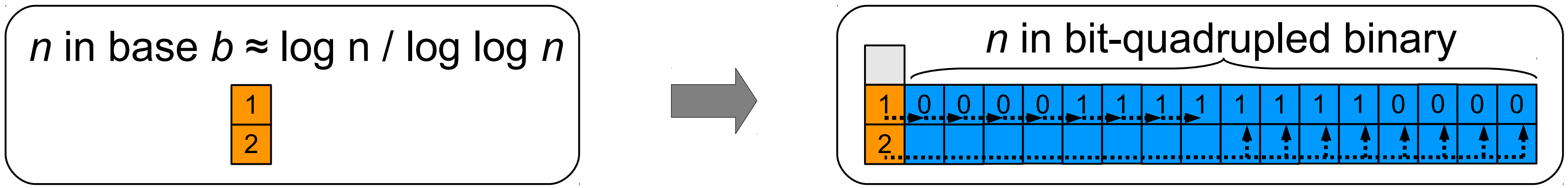

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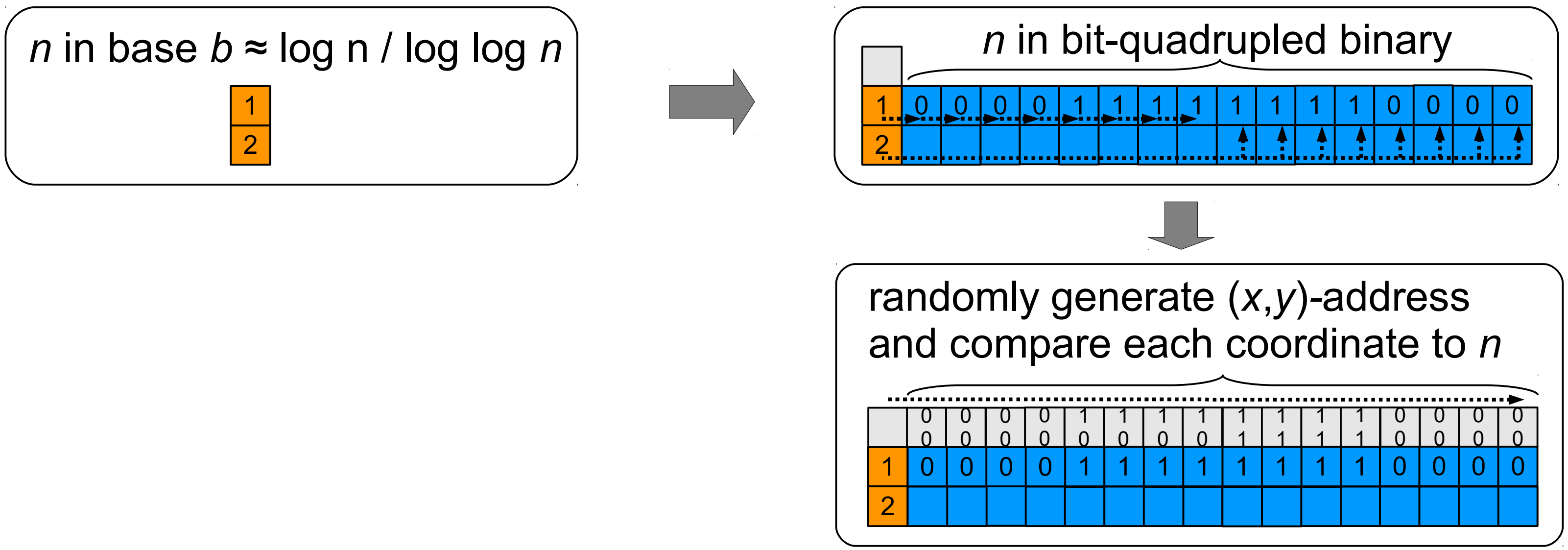

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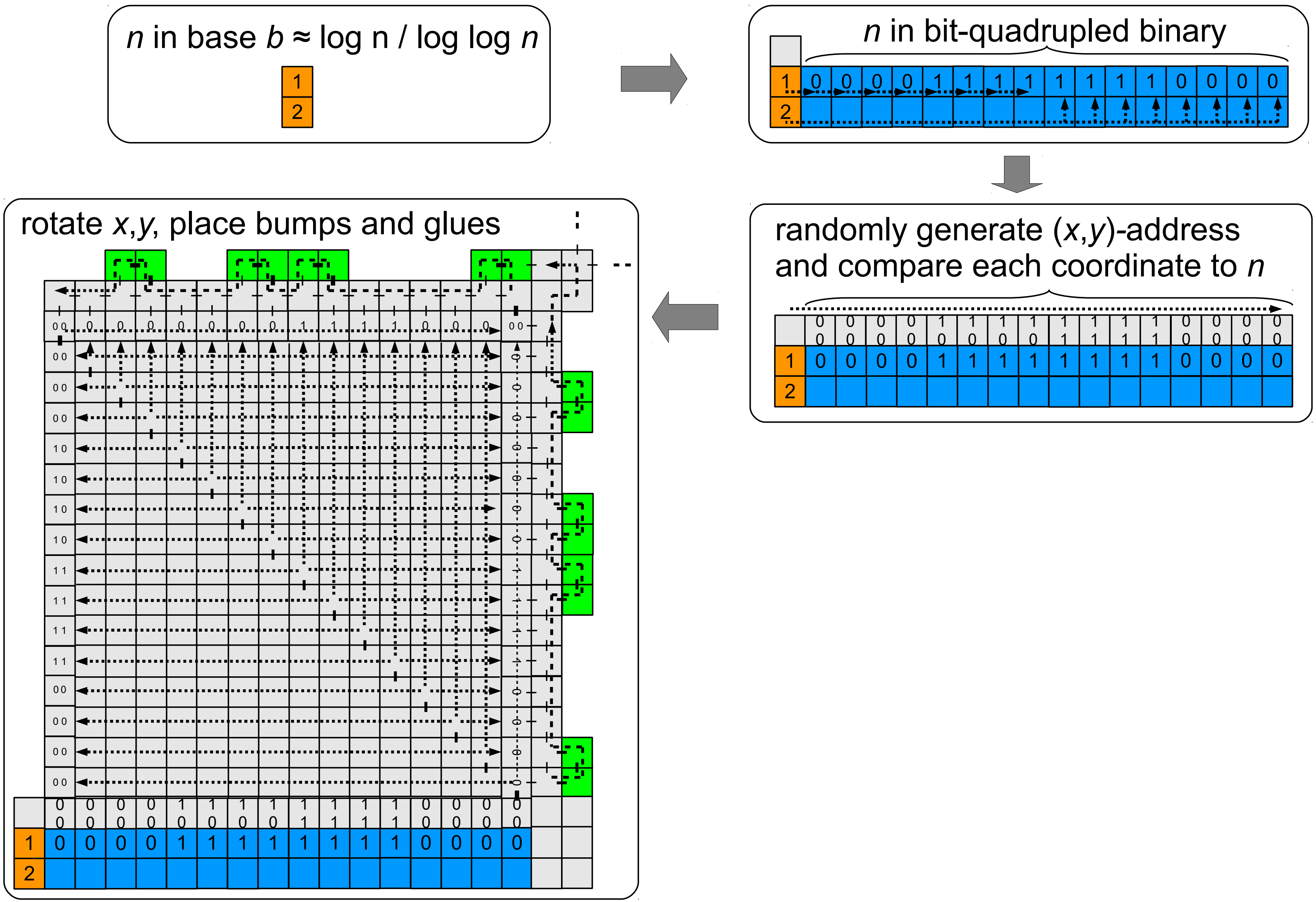

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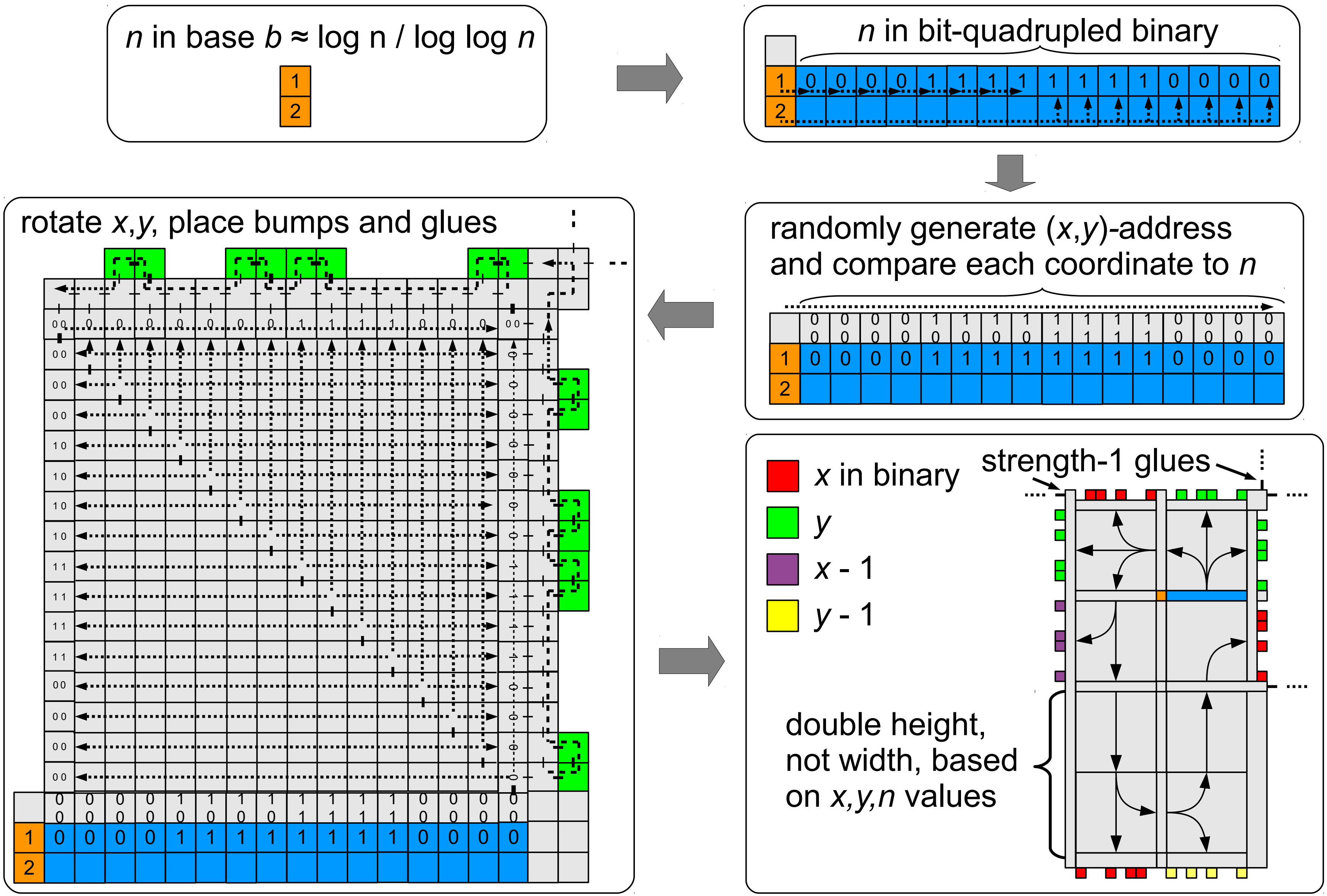

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The extra parallelism of the hierarchical model is **useless** for speeding up partial order systems.

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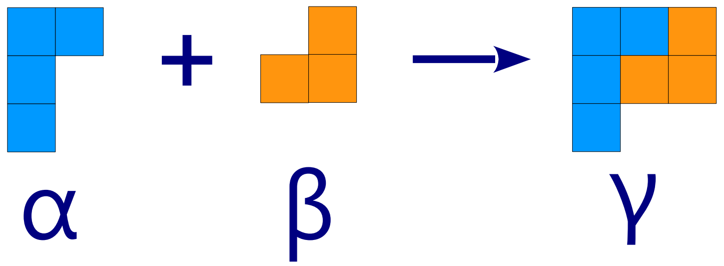

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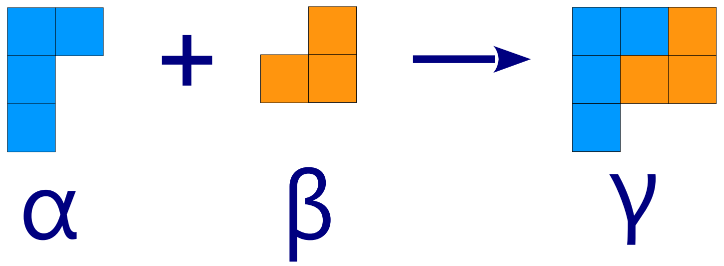

- Concentrations evolve by mass-action kinetics:

$$d[\alpha] / dt \;=\; \sum_{\gamma + \beta \to \alpha}[\gamma](t)\cdot[\beta](t) \;-\; \sum_{\alpha + \beta \to \gamma}[\alpha](t)\cdot[\beta](t)$$

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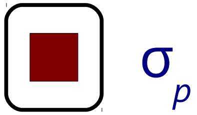

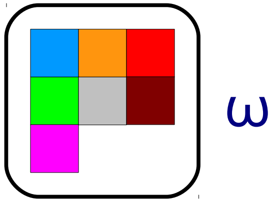

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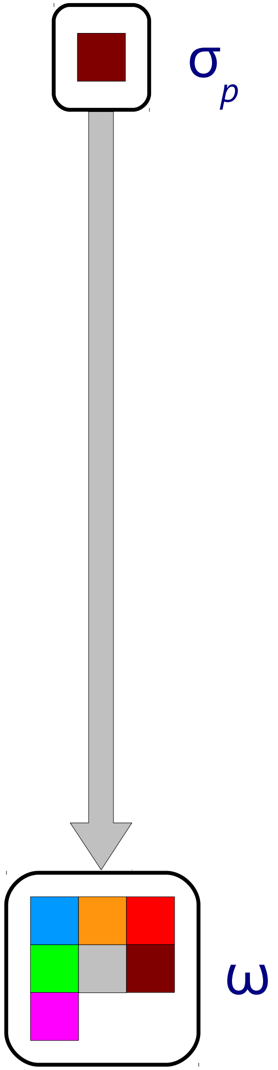

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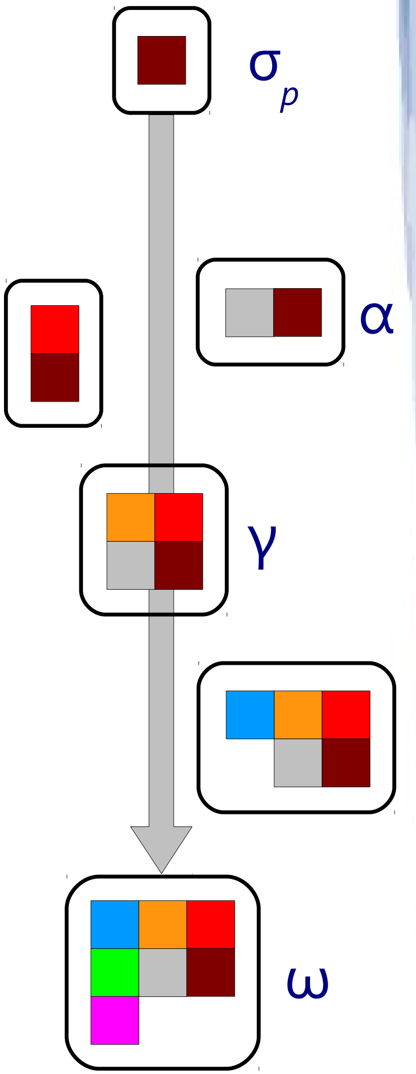

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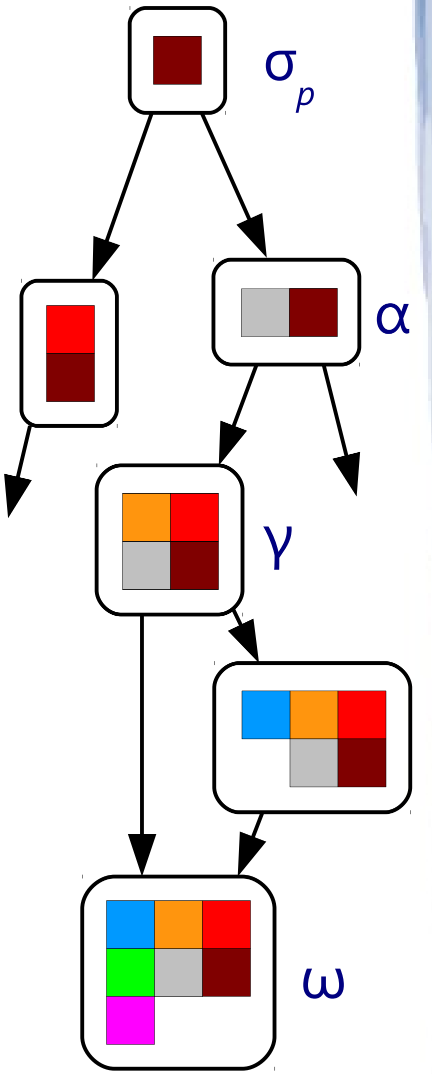

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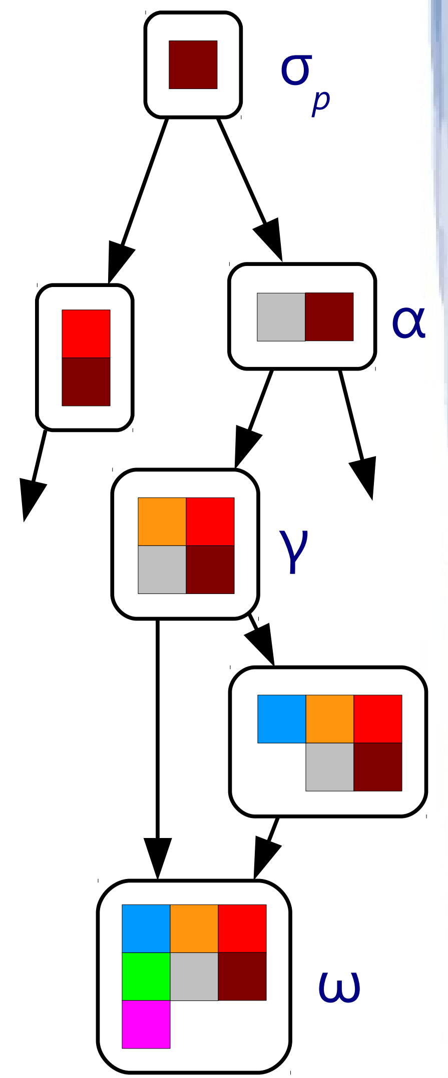

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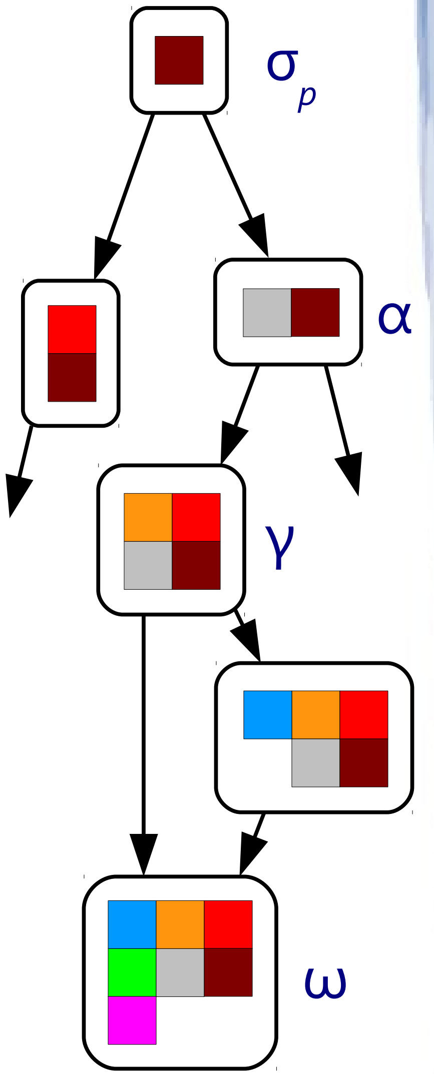

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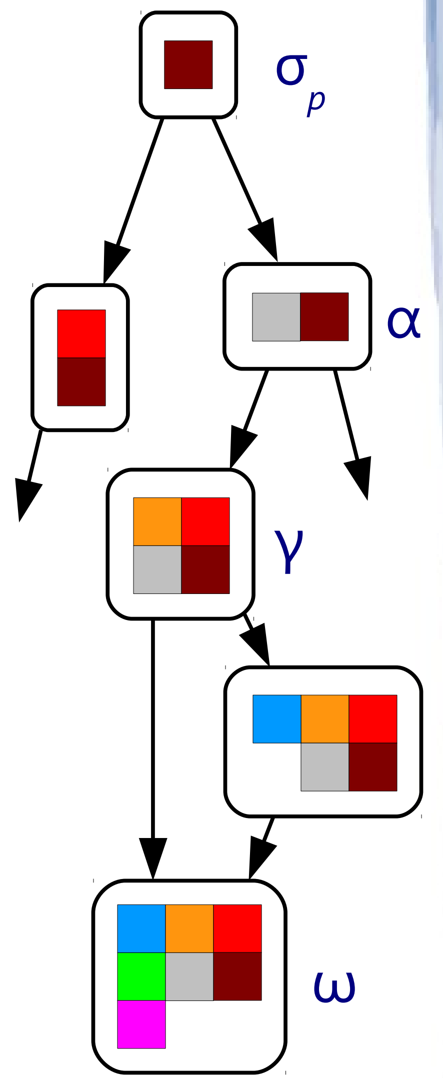

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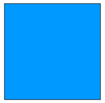
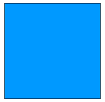
seeded



hierarchical



Main Proof Idea

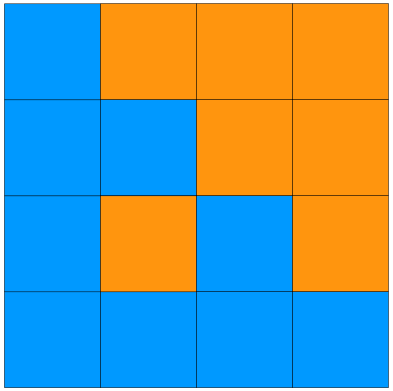
conservation of mass: assemblies of size *n* and *k* attach to create assembly of size *n* + *k*

→ ($t \geq 0$) $\sum_\alpha [\alpha](t) \cdot |\alpha| = 1$

→ assembly of size *k* has concentration ≤ 1/*k*

→ growing by size *k* in a single step takes expected time ≥ *k*

seeded



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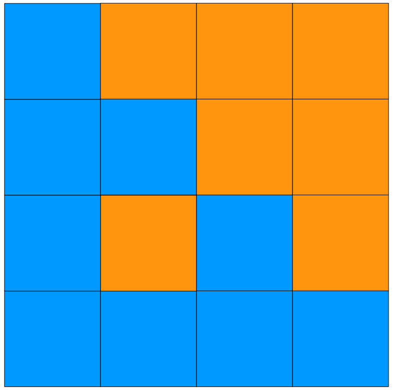

Why Partial Order Systems?

Argument breaks if a single assembly of size *k* could attach to many positions, any one of which suffices to proceed to terminal assembly.

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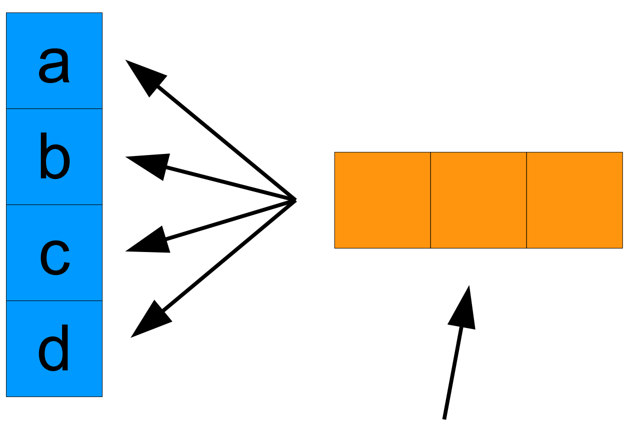

concentration ≤ 1/3

E[time to attach to a] ≥ 3

E[time to attach to any of a,b,c,d] ≥ 3 / 4

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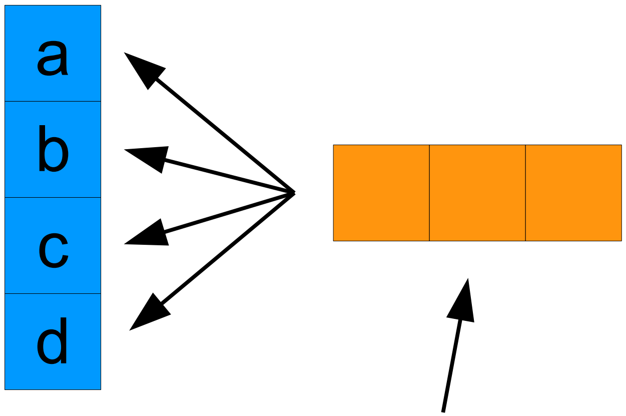

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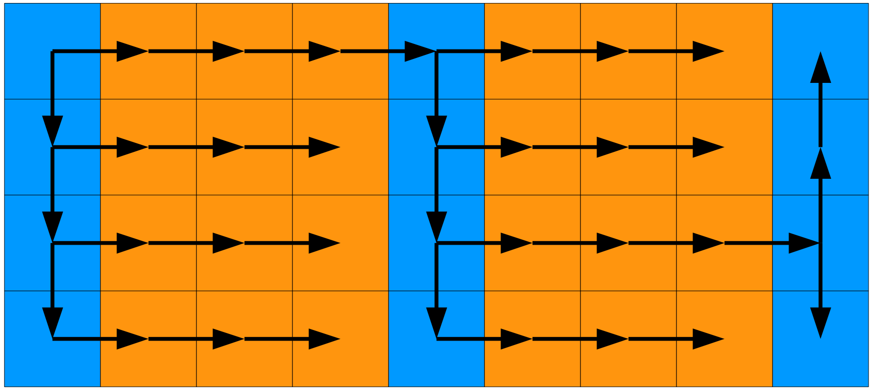
Any path in partial order DAG must assemble in order



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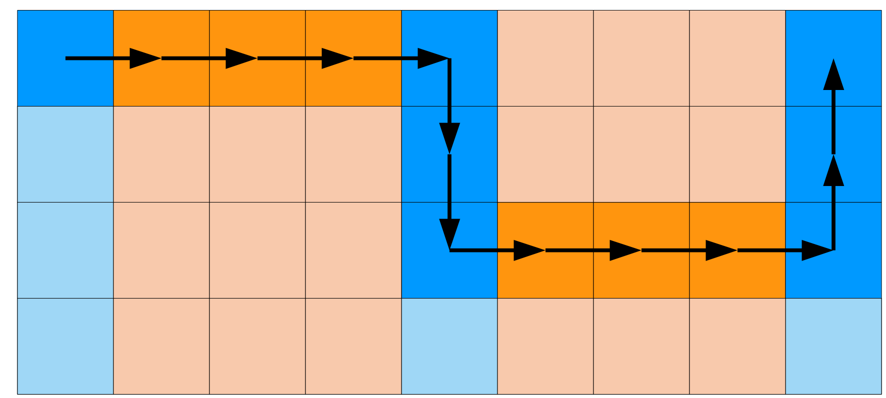

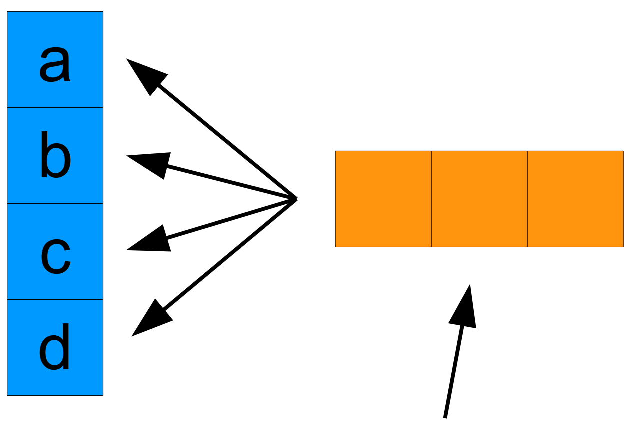

longest path has length ≥ diameter of shape

by concentration argument, path takes time *k* to grow by *k* tiles

concentration ≤ 1/3

E[time to attach to a] ≥ 3

E[time to attach to any of a,b,c,d] ≥ 3 / 4

Removing tiles (RNase model)

Removing Tiles

- aTAM is *monotone*: stably attached tiles do not detach
  - "Computation of a shape" with tiles may take a lot of space
  - Need large resolution loss to compute **within** the shape
  - kinetic model allows detachment but not controllable
- RNase model (Abel, Benbernou, Damian, Demaine, Demaine, Flatland, Kominers, Schweller)
  - make some tile types from RNA and some from DNA
  - after some time, add RNase enzyme to dissolve RNA tiles
  - only subassemblies made of DNA tiles remain

Shape-Building with Small Resolution Loss and Optimal Tile Complexity

Demaine, Patitz, Schweller, Summers (STACS 2011)*:*

given: finite shape *S*, |*S*|=*n*

there is a TAS T, |T| ≈ K(*S*), that assembles S at scale factor ≈ log *n*, with one step of dissolving RNA tiles

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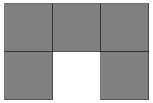
program *p* that prints *S*

S = 

RNA tiles:

DNA tiles:

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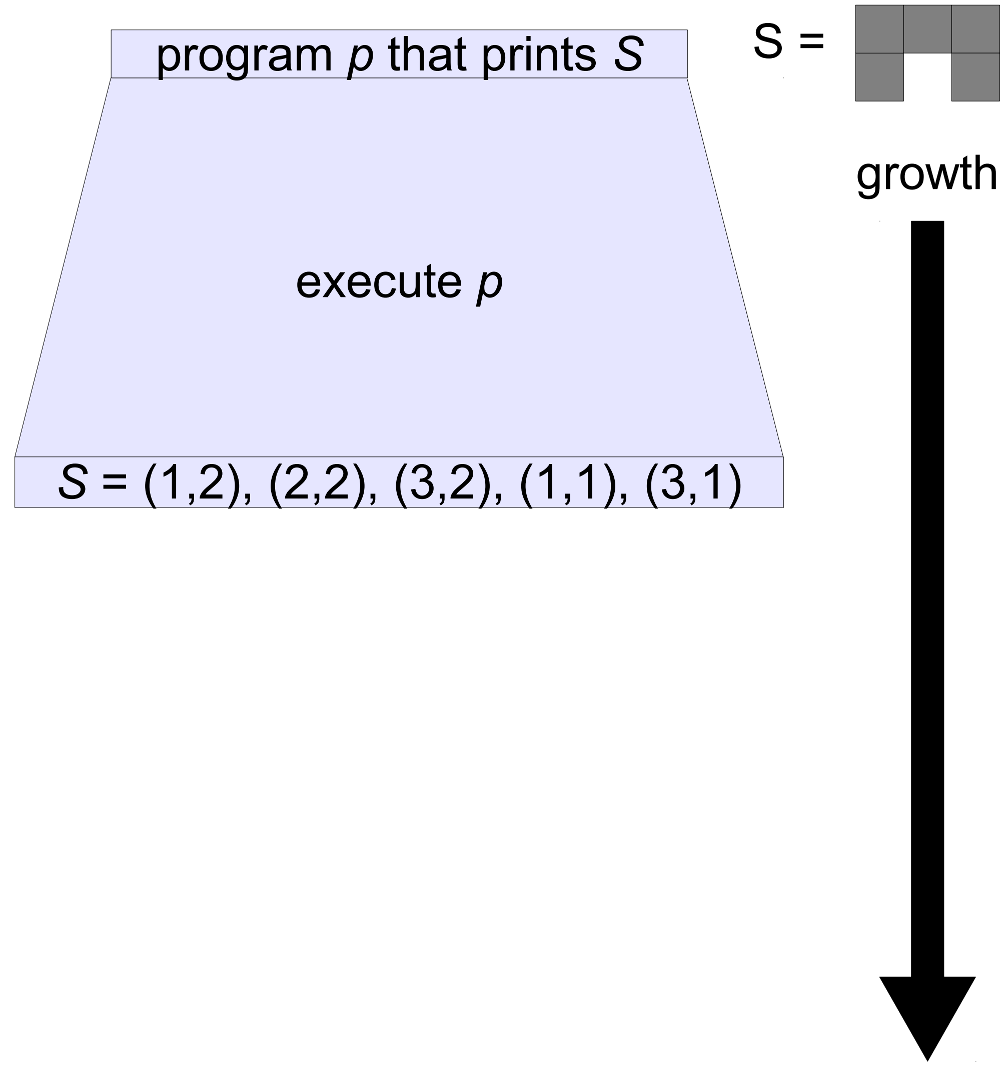

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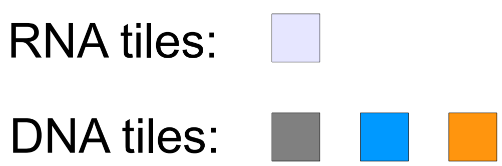

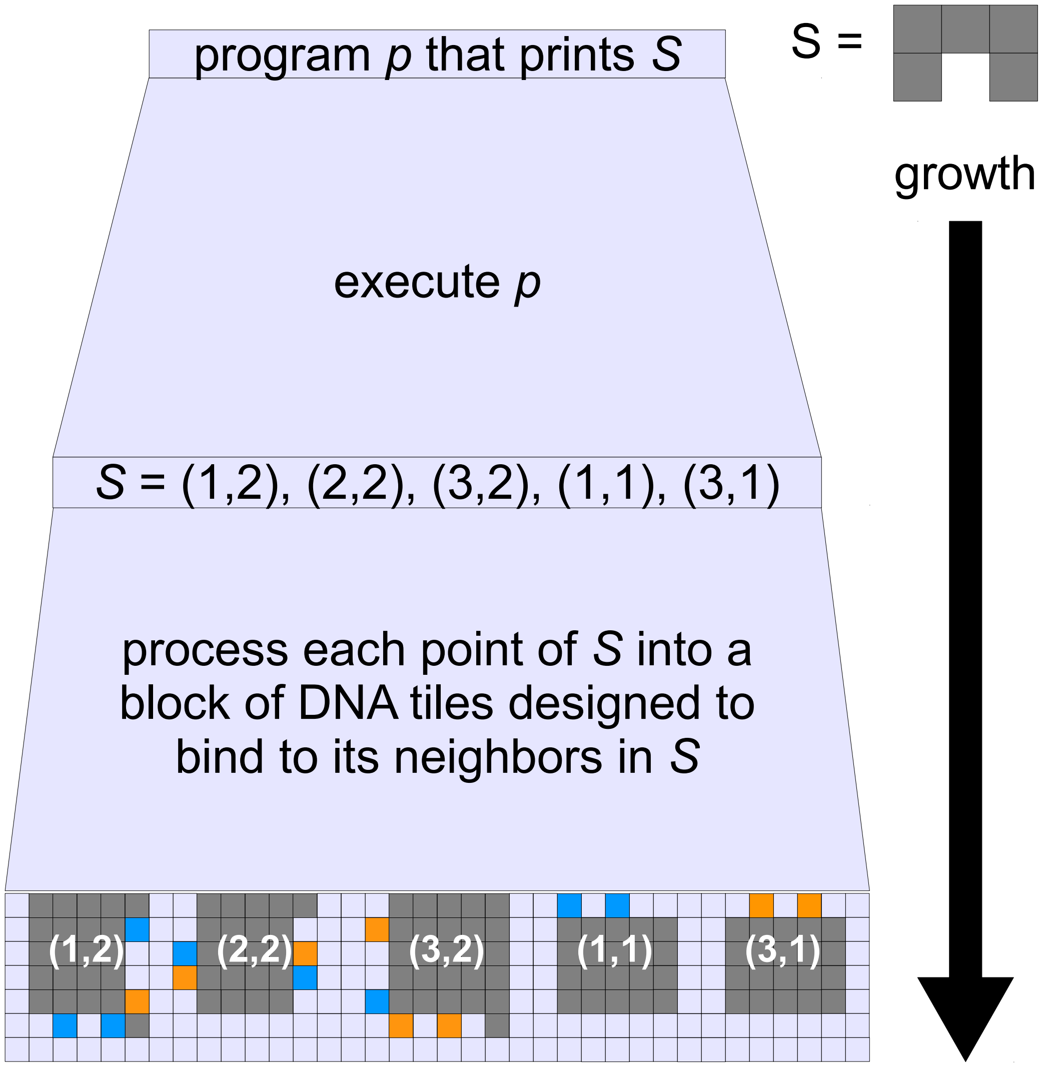

Shape-Building with Small Resolution Loss and Optimal Tile Complexity

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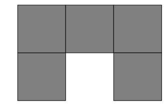
given: finite shape *S*, $|S|=n$

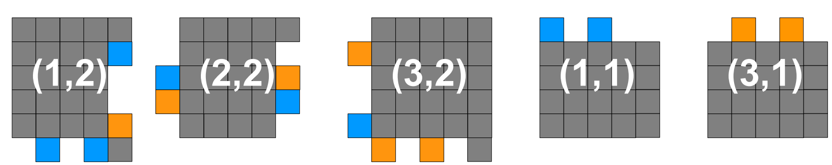
there is a TAS T, $|T| \approx K(S)$, that assembles S at scale factor $\approx \log n$, with one step of dissolving RNA tiles

S = 

dissolve RNA

RNA tiles:

DNA tiles:



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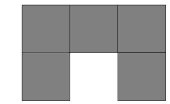
S = 

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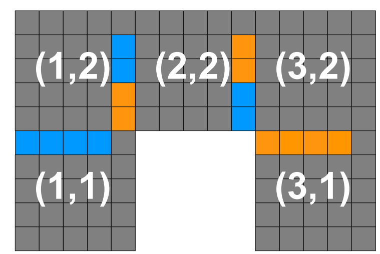

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DNA tiles: