Memory Consistency Conditions for Self-Assembly Programming

Aaron Sterling

Laboratory for Nanoscale Self-Assembly

Department of Computer Science

Iowa State University

Take-away message

- Self-assembling systems can be simulated by models of distributed shared memory.
- Types of error unique to algorithmic DNA self-assembly can be simulated by weak memory consistency conditions for those DSM models.
- Hence, the theory of memory consistency, and the theory of self-stabilization, can be productively applied to questions of algorithmic self-assembly.

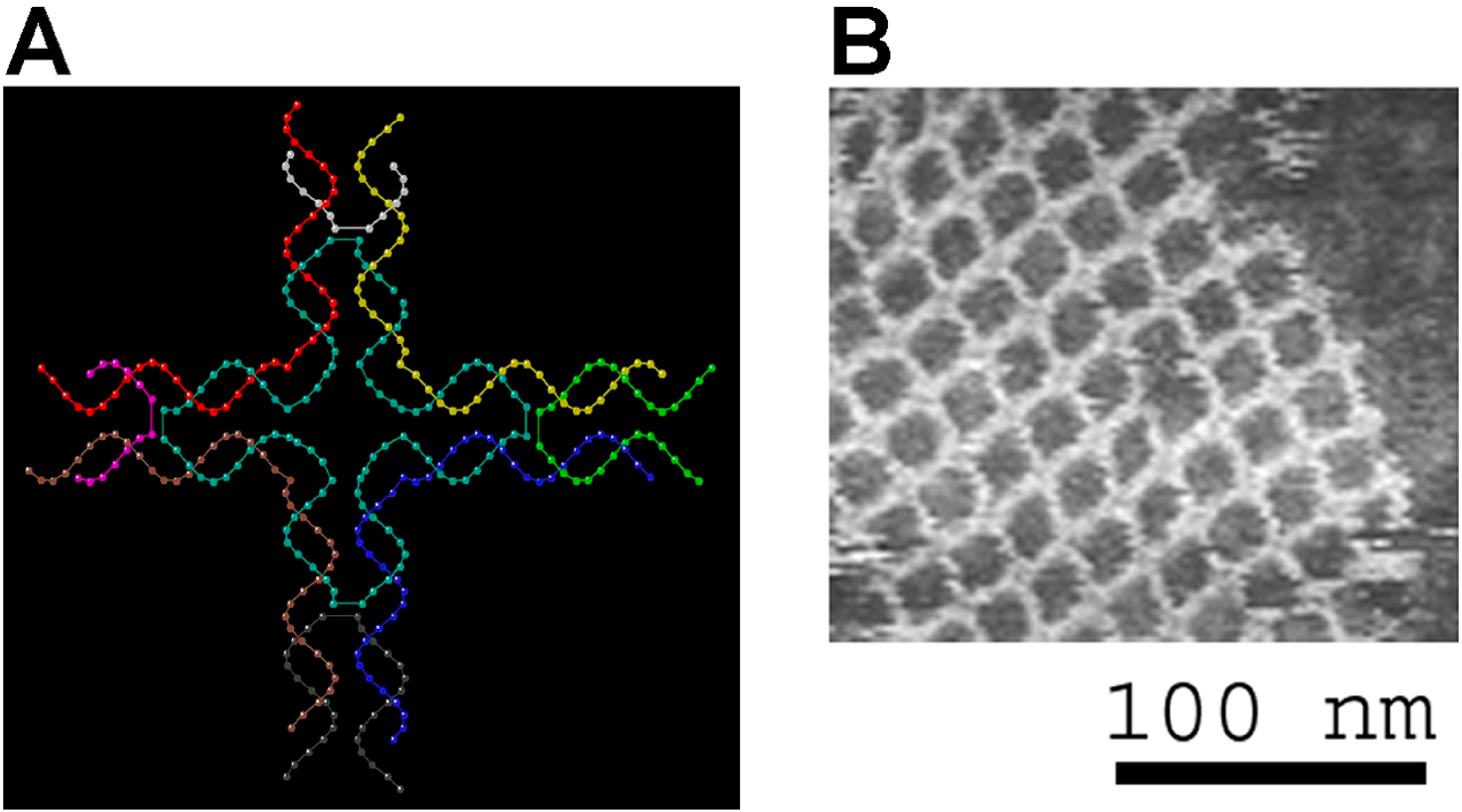
Take-away message

- The theory of multiprocessor architecture can be productively applied to biomolecular computing architecture!

Overview

- Introduction to algorithmic DNA self-assembly
- Introduction to distributed shared memory, and memory consistency conditions
- Sketch of reduction from self-assembly models to DSM models
- Two applications
- Conclusion, and preview of future work

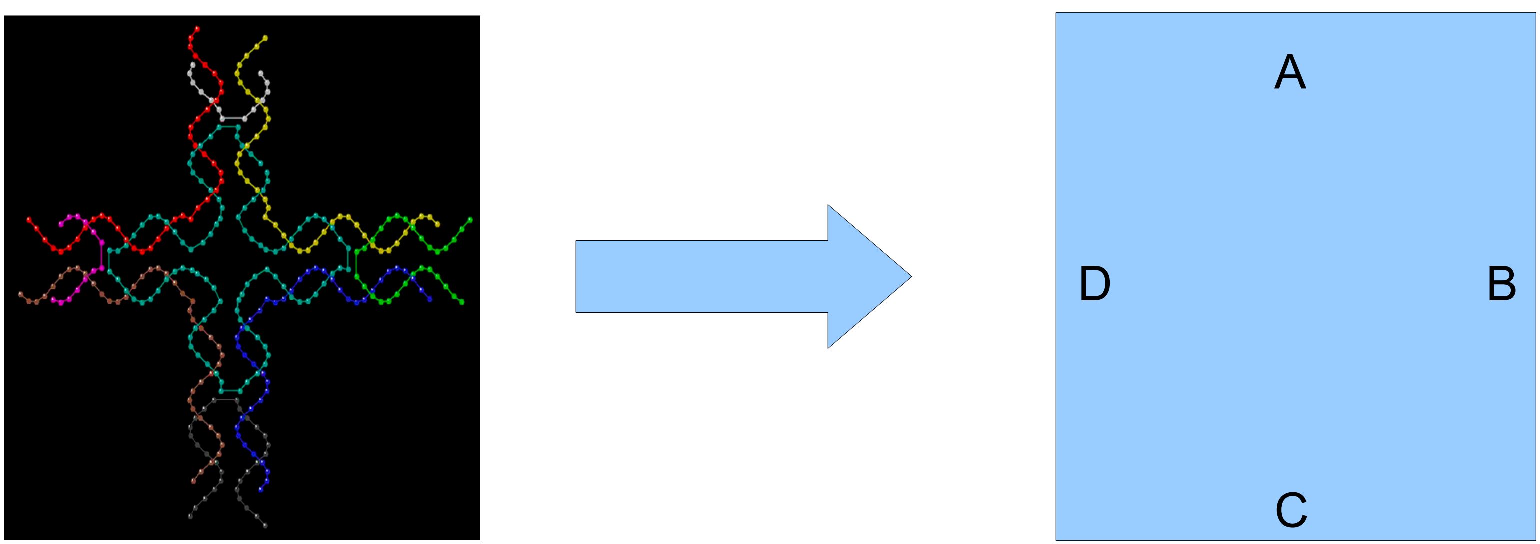
DNA self-assembly



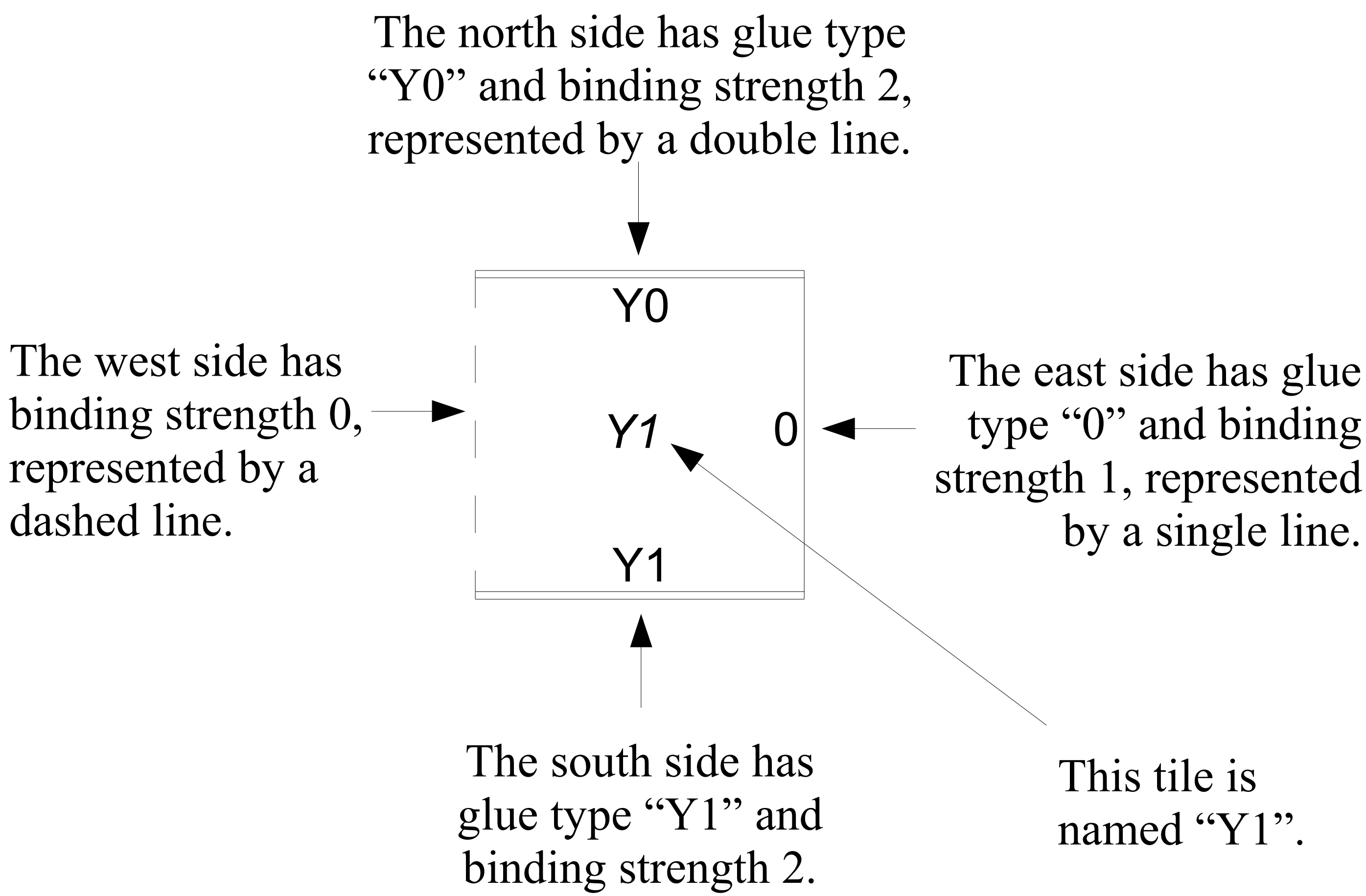
Source: Strong 2004

Algorithmic DNA self-assembly

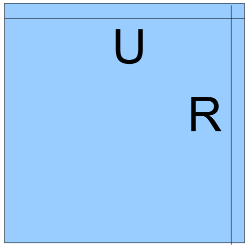
- Winfree's key insight [1995-8]:
  - DNA nanostructures with four “sticky ends” [Seeman] could be programmed by approximating them as a model of effectivized Wang tiling on the integer plane.



DNA tile self-assembly



Programmable Self-Assembly



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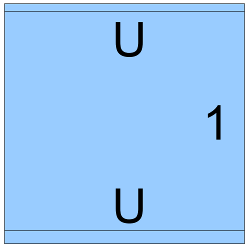

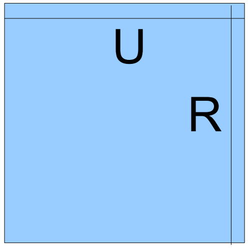

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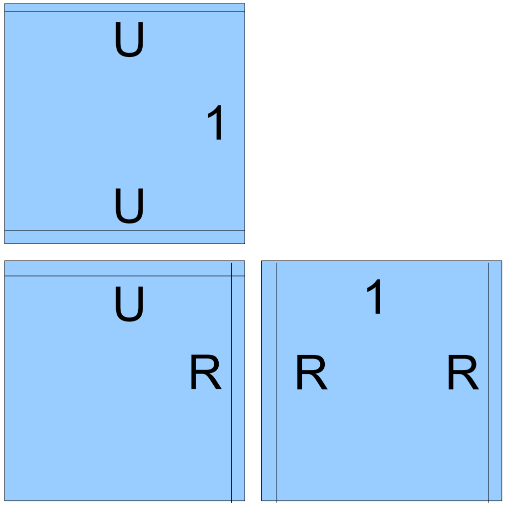

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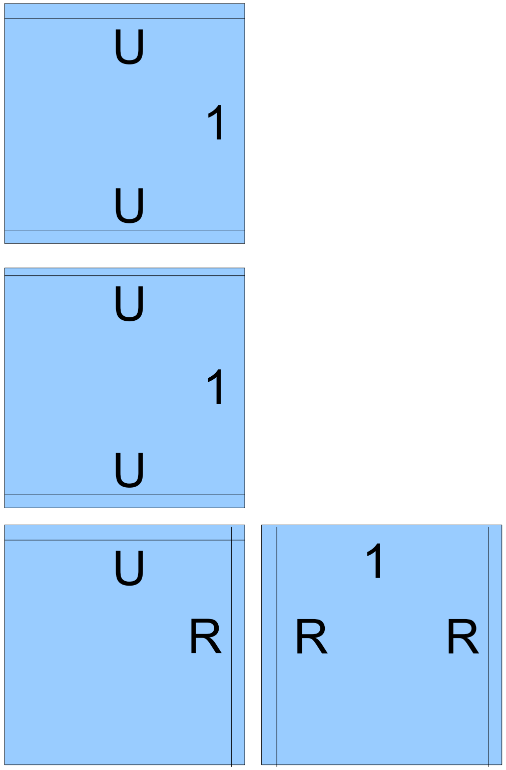

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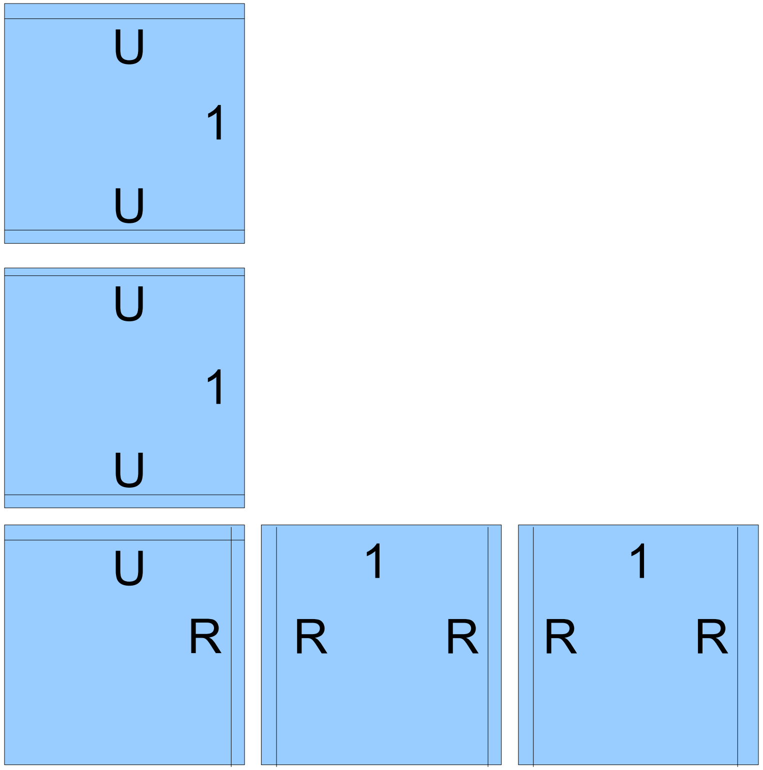

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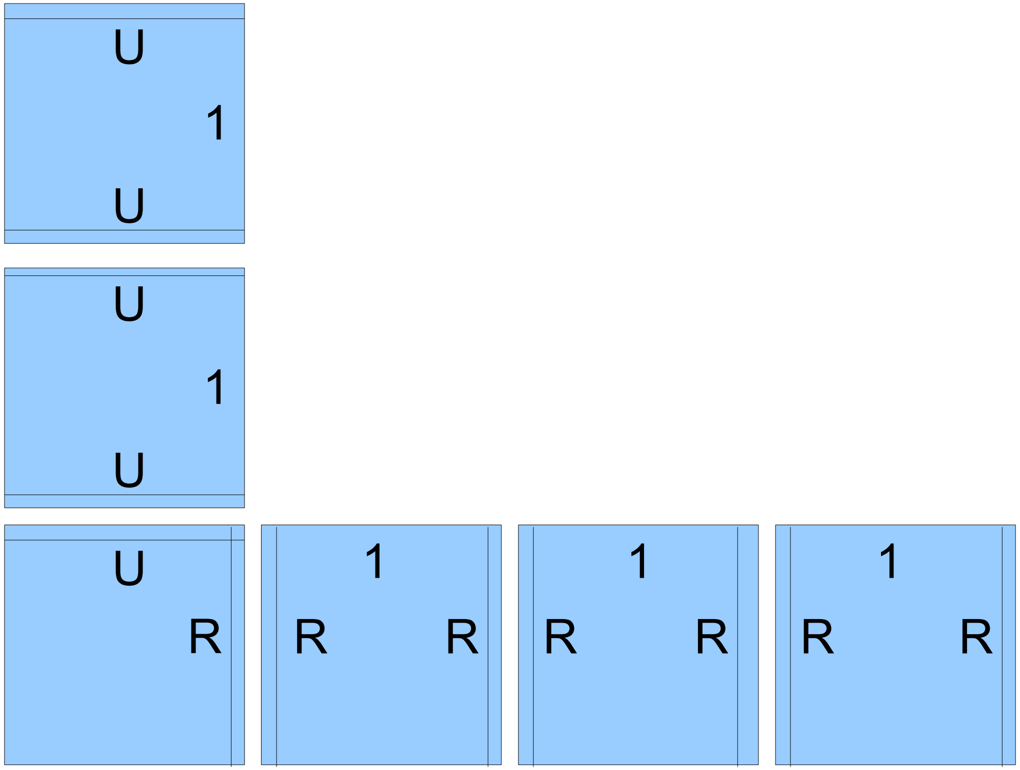

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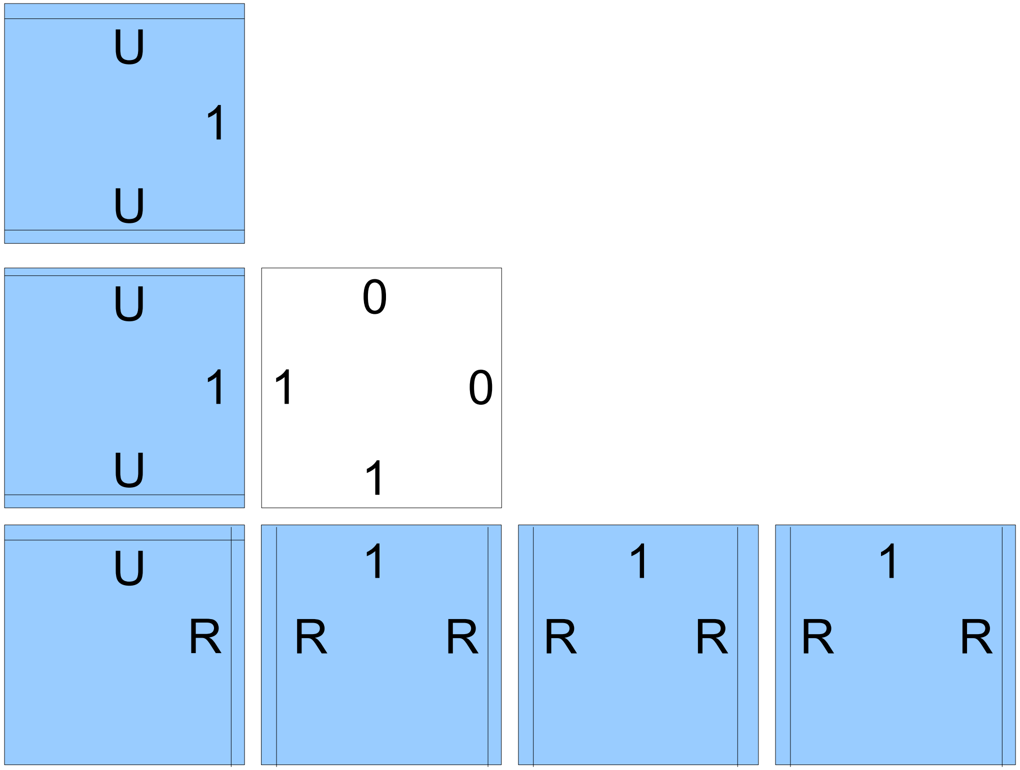

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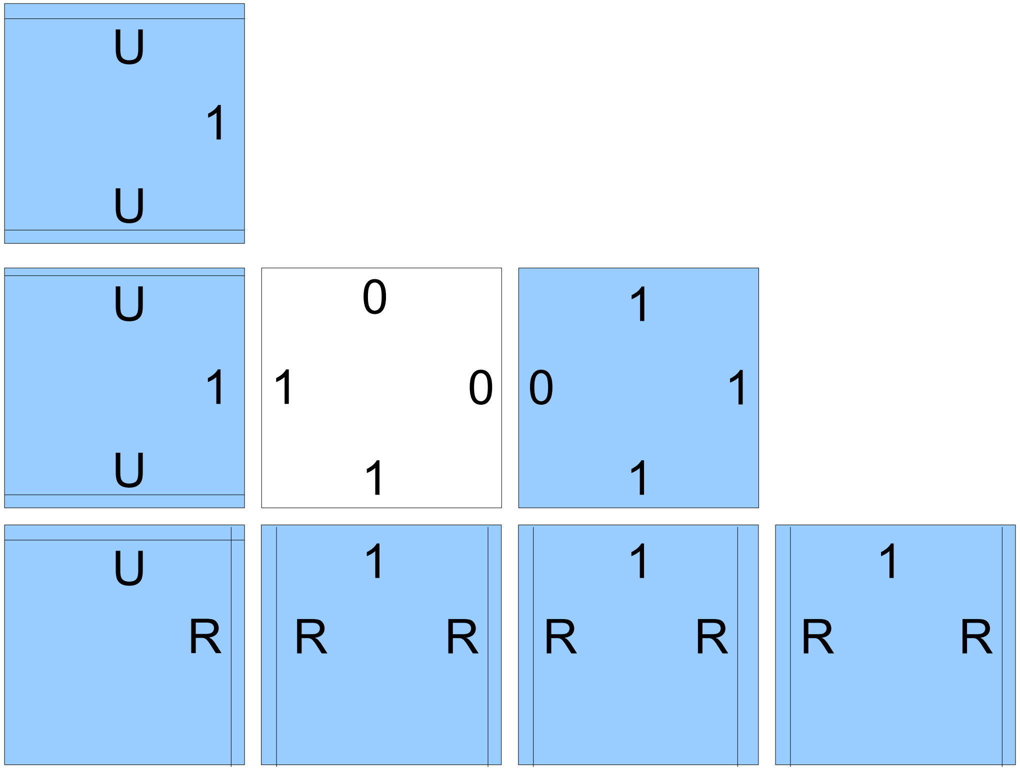

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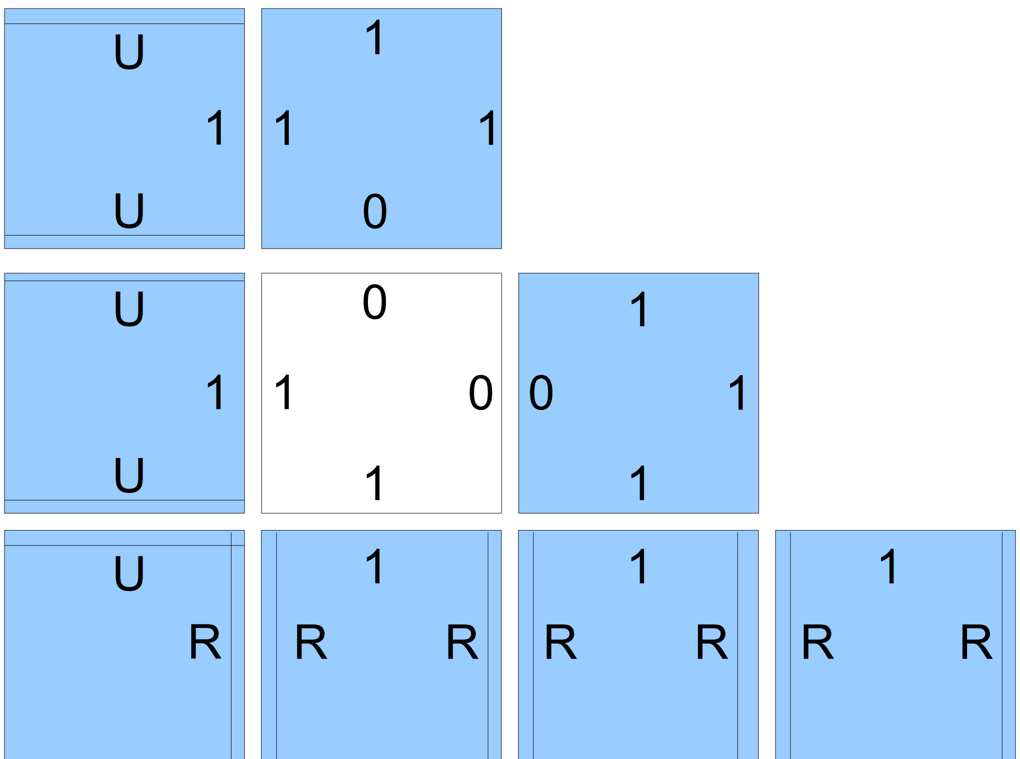

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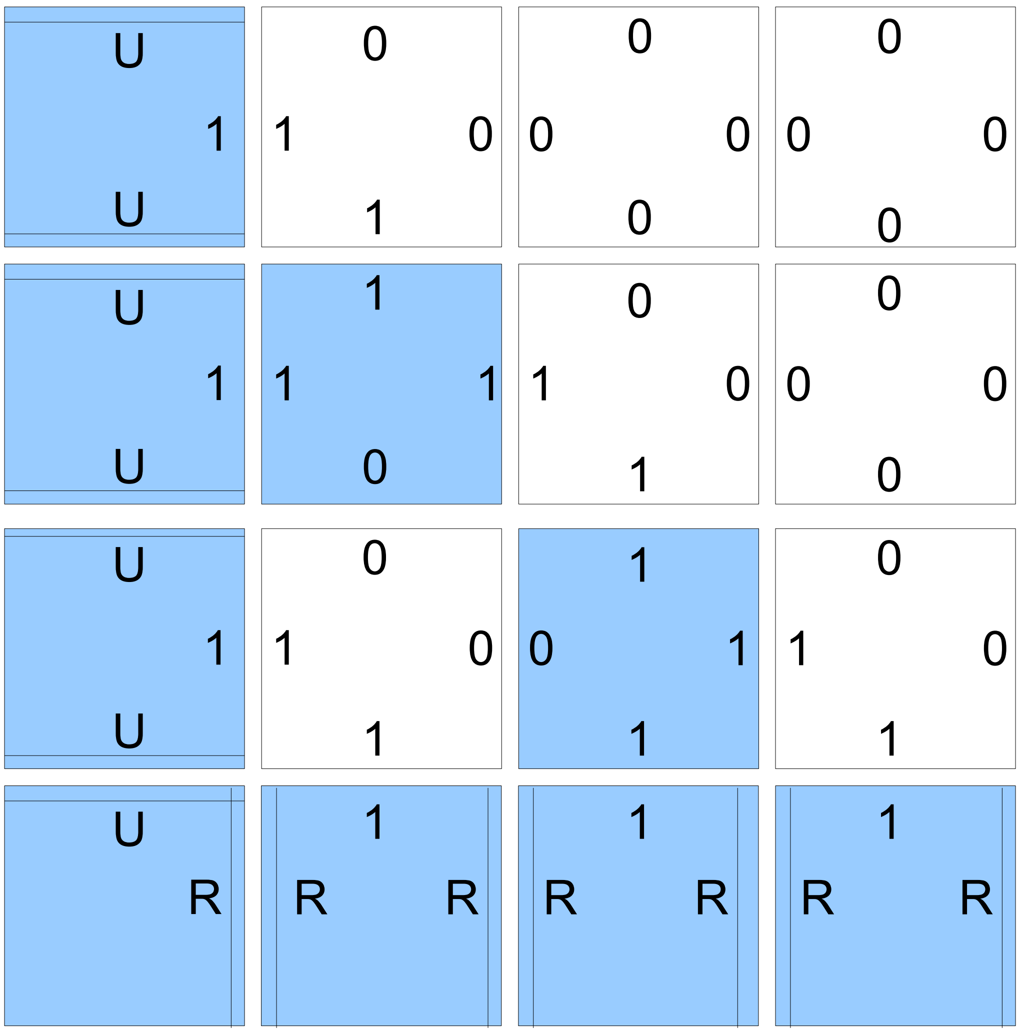
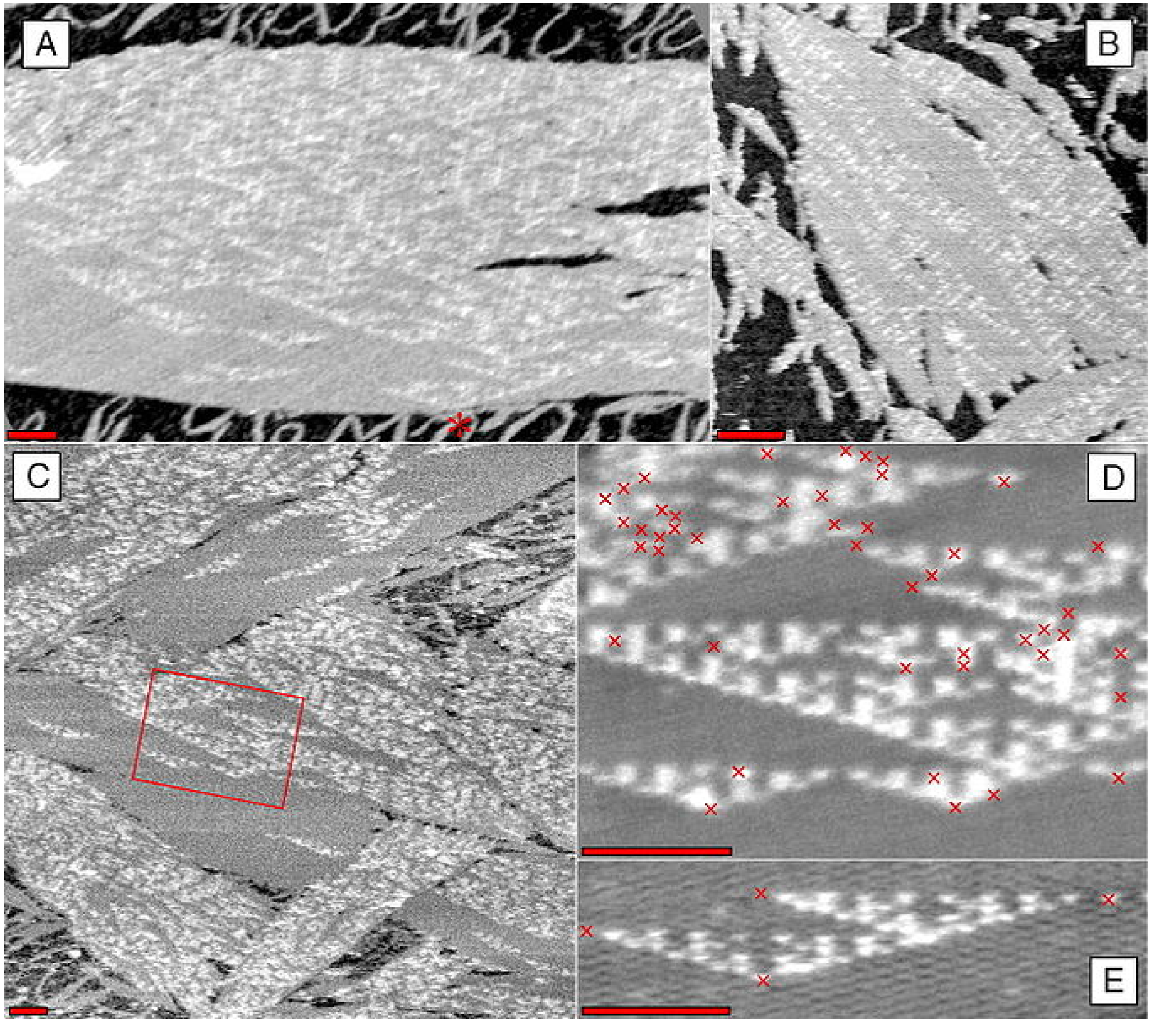


This set of eight tiles computes exclusive-or (addition mod 2), and is colored only if the output of the function is 1.

Programmable Self-Assembly



Rothemund et al., 2004

Tile Assembly Models

- Abstract Tile Assembly Model (aTAM) [Rothemund and Winfree]
  - Nondeterministic and error-free
  - At each time step, one tile is placed nondeterministically at the frontier
- Kinetic Tile Assembly Model (kTAM) [Winfree]
  - Probabilistic and error-permitting
  - At each time step, tiles on the frontier can bind or dissociate, with probabilities based on rate equations from chemical kinetics

Fundamental Questions

- Necessary and sufficient conditions to produce a unique terminal assembly
- Fault tolerance / error correction

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  - Local determinism [Soloveichik and Winfree]
- Fault tolerance / error correction
  - Proofreading [ChenGoel], [Soloveichik *et al*.]
  - Protected Tile Mechanism [Fujibiyashi *et al*.]

Tile Assembly as Distributed System

- Each agent has only local knowledge
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- Behavior is asynchronous
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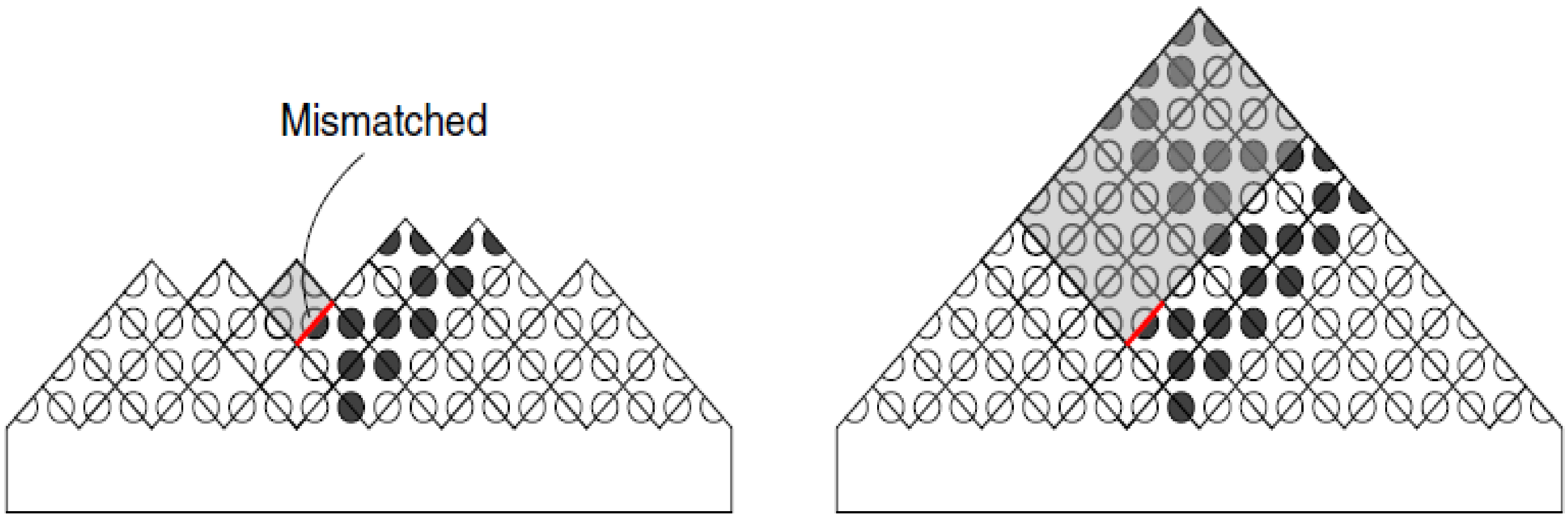
- Researchers in distributed systems have been designing algorithms for fault-tolerance for thirty years.
- Binding errors in self-assembly are fundamentally different from faults in previously-studied distributed systems.

Tile Binding Errors



A mismatched tile is trapped in the assembly before it can dissociate. [Fujibayashi *et al*.]

Binding Errors as Inconsistent Registers

- Metaphor: an agent approaches the assembly, “asks” whether the bonds in a location are correct, “hears” incorrectly what the bonds are, and binds at that location.

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- Metaphor: an agent approaches the assembly, “asks” whether the bonds in a location are correct, “hears” incorrectly what the bonds are, and binds at that location.
- Mathematics: simulate tile assembly systems with systems of distributed processors. The registers of these processors can be faulty, *i.e.*, can return inconsistent values, to model binding errors

Memory Consistency Conditions

- Multiprocessor programming, and architecture theory, have dealt with this type of problem for years.
- Just because a processor “writes” to a register, the register may not return that value. For example, the value may be in a cache, to be written to the register later.
- Programmers want guarantees of consistency; designers of architecture and compilers want flexibility for optimization.

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- *Sequentially consistent*: operations of all processors executed in sequential order, and ops of each processor appear in the order specified by its program.
- *Causally consistent*: for each processor, the ops of that processor plus all writes known to that processor appear in a total order that respects potential causality.

Examples

Causally consistent, not sequentially consistent:

p_1: $WRITE_x(0)$ $READ_x(1)$

p_2: $WRITE_x(1)$ $READ_x(0)$

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Not causally consistent:

p_1: $WRITE_x(0)$ $WRITE_x(1)$

p_2: $READ_x(1)$ $WRITE_y(2)$

p_3: $READ_y(2)$ $READ_x(0)$

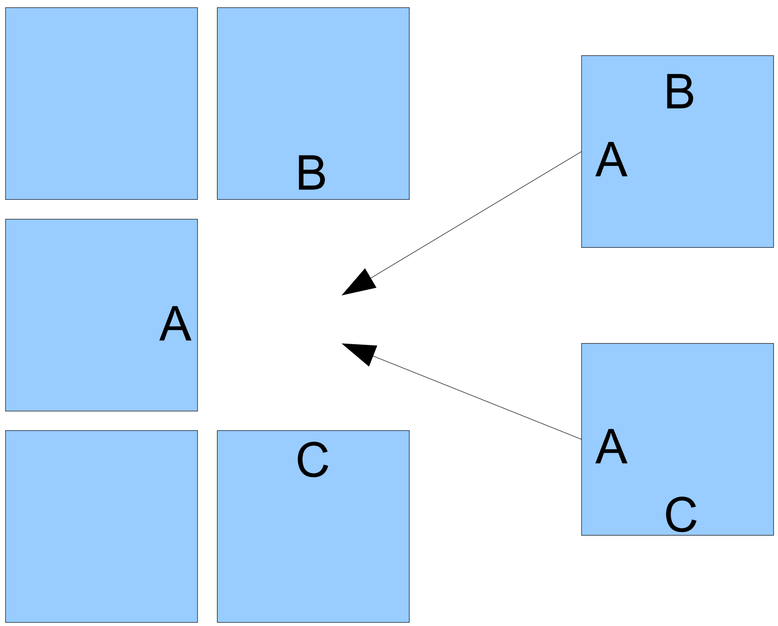
Simulation Theorem #1

- *Theorem*: There exists a class of causally consistent distributed processors that simulates the aTAM.
- “Simulate” means that each processor acts like a location on the assembly surface, and takes on a different state for each possible tile type, or “EMPTY” to simulate the absence of a tile.

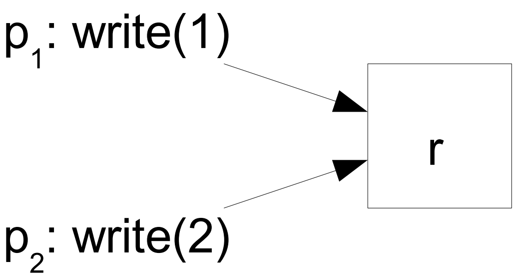
Application #1

- A tile assembly system is *locally deterministic* if, for any location in the assembly, a unique tile type can be placed legally in that assembly, given the neighboring tiles that were placed there previously in the assembly sequence.
- A multiprocessor program is *concurrent-write free* if no legal program execution permits conflicting writes to the same register.

Application #1



Not locally deterministic



Not concurrent-write free

Application #1

- *Theorem*: *T* is a locally deterministic tile assembly system iff it can be simulated by a concurrent-write free program on a system of distributed processors whose behavior is entirely determined by local binding rules.

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- *Consequence*: Programming language techniques (like types) to ensure concurrent-write freedom will also enforce local determinism when compiling tile assembly systems.

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- *Consequence*: Programming language techniques (like types) to ensure concurrent-write freedom will also enforce local determinism when compiling tile assembly systems.
- *Consequence*: Heuristics to check failure of concurrent-write freedom can be applied to self-assembly programming.

Simulation Theorem #2

- GWO ("global write-read-write order") is the condition that there is global agreement on the order of any two writes, when a processor can prove it has read one before the other.
- *Theorem*: There exists a class of GWO-consistent distributed processors that simulates the kTAM.

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- *Intuition*: In the kTAM, future bonds are causally related to past bonds. So writes are globally causally related, even though there is no guarantee that registers will return the values written.
- *Note*: This is the first “natural” distributed system shown to obey GWO, and not anything stronger. Errors in, *e.g.*, sensor networks or silicon architecture, are fundamentally different.

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- *Theorem*: There exists a polynomial-time algorithm that, given a locally deterministic *T* for the kTAM, outputs a self-healing, proofreading tile assembly system *T'*.

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- *Theorem*: There exists a polynomial-time algorithm that, given a locally deterministic T for the kTAM, outputs a self-healing, proofreading tile assembly system T'.
- *Note*: This was already known, though not published in this general form. The new contribution is the proof technique of self-stabilization.

Future Work

- “The greatest promise [of algorithmic DNA self-assembly] may lie in applications where DNA nanostructure templates have been used to assemble other inorganic components and functional groups.” [Nanofabrication by DNA self-assembly, Li *et al*.]

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  - Models of “mixed media” self-assembly

Future Work

"For the forseeable future, self-assembly has to deal with a significantly higher defect rate than etching and similar methods; this presumably has to be dealt with at the algorithmic level. Thus we need a theory of fault-tolerant assembly, as well as new fault-tolerant algorithms and architectures for these models." [The Computational Worldview and the Sciences, Arora *et al*.]

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- Self-stabilizing algorithms for self-assembling agents with binding errors

Thank you!