Aalto University
School of Science
and Technology

Combinatorial optimization in pattern assembly (extended abstract)

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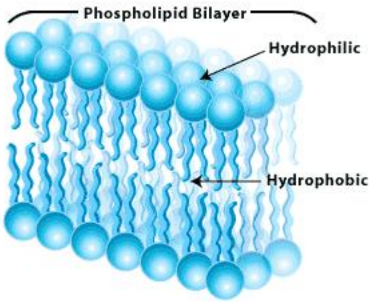
Talks at UCNC 2013 (Milan, Italy, July 1-5th, 2013)

An example of self-assembly

Lipid bilayer



The water, external environment, affects components (lipids), but does not intend to lead them to the membrane structure.

Other examples of self-assembly

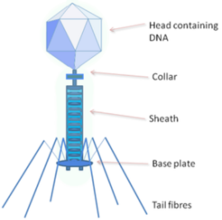
Self-assembly is an omnipresent phenomenon:

snow crystal

garaxy

pattern

city



virus capsid

Molecular assembly

Engineering Goal

DNA self-assembly

Why DNA?

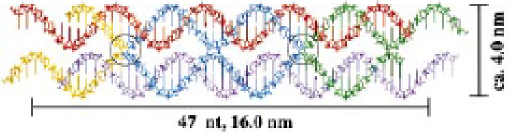
DNA is the molecule of choice in many labs [Doty 2012]:

- it is easy to synthesize
- its physical properties are well-understood
- due to its information-bearing properties

DNA self-assembly

DNA tile implementation

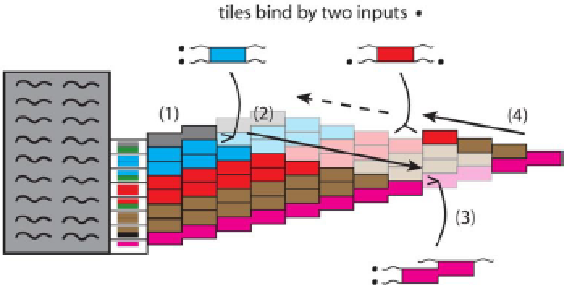
Winfree, Liu, Wenzler, and Seeman implemented **interactive DNA tiles** *in vitro* [Winfree et al. 1998] as a DNA double-crossover molecule:



4 single strands (red, yellow, purple, green), called **sticky ends** provide this “tile” with the capability of interacting with other “tiles”.

DNA self-assembly

Binary counter assembles from DNA tiles [Barish et al. 2009]



The gray box to the left is the *seed* (starting point of assembly process) made of **DNA origami** [Rothemund 2006].

DNA self-assembly

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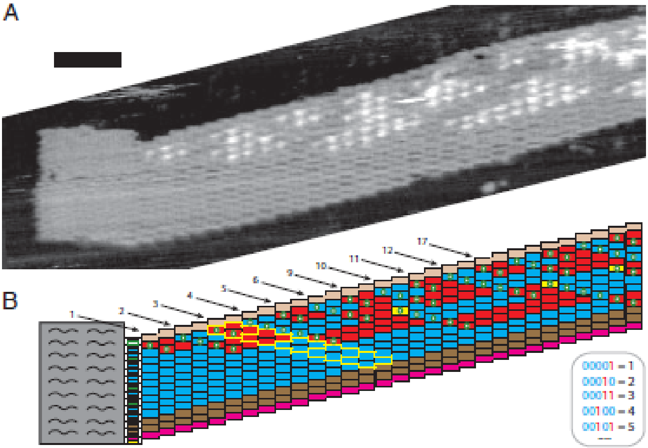
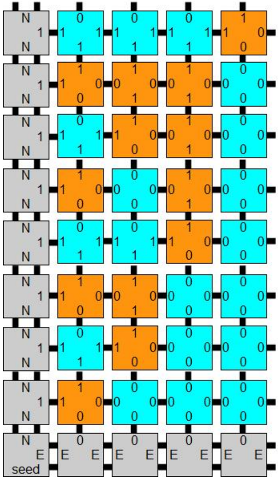


Pattern assembly

What is a pattern?

For $h, w, k \geq 1$, a **k-colored $(w \times h)$-pattern** P is a function from the region $\{(x, y) \mid 0 \leq x < w, 0 \leq y < h\}$ to the color set $\{1, 2, \ldots, k\}$.



Example

The right is a 3-colored (gray, blue, orange) 5×9-pattern, which is the well-known **binary counter pattern**.

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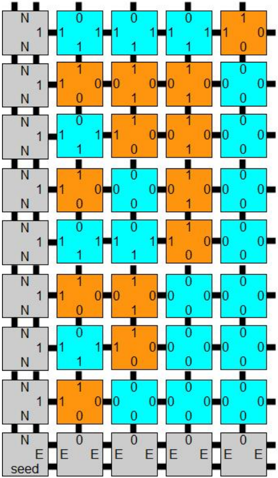

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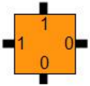
Pattern assembly

Rectilinear TAS

A **tile type** $t \in T$ is a DNA tile abstracted to be a square of specific color:



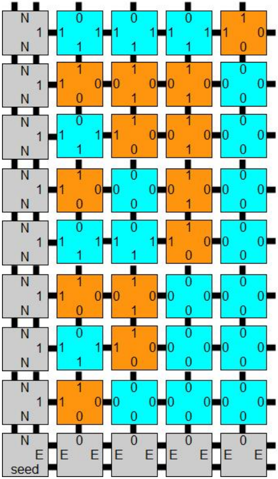
Each side has a label $(0, 1, \dots)$ that models a kind of sticky ends.

Rectilinear Tile-Assembly System (RTAS)

An RTAS is a pair (T, σ_L), where

T a finite set of tile types;

σ_L an L-shape seed.



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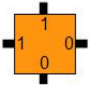

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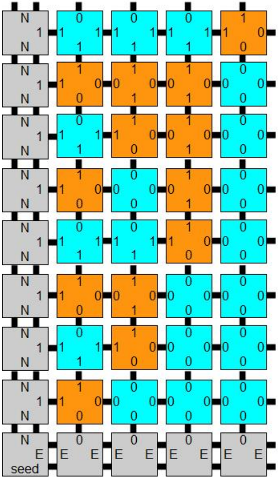
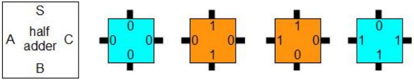


Pattern assembly

Rectilinear TAS

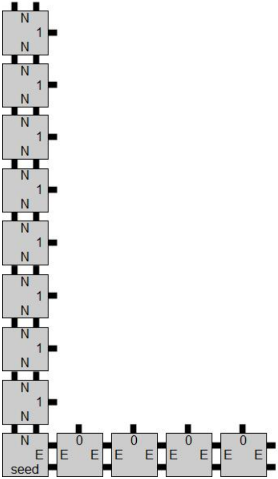
An RTAS with the following 4 tile types



assembles the binary counter pattern.

RTAS' attachment rule

- Assembly begins with the L-shape seed;
- A tile attaches if both of its west and south glues match.
- Assembly proceeds rectilinearly, from south-west to north-east.



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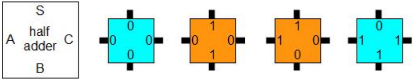

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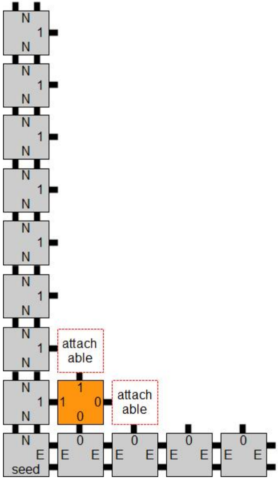

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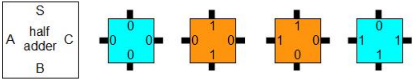

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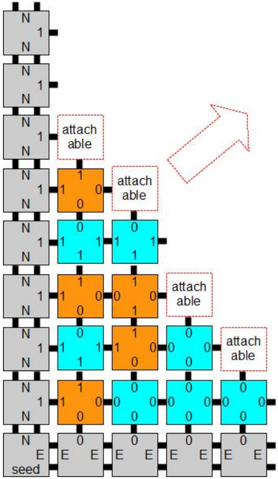

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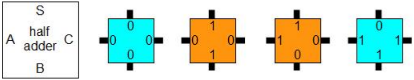

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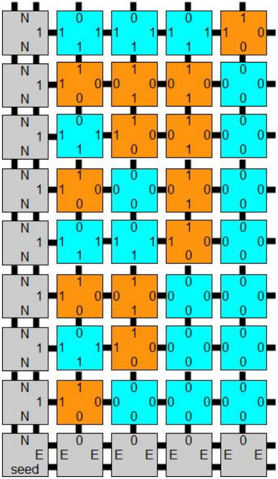


Pattern Assembly

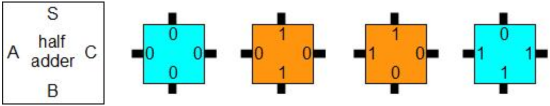
Rectilinear TAS

2-in 2-out logic gates

RTAS can have 4 tile types implement various 2-in 2-out logic gates such as `AND`, `OR`, `XOR`, and half-adder.

Example

The 4 tile types for counter pattern assembly implement **half-adder**.



Directed RTAS

Definition

An RTAS (T, σ_L) is **directed** if for any distinct $t_1, t_2 \in T$,

- their west glues are different, **or**
- their south glues are different.

Unique pattern assemblability

A directed RTAS assembles a unique pattern.

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PATTERN SELF-ASSEMBLY TILE SET SYNTHESIS (PATS)
[Ma & Lombardi 2008]

GIVEN: a pattern P
FIND: a directed RTAS with min # of tile types
that assembles P.

Theorem ([Czeizler & Popa 2012])

PATS *is* NP*-hard.*

Proof. It is due to a polynomial-time reduction from 3SAT. Its concise proof can be found in [Kari, Kopecki, S. 2013].

Constant colored PATS

Definition

"Any given logic circuit can be formulated as a colored rectangular pattern with tiles, using only a constant number of colors [Czeizler & Popa 2012]".

k-colored PATS(k-PATS)

GIVEN: a ***k*-colored** pattern P

FIND: a directed RTAS with min # of tile types that assembles P.

Constant colored PATS

Our contribution

Main Theorem

60-PATS is NP-hard.

Proof.

A given 3SAT instance ϕ is reduced to a 60-colored pattern $P(\phi)$ in a polynomial-time such that:

ϕ is satisfiable $\iff$ a directed RTAS assembles $P(\phi)$ using at most 84 tile types.

□

Proof idea

$P(\phi)$ consists of the following sub-patterns:

- MAIN CIRCUIT (evaluating 3SAT)
- GADGETS

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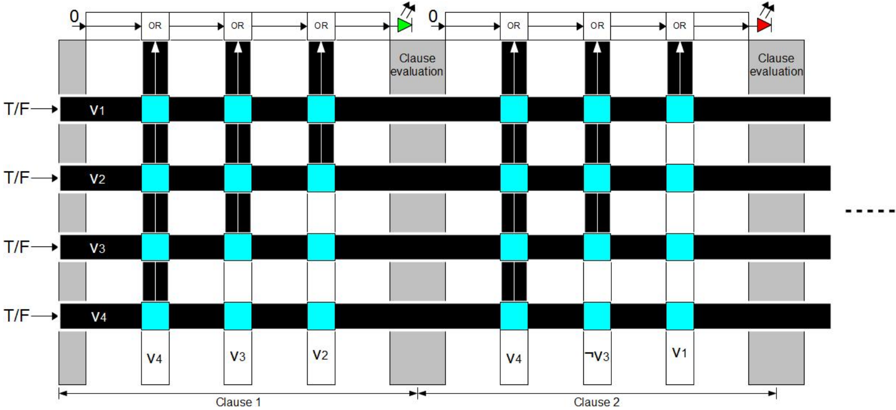
Proof idea

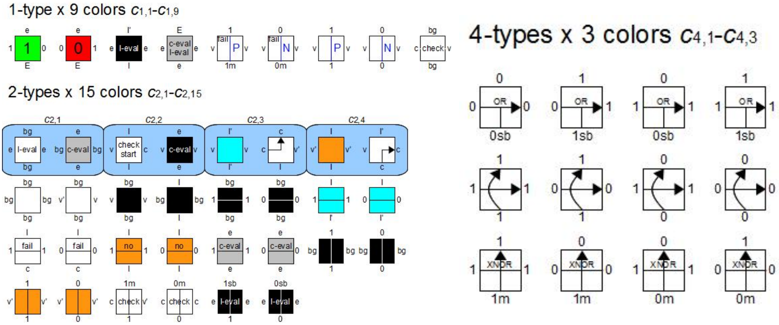
Circuit for evaluating 3SAT instance

The 3SAT instance ϕ can be evaluated using **2-in 2-out** logic gates (OR, XNOR, and intersection).



Proof idea

Set T_{3SAT} of 51 tile types for MAIN CIRCUIT



Tiles of these types evaluate ϕ according to the assignment, which are encoded on the L-shape seed σ_L.

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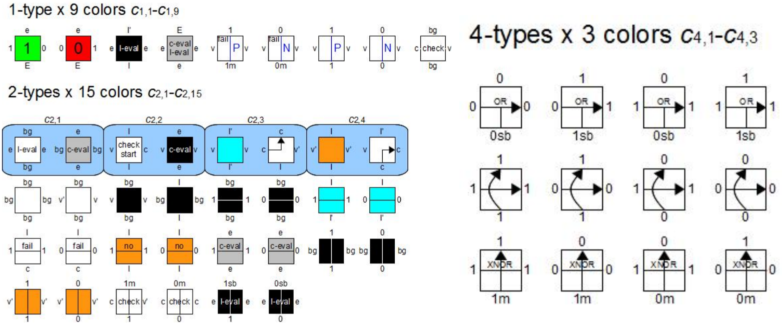

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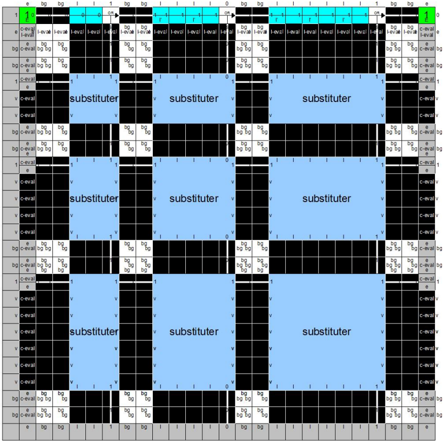
MAIN CIRCUIT



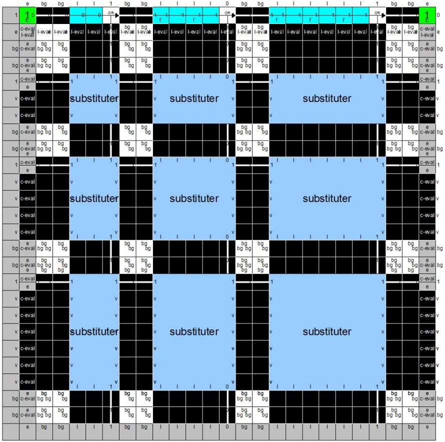
MAIN CIRCUIT is intuitivevly a snapshot of the evaluator circuit when all LEDs flush **green**, that is, ϕ **is satisfied**.

Satisfiability $\rightarrow$ assemblability

If ϕ is satisfiable, then encode a satisfying assignment on the L-shape seed and tiles in T_{3SAT} self-assemble MAIN CIRCUIT.

Proof idea

Main Circuit



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Satisfiability $\rightarrow$ assemblability

If ϕ is satisfiable, then encode a satisfying assignment on the L-shape seed and tiles in T_{3SAT} self-assemble Main Circuit.

Proof idea

Reduction

Satisfiability $\rightarrow$ 84 tile types are enough

84 tile types are enough:

- T_{3SAT} (of 51 tile types) for MAIN CIRCUIT;
- 33 tile types for 33 auxiliary colors (1 type per color) in GADGET.

We need to prove:

Unsatisfiability $\rightarrow$ need for 85 tile types

With T_{3SAT}, some LED position flushes red no matter what seed is, that is, MAIN CIRCUIT would not self-assemble. If 84 were enough, we must find something but T_{3SAT}.

Proof idea

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Proof idea

Role of GADGET

GADGET endows $P(\phi)$ with the following property:

Lemma

In order for a directed RTAS to self-assemble $P(\phi)$ using 84 tile types, the set T_{3SAT} must be used.

Corollary

If ϕ is not satisfiable, then no directed RTAS with 84 tile types can self-assemble $P(\phi)$.

Corollary

60-PATS is NP-hard.

Proof idea

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Corollary

60-Pats is NP-hard.

Approximability and PTAS

Corollary

For any $c \geq 60$*, there is no polynomial-time algorithm for* c-PATS *with approximation ratio* $\frac{85}{84}$*.*

Corollary

For any $c \geq 60$*,* c-PATS *does admit any polynomial-time approximation scheme (PTAS).*

Recent Developments

Theorem ([Johnsen, Kao, S. 2013])

29-PATS is NP-hard.

Proof.

This is due to a polynomial-time reduction from SUBSET SUM ψ to a 29-colored pattern $P(\psi)$ as: ψ is summable iff there is a directed RTAS with 46 tile types that self-assembles $P(\psi)$. □

Corollary

For any $c \geq 29$, there is no polynomial-time algorithm for c-PATS with approximation ratio $\frac{47}{46}$.

Corollary

For any $c \geq 29$, c-PATS does admit any PTAS.

Recent Developments

Theorem ([Johnsen, Kao, S. 2013])

*29-*PATS *is* NP*-hard.*

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Corollary

For any $c \geq 29$*,* c-PATS *does admit any PTAS.*

Future Works

- finding the minimum c such that c-PATS remains NP-hard (conjectured to be 2).
- the design of good approximation algorithms for constant colored PATS.

Acknowledgements

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- Department of Information and Computer Science, Aalto University

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