DNA Tile Self-Assembly

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Department of Computer Science

Natural Computing, Winter Term 2013/2014
(I) Self-Assembly Systems with a Temperature

(II) Directed vs. Undirected Self-Assembly Systems

(III) Staged Self-Assembly

(IV) Assembly of Patterns

(V) Assembly of “Smart Tiles” and “Smart Structures”
The abstract tile self-assembly model was defined in order to capture the process of DNA self-assembly in a simplified formal model. An aTAM consists of

- finite set of *tile types* $T$ with *glues* from $\Gamma$,
- *temperature* $\tau \in \mathbb{Z}^+$,
- glue strength function $g : \Gamma \rightarrow \mathbb{N}$, and
- *seed* tile (or structure) $\sigma$. 

A tile can attach to the growing structure if its binding strength is at least the temperature $\tau$. 

Let $\tau = 2$. 

An assembly is *terminal* if no further tiles can be attached.
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![Diagram of tile types and glue interactions]
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![Diagram of aTAM components: a seed tile $\sigma$, tiles with glues, and connecting structures.](image-url)
Abstract Tile Self-Assembly Model (aTAM)  
Winfree (1998)

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![Diagram of aTAM](image)
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Glues are implemented by complementary DNA sticky ends $u$ and $u^*$. The glue strength is the energy needed to break the hydrogen bonds between the sticky ends.

- the length of the sticky ends,
- G, C-content ($G - C$ pairs 3 hydrogen bonds whereas $A - T$ pairs have 2),
- possible mismatches in $u$ and $u^*$.
Modeling of Chemical Properties

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Depending on the *temperature* of the solution “weak bonds” will frequently assemble and disassemble, but will not be stable.

Other factors can influence the glue strength, like solvents (often salts) in the solution.
Self-Assembly of a Counter at Temperature $\tau = 2$

Seed

Frame

Half-adder

$g(\uppi) = 2$
$g(0) = g(1) = 1$
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\[ g(0) = g(1) = 1 \]

sum $a \oplus b$

input $a$

input $b$

carry $a \land b$
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- $g(0) = g(1) = 1$

$g(n) = 2$

$g(0) = g(1) = 1$

Sum $a \oplus b$

Input $a$

Input $b$

Carry $a \land b$
Self-Assembly of a Counter at Temperature $\tau = 2$

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<tr>
<th>Seed</th>
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<th>Half-adder</th>
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<tbody>
<tr>
<td>$= \sigma$</td>
<td>$= = = = = = = = $</td>
<td>sum $a \oplus b$</td>
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<td>$= = = = = = = = $</td>
<td>$= = = = = = = = $</td>
<td>input $a$</td>
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Rothemund, Papadakis, Winfree (2004)
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Self-Assembly of Sierpinski Triangles

output \( a \oplus b \)

output \( a \oplus b \)

input \( b \)

input \( a \)
Self-Assembly of Sierpinski Triangles

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<tr>
<th>Input a</th>
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<th>Output a ( \oplus ) b</th>
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An aTAM is *directed* (a.k.a. deterministic) if it forms one unique terminal assembly, where an assembly is defined by which tile type is placed at each position.
Directed Self-assembly Systems

An aTAM is *directed* (a. k. a. deterministic) if it forms one unique terminal assembly, where an assembly is defined by which tile type is placed at each position.

An aTAM *strictly self-assembles* a shape if all of its terminal assemblies are guaranteed to have that shape, although some of the assemblies may have different tile types at the same position.
Theorem

For \( n \in \mathbb{N} \), there is a finite shape \( S \) that is strictly self-assembled by an aTAM with \( c \) tile types, but every directed aTAM that (strictly) self-assembles \( S \) requires at least \( c + n \) tile types.
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For $n \in \mathbb{N}$, there is a finite shape $S$ that is strictly self-assembled by an aTAM with $c$ tile types, but every directed aTAM that (strictly) self-assembles $S$ requires at least $c + n$ tile types.
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\[
\begin{array}{cccc}
A_n & C_n & A_n & B_n \\
A_{n-1} & C_{n-1} & A_{n-1} & B_{n-1} \\
\vdots & \vdots & \vdots & \vdots \\
A_3 & C_3 & A_3 & B_3 \\
A_2 & C_2 & A_2 & B_2 \\
A_1 & C_1 & A_1 & B_1 \\
\end{array}
\]

### Theorem

There is an \textit{infinite} shape \( S \) such that some aTAM strictly self-assembles \( S \), but no directed aTAM (strictly) self-assembles \( S \).
Theorem

The directed (zig-zag) aTAM at temperature $\tau = 2$ is Turing-universal.
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$$\cdots \square 001010111 \square \cdots$$

$s \quad \delta(s,0) = (p,1,R)$

$$\cdots \square 101010111 \square \cdots$$

$p \quad \delta(p,0) = (q,0,L)$

$$\cdots \square 101010111 \square \cdots$$

$q \quad \cdots$  

$$\cdots \square 0011101 \square \cdots$$

$f \quad \cdots$$
Universality of Directed aTAM with $\tau = 2$

**Theorem**

The directed (zig-zag) aTAM at temperature $\tau = 2$ is Turing-universal.

---

Let $s$ be the initial state with symbols $01010111$. The transition function $\delta$ is defined as follows:

- $\delta(s, 0) = (p, 1, R)$
- $\delta(p, 0) = (q, 0, L)$
- $\delta(q, 0) = (f, 1, L)$
- $\delta(f, 0) = (\star, 1, L)$

The final state is represented by the symbol $\star$. This demonstrates the Turing-universality of the directed aTAM at $\tau = 2$. 

---

**Open Problem**

Is the directed aTAM Turing-universal at temperature $\tau = 1$?
Theorem

The directed (zig-zag) aTAM at temperature $\tau = 2$ is Turing-universal.

\[
\cdots \square 010111 \square \cdots \quad \delta(s, 0) = (p, 1, R)
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\[
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More external control is added to the assembly process by using different sets of tile types in each of several stages.

Start with a seed structure $\sigma$ and sets of tile types $T_1, \ldots, T_n$. For each stage $i = 1, \ldots, n$

1. add the tile types $T_i$ to the solution,
2. wait for a terminal structure to assemble,
3. then, “wash away” all unbound tile types.

After the $n$-th stage start over with the 1-st stage again.
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In biochemistry wet-labs the repeated process of mixing DNA structures (in our case tile types) into a solution and then purifying the solution to obtain certain structures is a commonly used technique.
Universality of Staged aTAM with $\tau = 1$

**Theorem**

The directed, staged aTAM at temperature $\tau = 1$ is Turing-universal.

Staged aTAM with $\tau = 2$ can simulate zig-zag aTAM with $\tau = 2$.

East-west glues are actual glues while north-south glues are simulated by the geometry of the tile.
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What are Nanoscopic Patterns?

“Molecular pegboards” (addressable nanoarrays), which are cheap to produce, for

a.) arranging nanoparticles (gold, silver, ...),

b.) molecular and logic circuits (*in vitro* and *in vivo*),

c.) enzyme interaction or enzyme detection,

d.) nano-factories like “artificial leafs”,

e.) quantum dot assembly.
Pattern Assembly

Pattern assembly is an aTAM where

→ the temperature is $\tau = 2$,
→ every tile type has a color,
→ every glue has strength 1, and
→ we start from an L-shaped seed.
Pattern Assembly

grid where every node has a property
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grid where every node has a property

pattern where every pixel has a color

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For a given pattern $P$, among all aTAMs which strictly self-assemble $P$, find an aTAM with the minimal number of tile types. Obvious bounds: $\#\text{colors} \leq \#\text{tile types} \leq \text{pattern size}$
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Theorem
A minimal tile set which strictly self-assembles a pattern $P$ is directed.

Theorem
It is NP-hard to find a minimal tile set that strictly self-assembles a given binary pattern $P$.

NP-hard: no algorithm is known which solves the problem efficiently.
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\[
\begin{array}{cccccccc}
7 & 6 & 1 & 3 & 2 & 1 & 2 \\
6 & 1 & 6 & 5 & 7 & 3 & 2 \\
1 & 2 & 4 & 1 & 2 & 5 & 7 \\
7 & 2 & 5 & 7 & 6 & 1 & 6 \\
7 & 6 & 1 & 2 & 1 & 2 & 1
\end{array}
\]

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Signals and Logic Gates on Tiles

Signal Passing

Attach *signals* on top of tiles which are triggered when the tile assembles. Signals can activate glues, deactivate glues, or trigger a signal on a neighbouring tile.
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![Diagram of signal passing on DNA tiles](image-url)
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**Logic Gates**

Several signals on one tile can be combined via *logic gates*. 
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Several signals on one tile can be combined via *logic gates*.

Signals and logic gates can be implemented using *strand displacement*. 
Signal Passing for Tile Self-Assembly
Padilla, Liu, Seeman (2011)
Smart tiles which can interactively self-assemble larger structures are in turn self-assembled from smaller “DNA structures”.

Robot Pebbles a. k. a. “Smart Sand”
Gilpin, Rus et al. (2009–2012)

http://www.youtube.com/watch?v=swxTTlHjN5Q
Logic-Gated Nanorobot for Targeted Transport
Douglas, Bachelet, Church (2012)

Key (target)
Lock 1
Cargo
Hinge
Lock 2