Abstract Tile Self-Assembly Model and the Complexity of Self-Assembled Rectangles
Molecular Building Blocks
Molecular Building Blocks

[Reif’s Group, Duke University]
DNA Scaffolding

[Sung Ha Park, Constantin Pistol, Sang Jung Ahn, John H. Reif, Alvin R. Lebeck, Chris Dwyer, and Thomas H. LaBean, 2006]
Self-Assembly for Circuit Patterns

[Cook, Rothemund, and Winfree, 2003]
More Examples of DNA Tiles

[Winfree’s Group, Cal Tech]
2D Self-Assembly for Turing Machines

[Winfree, Yang, and Seeman, 1998]
Simulation of Cellular Automata


340nm
Example of 3D Self-Assembly

[Shaw, University of Southern California]
3D DNA Cube

[Seeman, New York University]
3D DNA Truncated Octahedron

[Seeman, New York University]
Clonable DNA Octahedron

[Shih, Quispe, Joyce, 2004]
Outline

• Background, Motivation
• Model
• Rectangle
Tile Model of Self-Assembly
(Rothemund, Winfree STOC 2000)

Tile System: \( \{ t, G, T, s \} \)

- \( t \): temperature, positive integer
- \( G \): glue function \( G: \Sigma \times \Sigma \rightarrow \{0,1,\ldots,t\} \)
- \( T \): tileset \( \{ b, y, y, w, b, \ldots \} \)
- \( s \): seed tile
How a tile system self assembles

\[ T = \begin{align*}
S & \quad a & \quad b \\
 x & \quad c & \quad d
\end{align*} \]

\[ G(y) = 2 \quad G(g) = 2 \quad G(r) = 2 \quad G(b) = 2 \quad G(p) = 1 \quad G(w) = 1 \]

\[ t = 2 \]
How a tile system self assembles

\[ T = \begin{array}{ccc}
S & a & b \\
x & c & d
\end{array} \]

\[
\begin{align*}
G(y) &= 2 \\
G(g) &= 2 \\
G(r) &= 2 \\
G(b) &= 2 \\
G(p) &= 1 \\
G(w) &= 1 \\
t &= 2
\end{align*}
\]
How a tile system self assembles

\[ T = \begin{array}{ccc}
S & a & b \\
\times & c & d \\
\end{array} \]

\[
\begin{align*}
G(y) &= 2 \\
G(g) &= 2 \\
G(r) &= 2 \\
G(b) &= 2 \\
G(p) &= 1 \\
G(w) &= 1 \\
\end{align*}
\]

\[ t = 2 \]
How a tile system self assembles

\[ T = \begin{array}{c}
S \quad a \quad b \\
\hline
x \quad c \quad d \\
\end{array} \]

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

\[ t = 2 \]
How a tile system self assembles

\[ T = \begin{array}{ccc}
S & a & b \\
x & c & d
\end{array} \]

\[
T = \begin{cases}
G(y) = 2 \\
G(g) = 2 \\
G(r) = 2 \\
G(b) = 2 \\
G(p) = 1 \\
G(w) = 1
\end{cases}
\]

\[ t = 2 \]
How a tile system self assembles

\( T = \)

\[
\begin{array}{ccc}
S & a & b \\
x & c & d \\
\end{array}
\]

\[
\begin{array}{ccc}
d & c & x \\
a & b & \\
\end{array}
\]

\[
T = \begin{array}{c}
S \\
a \\
b \\
x \\
c \\
d \\
\end{array}
\]

\[
\begin{array}{c}
d \\
c \\
x \\
S \\
a \\
b \\
\end{array}
\]

\[
\begin{array}{c}
G(y) = 2 \\
G(g) = 2 \\
G(r) = 2 \\
G(b) = 2 \\
G(p) = 1 \\
G(w) = 1 \\
\end{array}
\]

t = 2
How a tile system self-assembles

\[ T = \begin{array}{ccc} S & a & b \\ x & c & d \end{array} \]

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

\[ t = 2 \]
How a tile system self assembles

\[ T = \begin{array}{ccc}
S & a & b \\
x & c & d \\
\end{array} \]

\[
T = \begin{array}{ccc}
S & a & b \\
x & c & d \\
\end{array}
\]

\[
G(y) = 2 \\
G(g) = 2 \\
G(r) = 2 \\
G(b) = 2 \\
G(p) = 1 \\
G(w) = 1 \\
t = 2
\]
How a tile system self assembles

\[ T = \begin{array}{ccc}
S & a & b \\
& x & c & d \\
S & a & b
\end{array} \]

\[
\begin{align*}
G(y) &= 2 \\
G(g) &= 2 \\
G(r) &= 2 \\
G(b) &= 2 \\
G(p) &= 1 \\
G(w) &= 1
\end{align*}
\]

\[ t = 2 \]
Efficient Assembly of Shapes

• Given a Shape:

• Design an **efficient** tile system that uniquely builds the shape:

\[ T = \]

- \[ S \]
- \[ a \]
- \[ b \]
- \[ x \]
- \[ c \]
- \[ d \]

\[ G(y) = 2 \]
\[ G(g) = 2 \]
\[ G(r) = 2 \]
\[ G(b) = 2 \]
\[ G(p) = 1 \]
\[ G(w) = 1 \]
Alphabet of Shapes, Built with DNA Tiles

[Bryan Wei, Mingjie Dai, Peng Yin, Nature 2012]
Outline

- Background, Motivation
- Model
- Rectangles
Building 1xn Lines
Building 1xn Lines
Building 1xn Lines
Building 1xn Lines
Building 1xn Lines

Tile Complexity: $n$
Building 2xn Rectangles

n
Building 2xn Rectangles

A

A

n
Building 2xn Rectangles
Building 2xn Rectangles

A
B
C

n
### Building 2xn Rectangles

<table>
<thead>
<tr>
<th>A</th>
<th>B</th>
<th>A</th>
<th>B</th>
</tr>
</thead>
</table>

---

n
Building 2xn Rectangles

\[ \text{A}_1 \quad \text{A}_2 \]
\[ \text{B}_2 \quad \text{B}_1 \]

\[ n \]
Building 2xn Rectangles
Building 2xn Rectangles
Building 2xn Rectangles

Lower Bound: \( \sqrt{\frac{n}{2}} = \Omega(\sqrt{n}) \)
Building 2xn Rectangles

2 x n lines

Lower Bound         Upper Bound

$\Omega(\sqrt{n})$            $O(n)$
Building 2xn Rectangles

Can we do better than $O(n)$?
Building 2xn Rectangles

2 x n lines

Lower Bound  Upper Bound

$\Omega(\sqrt{n})$  $O(n)$  $O(\sqrt{n})$

Can we do better than $O(n)$?
-YES
Build a 2 x 16 rectangle: \[ t = 2 \]
Build a 2 x 16 rectangle: \[ t = 2 \]
Build a 2 x 16 rectangle: \[ t = 2 \]

\[ \text{S}_1 \quad \text{S} \quad \text{C}_0 \quad \text{C}_1 \quad \text{C}_2 \quad \text{C}_3 \]

\[ \text{S} \quad \text{C}_1 \quad \text{C}_2 \quad \text{g} \quad \text{g} \quad \text{p} \]
Build a $2 \times 16$ rectangle: $t = 2$
Build a 2 x 16 rectangle: 

\[ t = 2 \]
Build a 2 x 16 rectangle: \[ t = 2 \]
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Build a $2 \times 16$ rectangle: $t = 2$
Build a 2 x 16 rectangle: \( t = 2 \)
Build a 2 x 16 rectangle:  

\[ t = 2 \]
Build a 2 x 16 rectangle: $t = 2$
Build a 2 x 16 rectangle: t = 2
Build a 2 x 16 rectangle: $t = 2$
Build a 2 x 16 rectangle: 

\[ t = 2 \]
Build a 2 x 16 rectangle: \( t = 2 \)

\[
\begin{array}{ccccccccccccccc}
S_1 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 2 & 2 & 2 & 2 & 3 & 3 & 3 & P \\
S & C_1 & C_2 & C_3 & C_0 & C_1 & C_2 & C_3 & C_0 & C_1 & C_2 & C_3 & C_0 & C_1 & C_2 & C_3 \\
\end{array}
\]

2 x n lines

Lower Bound \( \Omega(\sqrt{n}) \) \hspace{1cm} Upper Bound \( O(\sqrt{n}) \)