Intrinsic universality and the computational power of self-assembly

Damien Woods

Caltech
Computation and geometry


Portion of a tiling of Robinson’s 10-tile aperiodic square tile set

Abstract tile assembly model. Winfree 1998

Nubots - From Woods, Chen, Goodfriend, Dabby, Winfree, Yin. ITCS 2013
Physical motivation

• Engineers are building nanoscale molecular (chemical) computers

• Nature computes
  “Indeed, if the physics of our universe could not support computation, it’s doubtful that it could support life”

• We need a computational theory of self assembly and molecular interactions
• Prediction in science
• More importantly (for us), we can find interesting theoretical problems involving computation, geometry, asynchronosity, kinetics and thermodynamics
Our journey

\[ \text{polygon} \]
\[ \text{TAM, } \tau = 2 \]
\[ \text{2HAM, } \tau = c^3 \text{ (IU [9])} \]
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\[ \text{hexagon} \]
\[ \text{TAM, } \tau = 2 \]
\[ \text{2HAM, } \tau = 2 \text{ (IU [9])} \]
\[ \text{aTAM, } \tau \geq 2 \text{ (IU [11])} \]

\[ \text{aTAM, } \tau = 1 \]
\[ \text{Locally consistent} \]
\[ \text{aTAM } \tau = 2 \text{ (IU [12])} \]
Our journey

\[ \text{aTAM, } \tau \geq 2 \text{ (IU [11])} \]
Abstract tile assembly model

- Finite set of unit-sized square **tiles**
  - non-rotatable, unlimited supply of each tile type
- Each side has a **glue** (a,b,c,d,...)
- Each glue has a **strength** (0,1,2,3,...)
- **Tile assembly system**: is a [tile set, seed tile, temperature (0,1,2,3,...)]
- Growth begins from the **seed** tile at (0,0) in $\mathbb{Z}^2$
- A tile **sticks** to an assembly if enough of its glues match so that the sum of the strengths of the matching glues is at least the **temperature**
- Asynchronous

Key definition: **Tile assembly system**: tile set, seed tile, temperature
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A tile assembly system is a \([\text{tile set, seed tile, temperature}]\)

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- Temperature = 2

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Damien Woods, MCU 2013
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Cooperation (adjacent sides)

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**Cooperation (adjacent sides)**

- Cooperation requires that the sum of the strengths of the matching glues is at least the temperature.
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Temperature = 2
Abstract tile assembly model

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Cooperation (opposite sides)

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<table>
<thead>
<tr>
<th>A</th>
<th>a</th>
<th>b</th>
<th>c</th>
<th>d</th>
</tr>
</thead>
<tbody>
<tr>
<td>b</td>
<td>A</td>
<td>a</td>
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<td>c</td>
</tr>
<tr>
<td>a</td>
<td>B</td>
<td>b</td>
<td>c</td>
<td>k</td>
</tr>
<tr>
<td>g</td>
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- Each glue has a **strength** (0, 1, 2, 3, ...)
- Growth begins from a **seed** tile
- Tiles **stick** to the growing assembly if their glues match, and are strong enough (sum of strengths is at least the **temperature**)
- **Finite** set of tile types, unlimited supply of each tile type

Order of tile placement is nondeterministic (asynchronous growth).
More than one tile type can go at a given position.

Temperature = 2
Abstract tile assembly model

- Square units called tiles (non-rotatable)
- Each side has a glue (a,b,c,d,...)
- Each glue has a strength (0,1,2,3,...)
- Growth begins from a seed tile
- Tiles stick to the growing assembly if their glues match, and are strong enough (sum of strengths is at least the temperature)
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Defn. Tile assembly system: tile set, seed tile, temperature

Order of tile placement is nondeterministic (asynchronous growth).
More than one tile type can go at a given position
Algorithmic self-assembly with tiles: computation and geometry

- Seeman built tiles out of DNA in the laboratory
- Winfree showed that DNA tiles can run algorithms (much like cellular automata, Wang tiles)
- A variety of algorithmic tile assembly systems have been built from DNA
Computation with tile assembly

- **Turing universality**  
  Winfree, 1998

- **Efficient assembly of simple shapes**  
  - E.g. $n \times n$ squares using $\Theta(\log n / \log \log n)$ tile types  
  Rothemund, Winfree. STOC 2000

- **Efficient assembly of complicated connected shapes using a number of tile types roughly equal to the Kolmogorov complexity of the shape**  
  Soloveichik, Winfree. SICOMP 2007
Intrinsic universality

http://otcametapixel.blogspot.com/
http://www.youtube.com/watch?v=xP5-ileKXE8
Intrinsic universality

http://otcametapixel.blogspot.com/
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Intrinsic universality

- Conway’s Game of Life is an intrinsically universal cellular automaton

http://otcametapixel.blogspot.com/
http://www.youtube.com/watch?v=xP5-ileKXE8

Durand, Roka, The game of life: universality revisited. 1999
Intrinsic universality

- An intrinsically universal CA is one that “simulates” any other:
  - Appropriate encoding
  - Encodes all properties of the simulated CA, up to rescaling

- Theory of intrinsic universality in CA

- Applications:
  - separating class of cellular automata based on their simulation abilities
  - use of non-intrinsic universality results to prove that certain cellular automata are “computationally weak”
Is the abstract tile assembly model intrinsically universal?
Is the abstract tile assembly model intrinsically universal?

Yes!
Is the abstract tile assembly model intrinsically universal?

Yes!

There is a single universal tile set $U$ that simulates any tile assembly system.

Doty, Lutz, Patitz, Schweller, Summers, Woods. FOCS 2012
Our journey

\[ a\text{TAM}, \tau \geq 2 \text{ (IU [11])} \]
Simulation definition

• We want a definition of simulation that captures the notion of one Tile Assembly System simulating the “behaviour” of another

• \( T \) is a (any) simulated tile assembly system,
  
  • \( T = (\text{tileset } T, \text{ seed assembly } \sigma, \text{ temperature } \tau) \)

• Tile assembly system \( U_T = (U, \sigma_T, 2) \) simulates \( T \) if:
  
  - Tiles from \( T \) are simulated by \( m \times m \) supertiles in \( U_T \), i.e., a representation function \( R \) maps supertiles in assemblies of \( U_T \) to tiles in \( T \). Oh, and \( R \) is “clean”.
  
  - The producible assemblies in \( U_T \) represent exactly the producible assemblies in \( T \).
  
  - Ignoring \( m \times m \) scaling, dynamics are equivalent in \( U_T \) & \( T \).
Simulation definition

- Preassembled seed structure (encodes simulated TAS)

- Tiles are simulated by supertiles
  - For each assembly sequence in the simulated tile system, there is an assembly sequence in the simulator, and vice-versa
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Universal (simulator) tile set

Simulated tile

Simulator supertile

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Ignoring \( m \times m \) scaling, dynamics are equivalent in the simulated system and simulator.

- Tiles are simulated by supertiles
- For each assembly sequence in the simulated tile system, there is an assembly sequence in the simulator, and vice-versa.

Simulated tile

Preassembled seed structure (encodes simulated TAS)

Simulator supertile

Universal (simulator) tile set

Temperature = 2

Seed
Simulation definition

- We want a definition of simulation that captures the notion of one Tile Assembly System simulating the “behaviour” of another.

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Is the abstract tile assembly model intrinsically universal?

Yes!

Theorem: There is a single universal tile set $U$ that simulates any tile assembly system

Doty, Lutz, Patitz, Schweller, Summers, Woods. FOCS 2012
Tiles from the universal tile set $U$ are arranged so that they encode some simulated tile assembly system $T$. 

Preassembled seed supertile
Superside

Encoded glue of this superside (e.g. “a”)

Encoding of the entire simulated tile assembly system written down using tiles from the simulator $U$

<table>
<thead>
<tr>
<th>frame</th>
<th>glue</th>
<th>tile lookup table</th>
<th>blank</th>
<th>probe region</th>
<th>probe table</th>
<th>tile lookup table</th>
<th>glue</th>
<th>frame</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>$O(\log</td>
<td>T</td>
<td>)$</td>
<td>$O(</td>
<td>T</td>
<td>^4 \log</td>
<td>T</td>
<td>)$</td>
</tr>
</tbody>
</table>

Encoding of tile type 1 from $T$

$|T|$ is number of tiles in the simulated tileset $T$. 
One-sided binding with a single strength-$\tau$ south superside

Supertile 1

Glue “a” is encoded here

Tile set $T$ is encoded here
One-sided binding with a single strength-$\tau$ south superside

Glue “a” is encoded here

Tile set $T$ is encoded here
One-sided binding with a single strength-τ south superside
One-sided binding with a single strength-τ south superside
One-sided binding with a single strength-$\tau$ south superside

Glue “a” is encoded here

“Genome” is copied

“Genome” is read

crawler encodes glue of south superside

Tile set $T$ is encoded here

Damien Woods
One-sided binding with a single strength-$\tau$ south superside

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Tile set $T$ is encoded here

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crawler encodes glue of south superside

“Genome” is copied

“Genome” is read

Tile set $T$ is encoded here

Glue “a” is encoded here
One-sided binding with a single strength-$\tau$ south superside

Nondeterminism

Rotations

crawler encodes

glue of south superside

“Genome” is copied

“Genome” is read
# Crawler doing a tile lookup

**Crawler encodes “input” glues**

**Tile lookup table**

**Address entry counts**

```
<table>
<thead>
<tr>
<th></th>
<th>#</th>
<th>#</th>
<th>#</th>
<th>#</th>
<th>#</th>
<th>random num selection</th>
<th>#</th>
<th>#</th>
<th>#</th>
<th>#</th>
<th>#</th>
<th>#</th>
<th>compute state</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>1</td>
<td>2</td>
<td>3</td>
<td>4</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>2</td>
<td>3</td>
<td>4</td>
<td>0</td>
<td></td>
</tr>
</tbody>
</table>
```

**Crawler encodes “output” tile type**

**Address entries**

```
crawler encodes
crawler
tile lookup
table
```

```
crawler encodes
“input” glues
```
Two-sided binding with adjacent cooperating supersides

Glue “c” is encoded here
Glue “a” is encoded here
Two-sided binding with adjacent cooperating supersides

Glue "c" is encoded here
Glue "a" is encoded here
Two-sided binding with adjacent cooperating supersides

Glue “c” is encoded here
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Damien Woods, MCU 2013
Two-sided binding with adjacent cooperating supersides

Glue “c” is encoded here
Glue “a” is encoded here
Two-sided binding with adjacent cooperating supersides

Glue “c” is encoded here

Glue “a” is encoded here
A key problem

Better luck next time!

Uh oh!

A tile fits, but the path to the right is blocked!
Two-sided binding with opposite cooperating supersides

<table>
<thead>
<tr>
<th>2</th>
<th>b</th>
</tr>
</thead>
</table>

| 1 | a |

<table>
<thead>
<tr>
<th>glue</th>
<th>tile lookup table</th>
<th>probe table</th>
<th>probe region</th>
<th>blank</th>
<th>tile lookup table</th>
<th>glue</th>
</tr>
</thead>
</table>

Collect north & south glues, & random number
Two-sided binding with opposite cooperating supersides

<table>
<thead>
<tr>
<th></th>
<th>glue</th>
<th>tile lookup table</th>
<th>probe table</th>
<th>probe region</th>
<th>blank</th>
<th>tile lookup table</th>
<th>glue</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>base</td>
<td>b</td>
<td>b</td>
<td>a</td>
<td>a</td>
<td>b</td>
<td>b</td>
</tr>
<tr>
<td>2</td>
<td>base</td>
<td>b</td>
<td>b</td>
<td>a</td>
<td>a</td>
<td>b</td>
<td>b</td>
</tr>
</tbody>
</table>
Two-sided binding with opposite cooperating supersides
Two-sided binding with opposite cooperating supersides

collect north & south glues, & random number
Two-sided binding with opposite cooperating supersides

collect north & south glues, & random number
3-sided "uh-oh" example: probes miss each other

uh oh!
3-sided “uh-oh” example: probes miss each other
3-sided “uh-oh” example: probes miss each other
3-sided “uh-oh” example: probes miss each other
3-sided “uh-oh” example: probes miss each other

continues here because probes will not meet

uh oh!
- Variety of cases for different orders of superside arrival
- Superside win/lose configurations and crawler initiation locations (green)
- Proof analogy:
  - Distributed game
  - Computation & geometry
  - Key challenge: make all the tricks work together
Is the abstract tile assembly model intrinsically universal?

Yes!

Theorem: There is a single universal tile set $U$ that simulates any tile assembly system.

Doty, Lutz, Patitz, Schweller, Summers, Woods. FOCS 2012
Our journey

\[ \text{aTAM, } \tau \geq 2 \text{ (IU [11])} \]
Theorem: There is a **single** rotatable polygon that simulates **all** tile assembly systems.

Theorem: For each (Wang) plane tile system there is one rotatable polygon that simulates it.

Robinson’s 10-tile aperiodic tile set

A rotatable polygon that simulates a tile set

• For each set of (possibly rotatable, flipable) Wang square/hexagon tiles there is a single rotatable tile that simulates it

Hexagon example

rotation 1 = t1
rotation 2 = t2
A rotatable polygon that simulates a tile set

- For each set of (possibly rotatable, flipable) Wang square/hexagon tiles there is a single rotatable tile that simulates it.

Hexagon example:

- Rotation 1 = \( t_1 \)
- Rotation 2 = \( t_2 \)

Robinson's 10-tile aperiodic tile set (complimentary matching constraint)
A rotatable polygon that simulates a tile set

- For each set of (possibly rotatable, and/or flipable) square or hexagon tiles, there is a single (rotatable, flipable) tile that simulates it.

Hexagon example

\[
\begin{array}{cccc}
  a & f & \\
  b & c & e & d \\
  u & v & z & w & y \\
  b & v & c & w & d & e \\
  u & a & z & f & \\
  v & y & & \end{array}
\]

\[
\text{rotation 1} = t_1 \quad \text{rotation 2} = t_2
\]

(other rotations may cause problems)

Robinson's 10-tile aperiodic tile set
(complimentary matching constraint)
• An aperiodic tile set with 1 tile!
• Small gaps in the tilings
• We have given a general method (a compiler) to convert any square/hexagon plane tiling tile set to a single tile that simulates it
• So we can have a single tile that is aperiodic, or a single tile that simulates a universal Turing machine, etc.
A harder challenge: one tile for all of tile self-assembly

- Simulating tile assembly systems is significantly trickier than plane (Wang) tiling systems
- We want to design a single rotatable, flipable tile that simulates any tile assembly system
- Strength tau glues on rotatable tiles => Argh! There’s pumpable junk everywhere!
- So let’s not use strength tau glues on The One.
- Maybe we could find an intrinsically universal square tile set with strength < tau glues?
  - No! Any such tile set with a finite seed can not leave the seed’s bounding box
  - Let’s try hexagons!
Low strength hexes simulate high-strength squares

- Strength 1 or 0 hexagon glues, simulating strength 2, 1 or 0 square glues

- The we can simulate a set of low-strength hexagons with a single rotatable polygon
  - Bumps and dents to stop incorrect orientations and incorrect bindings
  - Glues are carefully rearranged on the polygon to allow “self seeding”
  - Many details omitted!
Construction overview

Tile assembly system $T$ → Hexagonal tile assembly system that simulates $T$ (using low-strength glues) → One polygon that simulates $T$

Intrinsically universal tile set → The one
Construction overview

Tile assembly system $T$ → Hexagonal tile assembly system that simulates $T$ (using low-strength glues) → One polygon that simulates $T$

Intrinsically universal tile set

The one

http://oscarfarellano.deviantart.com/
To use The One, simply apply a sequence of tile assembly system “reductions”:

Tile assembly system $T$ → Tile assembly system $U_T$ over the intrinsically universal tile set $U$ → Hexagonal tile assembly system (with low strength glues) → A tile assembly system that simulates $T$ using the single rotatable flipable polygonal tile.
One tile to simulate them all

Intrinsically universal tile set

The one

http://oscarfarellano.deviantart.com/
Magic dust

http://nighthawk101stock.deviantart.com/
Our journey

polygon
TAM, \( \tau = 2 \)

hexagon
TAM, \( \tau = 2 \)

\[ \uparrow \text{[8]} \]

\[ \uparrow \text{[8]} \]

\[ \approx \]

\( \text{aTAM}, \tau \geq 2 \) (IU [11])

Intrinsically universal tile set
Our journey

- polygon TAM, \( \tau = 2 \)
- hexagon TAM, \( \tau = 2 \)
- aTAM, \( \tau \geq 2 \) (IU [11])

Intrinsically universal tile set?
Our journey

Intrinsically universal tile set

Temperature 1

polygon
TAM, τ = 2

hexagon
TAM, τ = 2

aTAM, τ ≥ 2 (IU [11])

[11] [9,3] [9]

Damien Woods, MCU 2013
Temperature 1 tile assembly

- Temperature 1 tile assembly systems:
  - Each glues has strength 0 or 1
  - Tile binds to an assembly if $\geq 1$ glues match with strength $= 1$
  - Snakes on a plane
Temperature 1 tile assembly

- Each glues has strength 0 or 1
- Tile binds to an assembly if $\geq 1$ glues match with strength $= 1$
- Snakes on a plane
Is temperature 1 computationally weak?

- It has been conjectured (since 2000) that temperature 1 systems are “computationally weak”

- Some negative results:
  - Temperature 1 systems that build **fully connected** $n \times n$ squares require at least $n^2$ tile types
  - **Pumpable** temperature 1 systems produce only periodic structures
  - Temperature 1 with **no mismatches** require $2n-1$ tile types to assemble an $n \times n$ square

- Positive results:
  - 3D deterministic temperature 1 simulates Turing machines
  - 2D temperature 1 simulates Turing machine, but with some error

- It remains open whether temperature 1 (aka noncooperative) tile assembly systems can simulate Turing machines deterministically in 2D, whether they can efficiently build squares or other shapes, etc.

- But can they do tile assembly? I.e. can they simulate cooperative tile assembly?
- No!

---

Rothemund, Winfree. STOC 2000
Doty, Patitz, Summers. TCS 2011
Cook, Fu Schweller. SODA 2011
Meunier, Patitz, Summers, Theyssier, Winslow, Woods. SODA 2014
Temperature 1 is not IU for the aTAM

- We will show that no temperature 1 system simulates the following simple temperature 2 system

![Diagram](image)

(a) Equal arm lengths

(b) Unequal arm lengths

Meunier, Patitz, Summers, Theyssier, Winslow, Woods. SODA 2014
Temperature 1 is not IU for the aTAM

• First we prove a kind of strong pumping lemma for tile assembly (that holds at any temperature)

• We then use this pumping lemma to “fool” any claimed temperature 1 simulator into exposing its inability to simulate cooperation
Temperature 1 is not IU for the aTAM

- There are simple temperature 2 systems that can not be simulated by any temperature 1 system

- First fully-general negative result on temperature 1

- This negative result holds in 2D and 3D

- Recall: Deterministic 3D temperature 1 systems can simulate Turing machines!

- So these Turing-universal (powerful!) tile assembly systems can not simulate tile assembly

- Turing universal algorithmic behavior in self-assembly provably does not imply the ability to simulate arbitrary algorithmic self-assembly processes

- We walked into Mordor, and survived
Our journey

TAM, $\tau = 2$

polygon

Locally consistent

aTAM, $\tau = 2$ (IU [11])

$U[8]$

hexagon

TAM, $\tau = 2$

aTAM, $\tau \geq 2$ (IU [11])

$[8]$

$[19]$

Locally consistent

aTAM $\tau = 2$ (IU [12])

$\neq$

$[19]$
Our journey

\[ \text{TAM, } \tau = 2 \text{ (IU [9])} \]

\[ \text{2HAM, } \tau = c^2 \text{ (IU [9])} \]

\[ \text{2HAM, } \tau = c^3 \text{ (IU [9])} \]

\[ \text{Locally consistent aTAM, } \tau = 2 \text{ (IU [12])} \]

\[ \text{Intrinsically universal tile set?} \]

\[ \text{Temperature 1} \]
Conclusions

- 1. There is an intrinsically universal tile set:
  - i.e. there is a single tile set that can simulate any tile assembly system
- 2. There is a single rotatable polygon that can simulate any tile assembly system, or Turing machine
- 3. There is an aperiodic rotatable polygonal tile
- 4. Intrinsic universality can be used to separate, and classify, the power of self-assembly systems:
  - Temperature 1 can not simulate temperature 2 and above
  - Infinite set, of infinite hierarchies of hierarchical self-assembly systems (2HAM)
  - Other cool results that I have not mentioned:
    • Simulations between tile assembly and CA
    • Two-handed 3D tile set is IU for the 2D Signal-Passing tile assembly model
    • 3D Temperature 1 can simulate 2D Temperature 1
    • The restricted “locally consistent” tile assembly systems are intrinsic universal

Hendricks, Patitz, MCU, 2013

Hendricks, Padilla, Patitz and Rogers, DNA, 2013

Meunier, Patitz, Summers, Theyssier, Winslow, Woods. SODA 2014

Doty, Lutz, Patitz, Summers, Woods, STACS 2010
Open questions

1. Are the following models intrinsically universal?
   - hexagonal tile assembly model, polygonal tile assembly model, nubots, signal-passing tile assembly model

2. Is there a tile set $U_{\text{crazy fool}}$ that does nothing but simulate members from a “large” class of tile assembly systems?

3. Can we show that no 2D temperature 1 system can deterministically (correctly) simulate temperature 2 “zig-zag” tile assembly systems?
Thanks!

The tile assembly model is intrinsically universal. Doty, Lutz, Patitz, Schweller, Summers, Woods. FOCS 2012


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fin?
Our journey must continue...

Temperature 1

TAM, $\tau = 2$ (IU [9])

2HAM, $\tau = c^3$ (IU [9])

2HAM, $\tau = c^2$ (IU [9])

2HAM, $\tau = 2$ (IU [9])

aTAM, $\tau \geq 2$ (IU [11])

aTAM, $\tau = 1$ (IU [19])

Locally consistent aTAM $\tau = 2$ (IU [12])

Intrinsically universal tile set

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