## Theory and practice of algorithmic self-assembly

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## Structure

- Monday (lecture 1). Some high-level motivations, basic algorithmic selfassembly models (definitions) and very recent results on implementing algorithmic DNA nanotube circuits, a self-assembly model, in the wet-lab
- Tuesday (lecture 2): DNA sequence design and results on the DNA nanotube circuit model
- Wednesday (lecture 3). Complexity theory for self assembly.
- Theorem: The (cooperative, temperature >= 2) abstract tile assembly model is intrinsic universal
- Thursday (lecture 4). Complexity theory for self assembly.
- Theorem: The noncooperative (temperature 1) abstract tile assembly model does not simulate the cooperative model


## Abstract tile assembly model

- Square tiles
- finite set of tile types, unlimited supply of each type, non-rotatable
- Each side has a glue (colour) and strength ( $0,1,2,3, \ldots$ )
- System has a temperature (e.g. 2)
- Simple local binding rule: A tile sticks to an assembly if enough of its glues match so that the sum of the strengths
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- Tile assembly system:
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More than one tile type can go at a given position


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## Computation with tile assembly: theory

- Turing universality

Winfree, PhD Thesis. 1998


- Efficient assembly of simple shapes: $n \times n$ squares using $\Theta(\log n / \log \log n)$ tile types

Adleman, Cheng, Goel, Huang STOC 2001 Rothemund, Winfree. STOC 2000


Evans. PhD Thesis 2014

- Efficient assembly of scaled complicated connected shapes using a number of tile types roughly equal to the Kolmogorov complexity of the shape


## Theory of algorithmic self-assembly

- Helps us understand the abilities and limitations of self-assembly
- Also, its fun!
- aTAM is Turing universal: can "run" any algorithm Winfree, PhD Thesis 1998.
- Efficiently assemble $n \times n$ squares and other simple shapes
- Using only $\Theta(\log n / l \log \log n)$ tile types

Rothemund, Winfree. STOC 2000

- Efficiently assemble arbitrary finite shapes
- Number of tile types is roughly the Kolmogorov complexity of the shape

Soloveichik, Winfree. SICOMP 2007

- aTAM is intrinsically universal: there is one tile set that can simulate any tile assembly system
- Shape complexity can be put into the seed

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

- Thinking about these topics leads to a kind of "complexity theory" for self-assembly



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- Efficient assembly of scaled connected shapes using a number of tile types roughly equal to the Kolmogorov complexity of the shape Soloveichik, Winfree. SICOMP $2007_{8}$


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## Computation with tile assembly: theory

- Many other theoretical questions have been asked
- What questions would you ask?
- The goal is to understand the capabilities of these systems!
- Another goal is to motivate what we should build in the lab!
- Next slide: Let's ask a question


## Intrinsic universality

# Is there a set of intrinsically universal tiles: a set of aTAM tiles $U$ that can act like any other tile set? 



One universal tile set to do everything

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One universal tile set to do everything

What does "act like" mean?



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



## Comparing tile assembly models

## Is there a set of intrinsically universal tiles that can simulate any tile set?


-What is it that tile assembly systems do?

- Make shapes and patterns
- Carry out a crystal-like growth process (dynamics)
- Let define simulate using these criteria that are intrinsic to the model


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## Simulation

- For (any) simulated tile assembly system $T$
- $T$ = (tileset $T$, seed assembly $\sigma$, temperature T )
- Tile assembly system $\mathcal{U}$ simulates $T$ if:
- Tiles from $T$ are represented by $\boldsymbol{m} \mathbf{x} \boldsymbol{m}$ supertiles in $\mathcal{U}$
- Assemblies produced by $\mathcal{U}$ represent exactly assemblies produced by $T$ (via a representation function R : Blocks of tiles from $U$-> tiles from T )
- Dynamics are equivalent in $U$ and $T$, ignoring $m \times m$ scaling


Simulated system


Simulator system
$\bigcup \quad \begin{gathered}m \times m \text { seed } \\ \text { assembly }\end{gathered}$


## Simulation

- For (any) simulated tile assembly system $T$
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Simulated system

Simulator system

$U \quad$| $m \times m$ seed |
| :---: |
| assembly |

## Simulation definition

# Universal <br> (simulator) tile set 



## Simulator supertile



- Green 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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Temperature $=2$


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TAS)

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Preassembled seed structure

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Preassembled seed structure

## Simulation definition

## Universal <br> (simulator) tile set

Preassembled seed structure

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## Universal <br> (simulator) tile set

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## Simulation definition

Ignoring $m \times m$ scaling, production \& dynamics are equivalent in the simulated system and simulator

## Universal

 (simulator) tile set

Damien Woods


TAS)


Simulated tile

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## tile <br> Simulated

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## Simulation definition

## Universal <br> (simulator) tile set

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TAS)


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## Is the abstract tile assembly model intrinsically universal?



## Is the abstract tile assembly model intrinsically universal? Yes!



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

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

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Simulated system


Simulator system


## Superside


$|T|$ is number of tiles in the simulated tileset $T$.


## Superside



Encoded glue of this superside
(e.g. "a")





## One-sided binding with a single strength-т south superside



## One-sided binding with a single strength-т south superside



## One-sided binding with a single strength-т south superside



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## One-sided binding with a single strength-т south superside



## Crawler doing a tile lookup



Two-sided binding with adjacent cooperating supersides


Two-sided binding with adjacent cooperating supersides


Two-sided binding with adjacent cooperating supersides


Two-sided binding with adjacent cooperating supersides


Two-sided binding with adjacent cooperating supersides


Two-sided binding with adjacent cooperating supersides


Two-sided binding with adjacent cooperating supersides


## A key problem



Better luck next time!


Uh oh!

Two-sided binding with opposite cooperating supersides


Two-sided binding with opposite cooperating supersides


Two-sided binding with opposite cooperating supersides


Two-sided binding with opposite cooperating supersides


Two-sided binding with opposite cooperating supersides


Two-sided binding with opposite cooperating supersides


Two-sided binding with opposite cooperating supersides


Two-sided binding with opposite cooperating supersides


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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


$===-$|  |  |  |  |  |  |  |  |  |  |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |

3-sided "uh-oh" example: probes miss each other


- 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





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## A zoo of self-assembly models

How to compare these models?
abstract tile
assembly model


## A zoo of self-assembly models

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## A zoo of self-assembly models

How to compare these models?
abstract tile assembly model
temperature 2

hierarchical

temperature 1

## A zoo of self-assembly models

How to compare these models?
abstract tile assembly model
temperature 2

hierarchical
polyomino
temperature 1
dupled (domino)

polygonal free-body
geometric


## A zoo of self-assembly models <br> How to compare these models?


dupled \& restricted glue

## A complexity theory for self-assembly

Intrinsic universality...requires cooperation. Meunier, Patitz, Summers, Theyssier, Winslow, Woods. SODA 2014

## A complexity theory for self-assembly



## A complexity theory for self-assembly

Gives a structure to the field of self-assembly - a way to compare models

One Tile to Rule Them All. Demaine, Demaine, Fekete, Patitz, Schweller, Winslow, Woods. ICALP 2014.

Intrinsic universality...requires cooperation. Meunier, Patitz, Summers, Theyssier, Winslow, Woods. SODA 2014

Magic dust


## Result 1: There is a single rotatable polygon that simulates all tile assembly systems



Result 2: For each (e.g. Wang) plane tile system there is one rotatable polygon that simulates it
Theorem 7.1 Each colored square and hexagon plane tiling system in the families $\left(\left\}, c_{m}\right),\left(\left\{t_{r}, t_{f}\right\}\right.\right.$, $\left.c_{m}\right),\left(\{ \}, c_{c}\right)$ and $\left(\left\{t_{r}, t_{f}\right\}, c_{c}\right)$ is simulated by an $n$-gon nearly-plane tiling system.


Robinson's 10-tile aperiodic tile set

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



Robinson's 10-tile aperiodic tile set



Portion of a tiling of Robinson's 10-tile aperiodic square tile set (with rotations)

- Wang plane tiling system:
- Try to fill the plane with tiles.
- All sides must match.
- We care about the existence of tilings, but not how we made the tiling


## 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



## A rotatable polygon that simulates a tile set

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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

- An aperiodic tile set with 1 tile!
- Small gaps (<1 tile in size) 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




## 1 aperiodic tile

- 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



## 1 aperiodic tile

- Socolar-Taylor disconnected tile. 2012
- Aperiodic
- Rotations + flips

- Open question: Is there a single aperiodic connected 2D tile that makes gap-free tilings of the plane?


## But this is not (yet) magic dust



## 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 (Note that as a corollary this gives a single tile that simulates any algorithm)
- Problem 1:
- Strength tau glues on rotatable tiles => Argh! There's pumpable junk everywhere!
- 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
- Lets try hexagons!


## Low strength hexes simulate high-strength squares

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

- Then 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)
$\longrightarrow$ One polygon that simulates $T$


Tile set


The one

To use The One, simply apply a sequence of tile assembly system simulations:



Intrinsically
universal tile set
Intrinsically
universal tile set


The one

To use The One, simply apply a sequence of tile assembly system simulations:

$$
\begin{gathered}
\text { Tile assembly } \\
\text { system } T
\end{gathered} \longrightarrow \begin{gathered}
\text { Tile assembly } \\
\text { system UT over the } \\
\text { intrinsically } \\
\text { universal tile set } U
\end{gathered} \longrightarrow \begin{gathered}
\text { Hexagonal tile } \\
\text { assembly system } \\
\text { (with low strength } \\
\text { glues) }
\end{gathered} \longrightarrow \begin{gathered}
\text { A tile assembly } \\
\text { system that simulates } \\
T \text { using the single } \\
\text { rotatable flipable } \\
\text { polygonal tile }
\end{gathered}
$$



Intrinsically universal tile set


## The one

## One tile to simulate them all



Intrinsically universal tile set


## The one

## One tile to simulate them all



Intrinsically universal tile set


## The one

Magic dust

http://nighthawk101stock.deviantart.com/

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## Acknowledgements




Erik
Demaine


Martin
Demaine


Sándor Fekete


Pierre-Etienne
Meunier


Guillaume Theyssier


Andrew Winslow
And many others

Open question: Probabilistically fair intrinsically universal tile set?


## Structure

- Monday (lecture 1). Some high-level motivations, basic algorithmic selfassembly models (definitions) and very recent results on implementing algorithmic DNA nanotube circuits, a self-assembly model, in the wet-lab
- Tuesday (lecture 2): DNA sequence design and results on the DNA nanotube circuit model
- Wednesday (lecture 3). Complexity theory for self assembly.
- Theorem: The (cooperative, temperature >= 2) abstract tile assembly model is intrinsic universal
- Thursday (lecture 4). Complexity theory for self assembly.
- Theorem: The noncooperative (temperature 1) abstract tile assembly model does not simulate the cooperative model



## Temperature 1 tile assembly

- Temperature 1 tile assembly systems:
- Tile binds to an assembly if $\geq 1$ side match
- Snakes on a plane


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## Is temperature 1 computationally weak?

Binding on 1 side seems much weaker than binding on 2 sides ... right?

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

Rothemund, Winfree. STOC 2000

- Some partial negative results:
- Temperature 1 systems that build fully connected $n \times n$ squares require at least $n^{2}$ tile types

Rothemund, Winfree. STOC 2000

- Pumpable temperature 1 systems produce periodic structures Doty, Patitz, Summers. TCS 2011
- Temperature 1 with no mismatches require $2 n-1$ tile types to assemble an $n \times n$ square Manuch, Stacho, Stoll. J Comp. Bio. 2010
- Positive results:
- 3D deterministic temperature 1 simulates Turing machines

Cook, Fu Schweller. SODA 2011

- 2D temperature 1 simulates Turing machine, but with some error

Adleman et al FOCS 2002

- 2D temperature 1 can grow large(r than tile set size) structures

Meunier. In submission. 2015

## On the blackboard: fully-connected square result

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Meunier. In submission. 2015

- But can temperature 1 aTAM systems simulate cooperative tile assembly?
- Answer: No!

On the blackboard: fully-connected square result

## Result

- Theorem 1. There is no tile set $U$, such that at temperature $1, U$ simulates all tile assembly systems.
- Theorem 2. There is a 2D temperature 2 tile assembly system $T$ that can not be simulated by any 2D, nor any 3D, temperature 1 tile assembly system.

bottom arm
(a)


Damien Woods
(c)

(b)

(d)

## Temperature 1 can not simulate temperature 2

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

bottom arm
(a)

(c)

Equal arm lengths

(b)

(d)

Unequal arm lengths

## Warm-up: two-seeded system

On the blackboard: a much easier warm-up result

## Simulation definitions

## Follows:

Definition $3.1(\mathcal{T}$ follows $\mathcal{U})$. We say that $\mathcal{T}$ follows $\mathcal{U}$ (under $R$ ) if for all $\alpha^{\prime}, \beta^{\prime} \in \mathcal{A}[\mathcal{U}]$ where $\alpha^{\prime} \rightarrow^{\mathcal{U}} \beta^{\prime}$, it is the case that $R^{*}\left(\alpha^{\prime}\right) \rightarrow^{\mathcal{T}} R^{*}\left(\beta^{\prime}\right)$, and $\alpha^{\prime} \in \mathcal{A}_{\square}[\mathcal{U}] \Longrightarrow R^{*}\left(\alpha^{\prime}\right) \in \mathcal{A}_{\square}[\mathcal{T}]$.

## Models:

Definition 3.2 (nicely fuzzy). We say that $\mathcal{U}$ is nicely fuzzy with respect to $T$ if for all $\alpha^{\prime \prime} \in \mathcal{A}[\mathcal{U}]$ there exists $\alpha^{\prime} \in \mathcal{A}[\mathcal{U}]_{\text {fuzz-free }}$ such that $\alpha^{\prime} \rightarrow^{\mathcal{U}} \alpha^{\prime \prime}$, where $R^{*}\left(\alpha^{\prime \prime}\right)=R^{*}\left(\alpha^{\prime}\right)=\alpha \in \mathcal{A}^{T}$.

Definition $3.4(\mathcal{U}$ models $\mathcal{T})$. We say that $\mathcal{U}=\left(U, \sigma_{\mathcal{U}}, \tau_{\mathcal{U}}\right)$ models $\mathcal{T}=\left(T, \sigma_{\mathcal{T}}, \tau_{\mathcal{T}}\right)$ (under $\left.R\right)$ if:
(1) $\mathcal{U}$ is nicely fuzzy with respect to $T$, and
(2) $R^{*}\left(\sigma_{\mathcal{U}}\right)=\sigma_{\mathcal{T}}$, and
(3) for all $\alpha, \beta \in \mathcal{A}[\mathcal{T}]$ such that $\alpha \rightarrow^{\mathcal{T}} \beta$ it is the case that for all $\alpha^{\prime} \in \mathcal{A}[\mathcal{U}]_{\text {fuzz-free }}$ where $R^{*}\left(\alpha^{\prime}\right)=\alpha$, there exists $\beta^{\prime} \in \mathcal{A}[\mathcal{U}]_{\text {fuzz-free }}$ such that $\alpha^{\prime} \rightarrow^{\mathcal{U}} \beta^{\prime}$ and $R^{*}\left(\beta^{\prime}\right)=\beta$.

## Simulates:

Definition 3.5. We say that $\mathcal{U}$ simulates $\mathcal{T}$ (under $R$ ) if $\mathcal{T}$ follows $\mathcal{U}$ (under $R$ ) and $\mathcal{U}$ models $\mathcal{T}$ (under $R$ ).

## Temperature 1 is not IU for the aTAM

- First we prove a simple and general pumping lemma for tile assembly at any temperature (the window movie lemma)

- We then use this pumping lemma to "fool" any claimed temperature 1 simulator into exposing its inability to simulate cooperation


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## 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 (i.e. no restrictions on the model)
- 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 behaviour in self-assembly provably does not imply the ability to simulate arbitrary algorithmic self-assembly processes. Temp 1 3D can compute, but can't handle geometry
- The proof had almost zero "temperature 1 craziness"
- Ongoing work: with Pierre-Étienne Meunier, \& by Damien Regnault and PierreÉtienne Meunier towards showing other negative results on temperature 1


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