Self-Assembly

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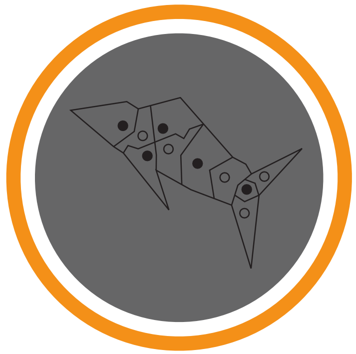

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Instructors

Dr. Navneet Bhalla has been conducting research in self-assembly for 10 years. His specialties include using evolutionary computing to design, and 3D printing to fabricate, self-assembling systems. His research interests include synthetic development; applying the principles of biological development to create evermore complex self-assembling systems. Dr. Bhalla is currently a Postdoctoral Fellow at Cornell University. He graduated with a B.Sc. in Computer Science from the University of Ottawa, an M.Sc. in Intelligent Systems from University College London, and a Ph.D. in Computer Science from the University of Calgary.

Instructors

Dr. Peter J. Bentley is an Honorary Reader at the Department of Computer Science, University College London (UCL). Peter runs the Digital Biology Interest Group at UCL. His research investigates evolutionary algorithms, computational development, artificial immune systems, swarming systems and other complex systems, applied to diverse applications including design, control, novel robotics, nanotechnology, fraud detection, mobile wireless devices, security, art and music composition. He has published over 200 scientific papers and is editor of the books "Evolutionary Design by Computers", "Creative Evolutionary Systems" and "On Growth, Form and Computers", and author of "The PhD Application Handbook" and the popular science books "Digital Biology", "The Book of Numbers", "The Undercover Scientist" and "Digitized."

Instructors

Prof. Marco Dorigo is the inventor of the ant colony optimization metaheuristic. His research interests include swarm intelligence, swarm robotics, and metaheuristics for discrete optimization. He is the Editor-in-Chief of Springer's journal "Swarm Intelligence". He is a Fellow of the IEEE and of the ECCAI, and was awarded the Marie Curie Excellence Award in 2003, the Dr. A. De Leeuw-Damry-Bourlart award in applied sciences in 2005, the Cajastur "Mamdami" International Prize for Soft Computing in 2007, and an ERC Advanced Grant in 2010.

Prof. Marco Dorigo received his PhD in electronic engineering in 1992 from Politecnico di Milano, Milan, Italy. From 1992 to 1993, he was a research fellow at the International Computer Science Institute, Berkeley, CA. In 1993, he was a NATO-CNR Fellow, and from 1994 to 1996, a Marie Curie Fellow. Since 1996, he has been a tenured researcher of the FNRS, the Belgian National Funds for Scientific Research, and a research director of IRIDIA, the artificial intelligence lab of the Université Libre de Bruxelles.

Agenda

- Introduction
- A Self-Reproducing Analogue
- DNA Nanotechnology and DNA Computing
- 3D Printed Self-Assembling Tiles
- Self-Assembling Robots
- Evolutionary Self-Assembly
- Staged Self-Assembly
- Conclusions

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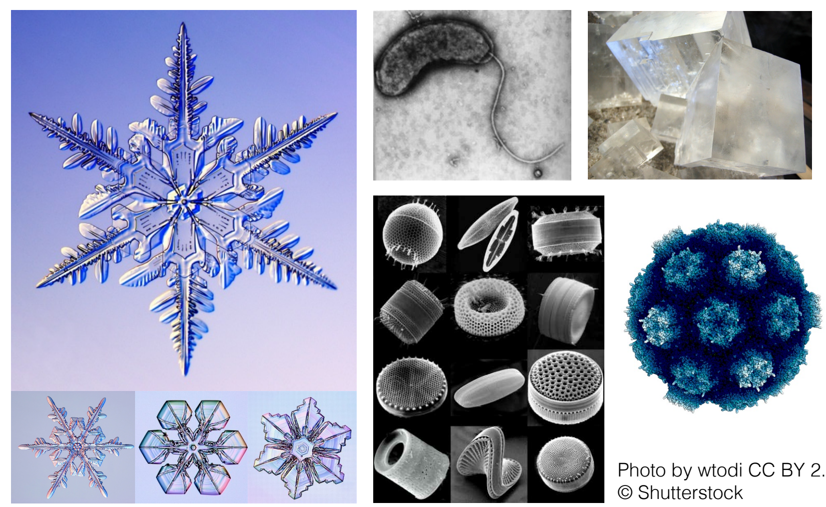
Self-Assembly

How do you design something that builds itself?

Self-Assembly in Nature



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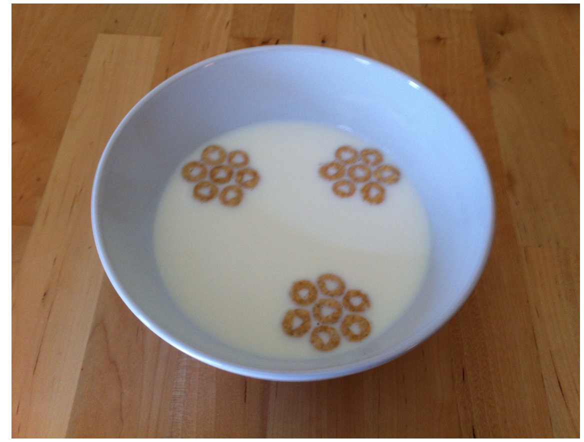
Motivation

- Self-assembly is considered to be a vital part to understanding the architecture of life [19]
- Self-assembly is viewed as an enabling technology for the creation of artificial systems [22]
- Engineering new technologies with natural characteristics, such as parallel construction, self-repair, reconfiguration, adaptability, and self-replication [16]

The "Cheerios Effect"



[27]

What is Self-Assembly?

- Origins in organic chemistry
- Self-assembly is not a formalized subject
- Self-assembly: autonomous "processes that involve pre-existing components (separate or distinct parts of a disordered structure), are reversible, and can be controlled by proper design of the components" [28]

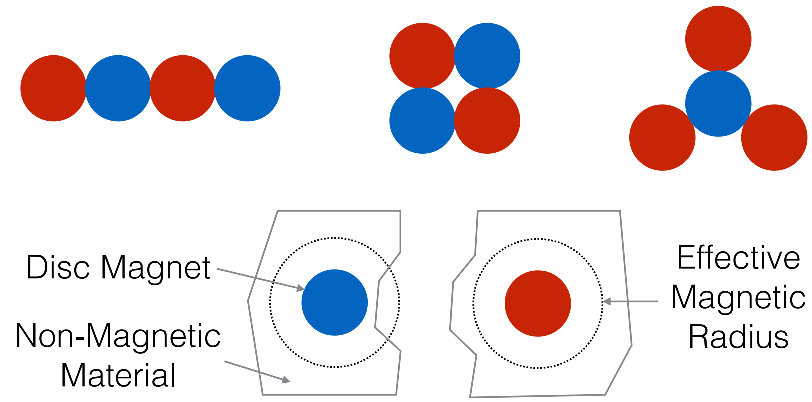
Types of Self-Assembly

- Static self-assembly: processes that lead to structures or patterns in local or global equilibrium and do not dissipate energy [28]
- Dynamic self-assembly: processes that lead to structures or patterns that can only occur while the system is dissipating energy [28]
- Further subcategories of self-assembly include: templated, biological, netted systems, hierarchical, algorithmic, and software [4]

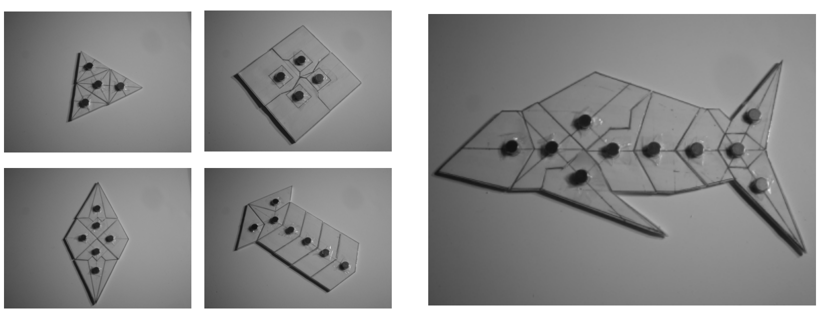
Designing Self-Assembling Systems

- Where do you start?
- How can you get two objects to assemble autonomously together?
- Could you extend your technique to multiple objects and create a variety of structures?

Example Using Magnets



Example Using Magnets



[3, 5, 20]

Forwards and Backwards Problems

- Forwards Problem: given a set of components, which self-assembled structures will result? [22]
- Backwards Problem: given a desired self-assembled target structure,what is the required set of components? [22]
- Other problems: yield, duration, scale, complexity, hierarchy of assembly methods…

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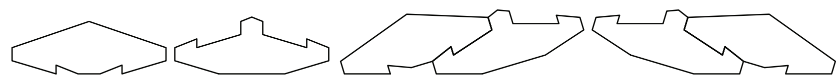
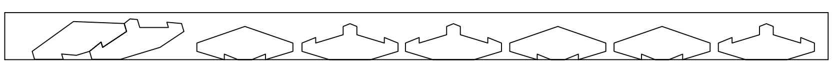
System Overview

- In 1957, L.S. Penrose and R. Penrose created the first artificial, mechanical, self-assembling systems [23]
- Their system could replicate a seed complex, simply by horizontally shaking a track

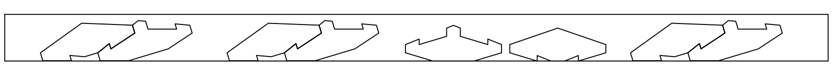


α β αβ complex βα complex

Example Scenario

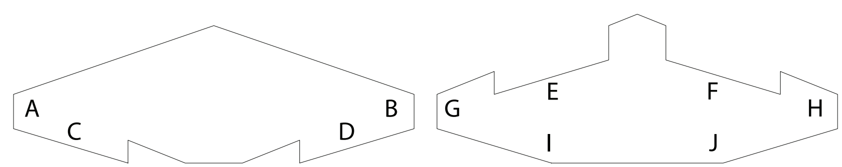


Initial Configuration

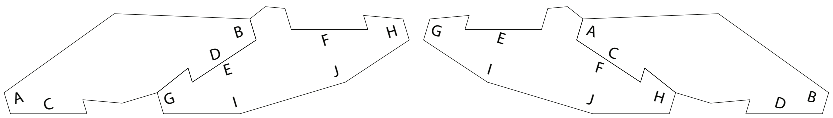


Final Configuration

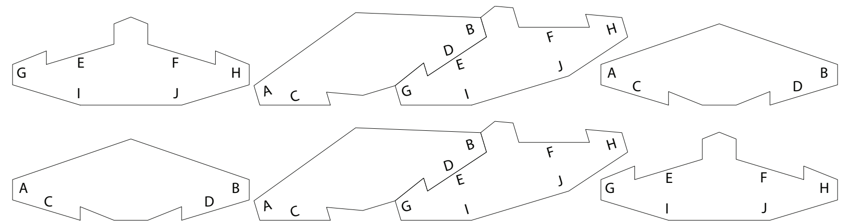
Physically Encoded Information



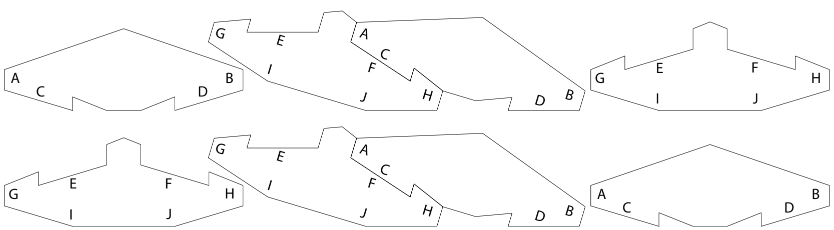
Assembly Rules



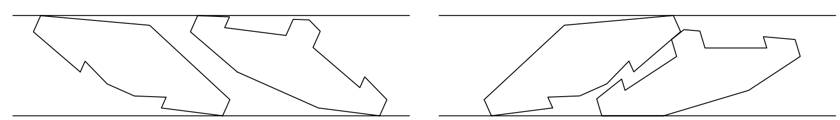
Rotation Rules



Rotation Rules



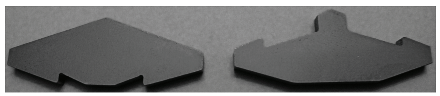
Environment Rules



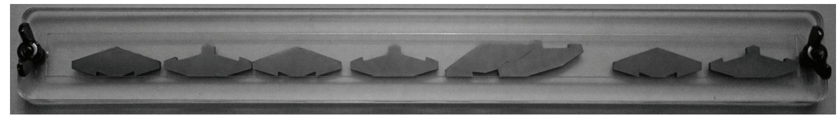
Autocatalysis Rules

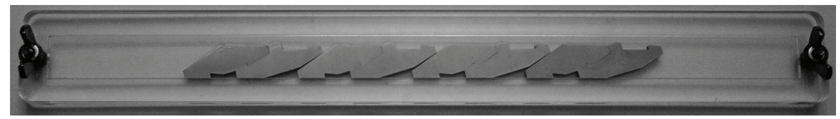
αβ autocatalysis $\alpha+\beta \rightarrow \alpha\beta; \alpha\beta$

βα autocatalysis $\beta+\alpha \rightarrow \beta\alpha; \beta\alpha$



Reversed Engineered Replica





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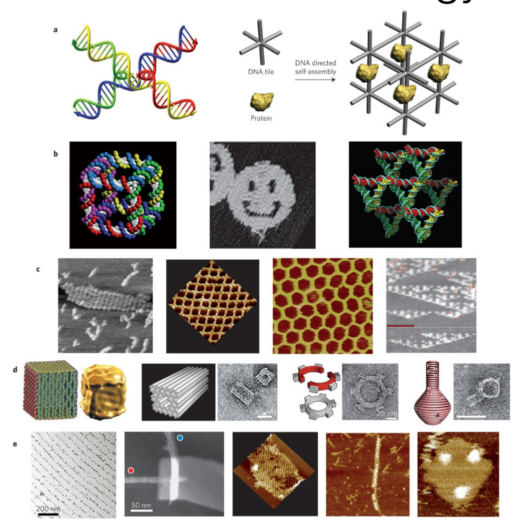
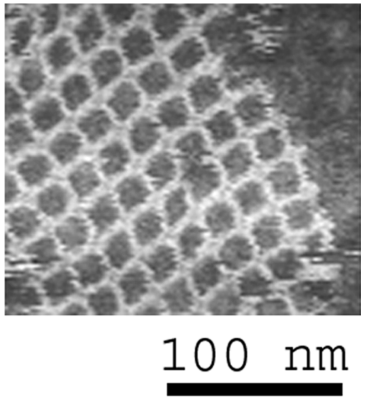
DNA Nanotechnology



[24]

DNA Computing



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abstract Tile Assembly Model (aTAM)

- A mathematical model, connecting computation with pseudo-crystalline growth [25]
- DNA tiles [29]
- Seed tile, environment temperature, co-operative binding

Extensions to the aTAM

- Tile Hard-coding Programming
- Staged Programming
- Tile Concentration Programming
- Temperature Programming

[14]

NP-Complete

- The aTAM has been used to investigate the complexity of self-assembly
- The problem of determining if a set of tiles self-assemble into a target structure is an NP-complete decision problem [1]
- The aTAM and its extensions have been used to investigate the algorithmic complexity of self-assembling a variety of target structure [15]

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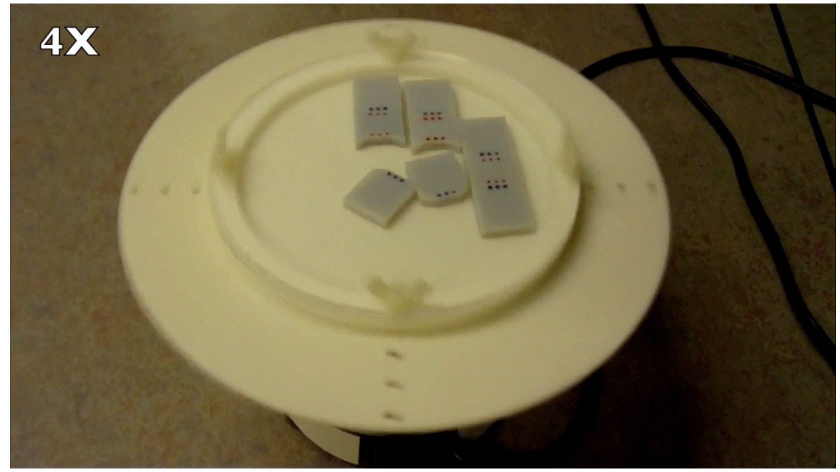
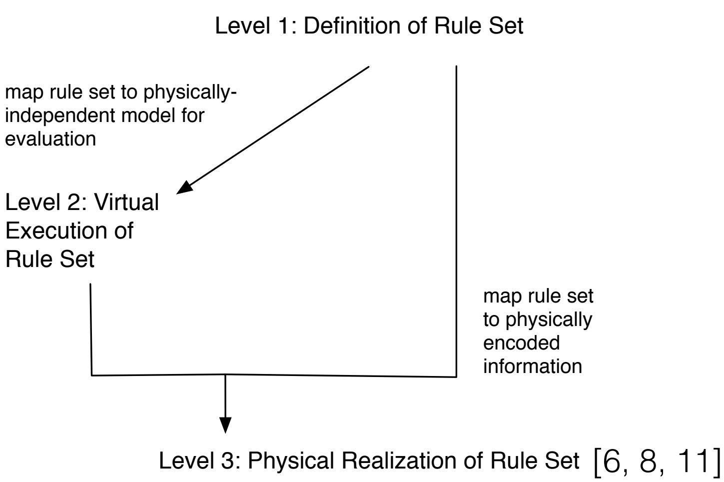
Video



Three-Level Approach



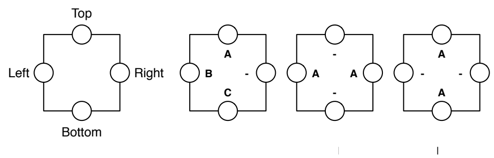
[6, 8, 11]

Level 1: Definition of Rule Set

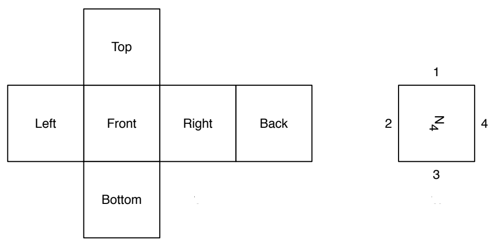
- Component Rules: specify the arrangement of component information
- Environment Rules: specify temperature and boundary constraints
- System Rules: specify the frequency of component types, and component-component and component-environment interactions

Level 1: Definition of Rule Set

2D Component



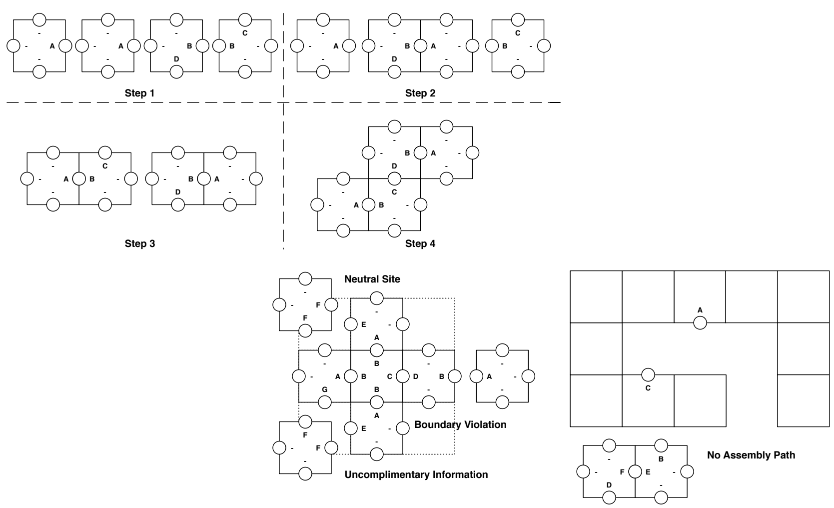
3D Component



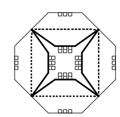
Level 2: Virtual Execution of Rule Set

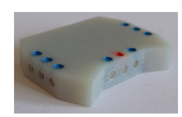
	Tiling Models	
Model Features	cTAM	aTAM
Seed Components	not required	required
Parallel Self-Assembly	yes	no
Number of Tile	multiple	one
2D/3D	2DcTAM/3DcTAM	2D
Rotations	2D/3D	no
One-Pot-Mixture	yes	yes
Error Checking	yes	no

Level 2: Virtual Execution of Rule Set

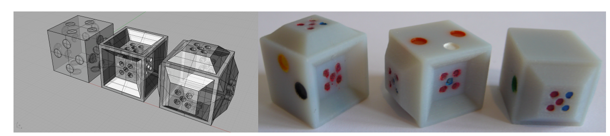


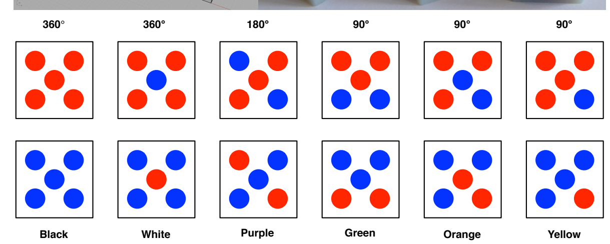
Level 3: Physical Realization of Rule Set





Locks	000	110	011	101
Keys	111	001	100	010





Physical Encoding Scheme

- Place 1 permanent magnetic disc in each bit location in a key
- Place 2 permanent magnetic discs in each bit location in a lock
- Strong key-lock binding, and weak key-key binding (break using environment temperature)
- Assign magnetic-bit patterns to keys and locks to prevent or reduce mismatch errors

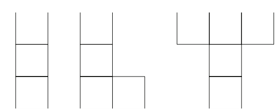
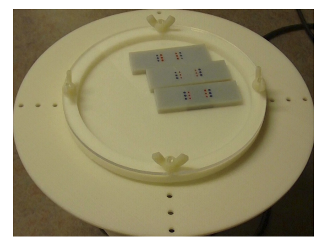
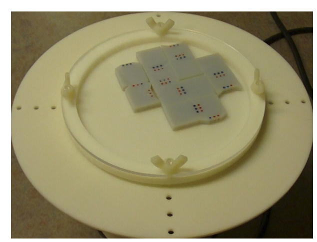
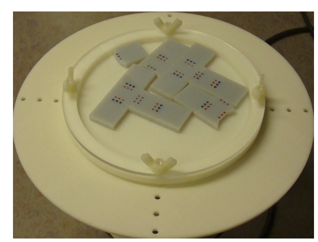
2D System Rules

Key/Lock	3-Bit	Label	Fits Rule	Breaks Rule
Lock	000	A	A fits B → A+B	ɸ
Lock	110	C	C fits D → C+D	ɸ
Lock	011	E	E fits F → E+F	ɸ
Lock	101	G	G fits H → G+H	ɸ
Key	111	B	B fits A → B+A	ɸ
Key	001	D	D fits C → D+C	ɸ
Key	100	F	F fits E → F+E	ɸ
Key	010	H	H fits G → H+G	ɸ

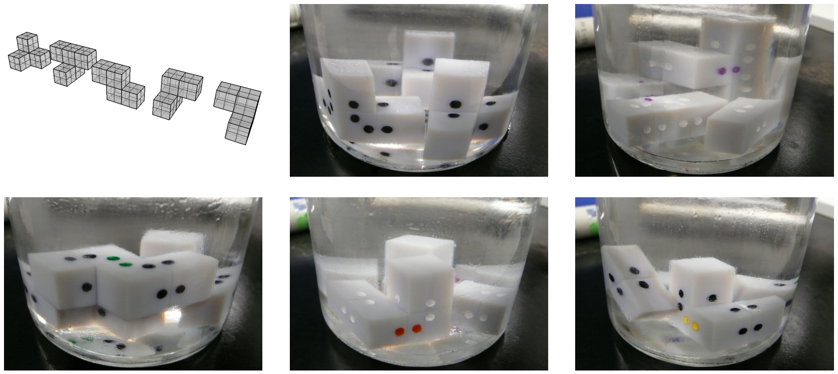
3D System Rules

Key/Lock	5-Bit	Label	Fits Rule	Breaks Rule
Lock	00000	I	I fits J → I+J	ɸ
Lock	10000	K	K fits L → K+L	ɸ
Lock	01010	M	M fits N → M+N	ɸ
Lock	10011	P	P fits O → P+O	ɸ
Lock	00111	R	R fits Q → R+Q	ɸ
Lock	10111	T	T fits S → T+S	ɸ
Key	11111	J	J fits I → J+I	ɸ
Key	01111	L	L fits K → L+K	ɸ
Key	10101	N	N fits M → N+M	ɸ
Key	01100	O	O fits P → O+P	ɸ
Key	11000	Q	Q fits R → Q+R	ɸ
Key	01111	S	S fits T → S+T	ɸ

2D Systems

3D Systems



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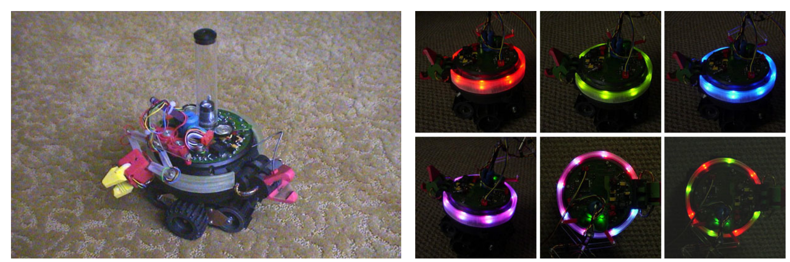
System Categories

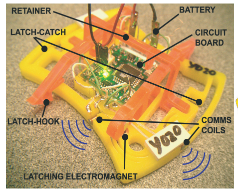
- Self-propelled
- Externally propelled:
  - Component directed
  - Environment directed

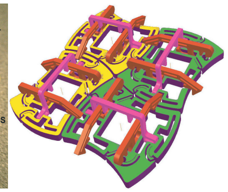
[18]

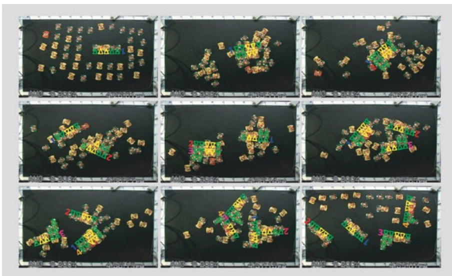
Self-Propelled



Component Directed

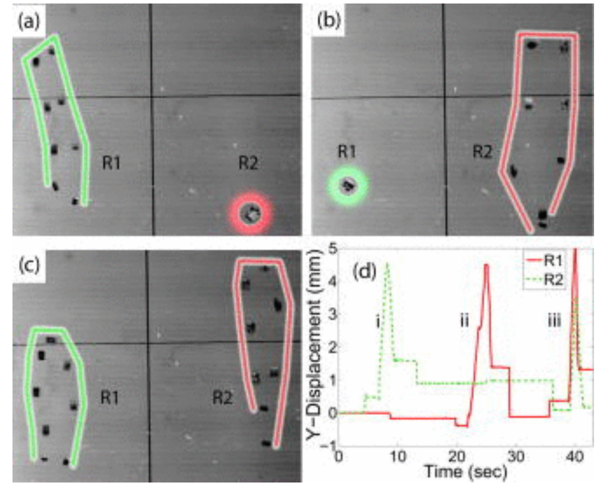






[17]

Environment Directed



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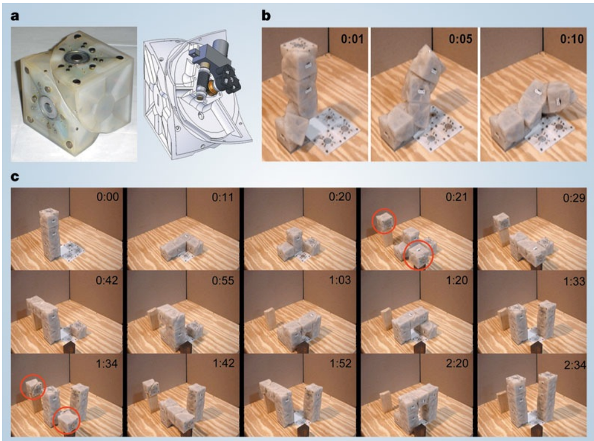
Evolving Self-Assembling Systems

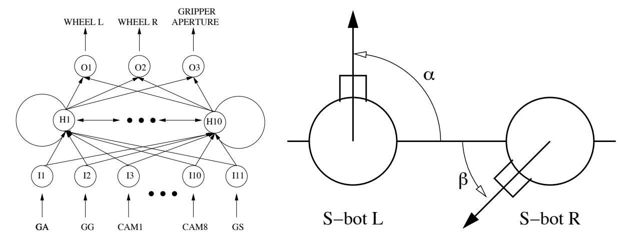
- Hierarchical processes
- Self-assembly protocols
- Component and environment information (forwards problem)
- Specific component sets (backwards problem)

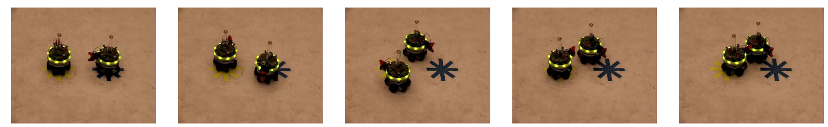
Evolving Self-Replication



[30, 31]

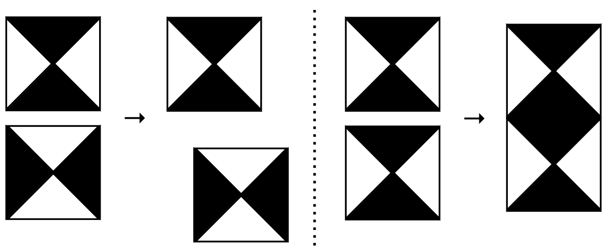
Evolving a Self-Assembly Protocol

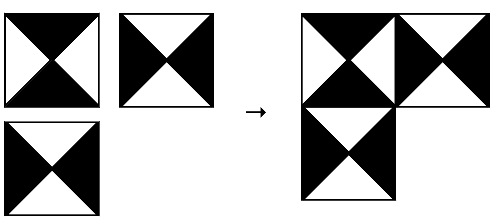




[2]

Evolving Virtual Tiles

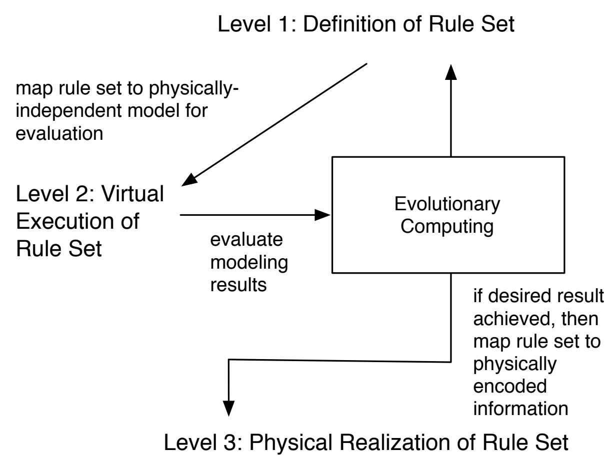




ϕ	W	B
W	2	3
B	3	6

[26]

Evolving Physical Tile Sets



[9, 11]

Evolving Physical Tile Sets

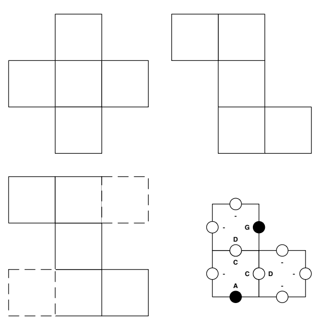
- Evolutionary unit is a single component
- Genotype is a variable-length list of components
- Phenotype is the resulting structure(s) from a set of components
- One genotype can have many phenotypes

Evolving Physical Tile Sets

- Generational genetic algorithm with elitism
- Roulette-wheel selection
- Variable-length crossover
- Duplication, deletion, and mutation
- Multi-objective fitness evaluation

Evolving Physical Tile Sets

	2D	3D
General Fitness	area perimeter Euler z-axis matches	volume surface area mean breadth Euler z-axis matches
Refined Fitness	locations error	locations error

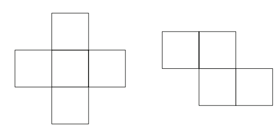


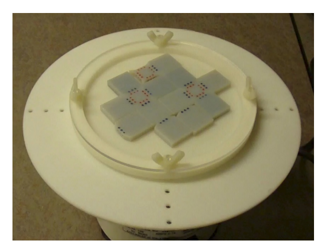
$$F2D = \left(0.18\sum_{i=1}^{5}|TOi - ANOi|\right) + 0.05(ANO6 + NO7)$$

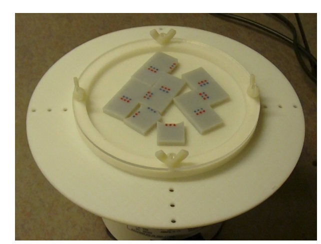
$$F3D = \left(0.15\sum_{i=1}^{6}|TOi - ANOi|\right) + 0.05(ANO7 + NO8)$$

	B (1,1,1)	D (0,0,1)	F (1,0,0)	H (0,1,0)
B (1,1,1)	0			
D (0,0,1)	5	2		
F (1,0,0)	5	4	2	
H (0,1,0)	4	3	3	4

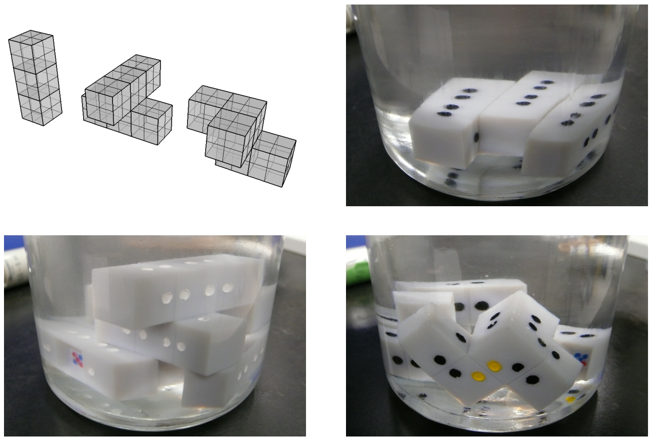
Evolving Physical Tile Sets







Evolving Physical Tile Sets



Agenda

- Introduction
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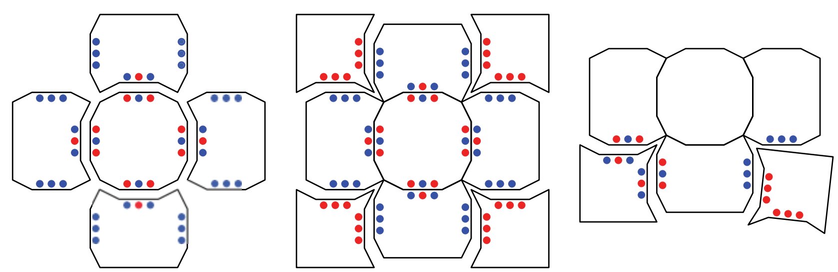
Leveraging Time

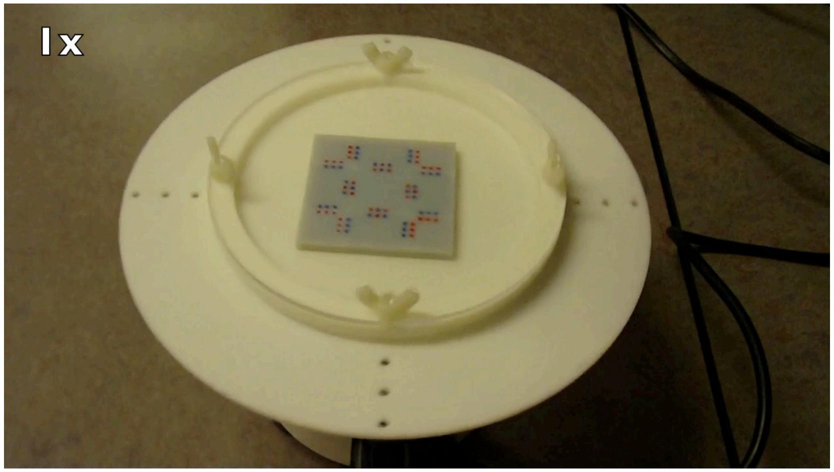
- Using components that cannot differentiate results in self-assembly being constrained to a limited set of components and their binding mechanisms
- Staging addresses this challenge by dividing the self-assembly process into time intervals, and encodes the construction of a target structure into the staging algorithm itself, and not exclusively into the design of the components [13]

Morphology and Error Prevention

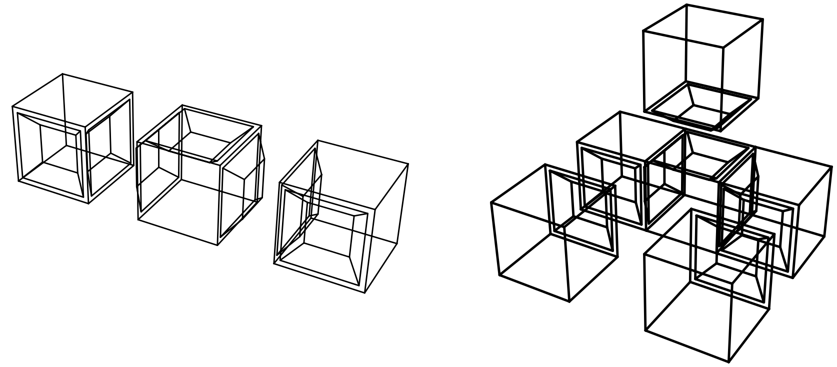


[10, 12]

2D Staged Self-Assembly

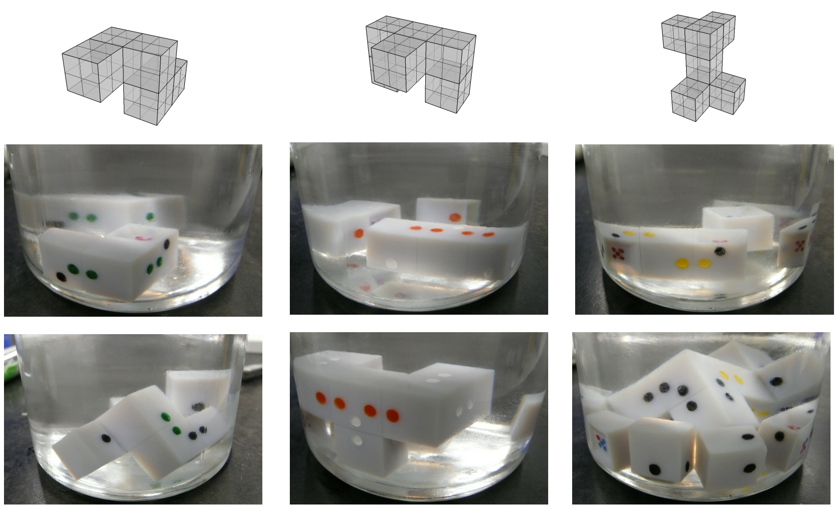


Synthetic Development



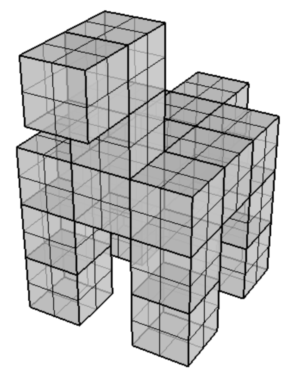
ψ_0 ψ_1

3D Staged Self-Assembly



Synthetic Development

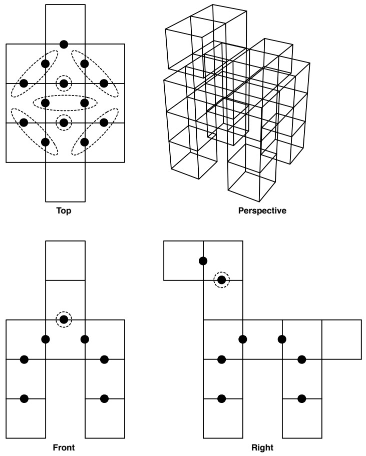
- Synthetic Development: applying the principles of evolution and biological development to the design and construction of self-assembling systems [7]



[12]

Synthetic Development

- 6 pairs of 90° degree rotational codes is required
- Only 3 pairs of 90° degree rotational codes in the 5-magnetic-bit physical encoding scheme

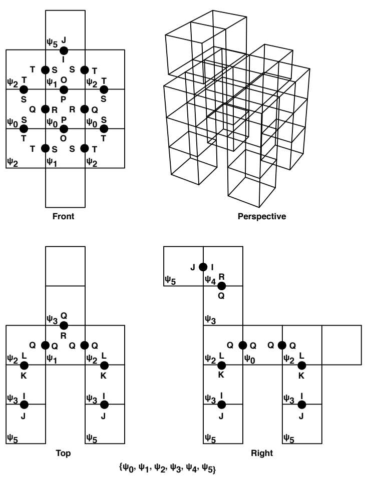


3D System Rules

Key/Lock	5-Bit	Label	Fits Rule	Breaks Rule
Lock	00000	I	I fits J → I+J	ϕ
Lock	01111	L	L fits K → L+K	ϕ
Lock	01010	M	M fits N → M+N	ϕ
Lock	01100	O	O fits P → O+P	ϕ
Lock	11000	Q	Q fits R → Q+R	ϕ
Lock	01111	S	S fits T → S+T	ϕ
Key	11111	J	J fits I → J+I	ϕ
Key	10000	K	K fits L → K+L	ϕ
Key	10101	N	N fits M → N+M	ϕ
Key	10011	P	P fits O → P+O	ϕ
Key	00111	R	R fits Q → R+Q	ϕ
Key	10111	T	T fits S → T+S	ϕ

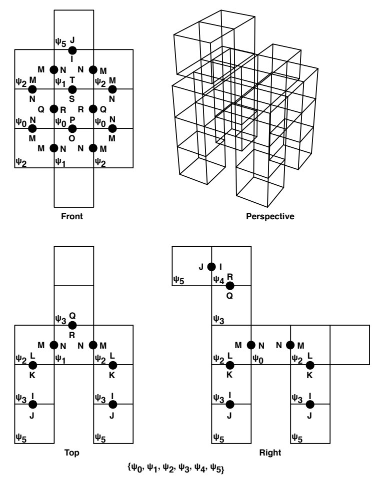
Synthetic Development

- Reintroduce component information used in a previous time interval
- Time intervals and component information to create a single target structure



Synthetic Development

- To create multiple target structures, use the morphology of the substructures to emulate a 90° rotational information



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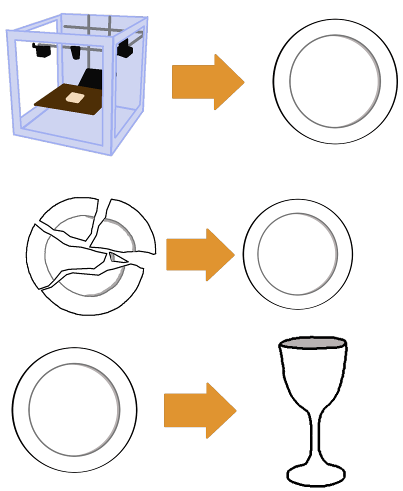
Conclusions

- Research in self-assembling systems is continuing to expand, within multiple disciplines
- One subfield that is still in its infancy is optimizing self-assembling systems, particularly applying evolutionary computation
- An area we believe to have tremendous promise is synthetic development

The Vision



Hybrid 3D printing and self-assembly to fabricate biomimetic products

Biomimetic products that self-repair

Biomimetic products that self-reconfigure

Acknowledgements

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