Artificial Life & Complex Systems

Lecture 13

Self-Assembly

June 8, 2007

Max Lungarella

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- What is self-assembly?
- Self-assembly in nature
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- Protocells and PACE
- Modular self-reconfigurable robots

What is Self-Assembly?

Self-assembly: no precise general definition

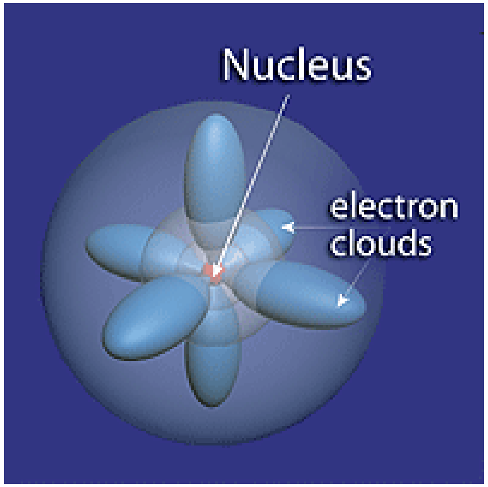
But roughly speaking:

- "process by which an organized structure can <u>spontaneously</u> form from simpler parts"
- "process in which components, either separate, or linked, <u>spontaneously</u> form ordered aggregates" *(G.M.Whitesides, PNAS, Vol.99, no.8, 2002)*

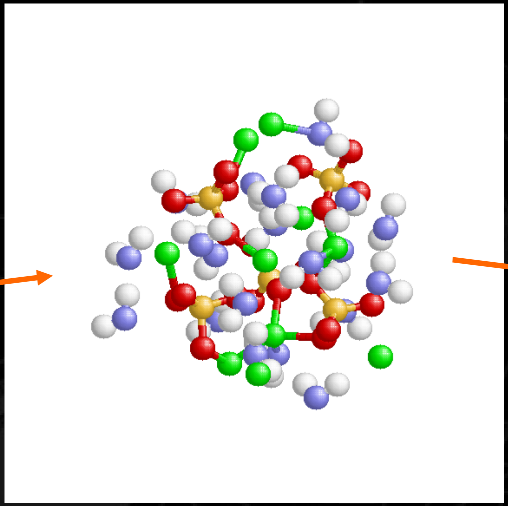
Most relevant research issues:

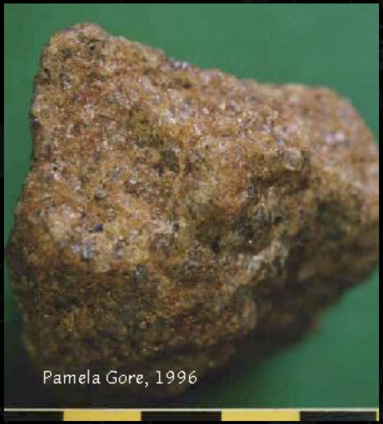
- Programming
- Complexity
- Fault-tolerance
- Self-healing
- Self-reproduction
- Evolution

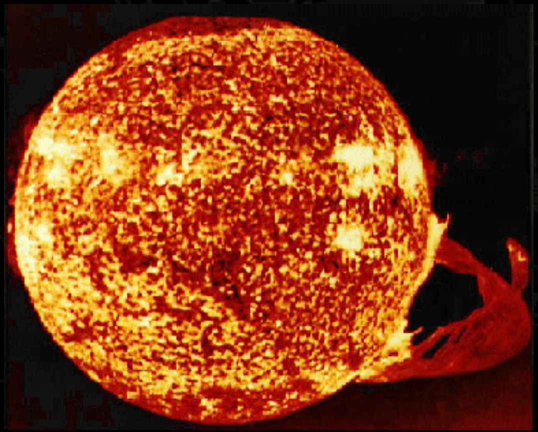
Self-Assembly in Nature (Uncoded)



Graphic Illustration by Sergio Salinas

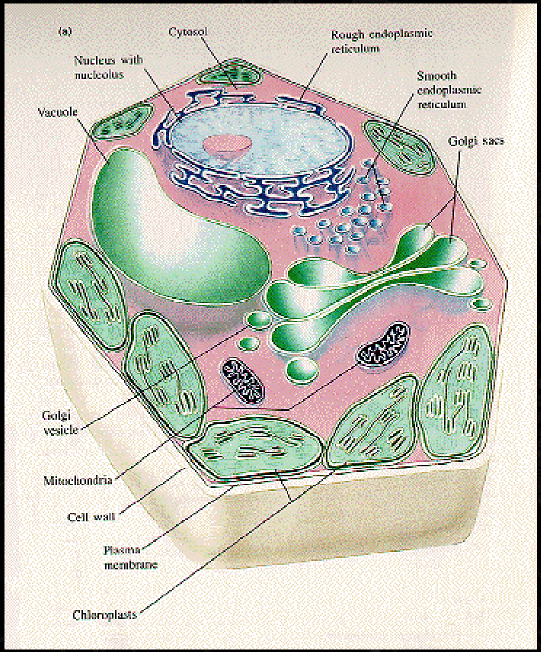




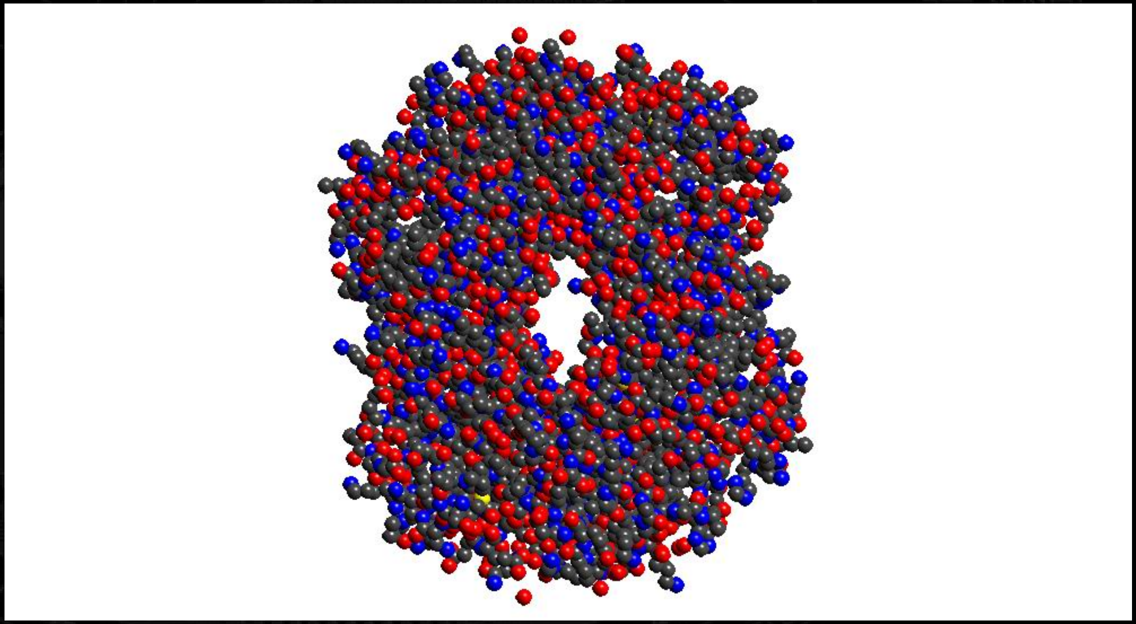


Self-Assembly in Nature (Coded)

Other structures that were self-assembled

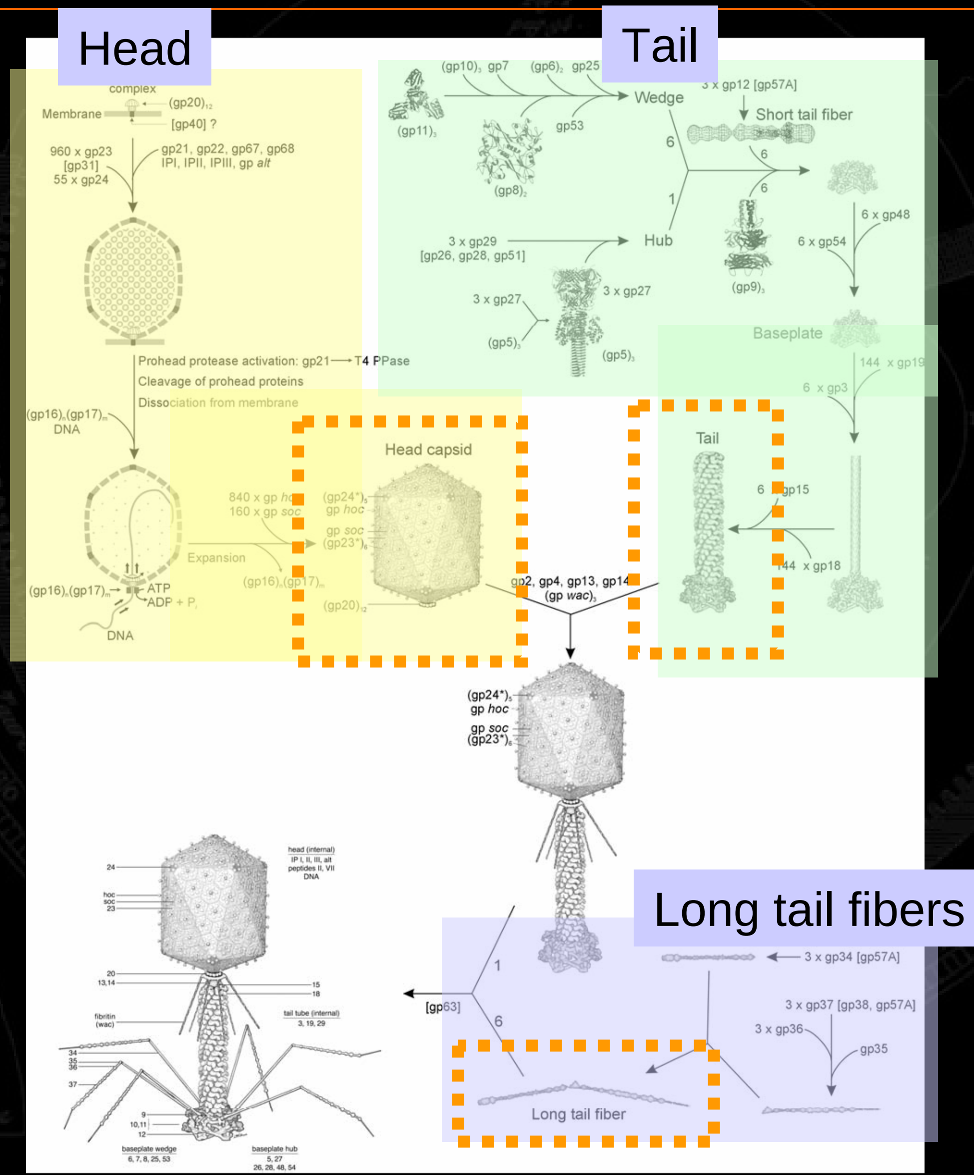


Plant Cell



Hemoglobin

Self-Assembly in Nature: Bacteriophage



Other Examples

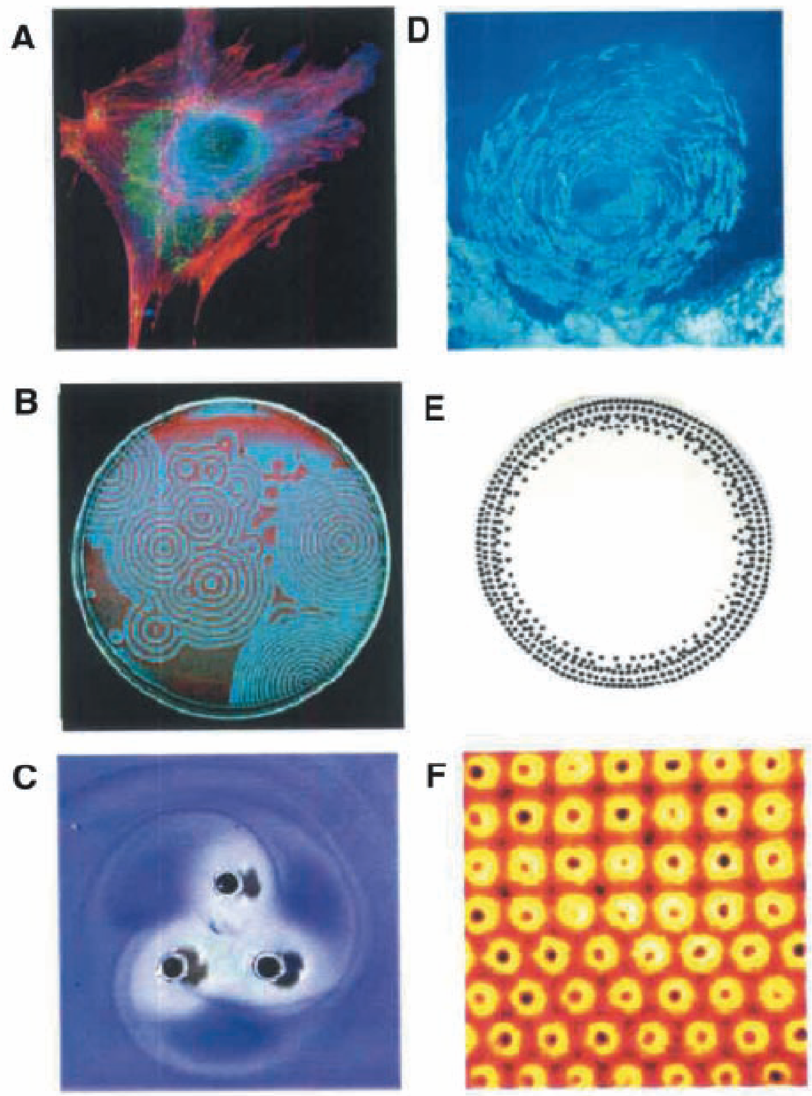


Fig. 2. Examples of dynamic self-assembly. (A) An optical micrograph of a cell with fluorescently labeled cytoskeleton and nucleus; microtubules (~24 nm in diameter) are colored red. (B) Reaction-diffusion waves in a Belousov-Zabatinski reaction in a 3.5-inch Petri dish. (C) A simple aggregate of three millimeter-sized, rotating, magnetized disks interacting with one another via vortex-vortex interactions. (D) A school of fish. (E) Concentric rings formed by charged metallic beads 1 mm in diameter rolling in circular paths on a dielectric support. (F) Convection cells formed above a micropatterned metallic support. The distance between the centers of the cells is ~2 mm. [Image credits: (A) from (*30*); (B) from (*26*); (C) from (*31*)]

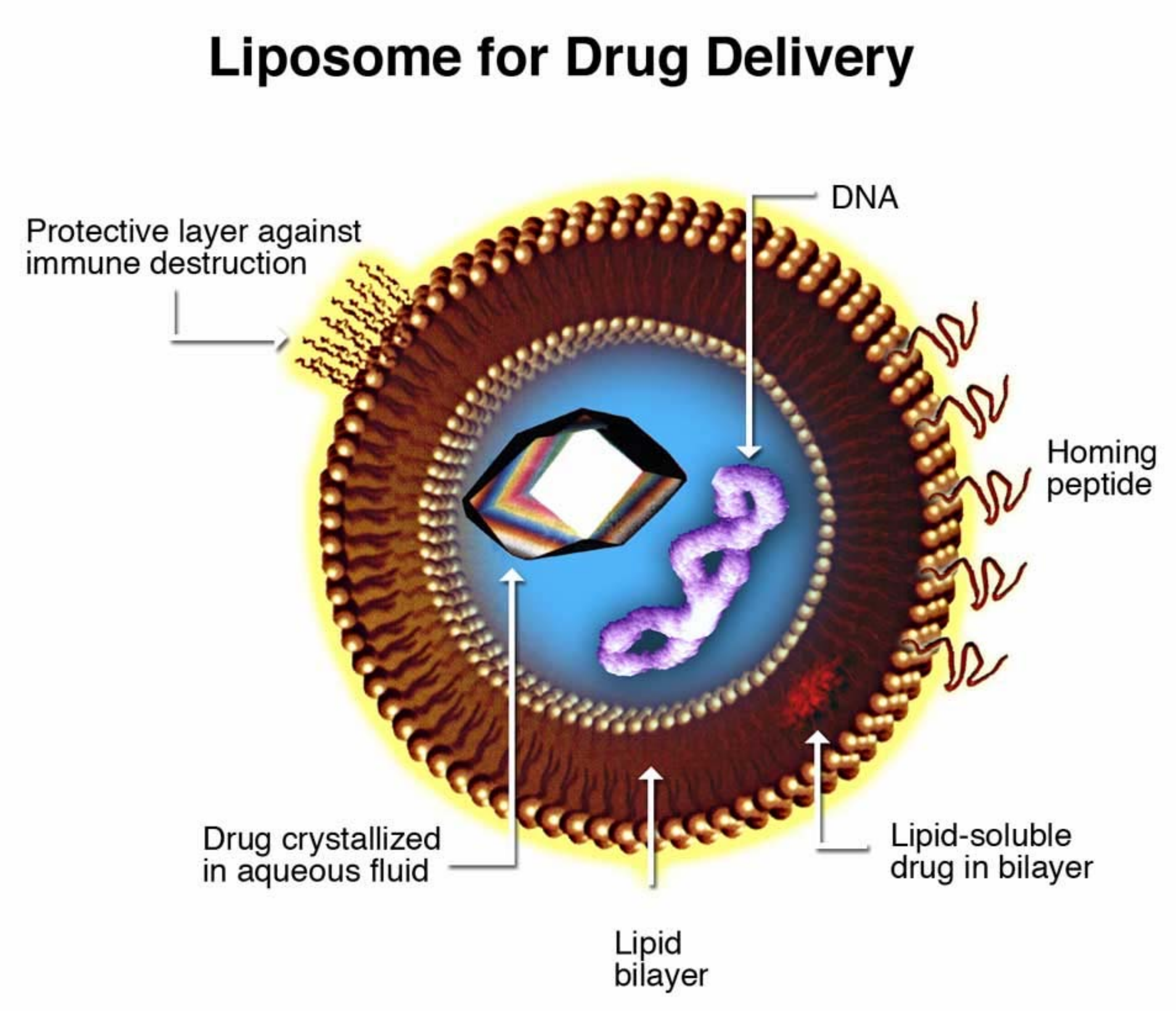
Whitesides and Grzybowski, 2002

Self-Assembly – Why Studying It?

- Self-assembly is about (spontaneous) transition of disorder to order
- Living cells self-assemble: understanding life will therefore require understanding self-assembly
- Self-assembly is one of the few practical strategies for making ensembles of nanostructures
- Manufacturing and robotics will benefit from self-assembly
- Self-assembly is common to many dynamic, multicomponent systems, from smart materials and self-healing structures to netted sensors and computer networks

Whitesides and Grzybowski, 2002

Self-Assembly: Early Success



More Recent Successes

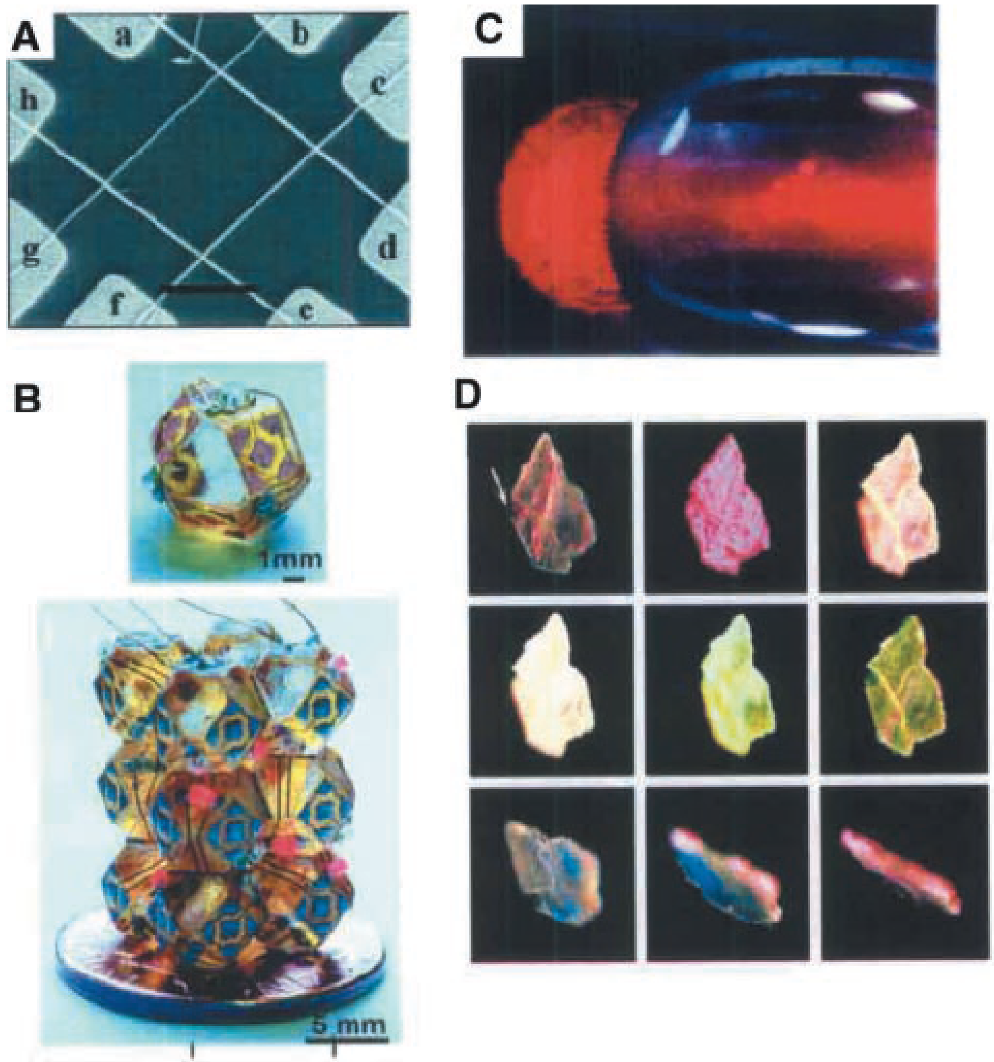


Fig. 3. Applications of self-assembly. **(A)** A 2 by 2 cross array made by sequential assembly of *n*-type InP nanowires with orthogonal flows. **(B)** Diffraction grating formed on the surface of a poly(dimethylsiloxane) sphere ~1 mm in diameter. The sphere was compressed between two glass slides, and its free surface was exposed to oxygen plasma. Upon release of compression, the oxidized surface of the polymer buckled with a uniform wavelength of ~20 μm. **(C)** Three-dimensional electronic circuits self-assembled from millimeter-sized polyhedra with electronic components (LEDs) embossed on their faces. **(D)** An artificial, ferromagnetic opal prepared by templated self-assembly of polymeric microbeads. The optical properties of the aggregate can be adjusted by modifying external magnetic field.

Whitesides and Grzybowski, 2002

Why Self-Assembly? Examples

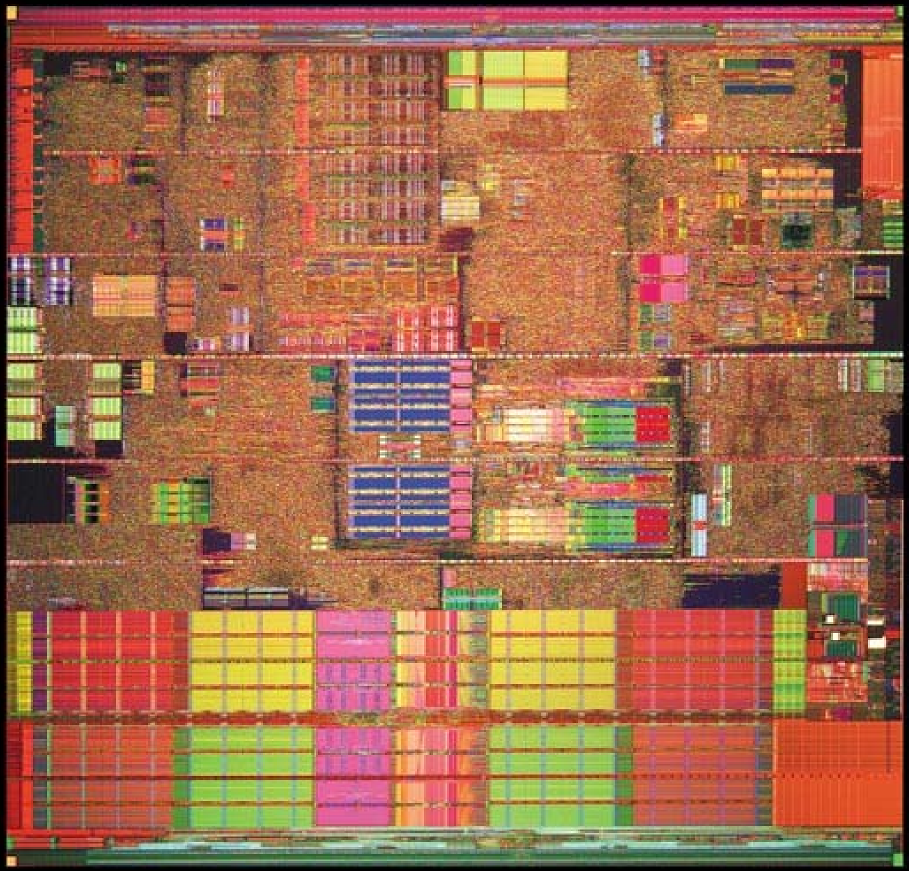
Movies:

Lego-car

Plane!

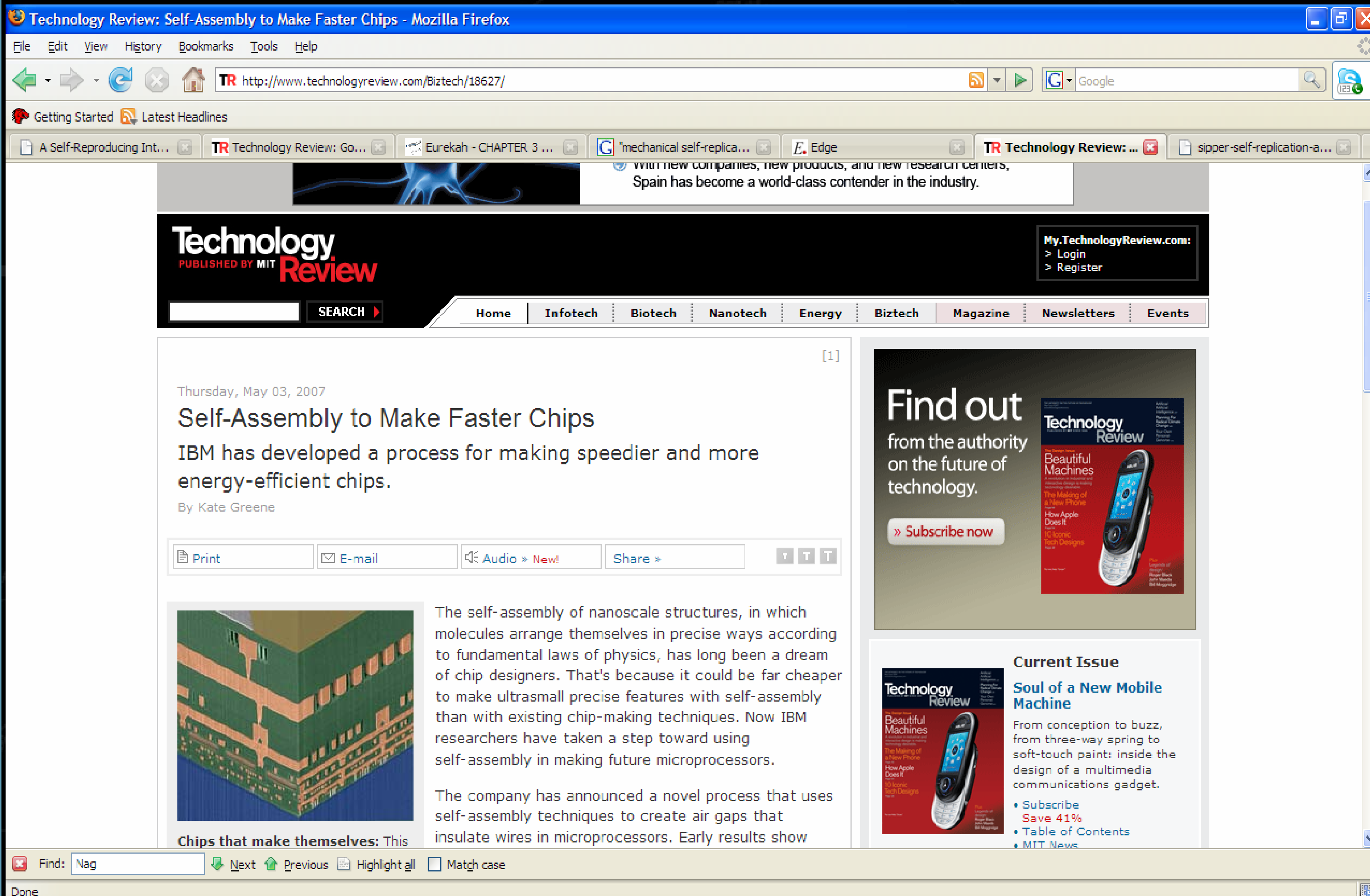
Why Self-Assembly?

Can this structure be made using self assembly?



Intel P4 (Prescott) CPU Die

Application



Features

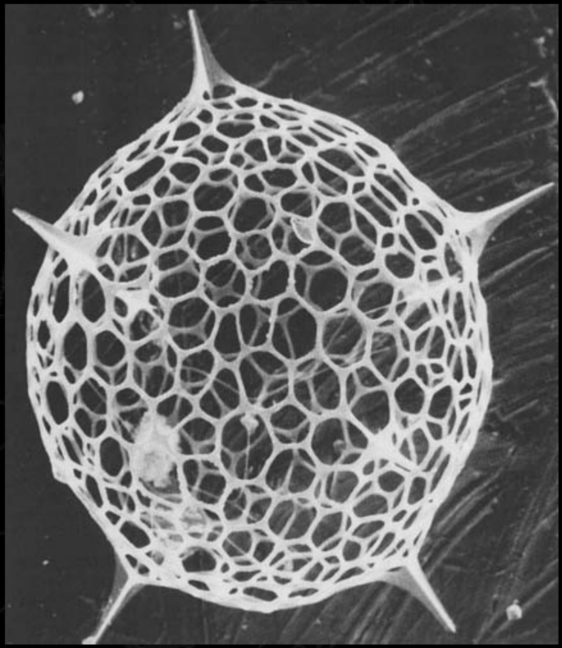
- Complex structure emerges from local interaction of (typically) independent entities without central control
- Interactions are typically random
- SA plays important role not only in origin of living systems but also their operation
- SA can be employed as a strategy to build nano-scale structures, such as thin films or molecular wires, or to solve computational problems

Self-Assembly

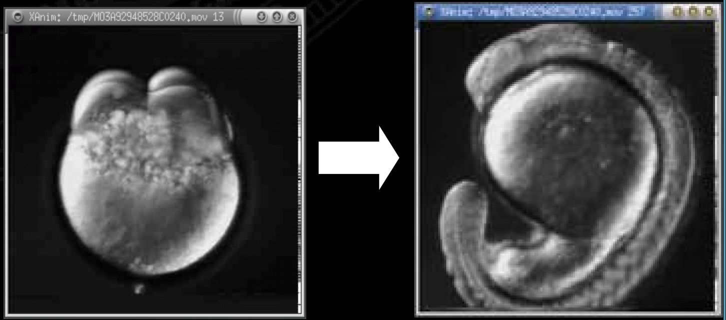
There is "prior art", SA is already present in nature

- Inside cells
- Generation of biochemical complexity
- Robust self-assembly of organisms over 18 orders of magnitude in volume (self-assembly at all scales!)

Non-trivial 3D self assembly



IL 33. Radiolara



Self-Assembly in Nature

T4 phage Movie

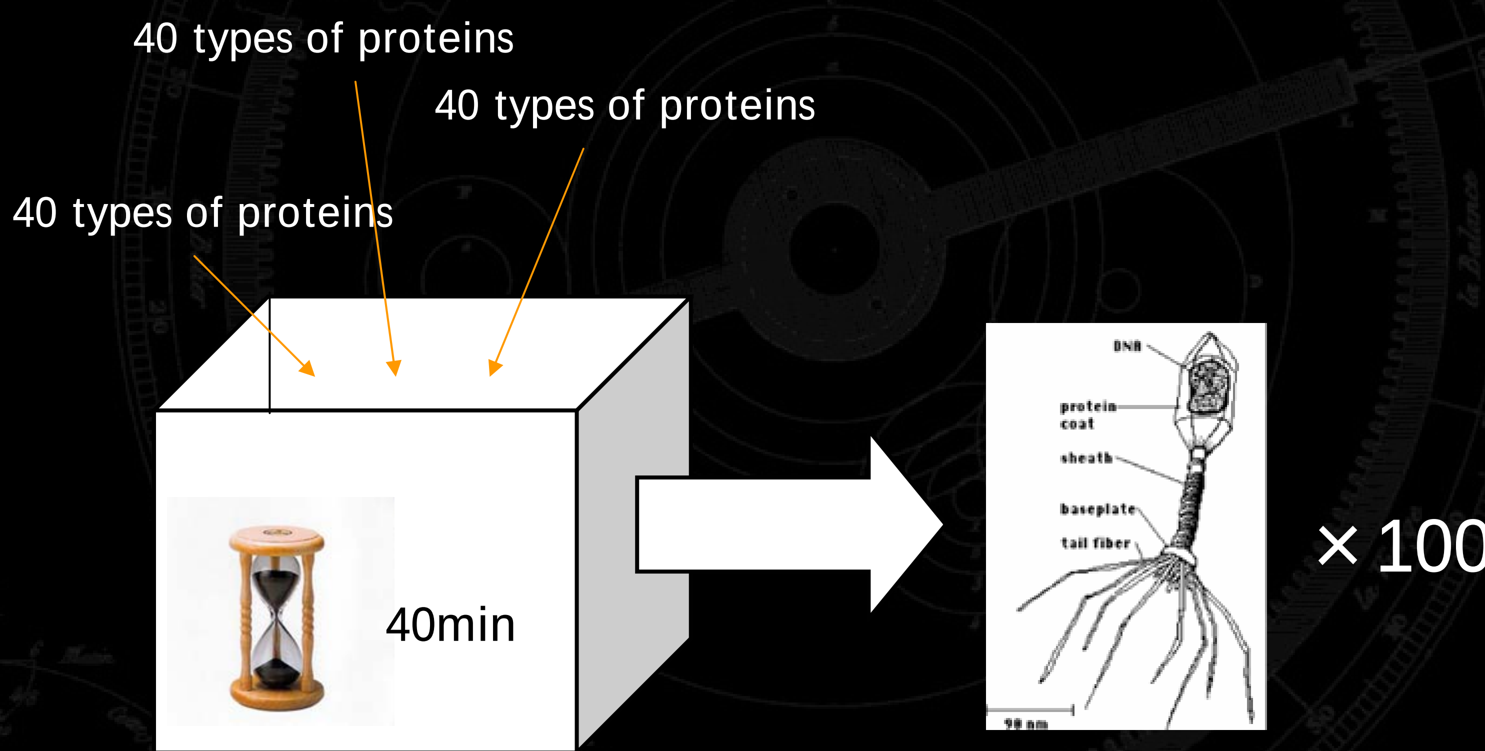
W. Scott Meadors

S. Lee Gooding

James A. Bartek

http://www.seyet.com/

Shaken Not Stirred ...



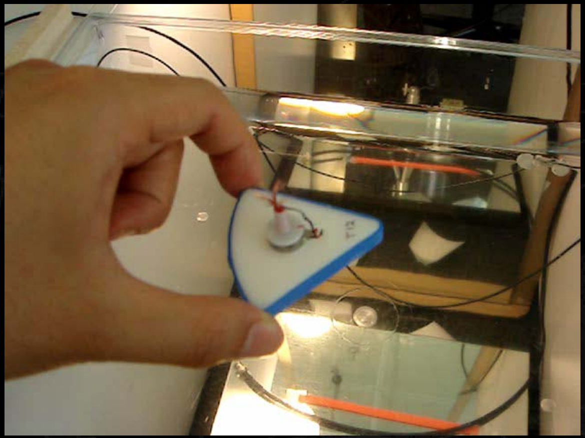
"shaking the box" of appropriate basic elements
can be sufficient for robust and efficient self-assembly

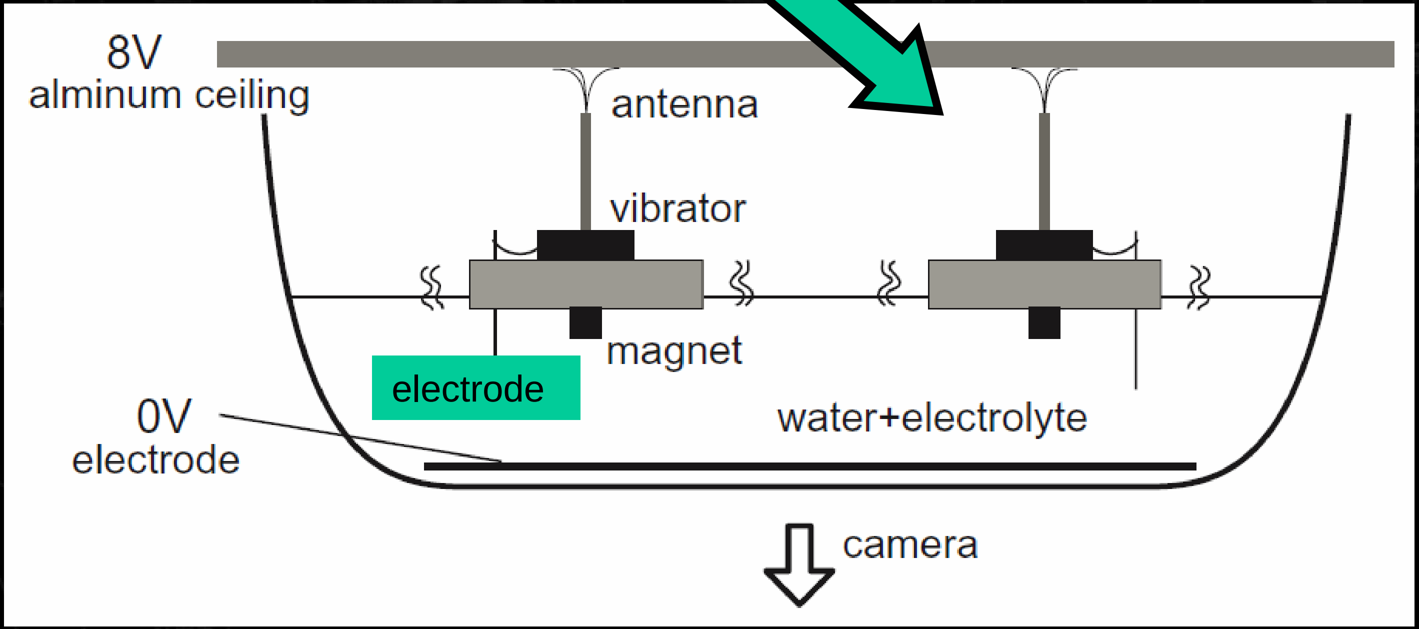
Self-Assembly

Bottom-up fabrication of complex structures:

- Arbitrary shapes can be self-assembled (2D)
- Enabled by DNA nanotechnology
- Meso-scale modeling

Tribolon: Directed Self-Assembly

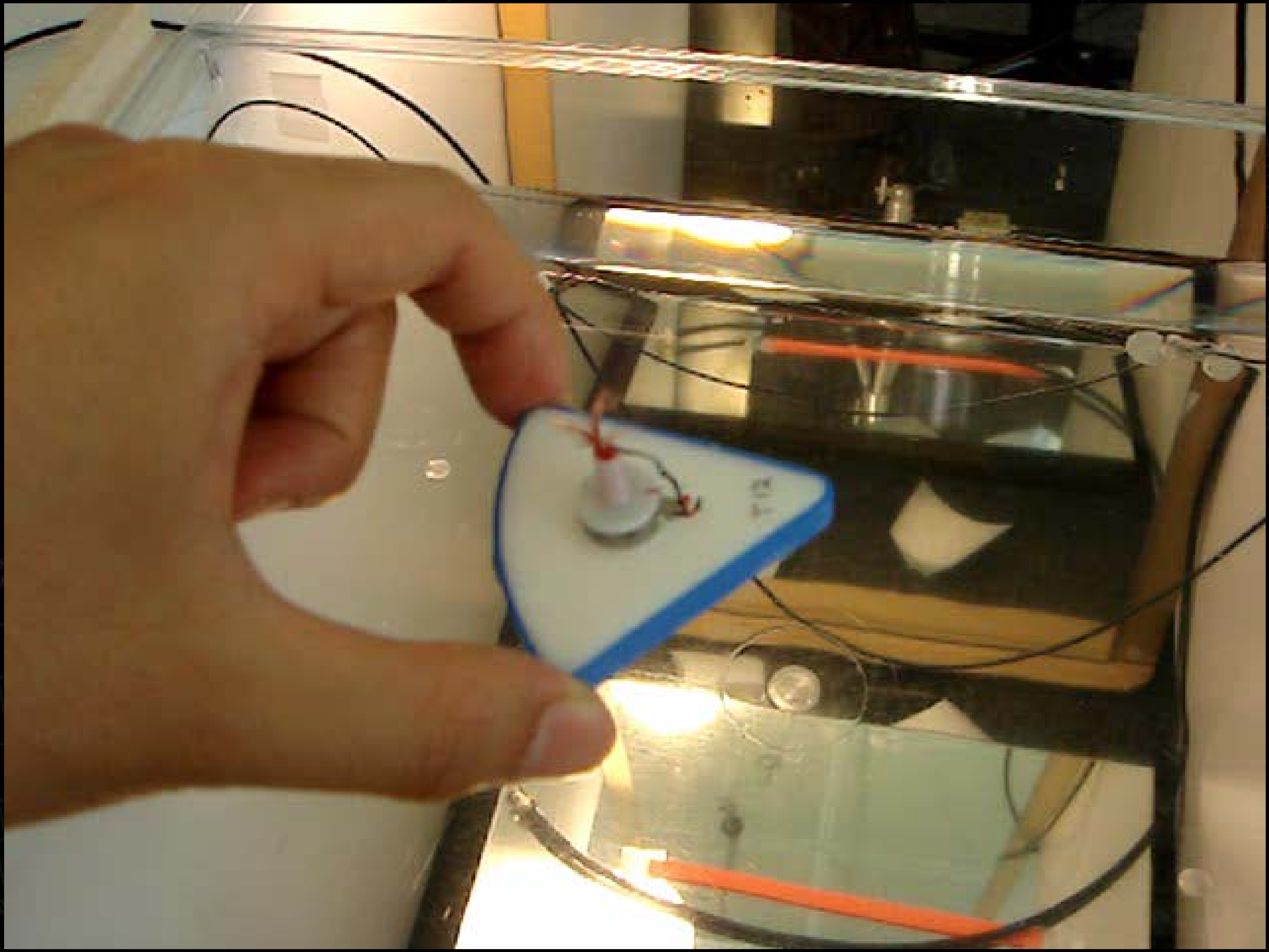




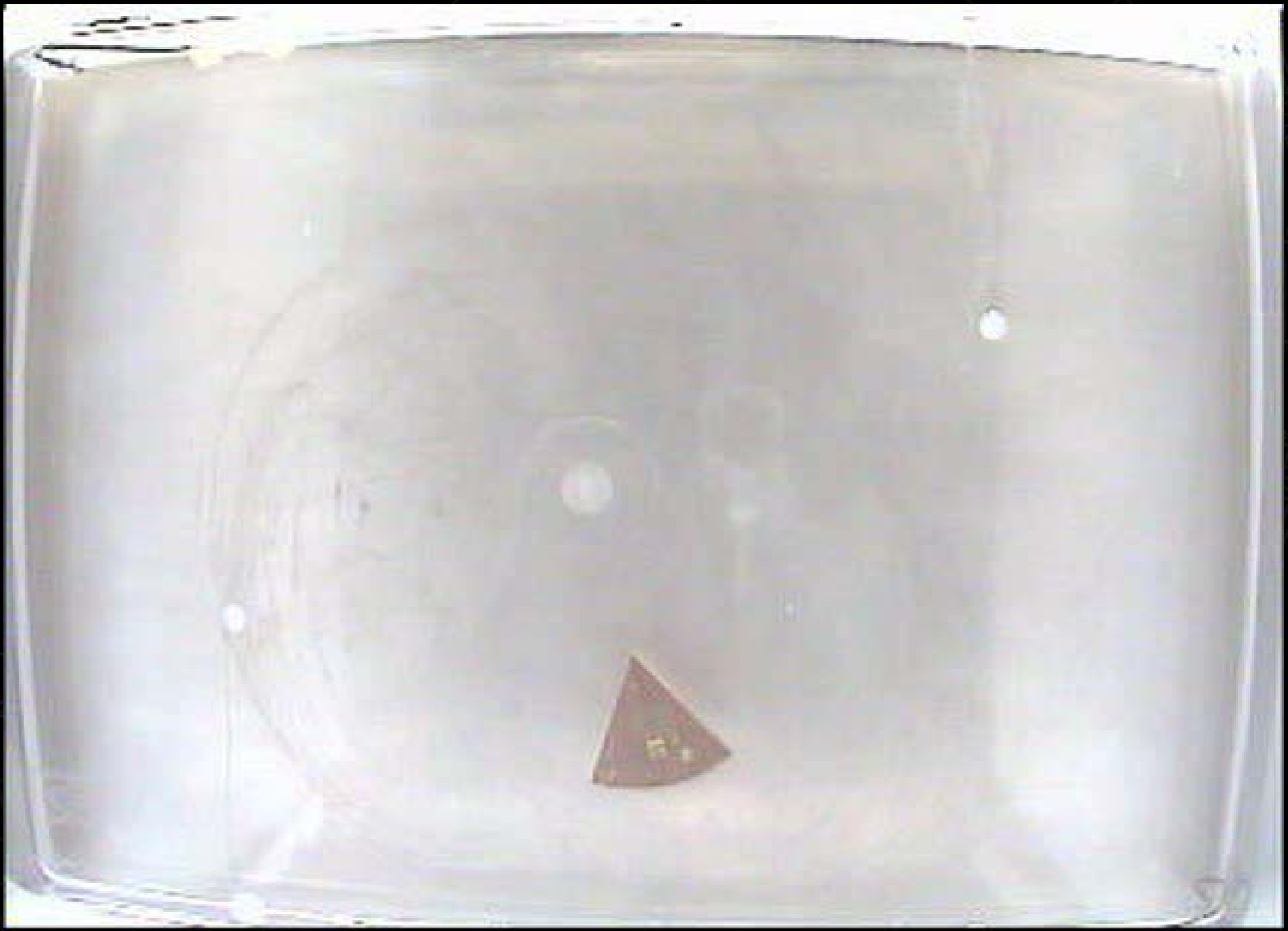
Miyashita, Hadorn, and Eggenberger, 2007

Inspiration

Tribolon



Wall Following



Miyashita, Hadorn, and Eggenberger, 2007

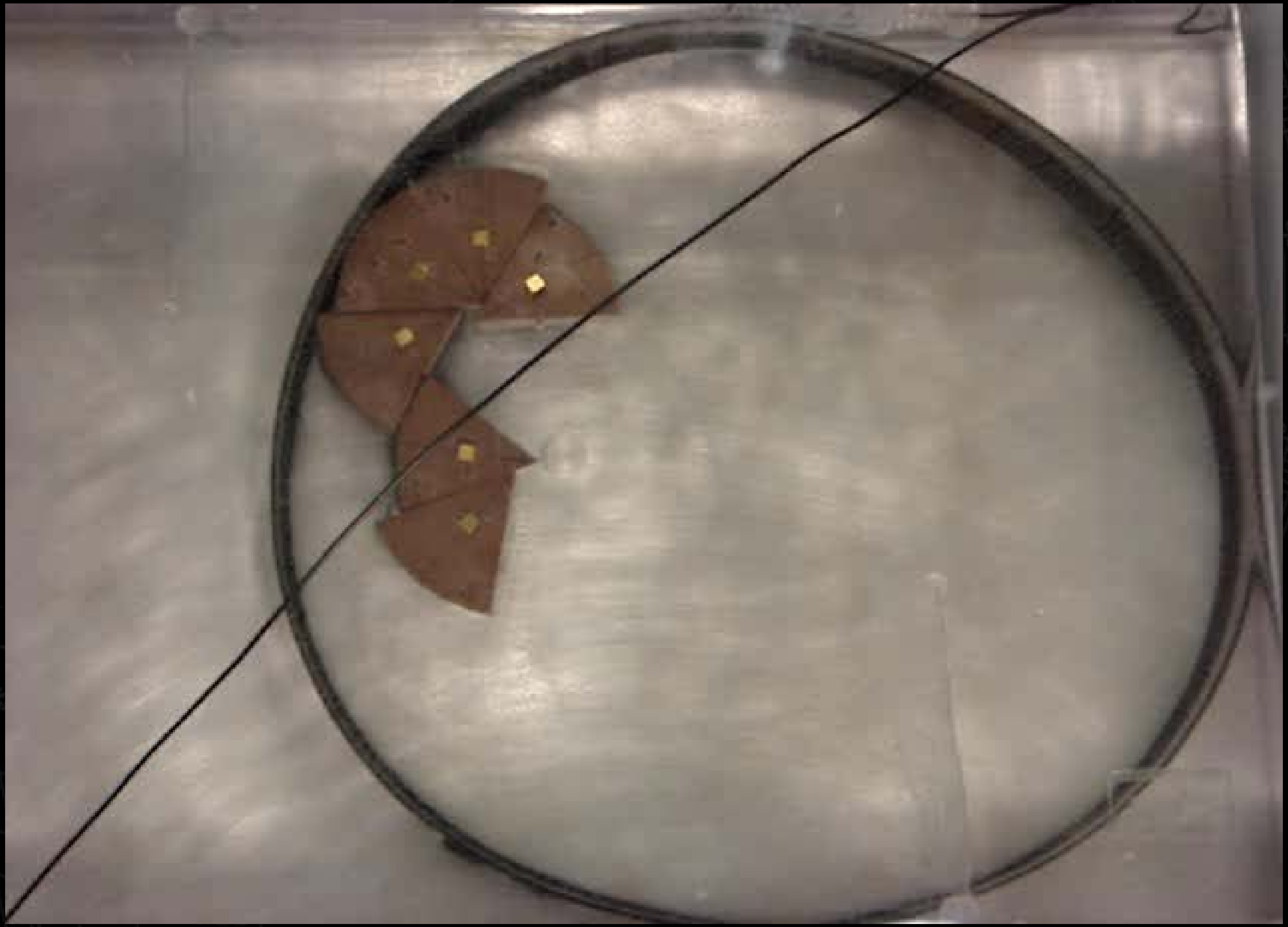
Unstable Relative Positions

Miyashita, Hadorn, and Eggenberger, 2007

Six Units

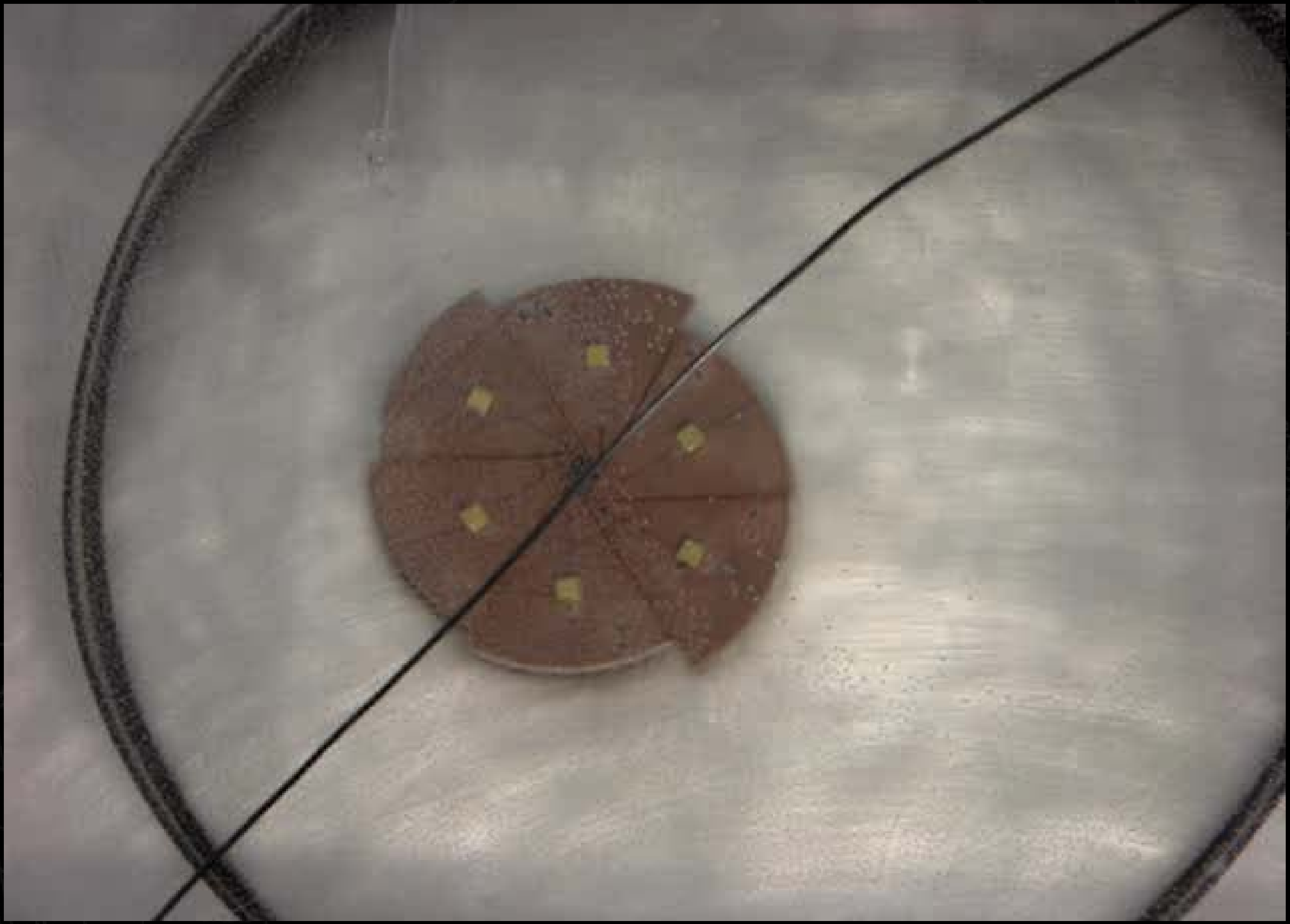
Miyashita, Hadorn, and Eggenberger, 2007

Hierarchical Aggregation



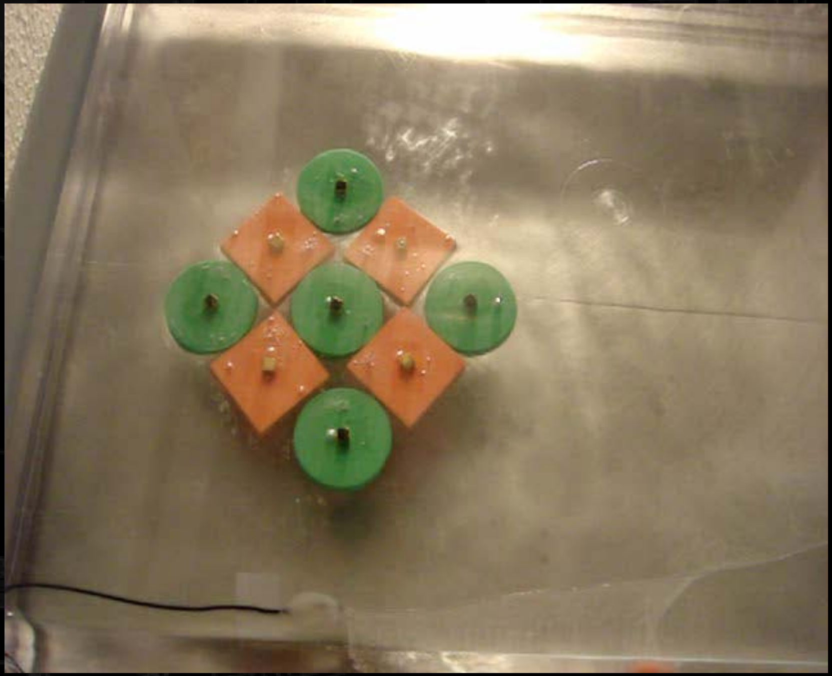
Miyashita, Hadorn, and Eggenberger, 2007

Hierarchical Aggregation



Miyashita, Hadorn, and Eggenberger, 2007

Heterogeneities



Miyashita, Hadorn, and Eggenberger, 2007

Programmable Self-Assembly

Original problem statement:

- How can we engineer complex global structures and patterns from local interactions?

New problem statement:

- How do we design local behavior that achieve particular global goals?
- What are the local and global programming paradigms?
- Can the individual components actively decide whether to bind with others?

Programmable Self-Assembly

Bishop, J., Burden, S. et al., 2005

Programmable Self-Assembly: Units

Fig. 1. Four programmable parts partially assembled into a triangle. The parts bind upon random collisions and communicate via IR, deciding whether to remain bound or to detach. A graph grammar stored on the microcontroller of each part determines the ultimate global structure that will emerge. The parts are not self-motive but instead are "mixed" on an air table by overhead oscillating fans.

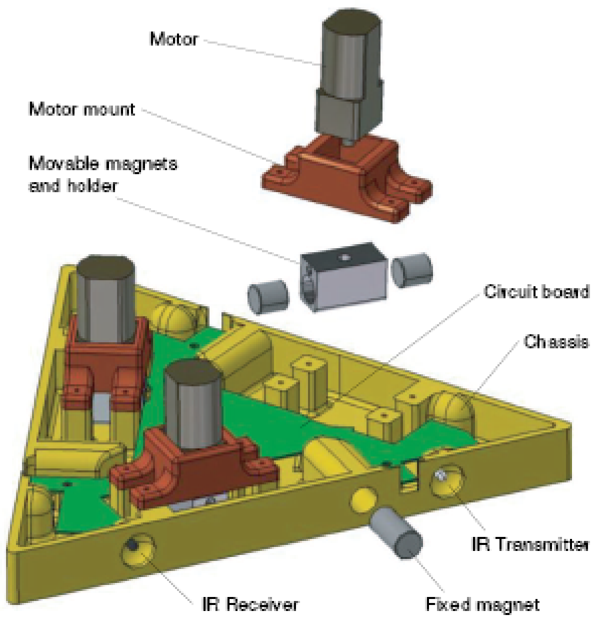
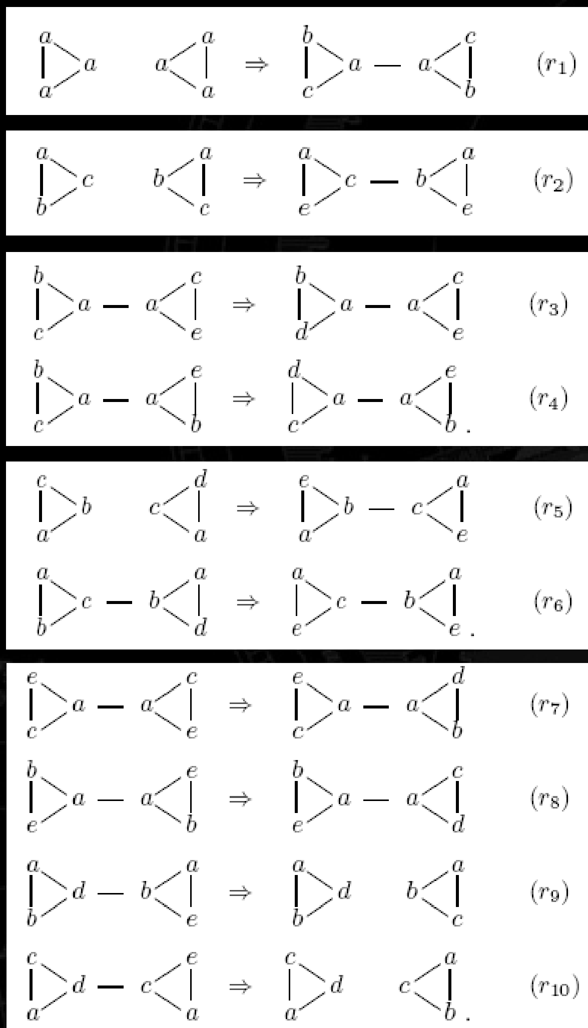


Fig. 2. The components of the programmable part include low power magnetic latches, infrared communications, and an on-board microcontroller.

Bishop, J., Burden, S. et al., 2005

Programmable Self-Assembly: Grammar



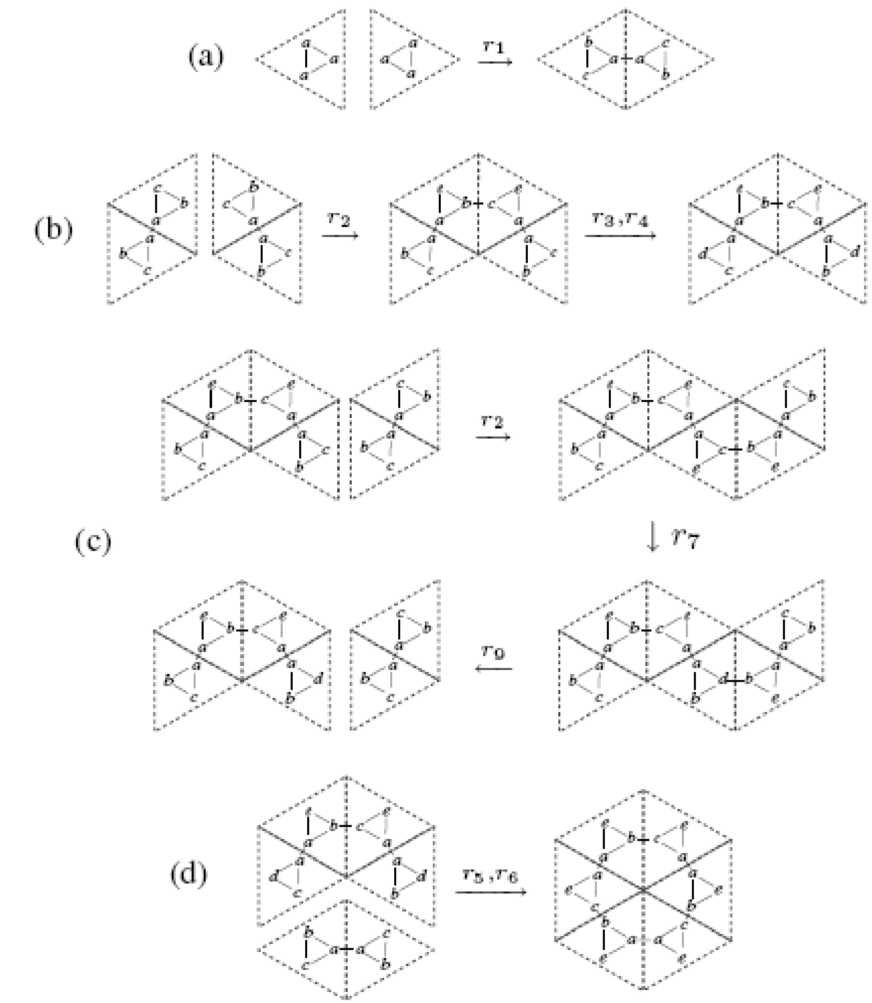


Fig. 3. The steps in the self-assembly of a hexagon using the rules described in Section V. Note that the geometry of the embedding represented here is for convenience. Graph grammars are purely topological, describing only the way the network topology of the system changes.

Bishop, J., Burden, S. et al., 2005

Programmable Self-Assembly

Self-Organizing Programmable Parts
Slow Hexagon Formation

Klavins Lab
University of Washington

J. Bishop S. Burden E. Klavins R. Kreisberg
W. Malone N. Napp T. Nguyen

UNIVERSITY OF WASHINGTON

NSF Grant # 0347955

NATIONAL SCIENCE FOUNDATION

http://faculty.washington.edu/klavins

March 2005

Programmable Self-Assembly

Self-Organizing Programmable Parts

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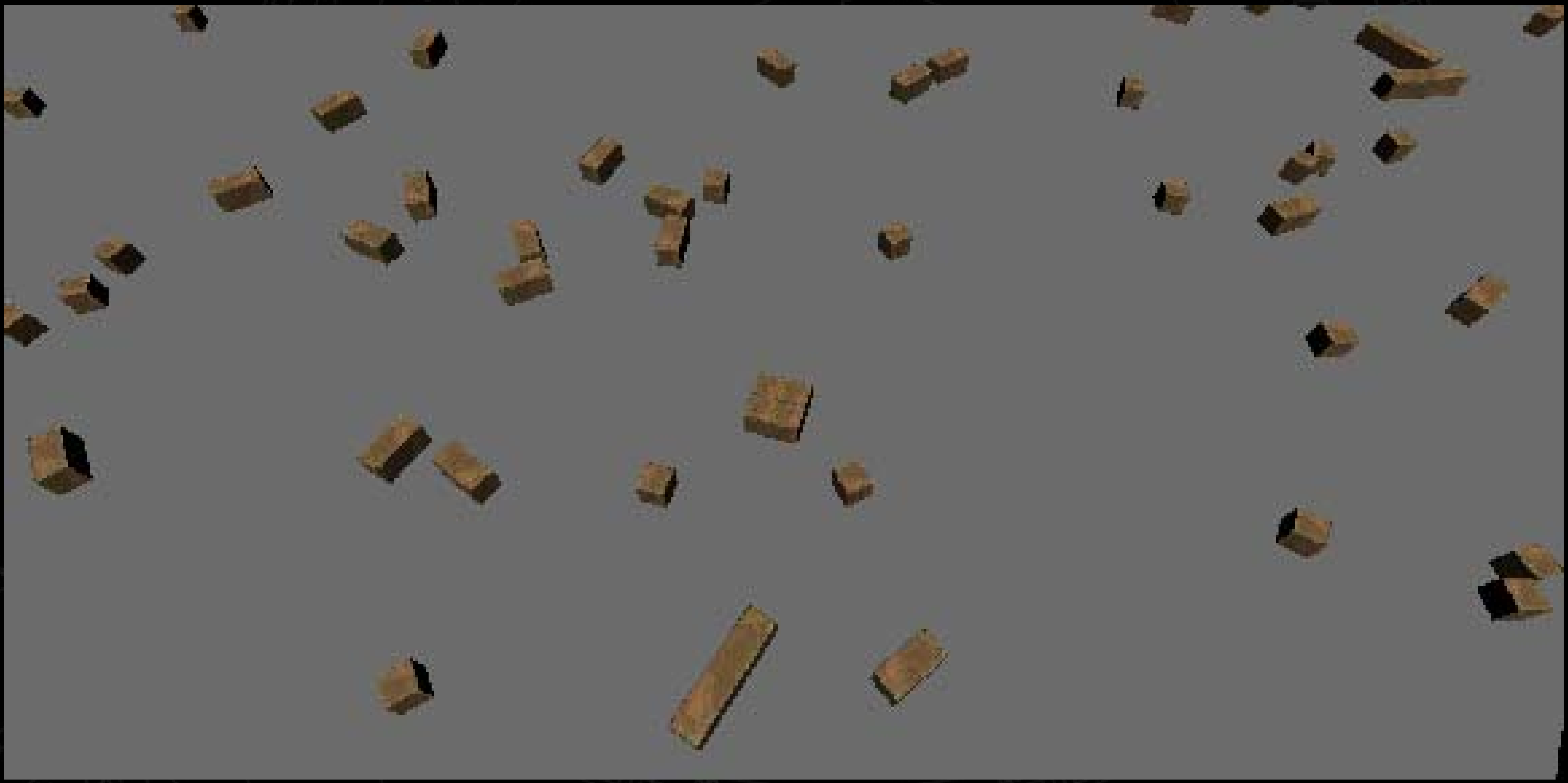
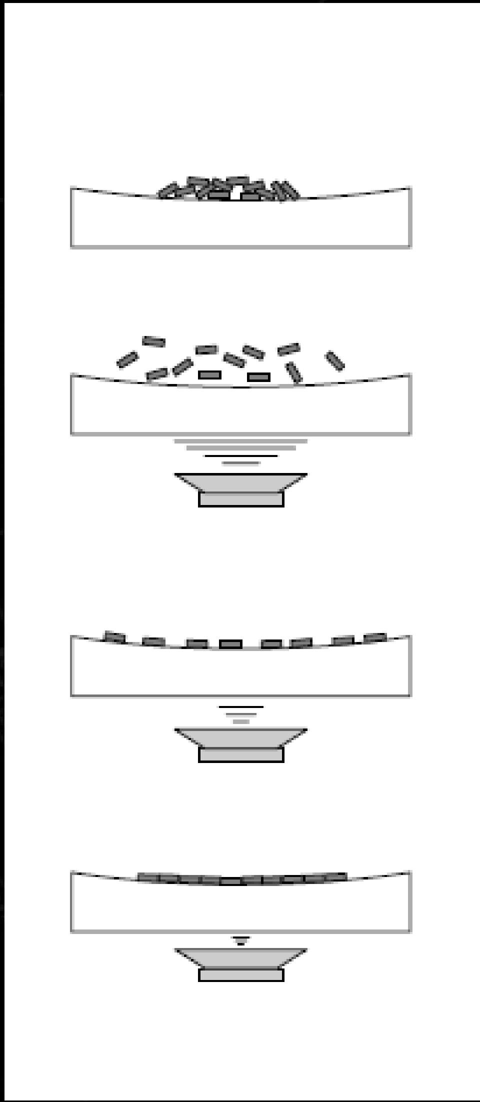
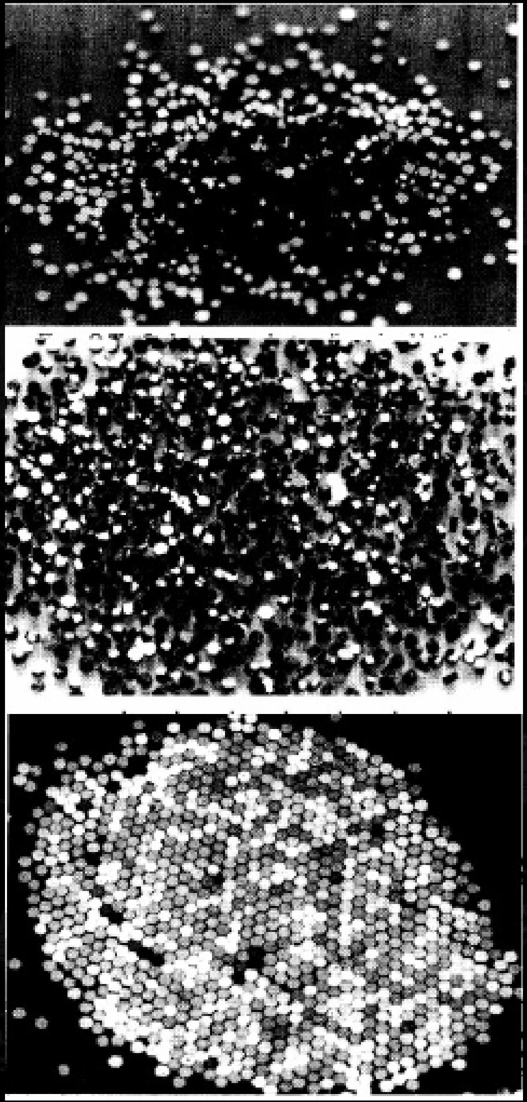
Klavins Lab, Univ. of Washington

Stochastic Self-Assembly



Stochastic Self-Assembly





Cohn, Kim, and Pisano (1991)

Bottom-Up Fabrication

Biology creates very complex objects – defined from the molecular scale up to meters – that construct themselves from elementary components, and sometimes even reproduce

Scaffolded Self-Assembly of DNA

Folding DNA to create nanoscale shapes and patterns

Paul W. K. Rothemund[1]

‘Bottom-up fabrication’, which exploits the intrinsic properties of atoms and molecules to direct their self-organization, is widely used to make relatively simple nanostructures. A key goal for this approach is to create nanostructures of high complexity, matching that routinely achieved by ‘top-down’ methods. The self-assembly of DNA molecules provides an attractive route towards this goal. Here I describe a simple method for folding long, single-stranded DNA molecules into arbitrary two-dimensional shapes. The design for a desired shape is made by raster-filling the shape with a 7-kilobase single-stranded scaffold and by choosing over 200 short oligonucleotide ‘staple strands’ to hold the scaffold in place. Once synthesized and mixed, the staple and scaffold strands self-assemble in a single step. The resulting DNA structures are roughly 100 nm in diameter and approximate desired shapes such as squares, disks and five-pointed stars with a spatial resolution of 6 nm. Because each oligonucleotide can serve as a 6-nm pixel, the structures can be programmed to bear complex patterns such as words and images on their surfaces. Finally, individual DNA structures can be programmed to form larger assemblies, including extended periodic lattices and a hexamer of triangles (which constitutes a 30-megadalton molecular complex).

(Rothermund, 2006)

Folding DNA to Create Nanoscale Shapes and Patterns

(Rothermund, 2006)

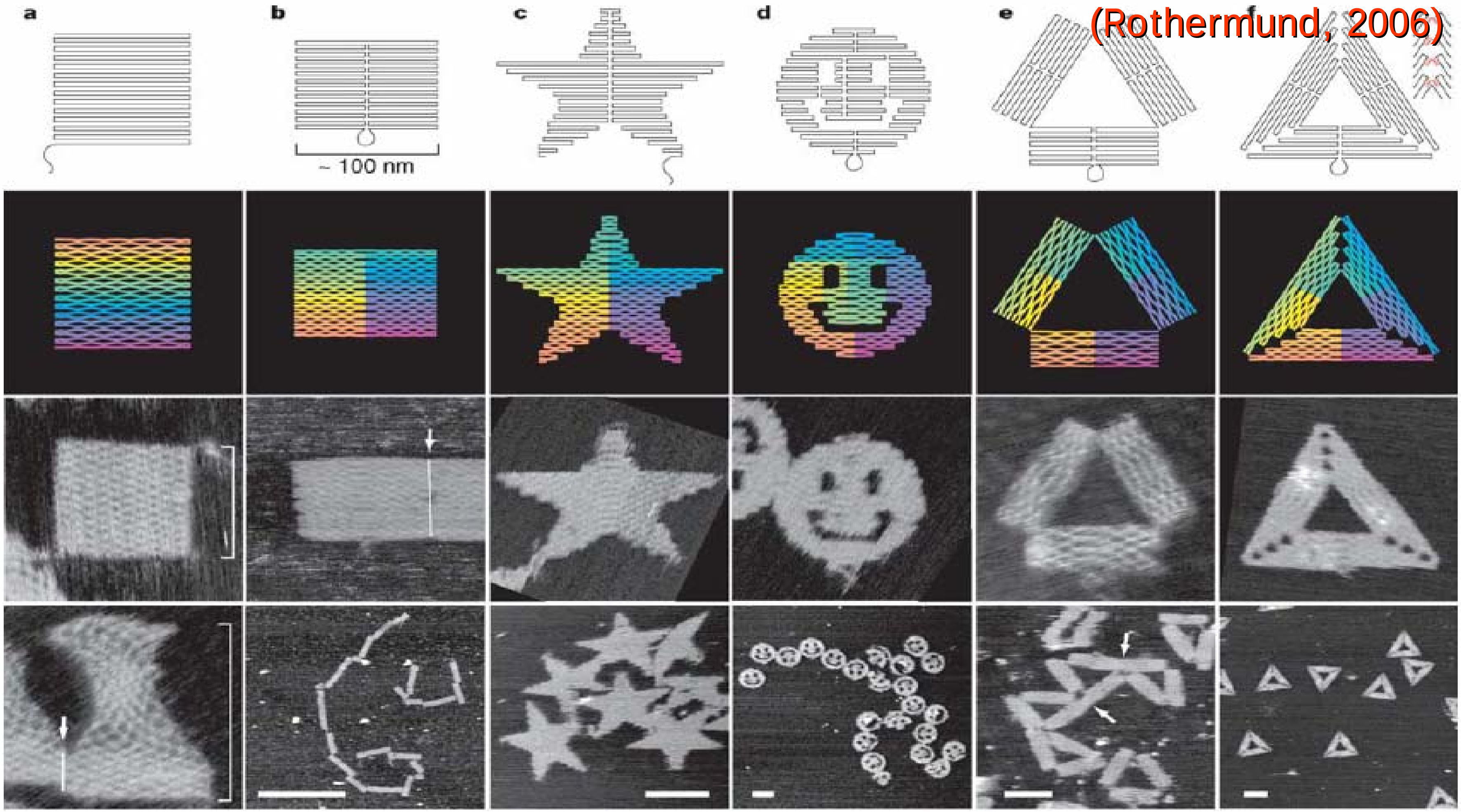
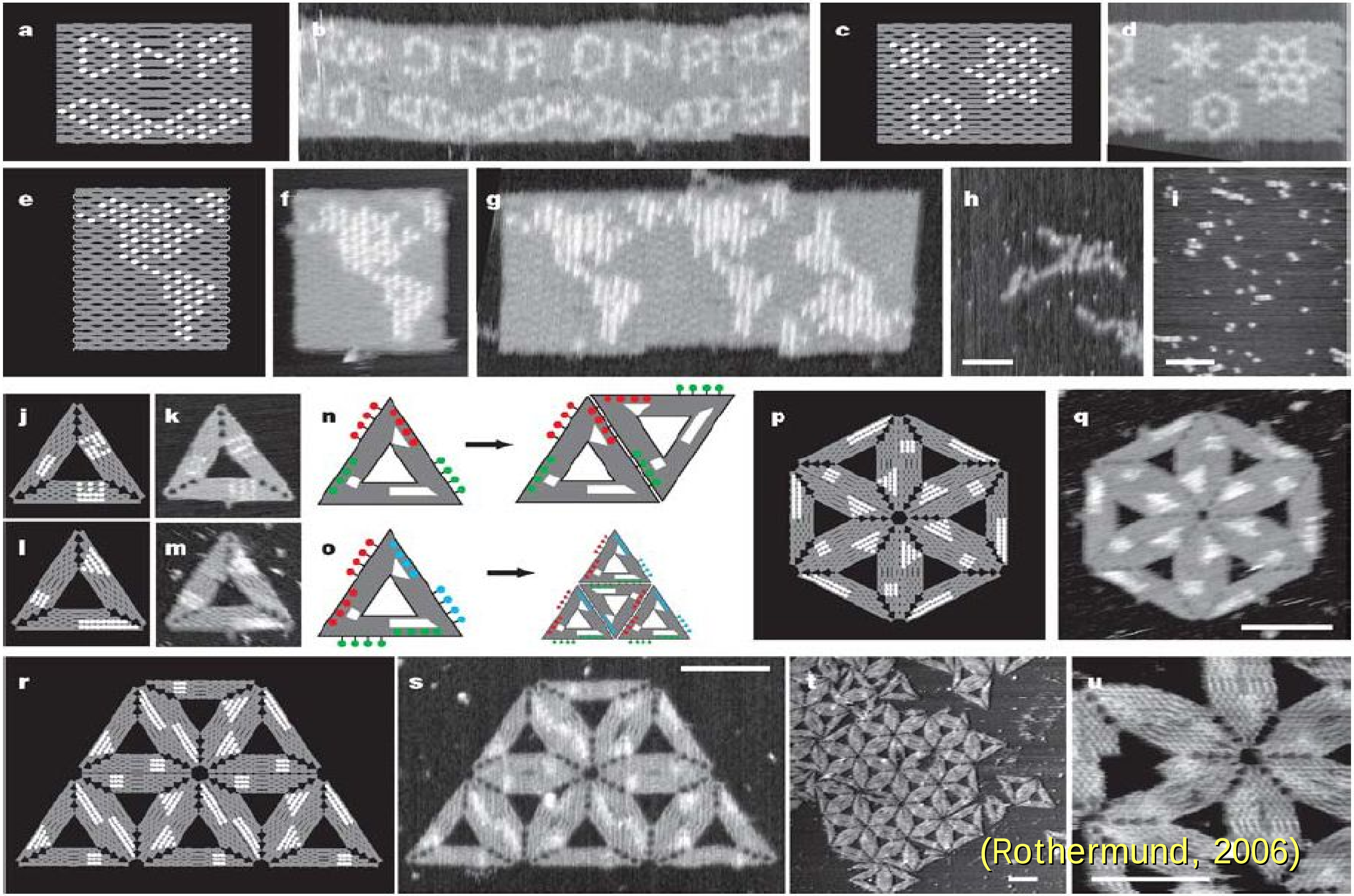


Figure 2 | DNA origami shapes. Top row, folding paths. **a**, square; **b**, rectangle; **c**, star; **d**, disk with three holes; **e**, triangle with rectangular domains; **f**, sharp triangle with trapezoidal domains and bridges between them (red lines in inset). Dangling curves and loops represent unfolded sequence. Second row from top, diagrams showing the bend of helices at crossovers (where helices touch) and away from crossovers (where helices bend apart). Colour indicates the base-pair index along the folding path; red is the 1st base, purple the 7,000th. Bottom two rows, AFM images. White lines and arrows indicate blunt-end stacking. White brackets in **a** mark the height of an unstretched square and that of a square stretched vertically (by a factor >1.5) into an hourglass. White features in **f** are hairpins; the triangle is labelled as in Fig. 3k but lies face down. All images and panels without scale bars are the same size, 165 nm × 165 nm. Scale bars for lower AFM images: **b**, 1 μm; **c**–**f**, 100 nm.

Folding DNA to Create Nanoscale Shapes and Patterns

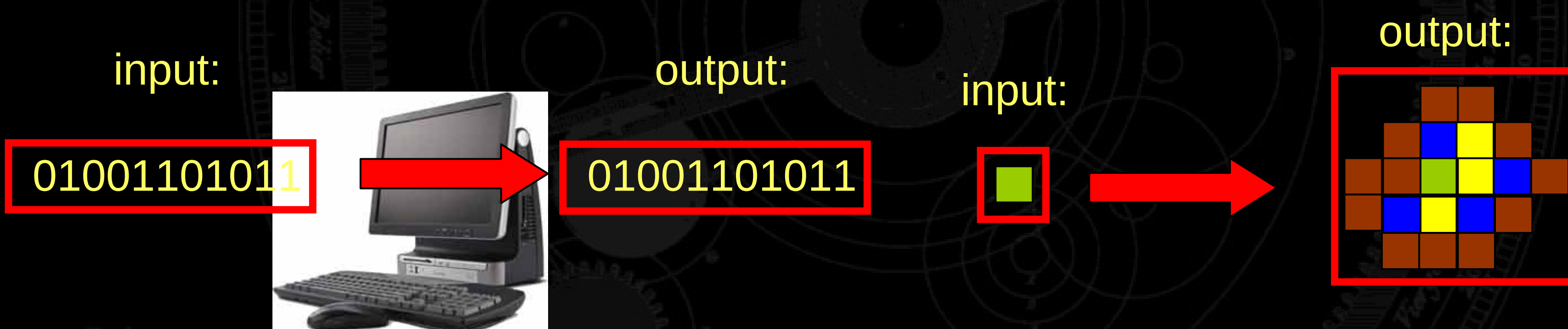


(Rothermund, 2006)

One Particular Motivation

Compute “along the way”

- The self-assembly of a crystal can resemble a program that leaves the traces of its operations embedded in it



- The assembly of a 2D crystal can simulate a universal Turing machine!

Motivation: Self-Assembly of DNA

	DNA	Current computer
Information density (bits/nm^3)	~1	~10^{-11}
Parallelism (operations/sec)	~10^{18}	~10^{12}
Energy expediture (J/operation)	~10^{-19}	~10^{-9}

Algorithmic Self-Assembly

First A Few Words on Tiles

- A tiling is an arrangement of tiles (shapes) that covers the plane
- Tiles fit together according to matching rules: their edges must have complementary shapes and must agree on additional markings such as colors
- Tiling problem: given a finite set of tiles, does there exist a valid tiling of the plane (proven unsolvable)

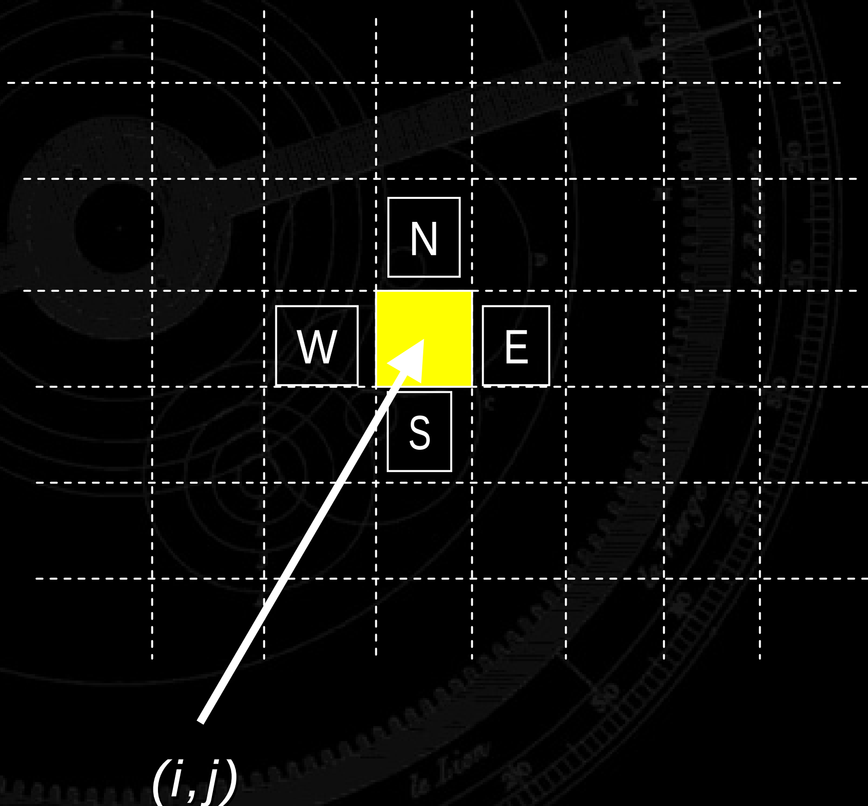
The Tile Assembly Model

Infinite lattice:

- Z x Z

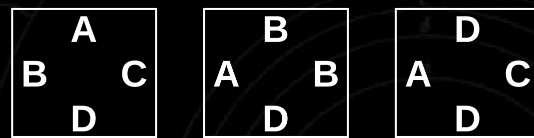
Every position in the grid has a relative position associated:

N$(i,j)=(i,j+1)$
S$(i,j)=(i,j-1)$
E$(i,j)=(i+1,j)$
W$(i,j)=(i-1,j)$



Bond Types and Tile Types

Our fundamental unit is a square tile with labeled edges, or bond types



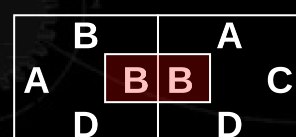
We consider a set of bond types Σ (e.g., Σ={A,B,C,D,*null*})

A reflection or rotation gives a different tile

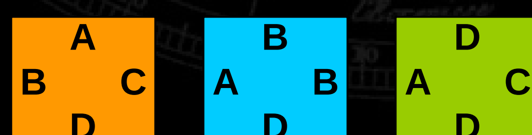
So a tile type is a quadruple: $\tilde{t} = (\sigma_N, \sigma_S, \sigma_E, \sigma_W) \in \Sigma^4$

and we have unlimited supply of them

Tiles types with identical edges can pair with each other



We will represent tile types with different colors. All tile types for the set *T*

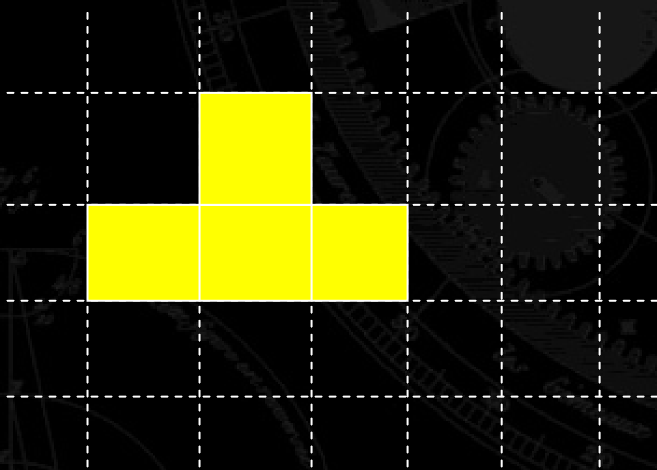


Tiles

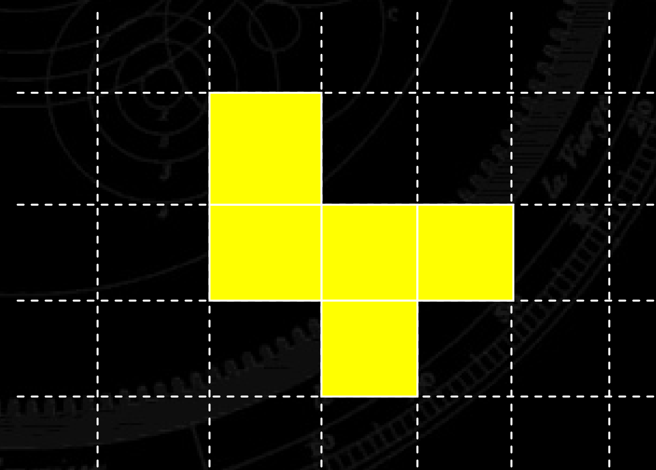
A *tile* is a pair $(\tilde{t}, (i, j)) \in T \times Z^2$

i.e., it corresponds to a tile with certain tile type located in a certain position in our grid

A configuration is a set of tiles, such that there is exactly one tile in every location



Configuration 1



Configuration 2

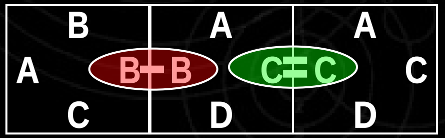
Interaction Between Tiles

A strength function $g : \Sigma \times \Sigma \to Z$ defines the interactions between two tiles.

We say a tile t_1 interacts with its neighbor t_2 with strength

$$\Gamma(t_1, t_2) = g(\sigma, \sigma')$$

g	A	B	C	D	null
A	1	0	0	0	0
B	0	1	0	0	0
C	0	0	2	0	0
D	0	0	0	1	0
null	0	0	0	0	0



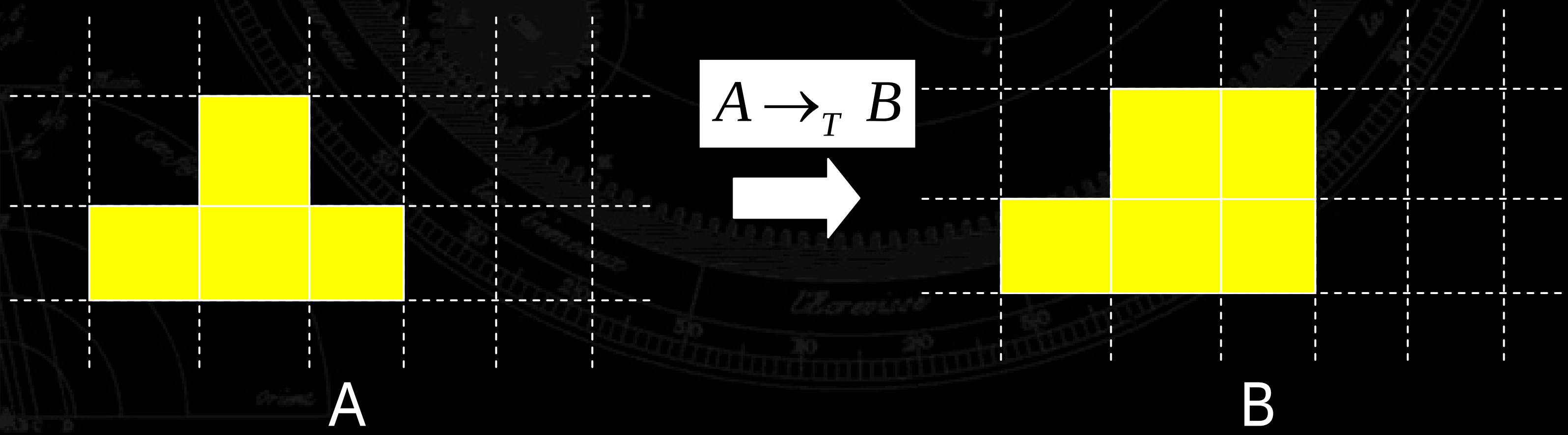
Usually, only diagonal strength functions are considered, and the range of g is {0,1,2}

The Tile Assembly Model (TAM)

A <u>tile system</u> is a quadruple (T, t_s, g, τ) i.e., it consist of

- a set of tile types
- a seed tile
- a strength function
- a binding threshold or “temperature”

Self-assembly is defined as a relation between configurations:

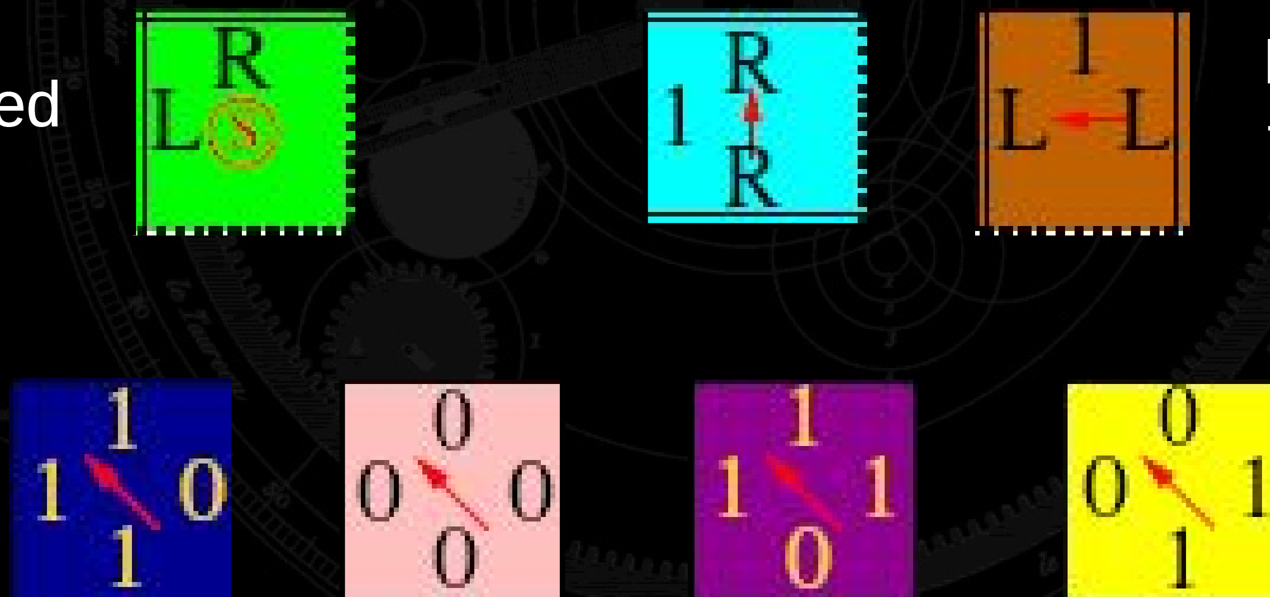


Examples of Tile Systems

Sierpinski tile set

- 7 types of tiles: 1 seed, 2 boundary (input) tiles, 4 rule tiles

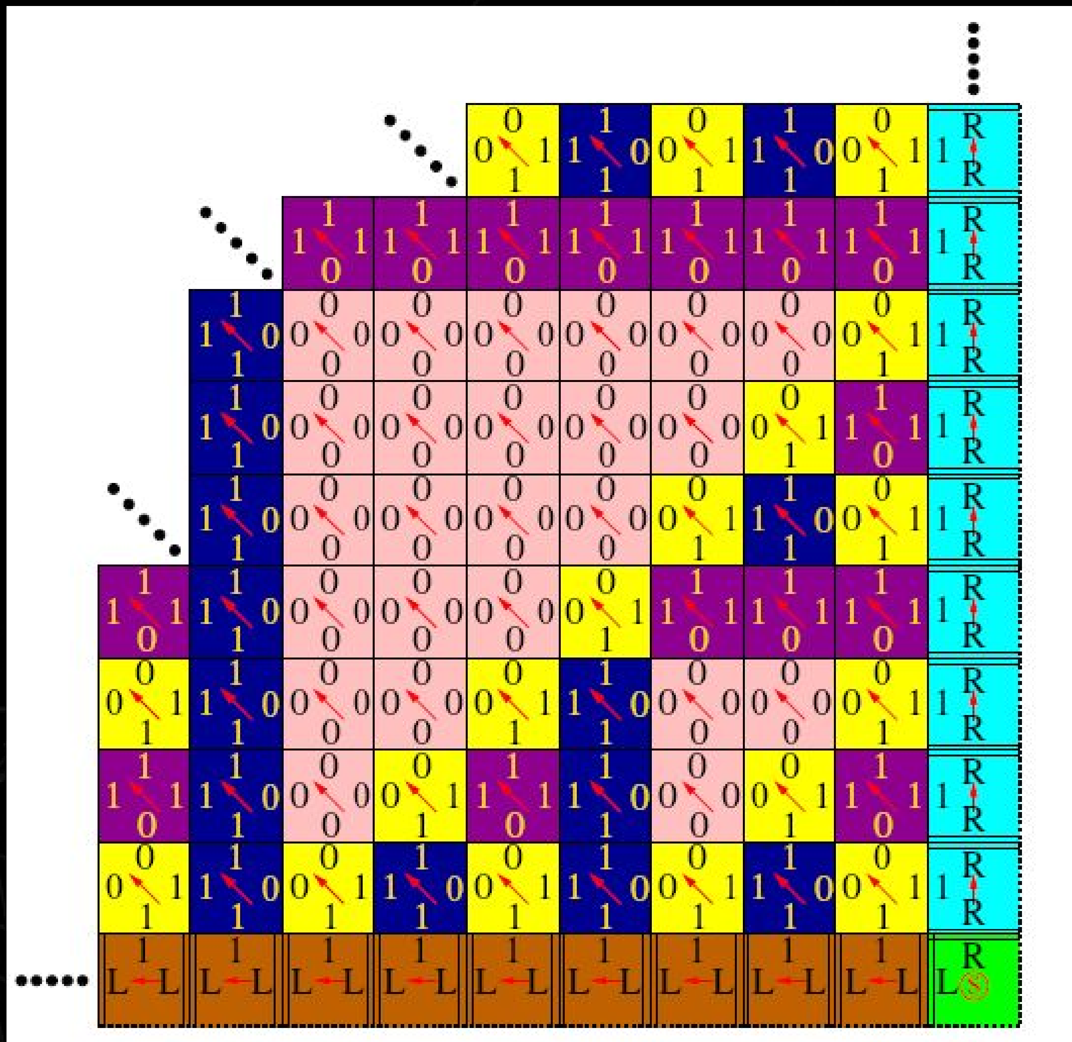
Seed



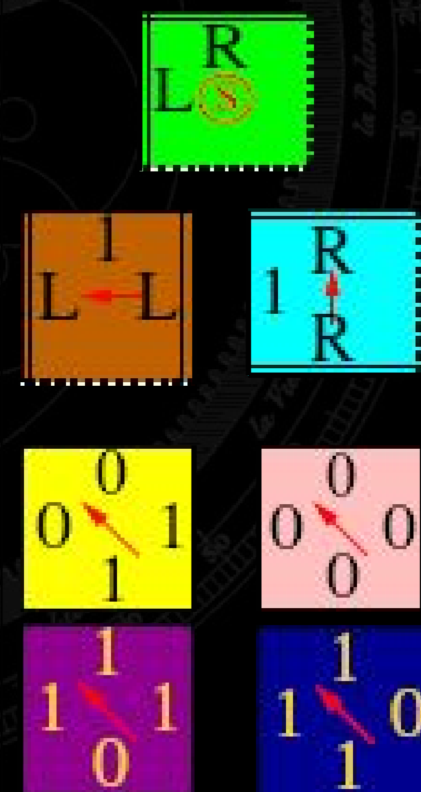
Boundary tiles

“Rule” tiles

Sierpinski Tile Set

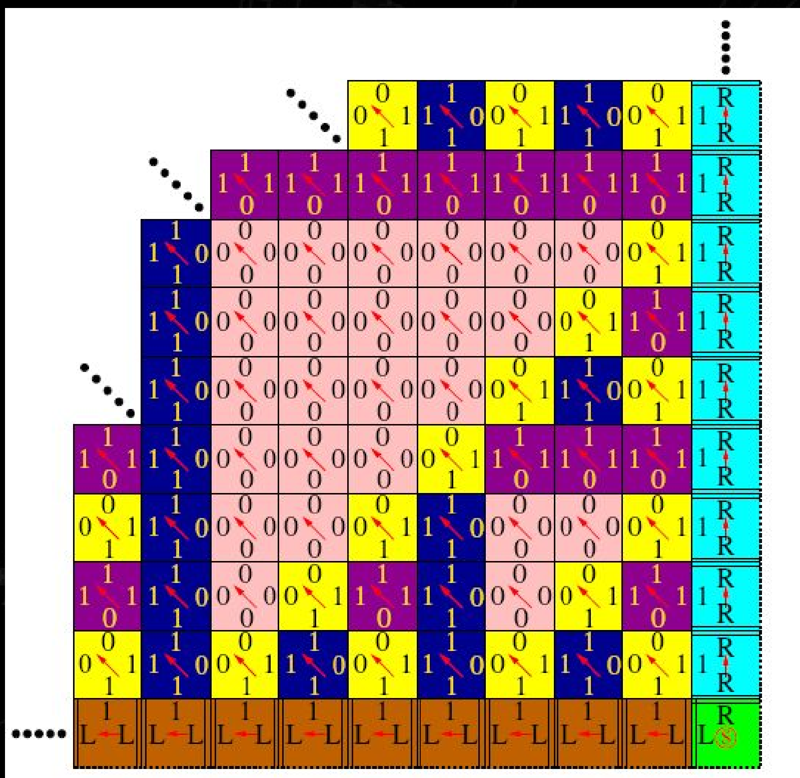


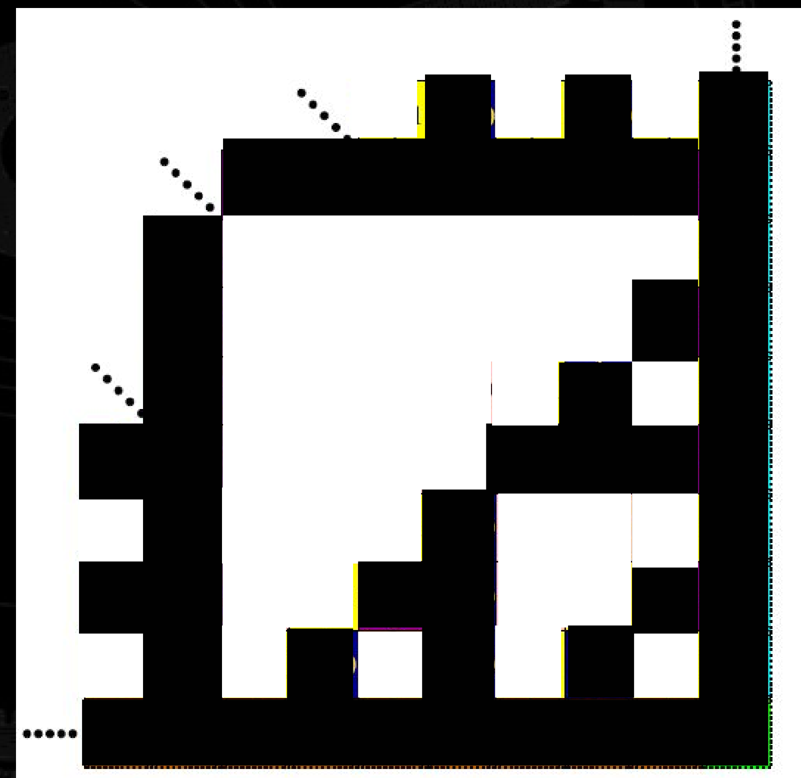
Tiles



See Winfree, Rothermund et al.

Sierpinski Tile Set

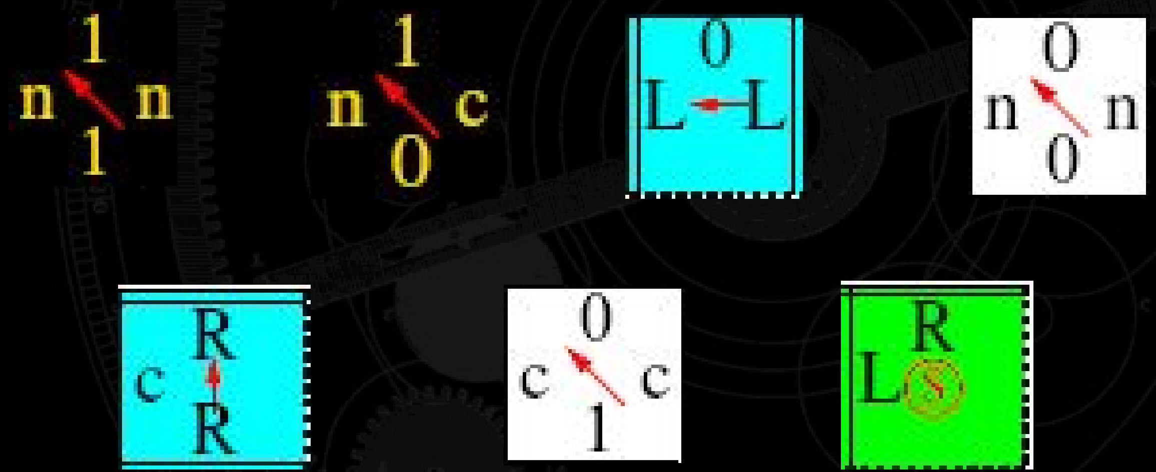




See Winfree, Rothermund et al.

Binary Counter

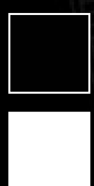
Tile types:



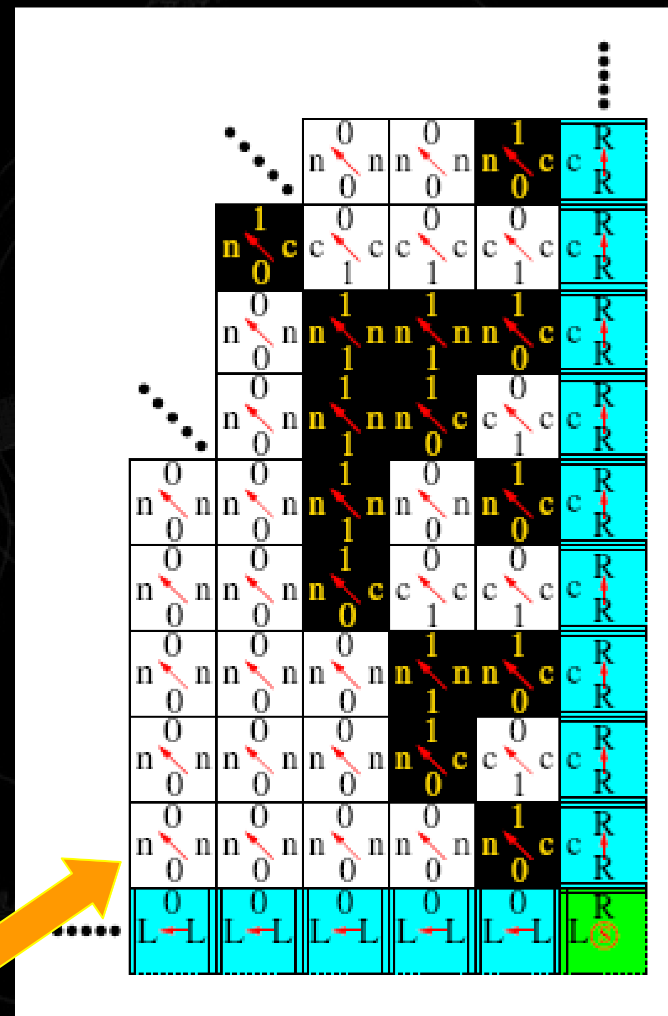
See Winfree, Rothermund et al.

Binary Counter

- Begin with seed
- Continue with boundary tiles
- Then “rule” tiles
- Count upwards (binary)

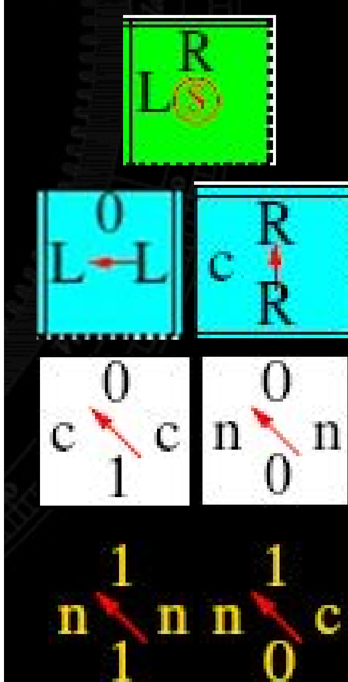

= 1

= 0



00001

Tiles

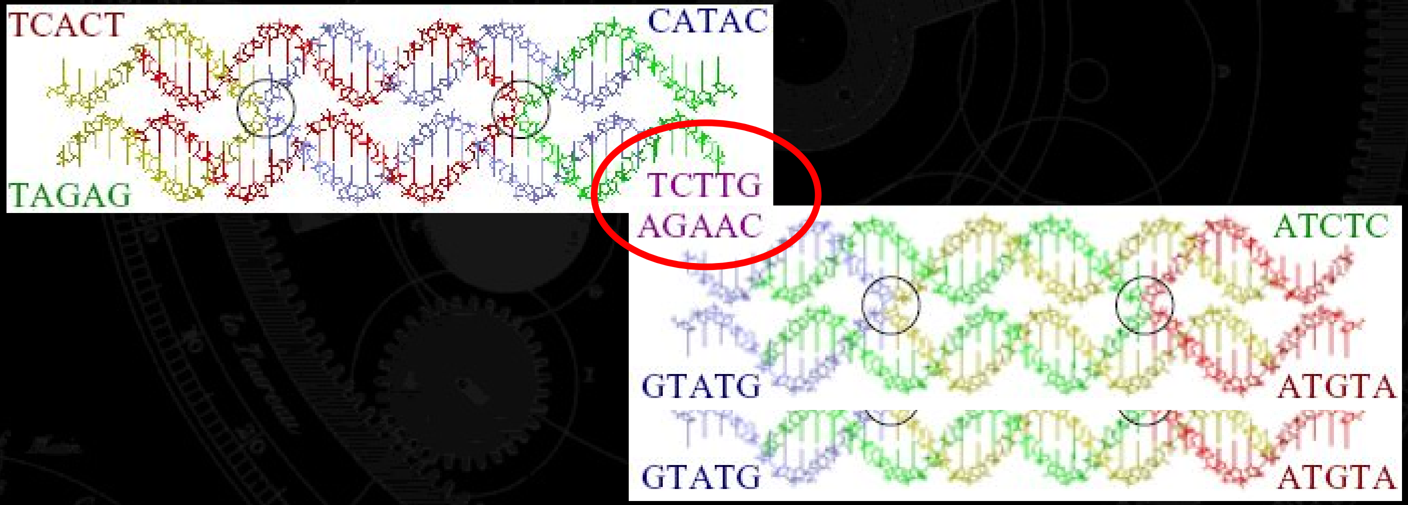


See Winfree, Rothermund et al.

From Theory to Practice (Biology)

Tiles are "do-able" in practice

DNA Nano-technology



Winfree, E. et al. (1998). Design and self-assembly of two dimensional DNA crystals

Protocell Assembly – Ongoing

- Question is not whether simple life-forms can be assembled but under which conditions it can occur
- Bottom-up routes to artificial (proto)cells
- Ultimate goal: living artificial cells made from non-living material

http://protocells.lanl.gov/

http://www.protocell.org/

http://bruckner.biomip.rub.de/bmcmyp/Data/PACE/WWW/PACE/index.html

PACE Project

Artificial cells = living matter

Computational aspects of living matter/artificial cells:

- Design of artificial cells (relies on self-assembly)
- Programming artificial cells (low-level assembly language still needs to be discovered)
- Computational potential of artificial cells (programmability of functionality; programmability of pattern)

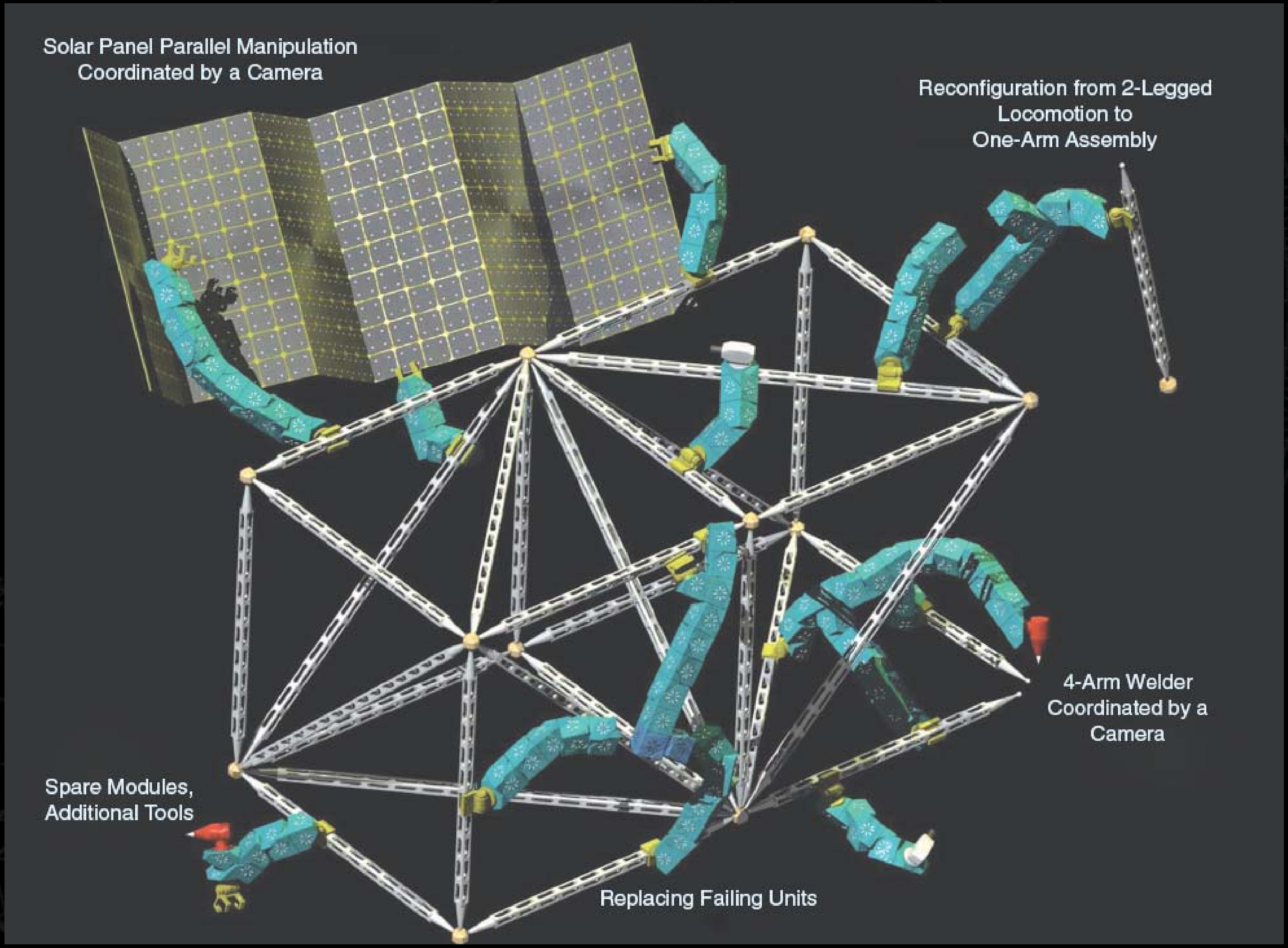
Synthetic/Systems Biology

Beginning of Norman Packard’s talk

Modular Self-Reconfigurable Robots

- Modules are connected
- Modules can change form (variable morphology)

Application Scenario



(Zykov et al., 2007)

The Robosphere

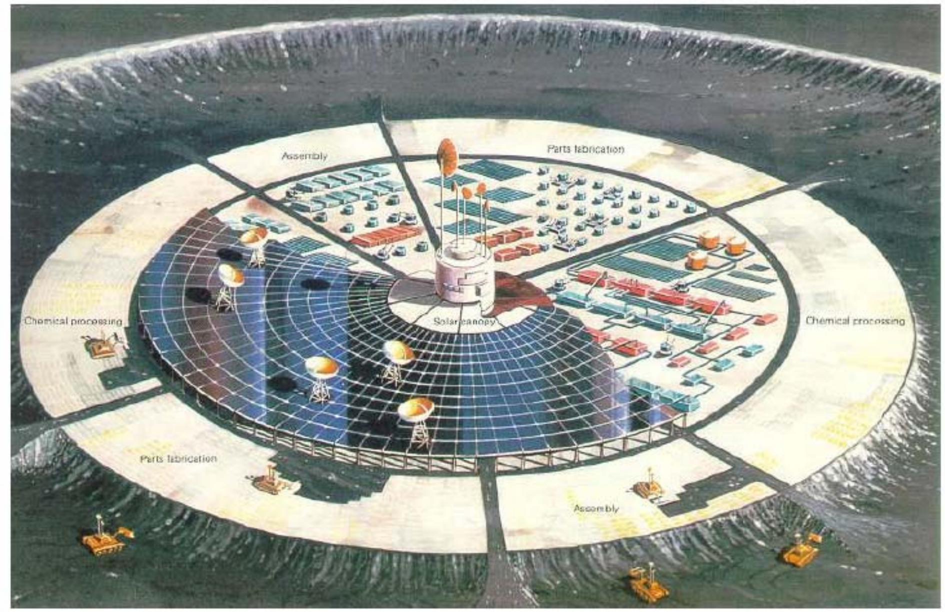


Figure 1: *Artists impression of self-replicating lunar factory.*

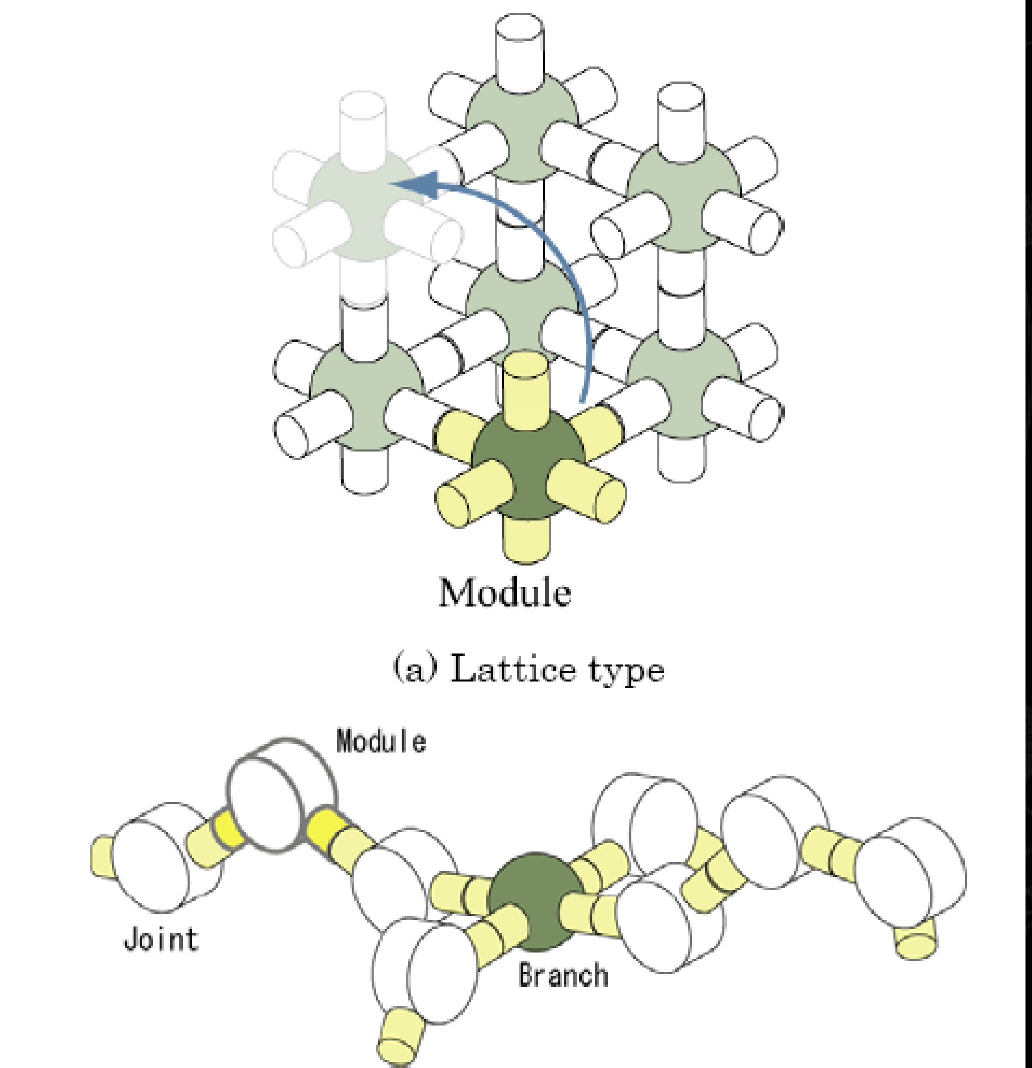
????

http://robosphere.arc.nasa.gov/

Motivation and Inspiration

- Versatility and adaptivity (new morphologies better suited for the task)
- Robustness (parts are interchangeable → self-repair)
- Low cost (many copies of a few types of modules)

Self-Reconfigurable Robots



(a) Lattice type

(b) Chain type

Murata and Kurokawa (2003) “Self-reconfigurable robots”

Self-Configurable Robots

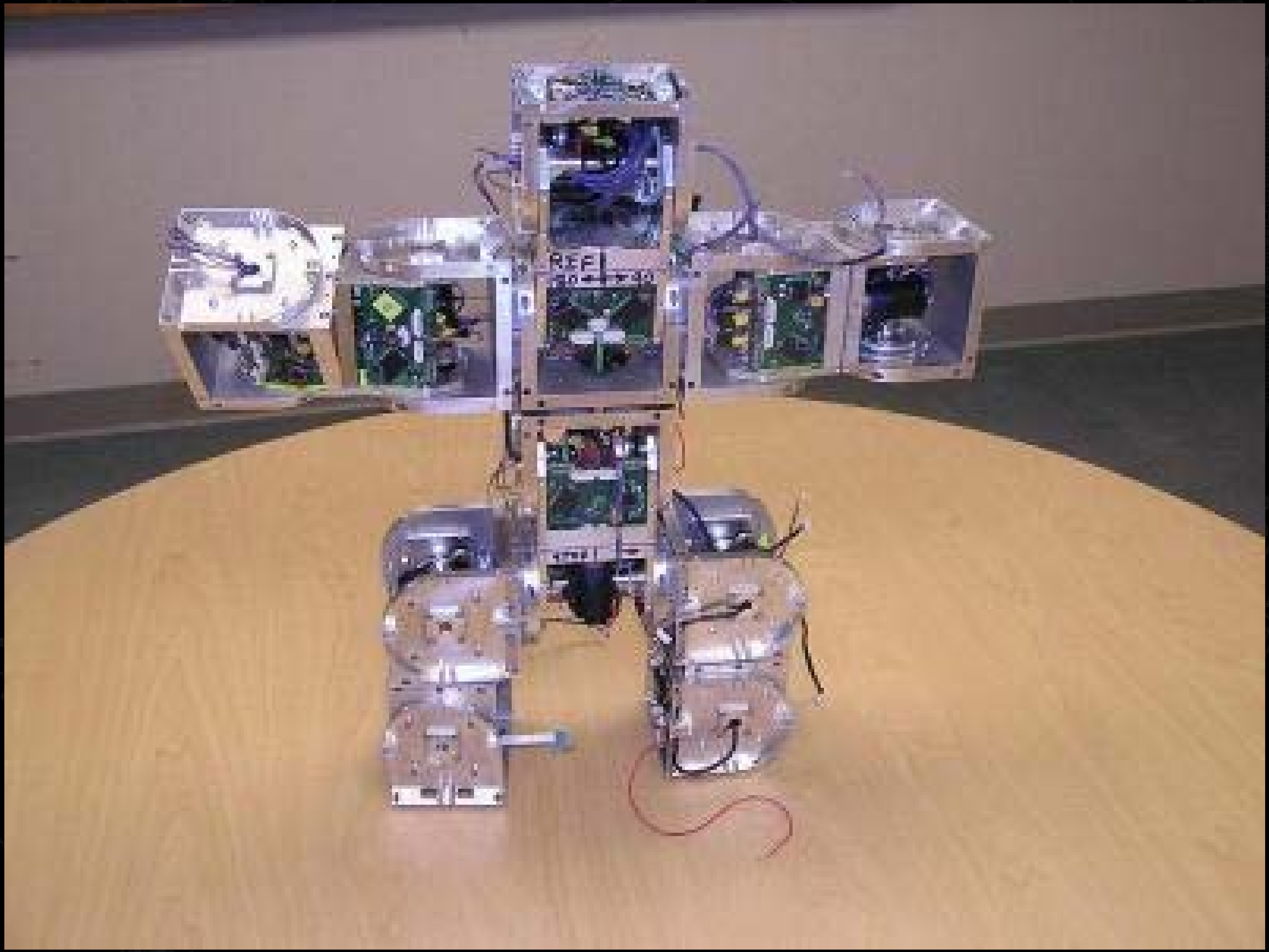
Kaspar Stoy (2004)

Hydra

"Living" building blocks for self-designing artifacts

Check out: http://hydra.mip.sdu.dk/

Superbot (2007)



http://www.isi.edu/robots/superbot.htm