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THE NANO GROUP



Nanoscale Sensor Networks

DNA: A New Paradigm for Communication at the Bottom

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Universität zu Lübeck

Institute of Telematics

May 25, 2021

Overview

- | | | |
|---------------------|-----------------------|-------------------|
| 1. The Nanogroup | 7. Big Problems | The Nanogroup |
| 2. What We Do | 8. The Nanoscale | What We Do |
| 3. Motivation | 9. DNA Basics | Motivation |
| 4. Applications | 10. Message Molecules | Applications |
| 5. State of the Art | 11. Conclusion | State of the Art |
| 6. Prediction | 12. Summary | Prediction |
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The Speaker



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CV:

- ▶ Born 1990 in Lübeck
- ▶ Abitur in 2009
- ▶ Bachelor in 2013 on P2P systems
- ▶ Master in 2016 on competitive analysis
- ▶ Conceptualized DNA-based nanonetworks
- ▶ Doctor in 2020 on nanonetworks with magna cum laude
- ▶ Postdoctoral researcher since 2020
- ▶ Workshop organizer WoNaN
- ▶ Author of nanonetwork lectures & seminars



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The Nanogroup



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Key Points:

- ▶ The Nanogroup was Founded in 2017
- ▶ We focus on:
 1. Nano-computation
 2. DNA-based nanonetworks
 3. Ethical, legal and social consequences
 4. Protocols
 5. Engineering aspects
 6. Simulation
 7. And many more topics



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Mindmap

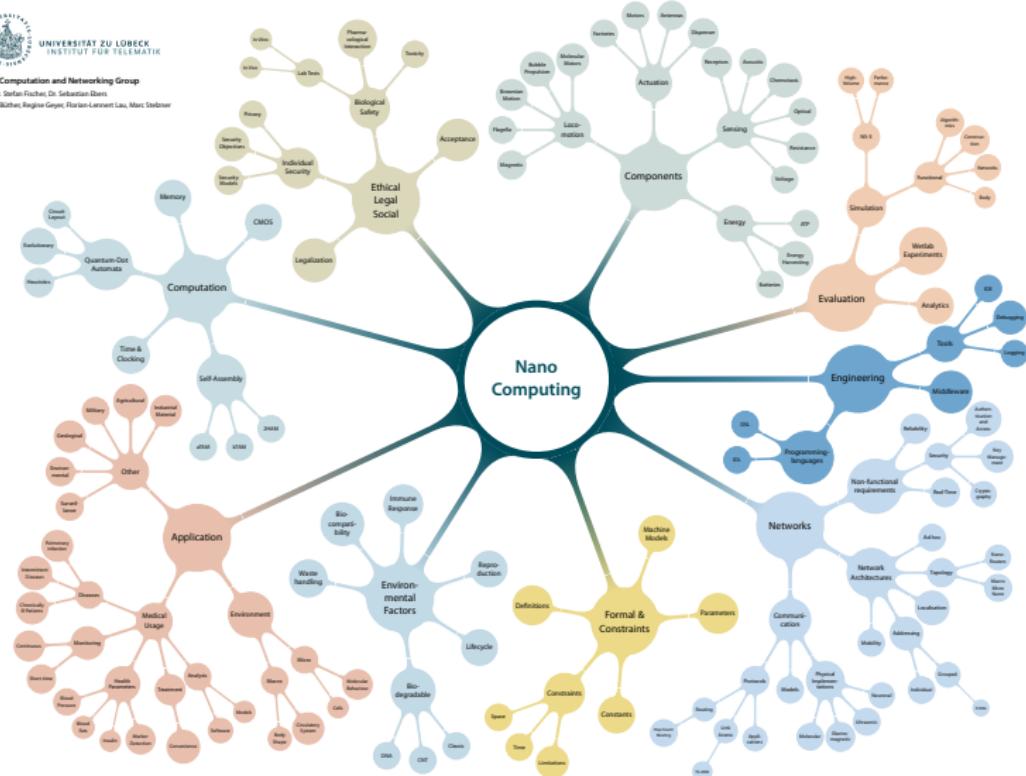


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Nano Computation and Networking Group
Prof. Dr. Stefan Fischer, Dr. Sebastian Ibars
Florian Büthe, Regine Geyer, Florian-Lennert Lau, Marc Stödter



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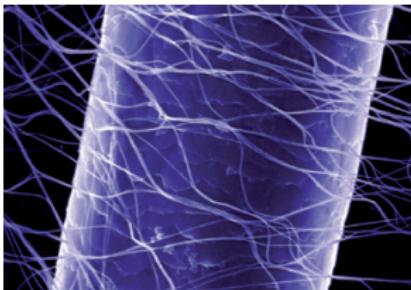
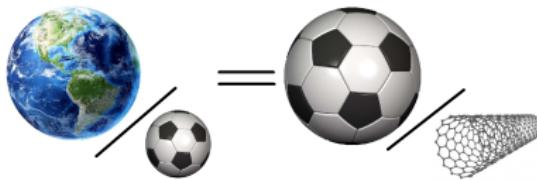
Origin



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Nanos = dwarf:

- ▶ **Atom** for the first time 500 BCE mentioned in Greece
- ▶ **Kalapas** 600 CE in Buddhist India
- ▶ 1–4000 nanometer = $1\text{--}4000 \times 10^{-9}\text{ m}$
- ▶ Hair:
 $20\,000\text{ nm}\text{--}200\,000\text{ nm}$
- ▶ Cell: 10 000 nm
- ▶ DNA-helix: 2 nm

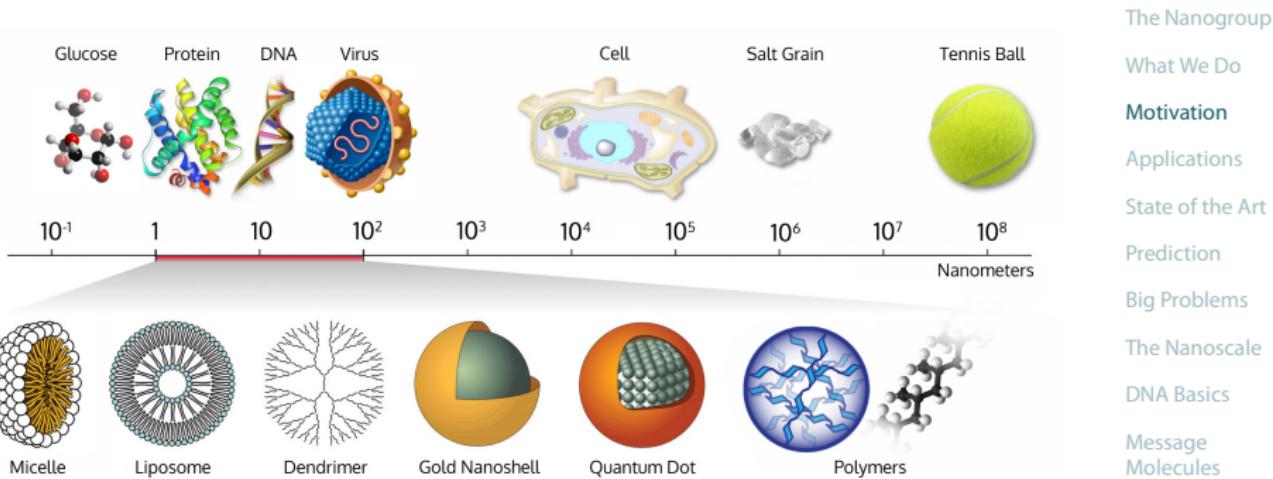


Hair vs. nano fibre.¹

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¹Nau 2016.

Size



Size comparison of various nanoscale objects and particles².

²wichlab 2017.

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Early Use

Germanic sword *Ulfberht*:

- ▶ 800–1100 BC
- ▶ Carbon reinforced steel
- ▶ Carbon source: *bones*
- ▶ *Carbonnanotubes* reinforcing steel
- ▶ *Misbelief* that the strength of animal or enemy passes from bones into the sword



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Applications

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Use Cases



- ▶ Medical surveillance of *health parameters*
- ▶ Military *communication monitoring*
- ▶ *Agricultural* efficiency enhancements through:
 - ▶ Destruents
 - ▶ Rhizomenetworks
 - ▶ Disease prevention or control
- ▶ Environmental control & regeneration
- ▶ Natural catastrophes warning systems

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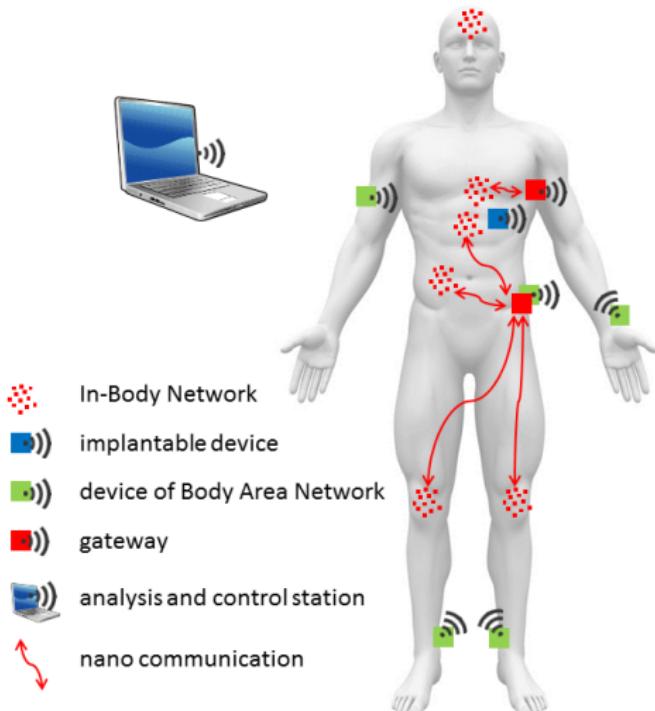
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Pulmonary Inflammation



Detection of pulmonary inflammation³:

- ▶ *Discovery* of disease markers through a Body Area Network (BAN)
- ▶ *Communication* of discoveries to other devices and to a *gateway*
- ▶ *Direct* treatment during the *emergence* possible
- ▶ *Local* treatment without damaging of the surrounding tissue possible

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³Stelzner et al. 2016.



State of the Art

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Research With Carryover



Interdisciplinary field of research:

- ▶ Sensor networks with *protocols* and *algorithms* The Nanogroup
- ▶ Mathematics with *analytical tools* and *simulations* What We Do
- ▶ Medicine with clinical trials Motivation
- ▶ Pharmacy with exploring medication Applications
- ▶ Bioengineering through construction of new nanostructures State of the Art
- ▶ Biology by exploring natural adaptive processes Prediction
- ▶ Chemistry & Physics by particle research Big Problems

Existing Nanostructures

What can already be created?



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- ▶ **Nanoparticles** for disease control
- ▶ Primitive **microbots**
- ▶ Primitive **transport structures**
 - ▶ Liposomes
 - ▶ DNA-boxes
 - ▶ „Dead“ bacteria
- ▶ DNA-Origami structures

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Gold Nanoparticles



For fighting cancer:

- ▶ „Coating“ of nanoparticles by *antibodies*
- ▶ *Binding* of nanoparticles to desired tissue
- ▶ *Heating* of nanoparticles via lasers
- ▶ Nanoparticles vibrate & *heat up*
- ▶ The heat *kills* cancer tissue

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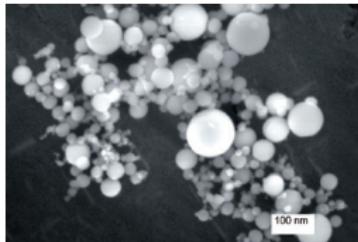
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Aluminum nanoparticles⁴.

⁴Nau 2016.

Magnetic Nanoparticles



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Magnetic particle imaging:

- ▶ Uses *iron oxide particles* the size of about 10 nm
- ▶ Assists in *visualizing* biological processes
- ▶ Activation of particles by *magnetic fields*
- ▶ Calculation of locations from *resonance*

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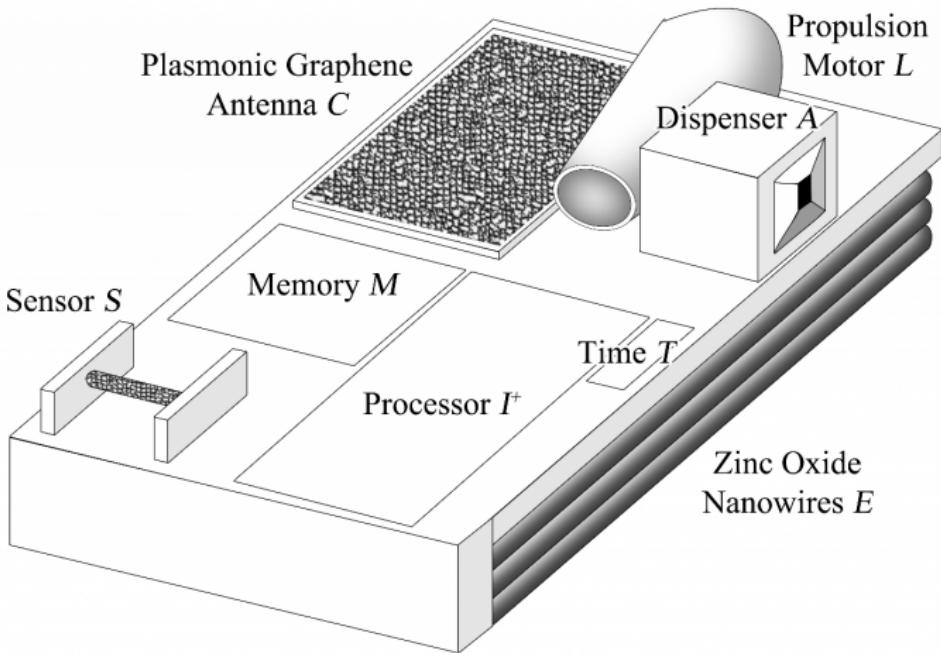
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Microbots I



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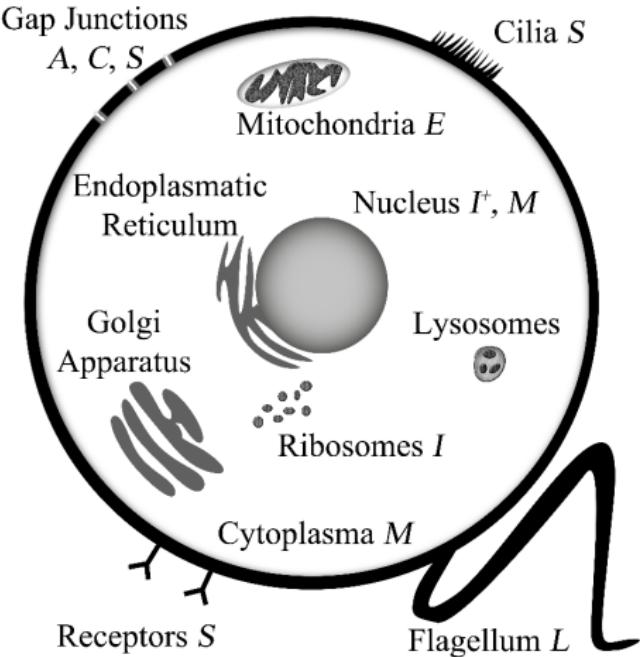
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Cell Bots



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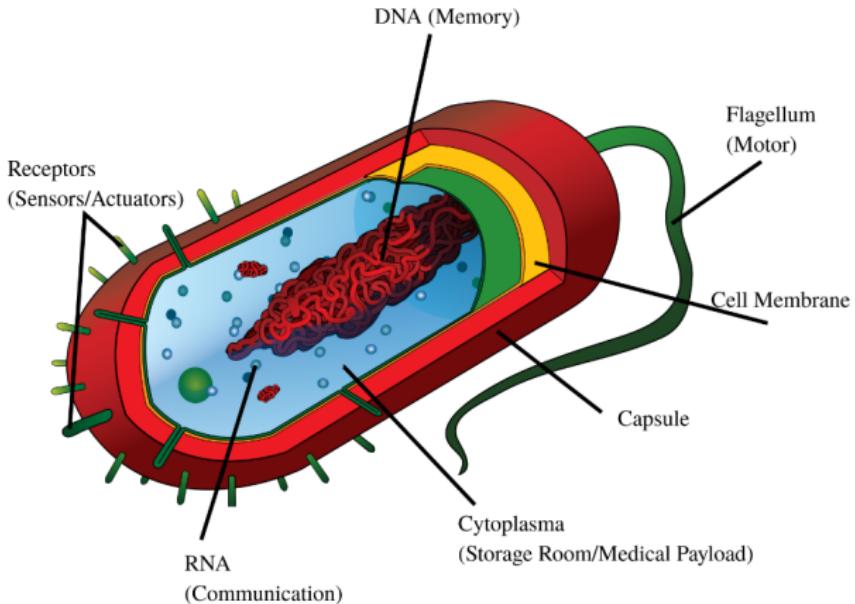
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Bacteria Bots



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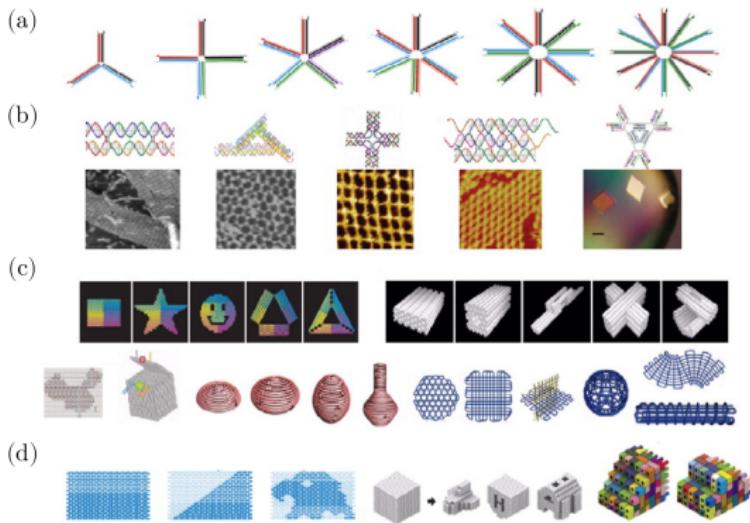
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DNA Nanosctructures



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Collection of already produced nanostructures⁵.

⁵Chao et al. 2015.



Prediction

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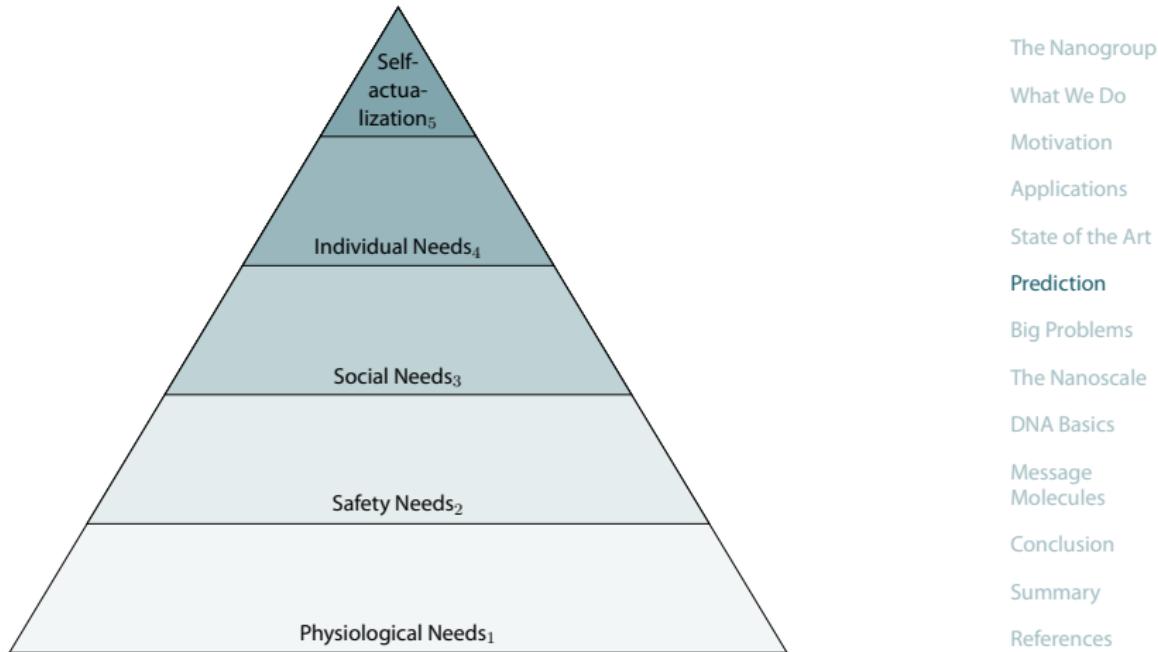
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Prognosis



Economics



Industry	GDP \$	% of GDP	Maslow	
Housing	1898	13 %	2	The Nanogroup
Local government	1336	9 %	2	What We Do
Finance	1159	8 %	2	Motivation
Health	1136	8 %	1	Applications
Durable products	910	6 %	4	State of the Art
Retail trade	905	6 %	4	Prediction
Wholesale	845	6 %	4	Big Problems
State government	658	5 %	2	The Nanoscale
Data	646	4 %	4	DNA Basics
Entertainment	591	4 %	3-5	Message Molecules
Construction	529	4 %	2	Conclusion
Disposal	448	3 %	2	Summary
Others Services	447	3 %	4-5	References
Services	297	2 %	4-5	
Mining	290	2 %	4	
Administration	284	2 %	4-5	
Education	174	1 %	1-5	
Agriculture	173	1 %	1	

Overarching Problems



Great unresolved problems in nanoresearch:

- ▶ ***Construction*** of nanoscale, functional components for nanodevices or nanonetworks
- ▶ ***Communication*** and communication mechanisms at the nanoscale
- ▶ ***Computations*** that take the restrictions at the nanoscale into account
- ▶ ***Compatibility*** of all sub-solutions for holistic, nanoscale functional units or nanonetworks

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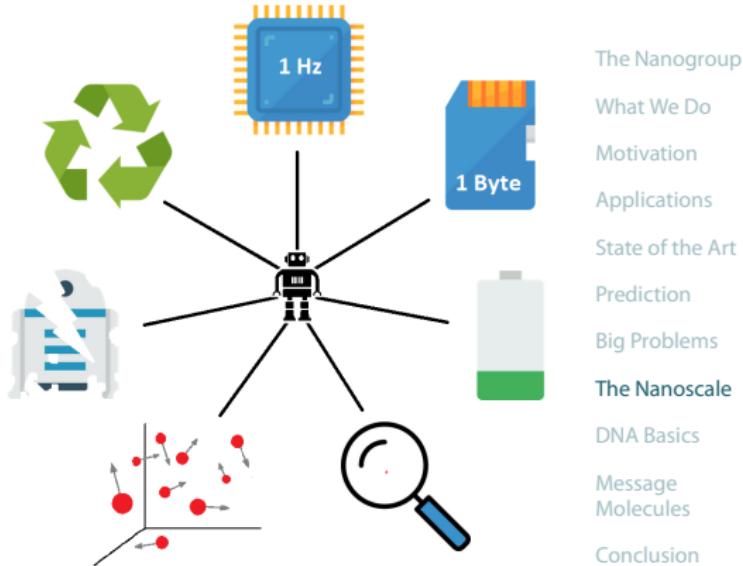
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Nanoscale Peculiarities



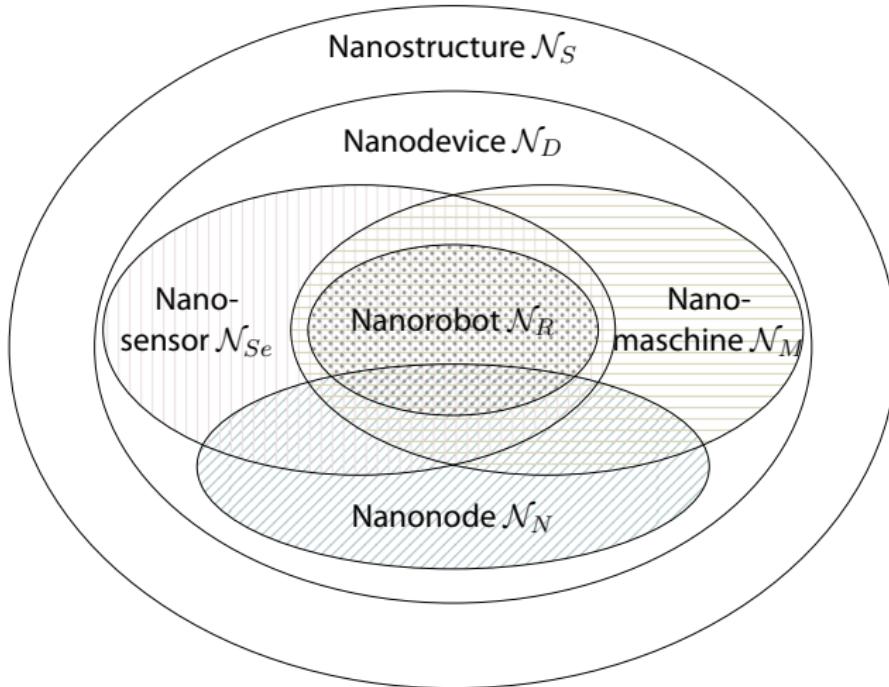
Unique Points:

- ▶ Extreme number of participants
- ▶ High topology dynamics
- ▶ Time/space restrictions
- ▶ Heterogeneity
- ▶ No central control instances
- ▶ No direct influence
- ▶ Biocompatibility
- ▶ Energy availability
- ▶ Waste disposal



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Machine Models



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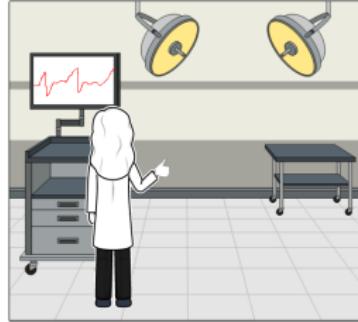
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Storyboard



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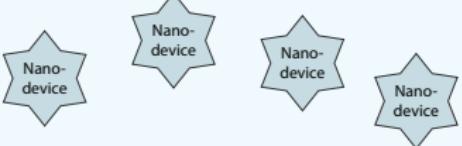
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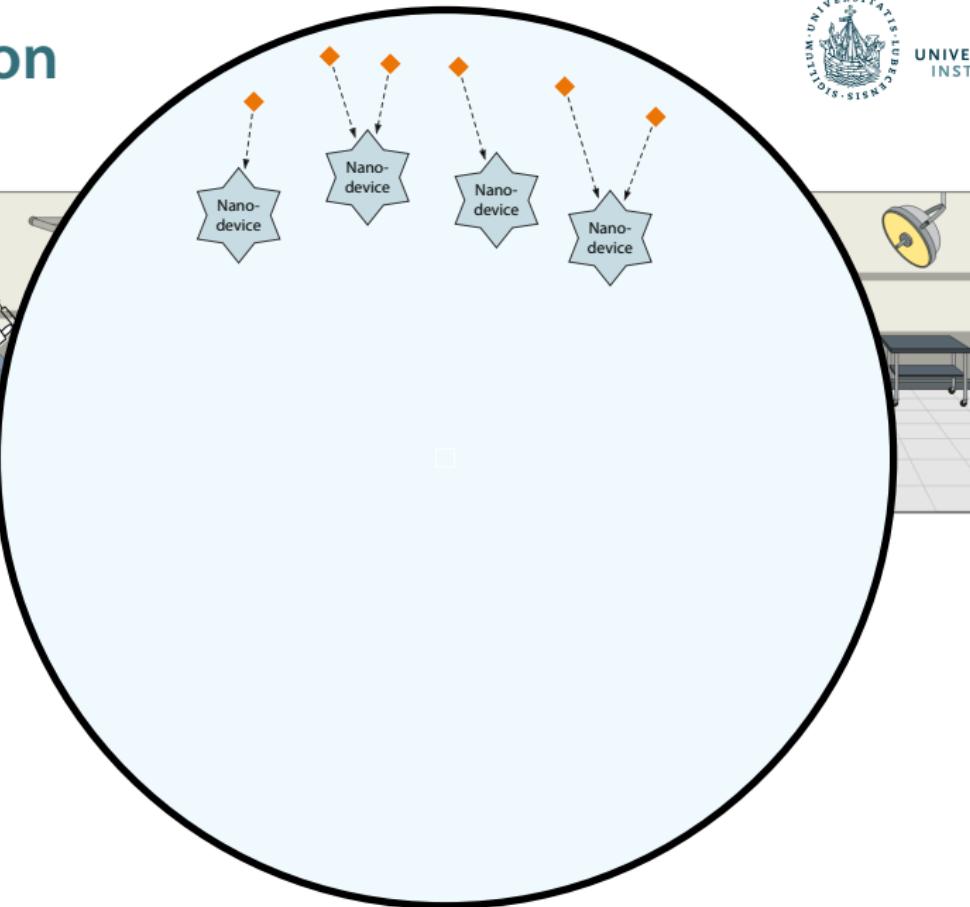
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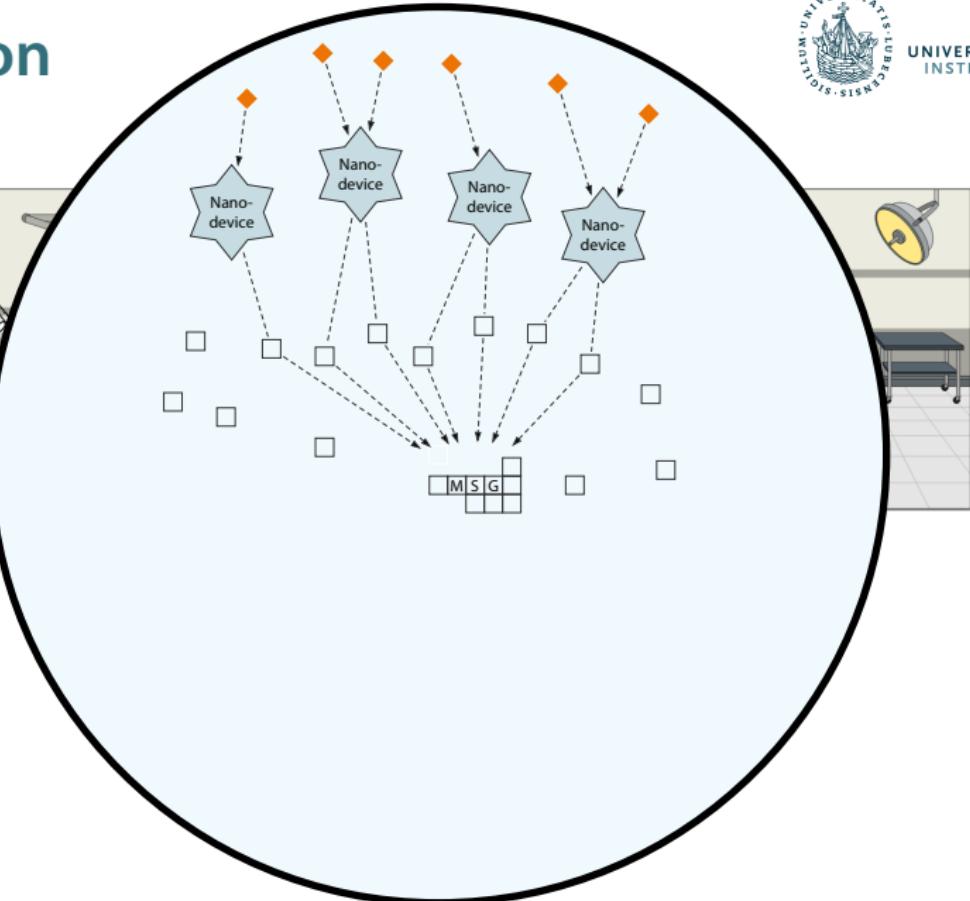
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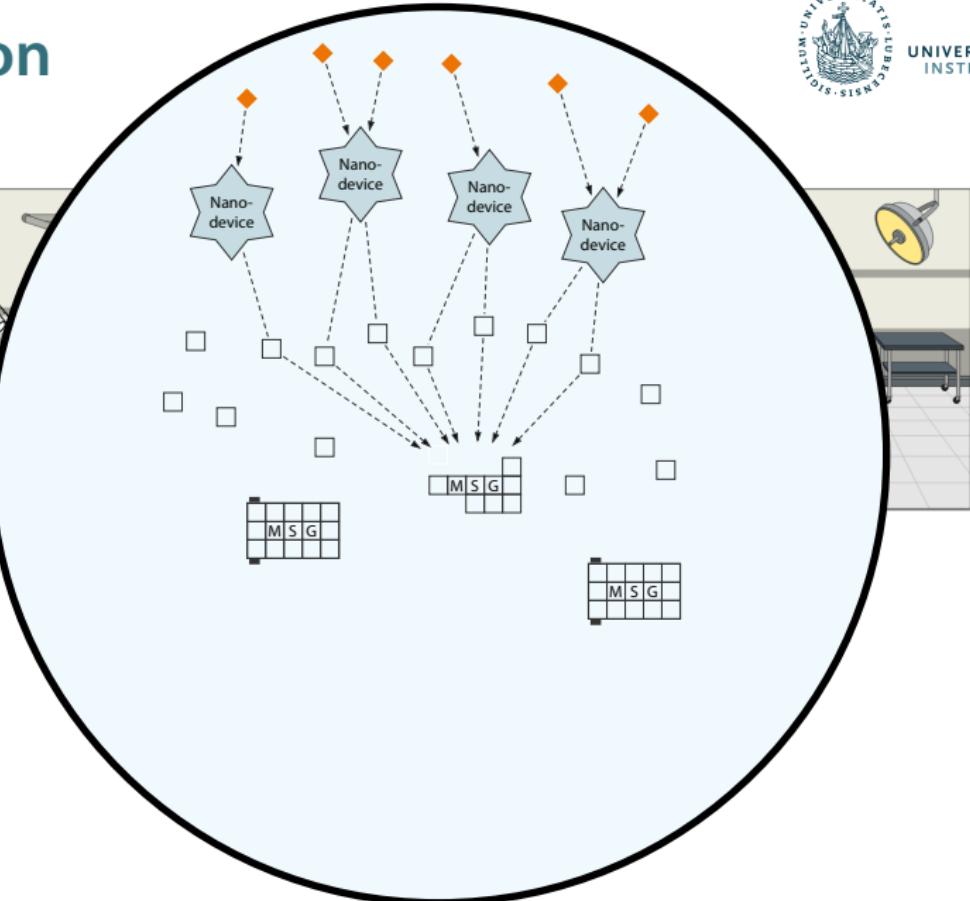
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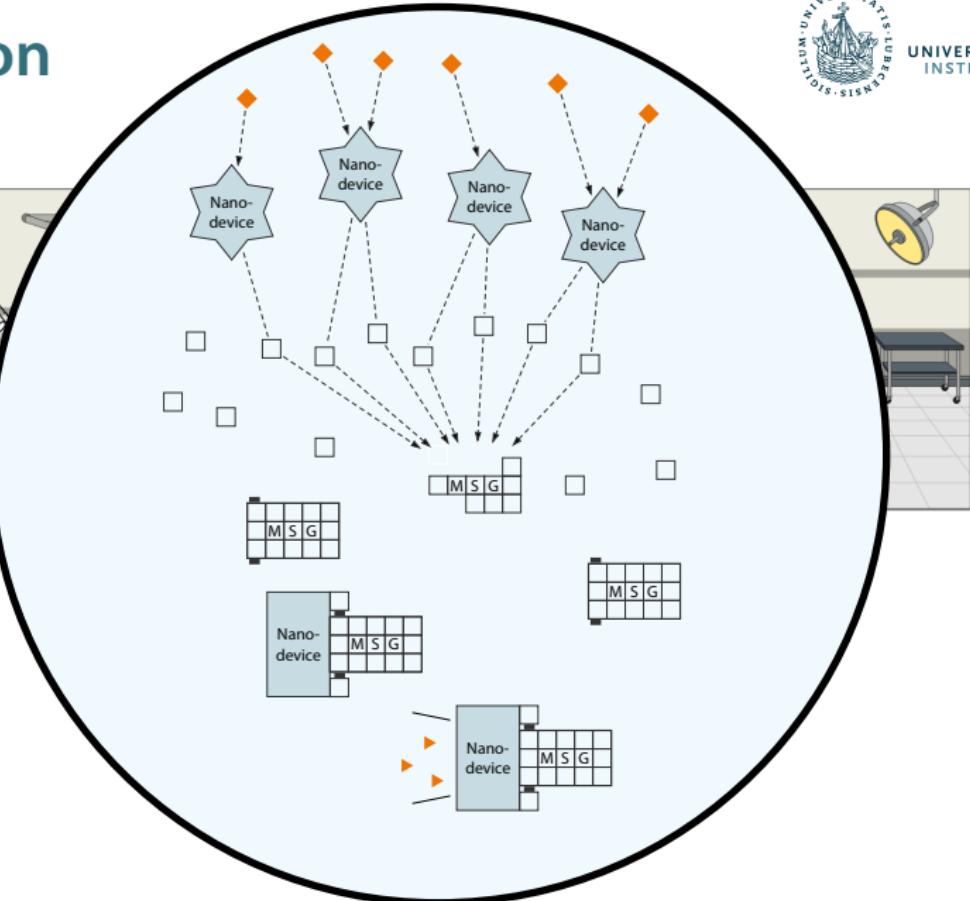
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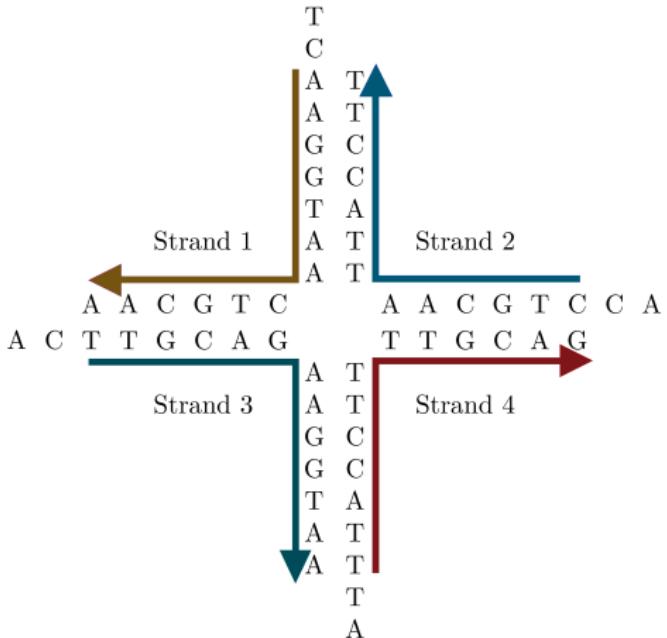
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DNA-Tiles



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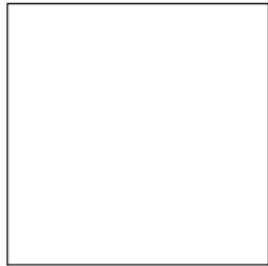
DNA-tile with glues in all directions

Model I



Formal definition of DNA-tiles⁶:

- ▶ Non-rotateable *blocks*



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⁶Lathrop, Lutz, and Summers 2007.

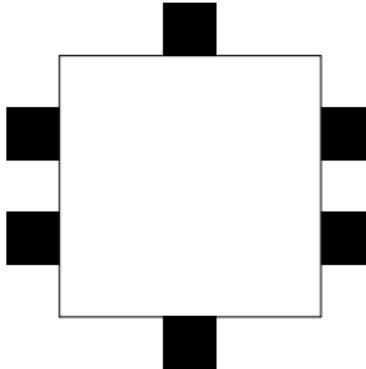
Model I



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Formal definition of DNA-tiles⁶:

- ▶ Non-rotateable *blocks*
- ▶ *Glues* on each side of different strength



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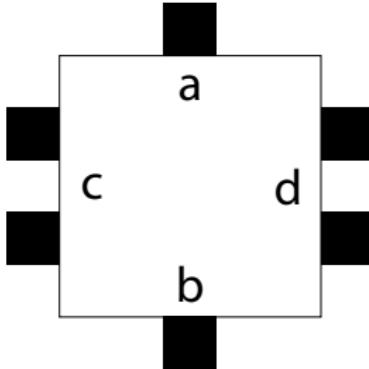
⁶Lathrop, Lutz, and Summers 2007.

Model I



Formal definition of DNA-tiles⁶:

- ▶ Non-rotateable *blocks*
- ▶ *Glues* on each side of different strength
- ▶ Glues have *labels*



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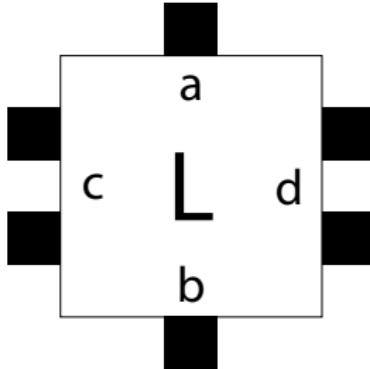
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Formal definition of DNA-tiles⁶:

- ▶ Non-rotateable *blocks*
- ▶ *Glues* on each side of different strength
- ▶ Glues have *labels*
- ▶ *Marker* in the middle



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⁶Lathrop, Lutz, and Summers 2007.

Model II



Important properties:

- ▶ Tiles can *compute* – they are Turing-complete³
- ▶ Tiles can *construct*⁴
- ▶ Tiles can *communicate* in networks⁵

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⁷Winfree et al. 1998.

⁸Patitz 2014.

⁹Lau, Büther, Geyer, et al. 2019.

Model II



Important properties:

- ▶ Tiles can *compute* – they are Turing-complete³
- ▶ Tiles can *construct*⁴
- ▶ Tiles can *communicate* in networks⁵
- ▶ Influenced by the *temperatur* τ

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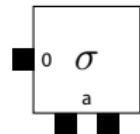
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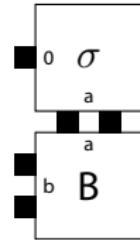
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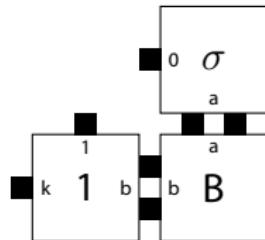
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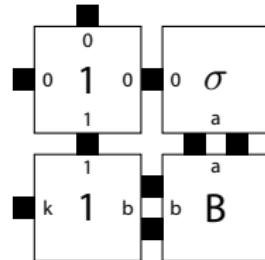
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⁷Winfree et al. 1998.

⁸Patitz 2014.

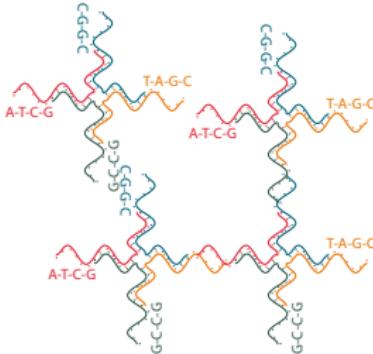
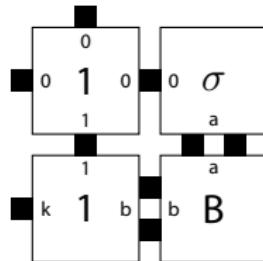
⁹Lau, Büther, Geyer, et al. 2019.

Model II



Important properties:

- Tiles can *compute* – they are Turing-complete³
- Tiles can *construct*⁴
- Tiles can *communicate* in networks⁵
- Influenced by the *temperatur τ*



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⁷Winfree et al. 1998.

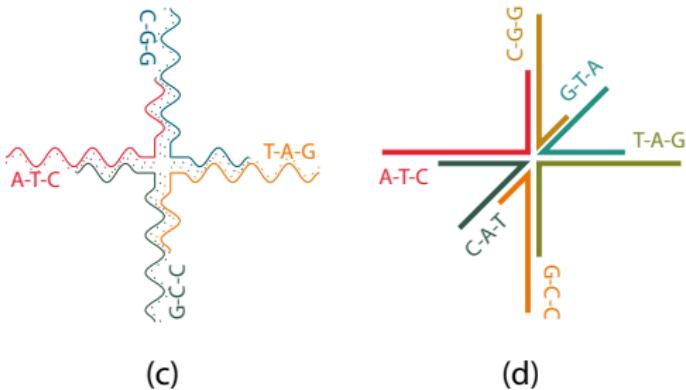
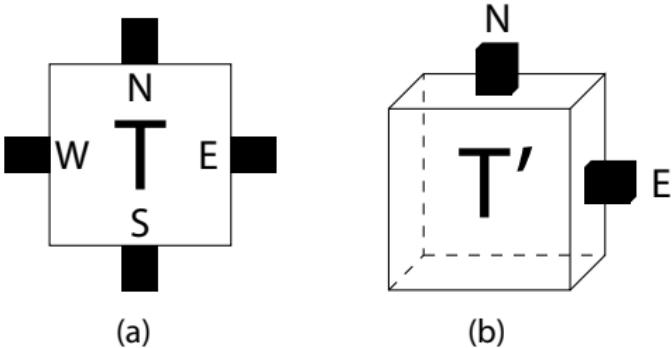
⁸Patitz 2014.

⁹Lau, Büther, Geyer, et al. 2019.

From 2D- to 3D-tiles



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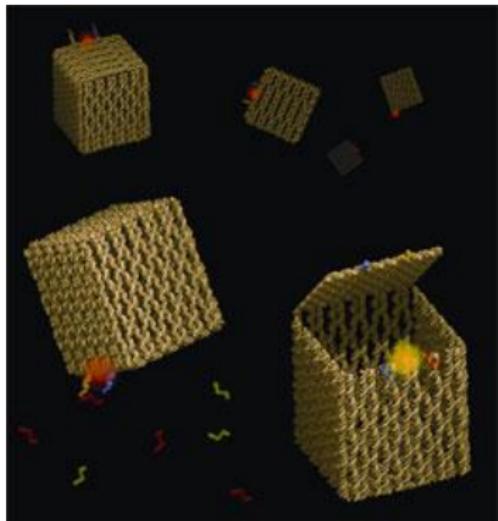


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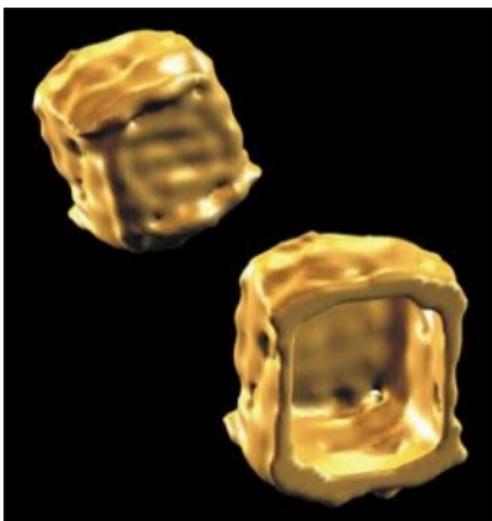
DNA-Origami-Nanobots



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Schematic DNA-Box



Realistic DNA-Box¹¹

¹¹ Andersen, Dong, Morten M. Nielsen, et al. 2009.

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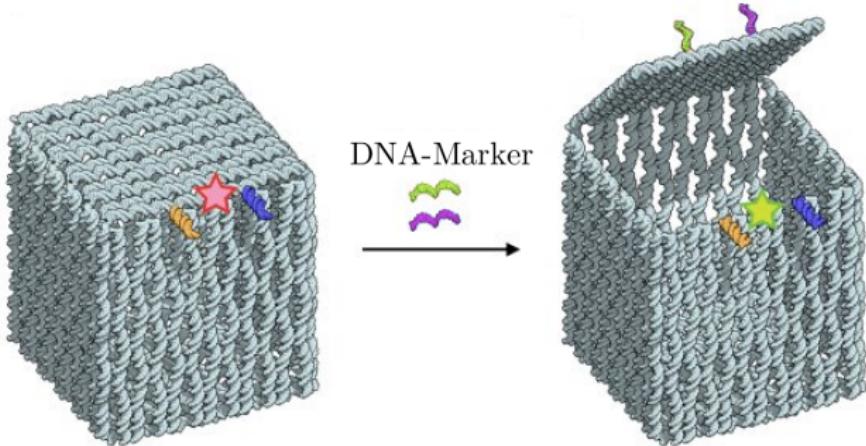
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Mechanism DNA-Box



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Mechanism of the DNA-Box

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¹¹ Andersen, Dong, Morten M. Nielsen, et al. 2009.

Interim Conclusion



Results to far:

- ▶ Until now showed what is possible *constructed*

How do we *compute* and *communicate*?

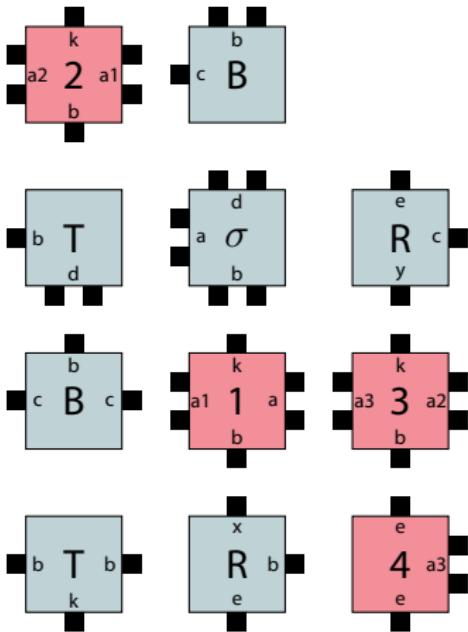
- ▶ Computations in *messages* instead of nanobots
- ▶ Computations via *conditional* assembly
- ▶ Input via *event based* release of specific tiles
- ▶ *Formation of a ligand* after a *successful* computation

⇒ Advantage: Fewer *resource constraints* in the channel!¹²

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¹²Lau, Büther, Geyer, et al. 2019.

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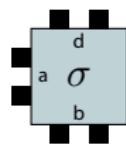
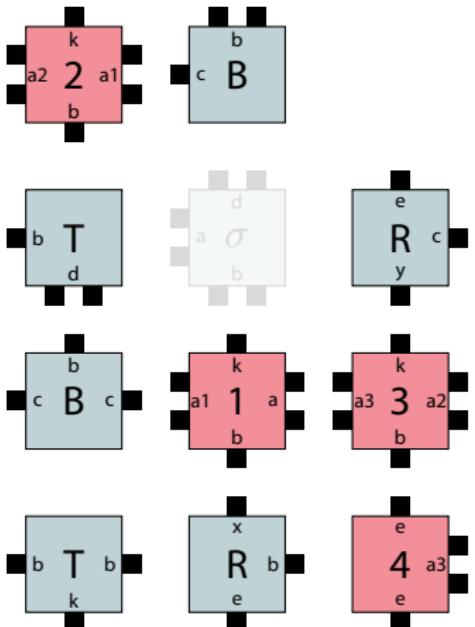
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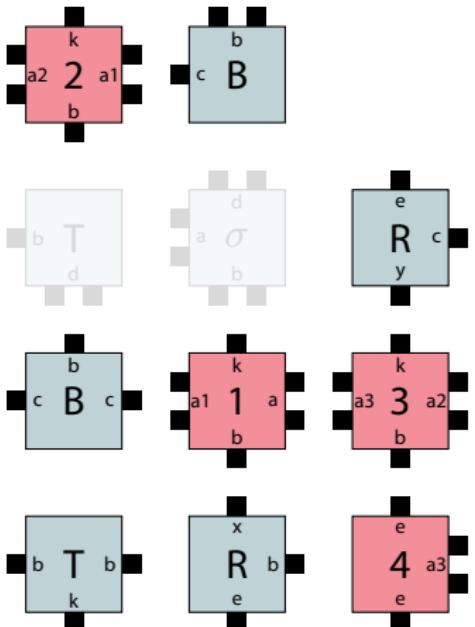
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¹²Lau, Büther, Geyer, et al. 2019.

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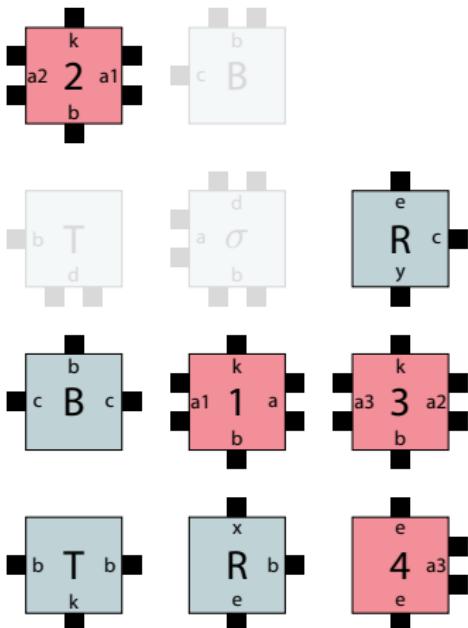
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¹²Lau, Büther, Geyer, et al. 2019.

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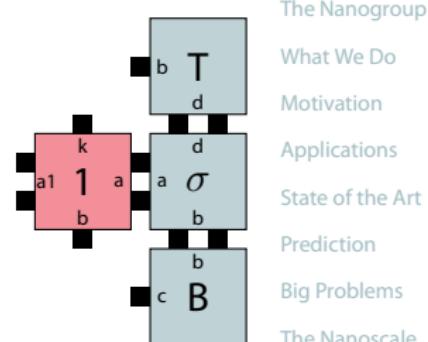
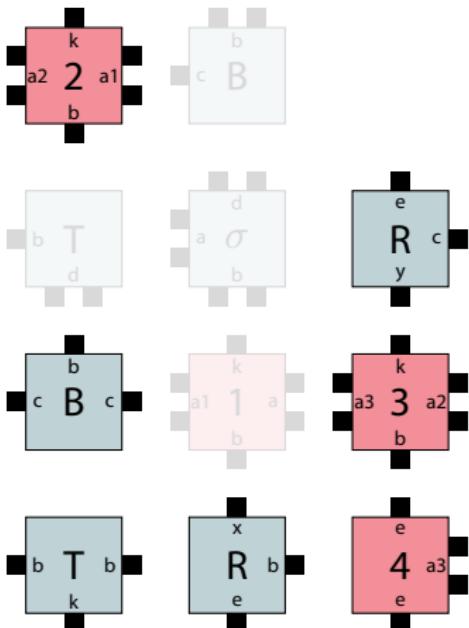
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¹²Lau, Büther, Geyer, et al. 2019.

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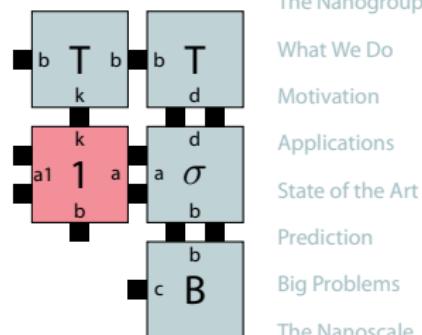
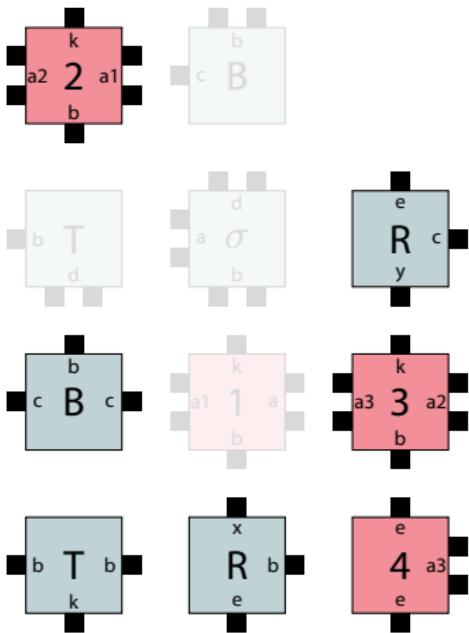
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¹²Lau, Büther, Geyer, et al. 2019.

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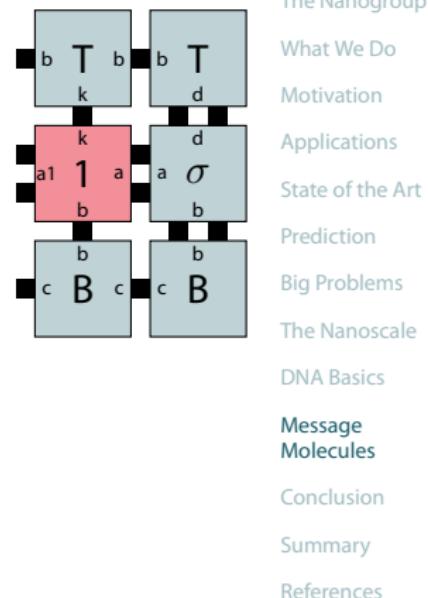
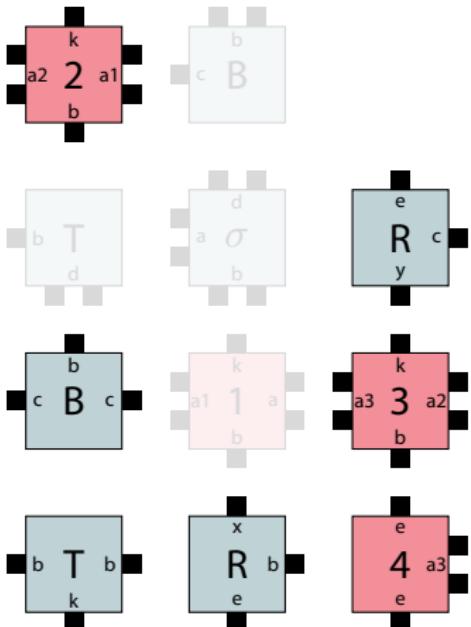
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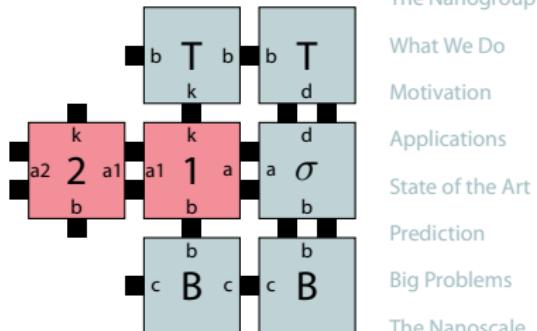
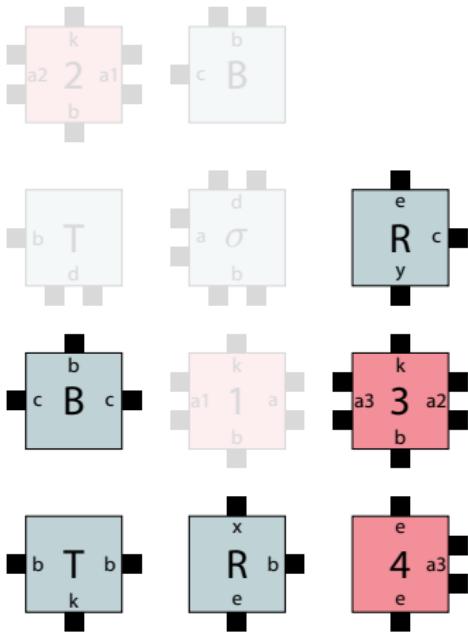
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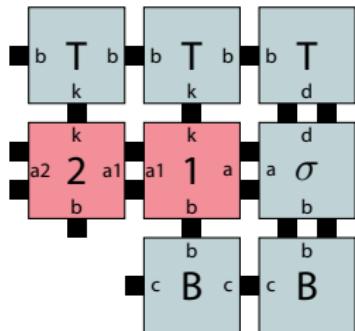
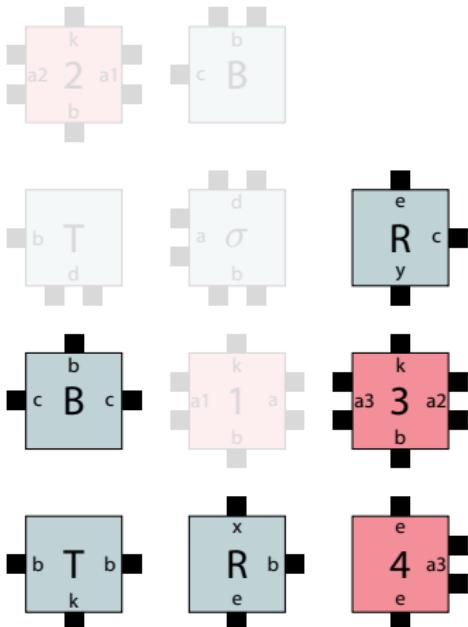
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¹²Lau, Büther, Geyer, et al. 2019.

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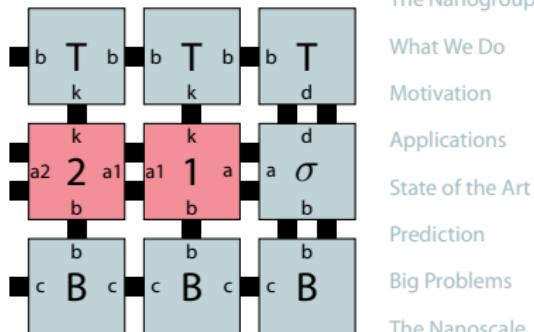
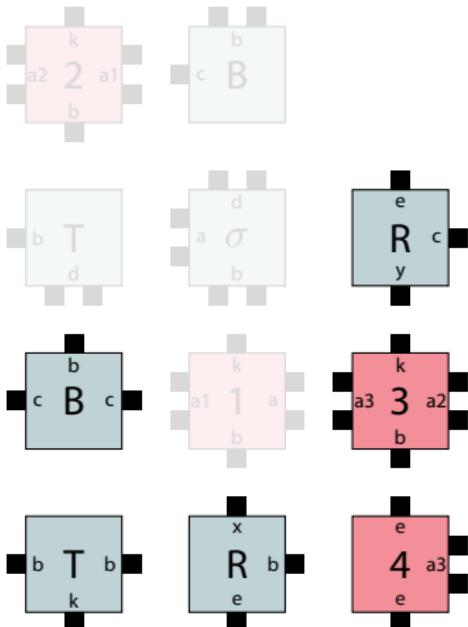
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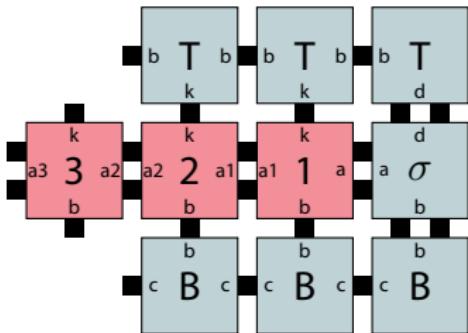
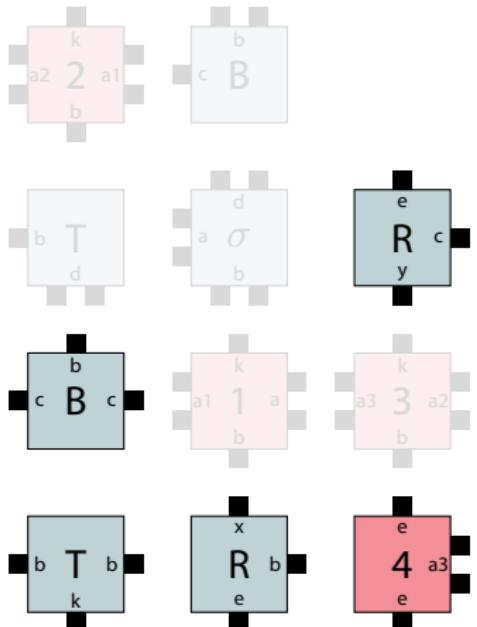
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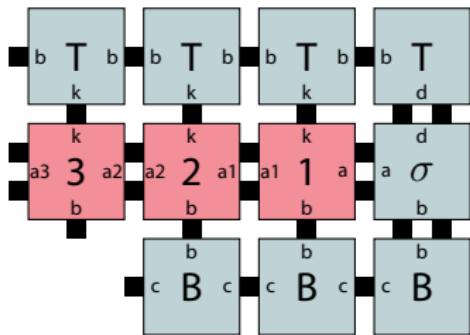
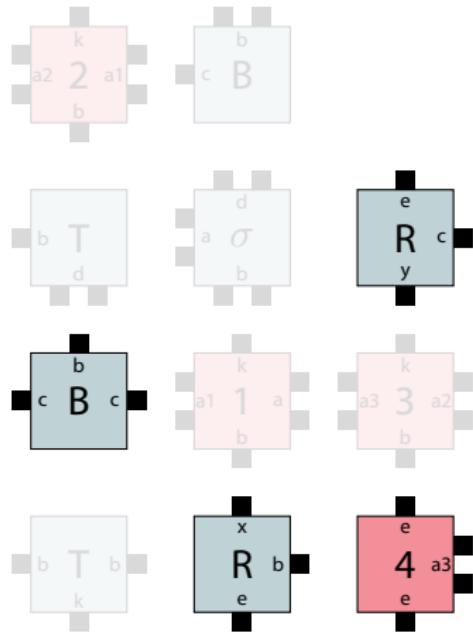
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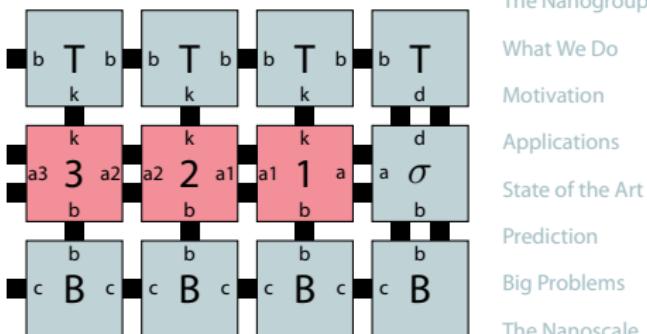
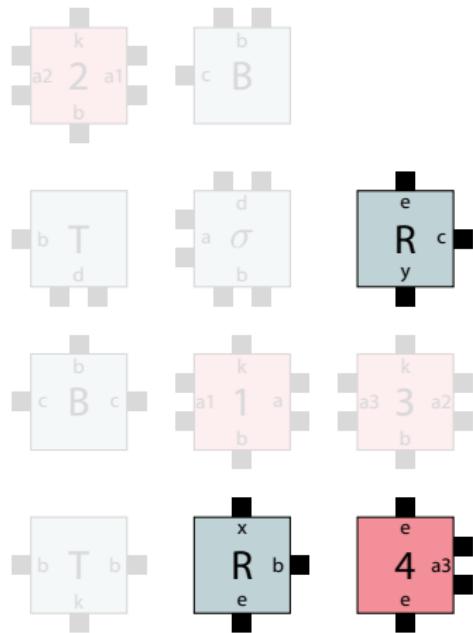
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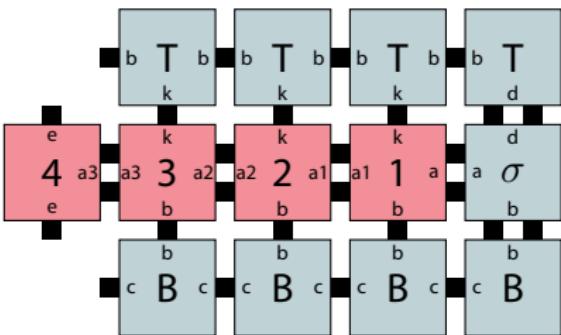
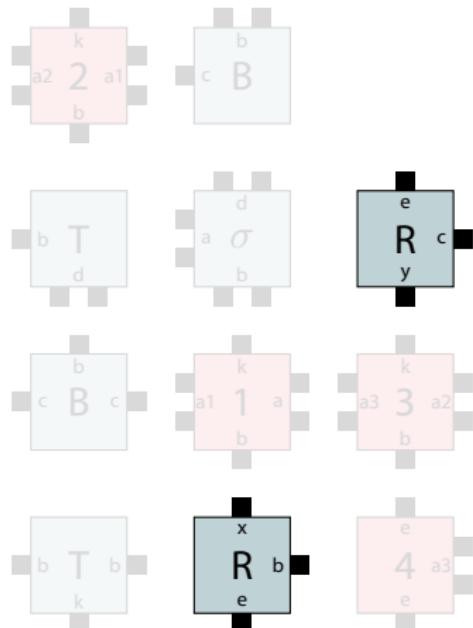
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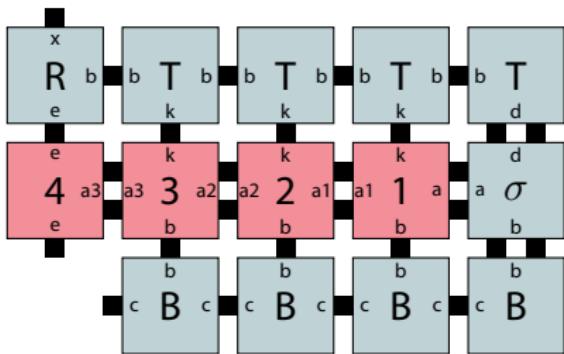
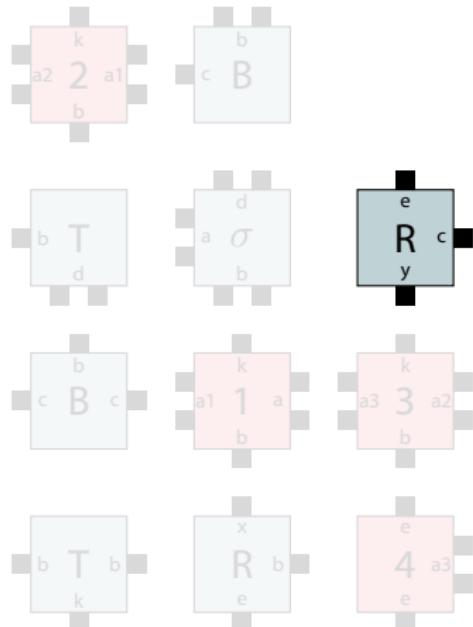
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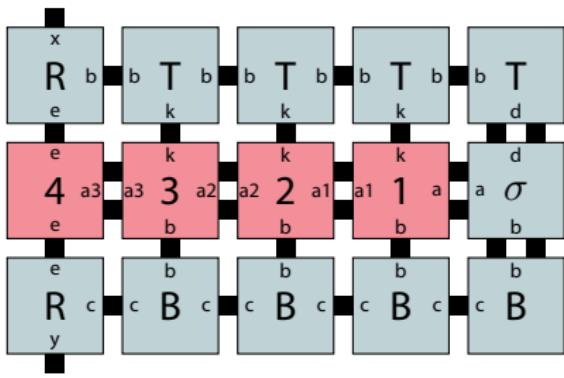
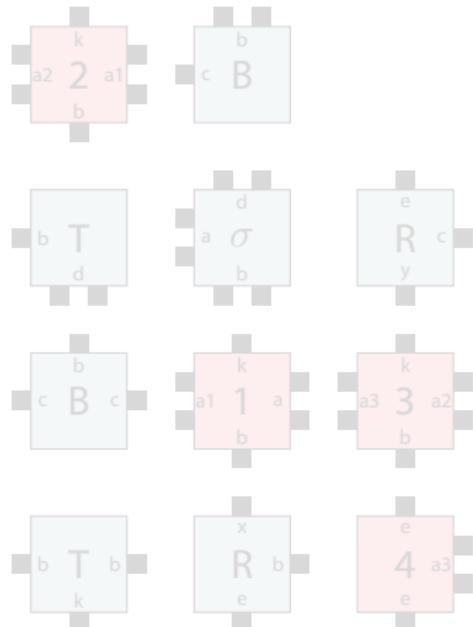
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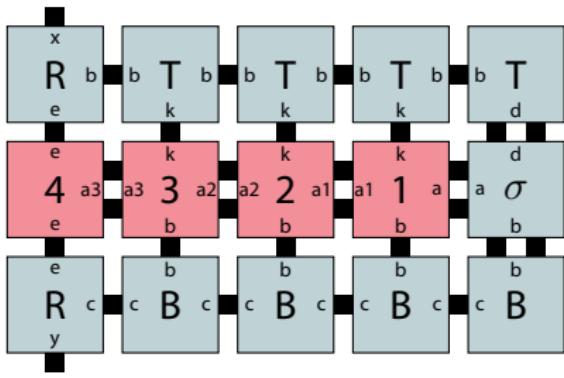
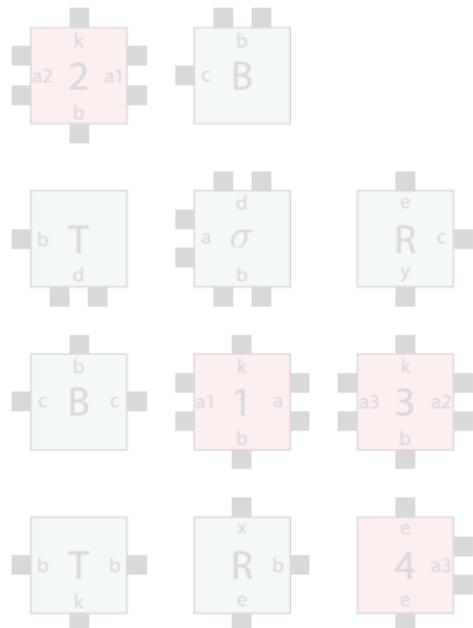
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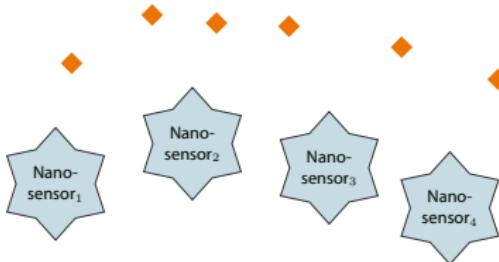
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⇒ Full assembly **only** when tiles 1–4 are present

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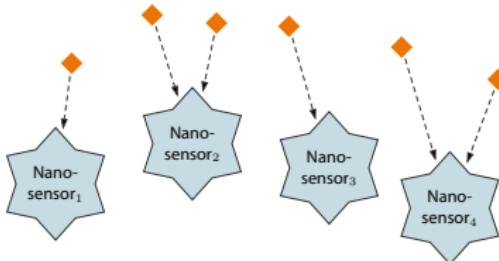
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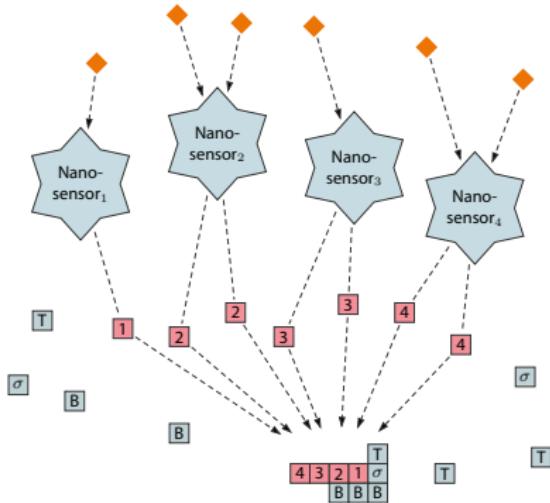
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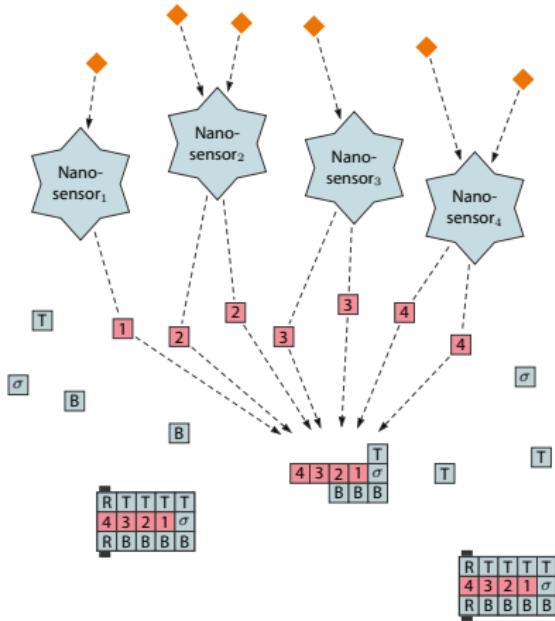
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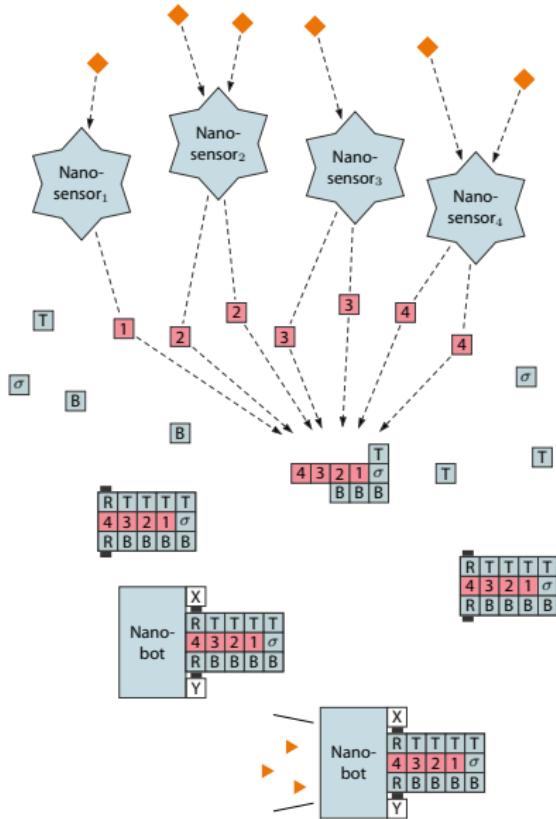
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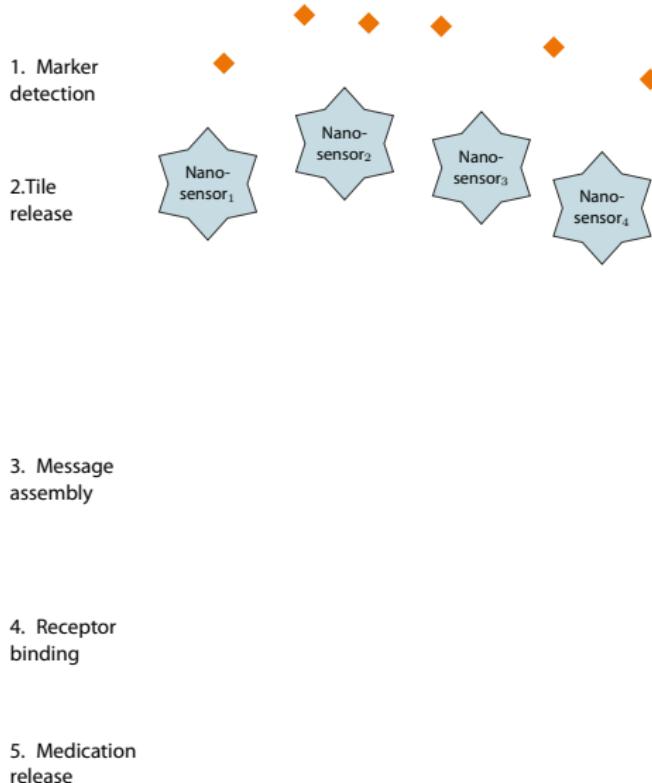
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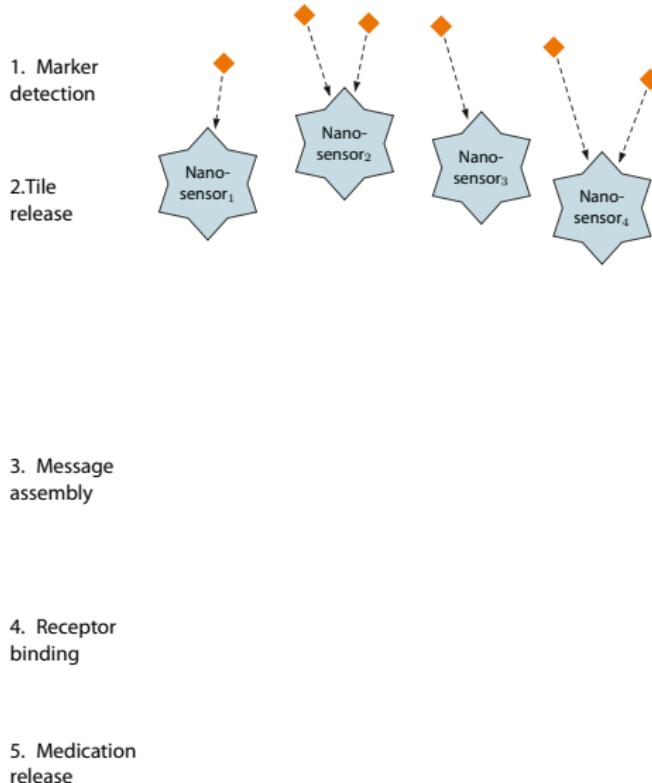
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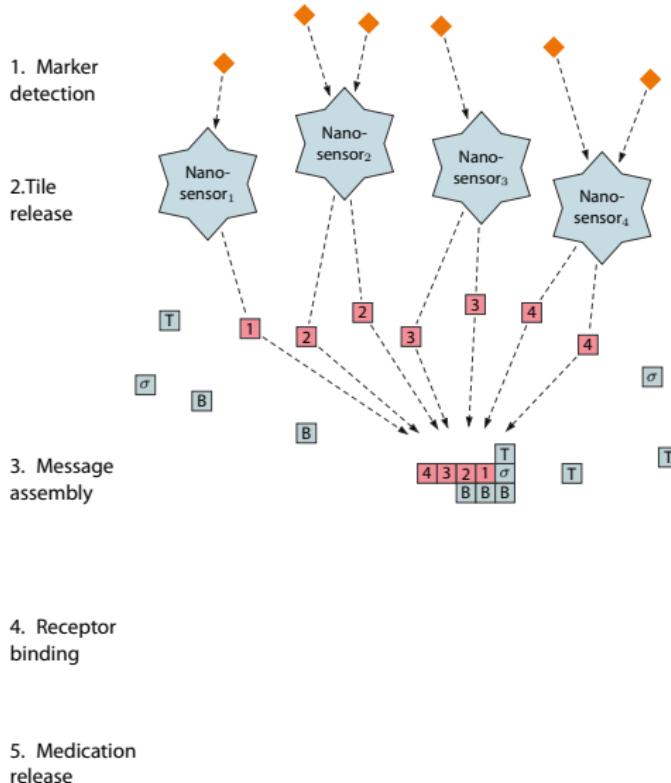
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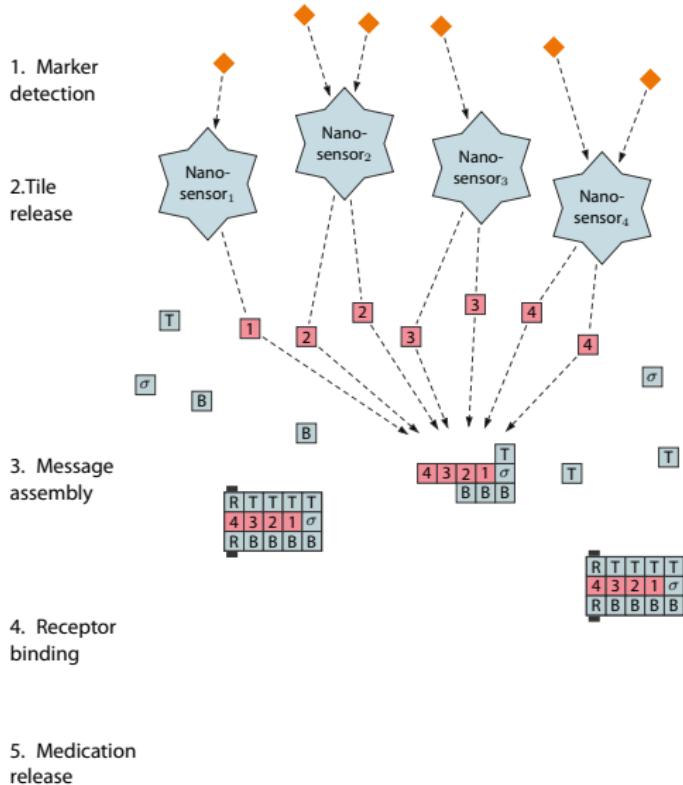
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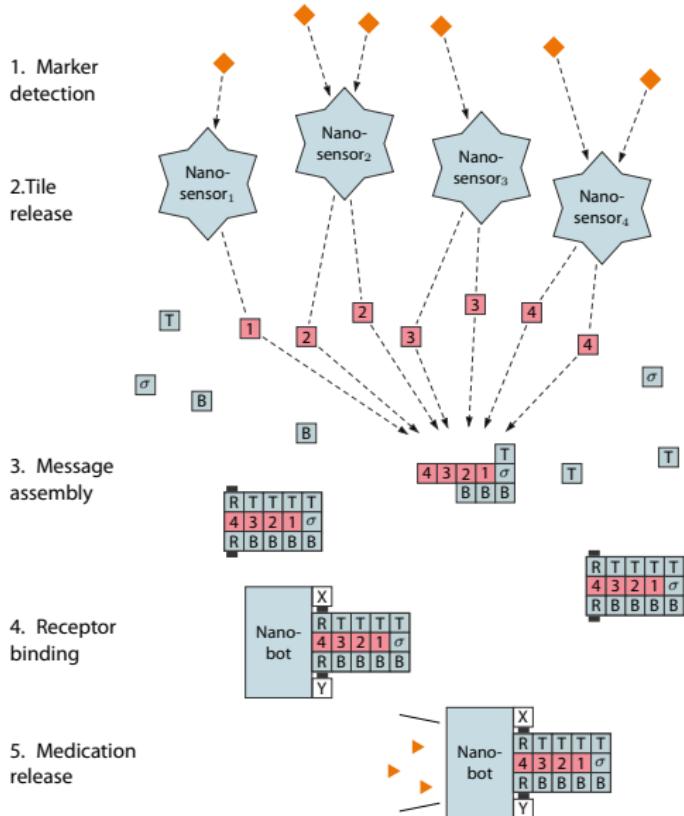
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Modularization



The following realizable *modules* exist:

1. Detecting a *arbitrary marker* through a nanosensor. Li et al. have already shown that medication can be released after the detection of markers¹³.
2. The *storage* of tiles and drugs in nanostructures¹⁴.
3. *Assembly* of message molecule in the laboratory¹⁵.
4. The attachment of message molecule to a nanobot¹⁶.
5. The *release* of tiles or drugs, see 1.¹⁷.

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¹³Li et al. 2018; Benenson et al. 2004.

¹⁴Li et al. 2018; Andersen, Dong, Morten M Nielsen, et al. 2009.

¹⁵Lee et al. 2004.

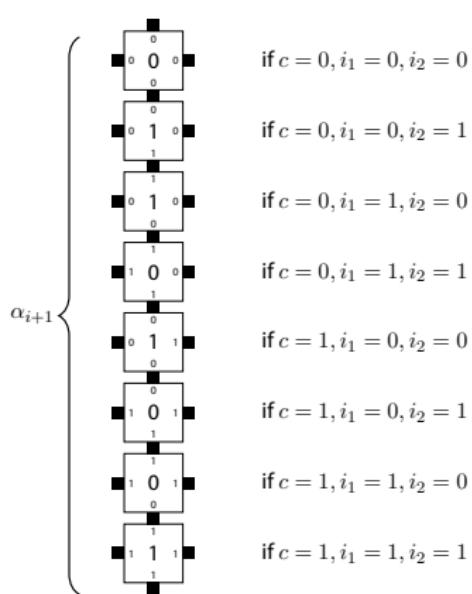
¹⁶Cheng et al. 2005.

¹⁷Li et al. 2018.

Add



Behavior ADD:



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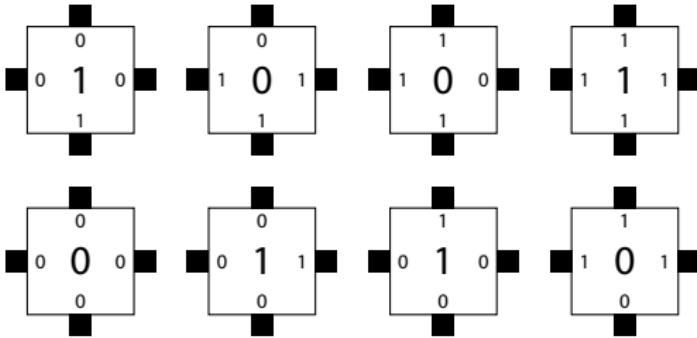
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Function Problem Add



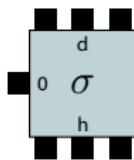
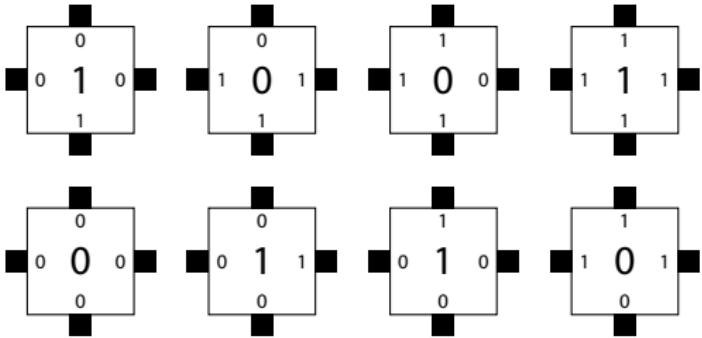
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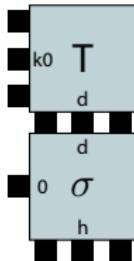
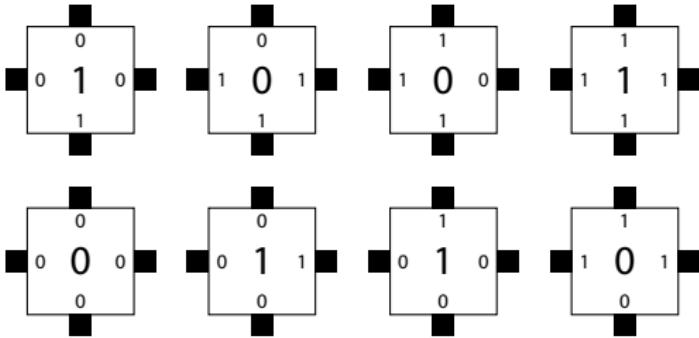
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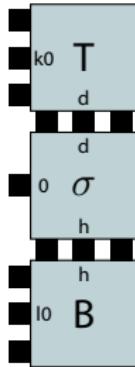
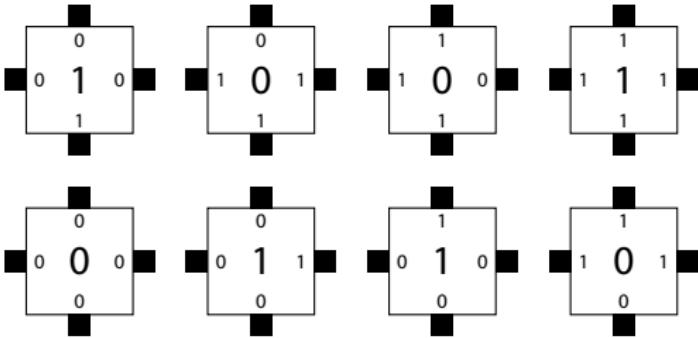
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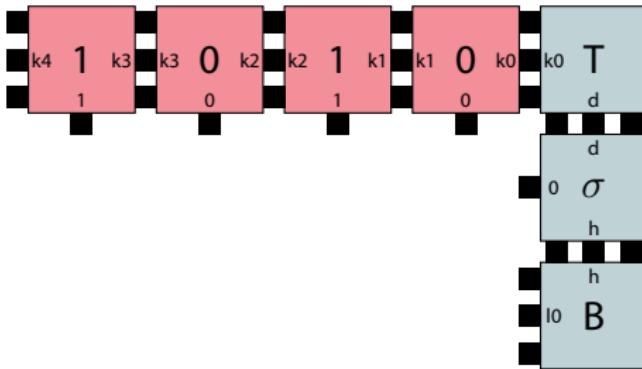
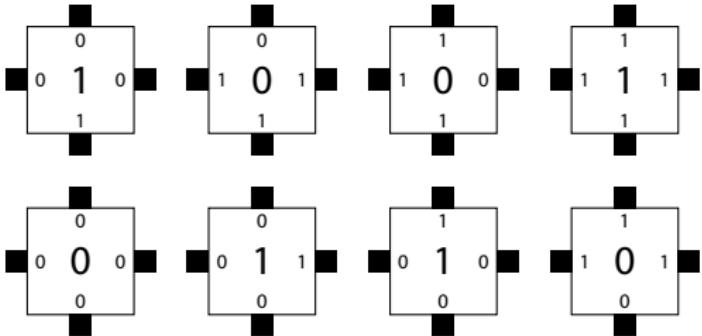
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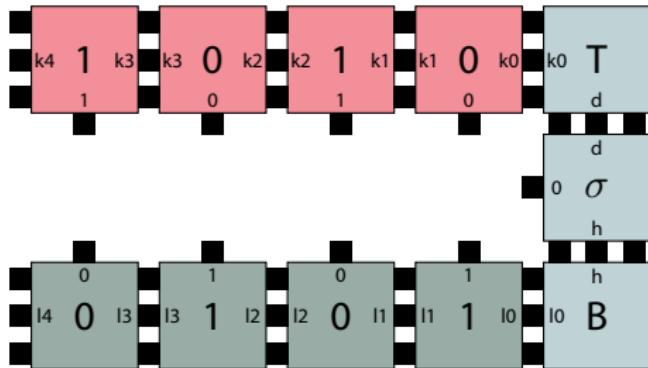
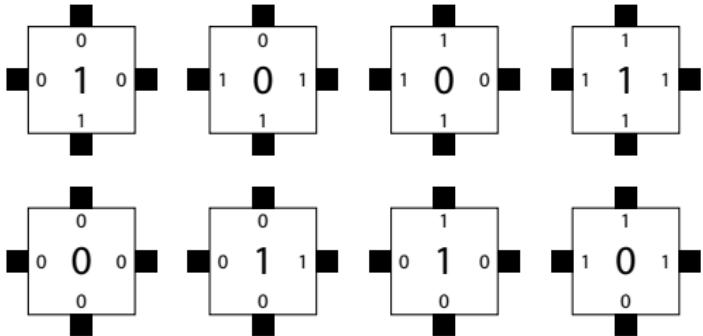
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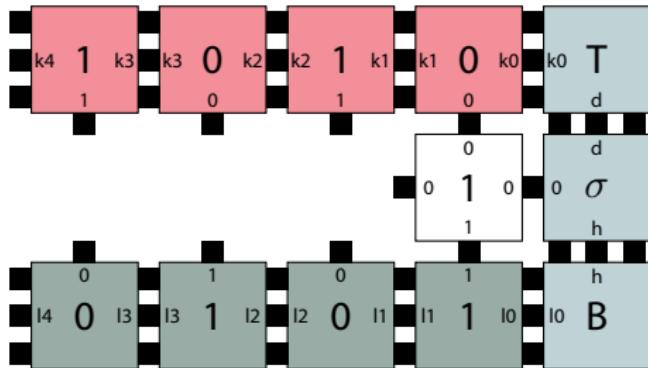
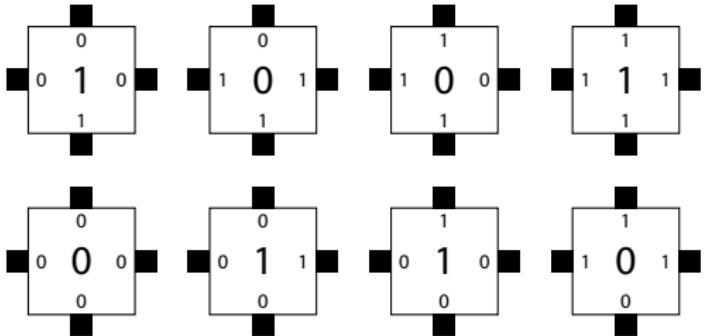
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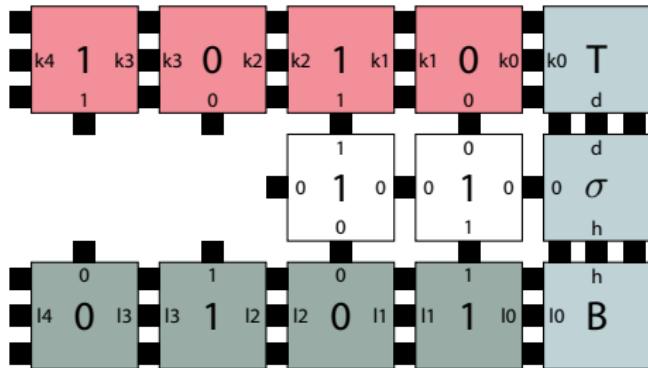
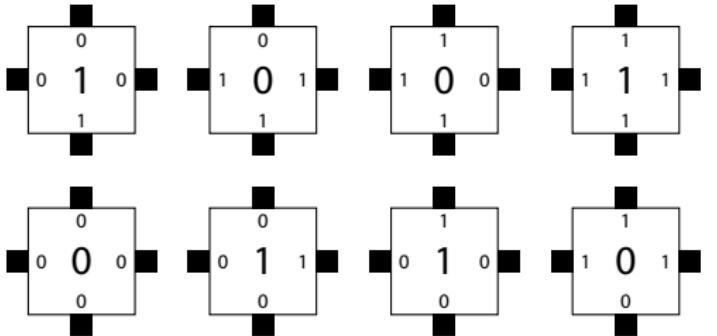
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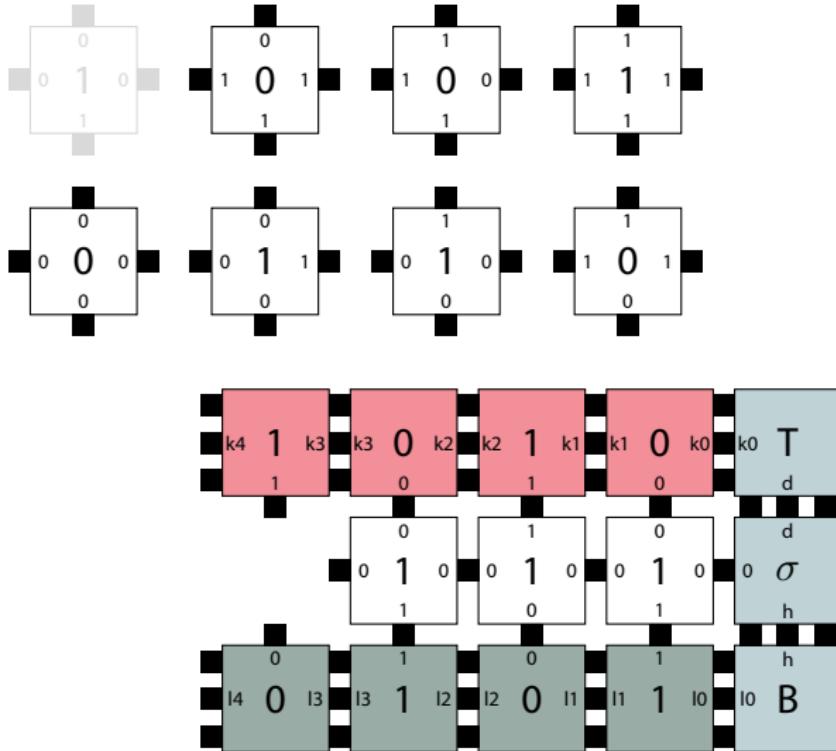
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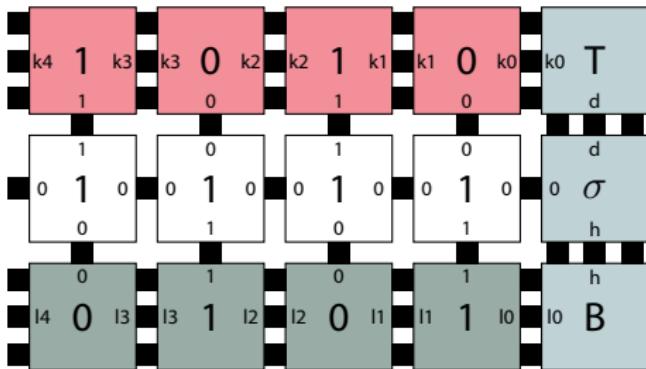
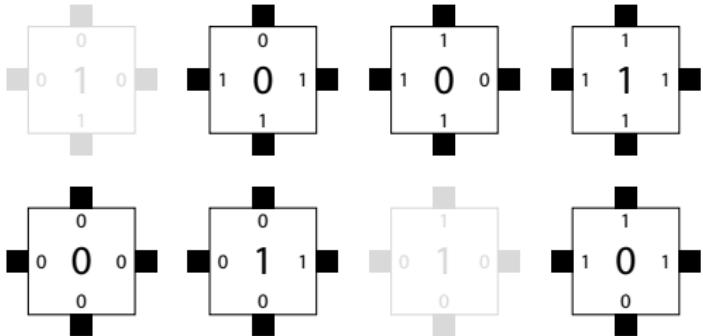
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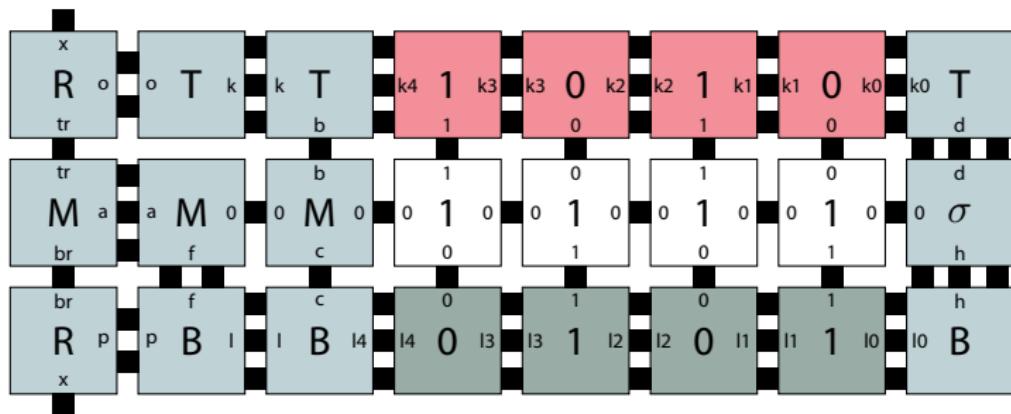
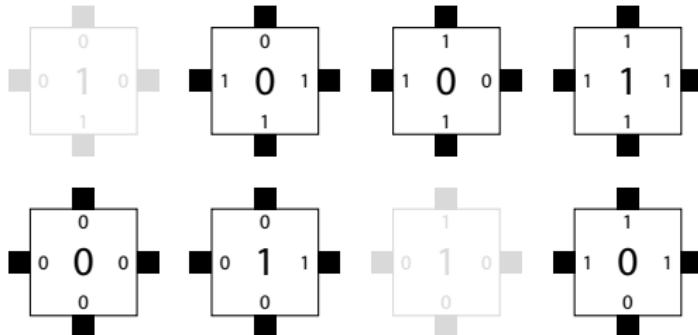
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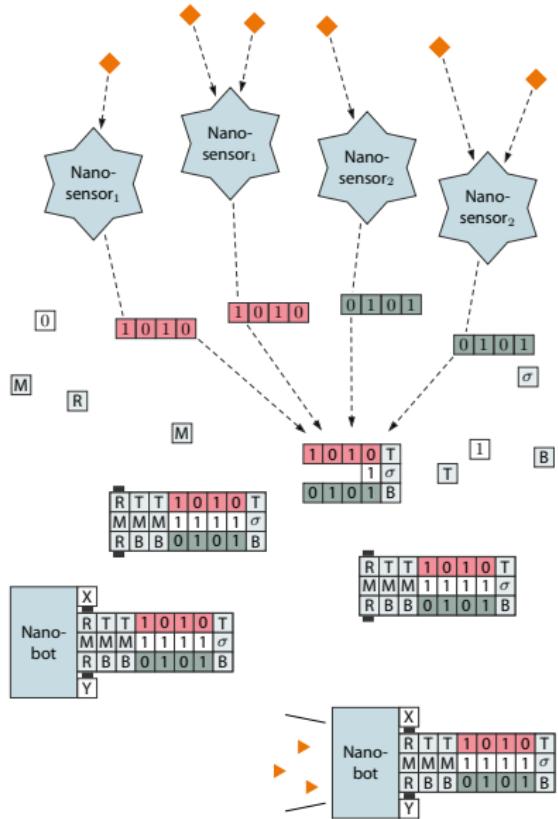
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Add-Nanonetwork



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Thres



Behavior THRES:

- ▶ Algorithm and input are identical
- ▶ Various molecules are formed
- ▶ These correspond to all *combinations* of a threshold size k
- ▶ In the example, a threshold value of 3 out of 4 input bits is calculated
- ▶ Message molecules are *different versions* of a AND molecule

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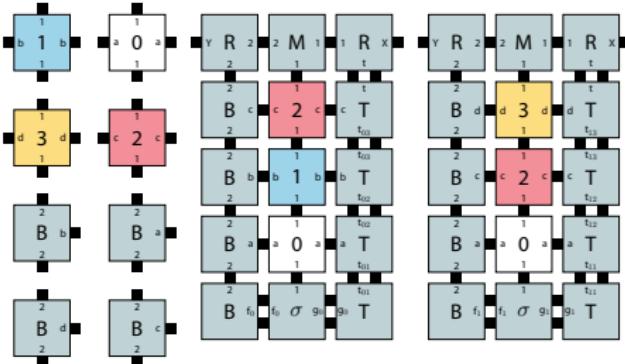
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Decision Problem Thres



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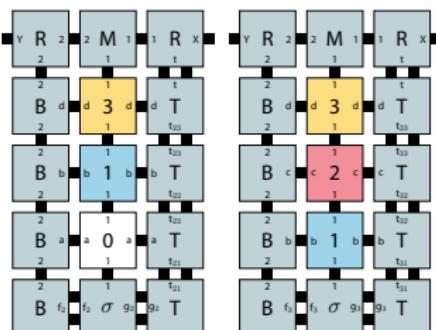
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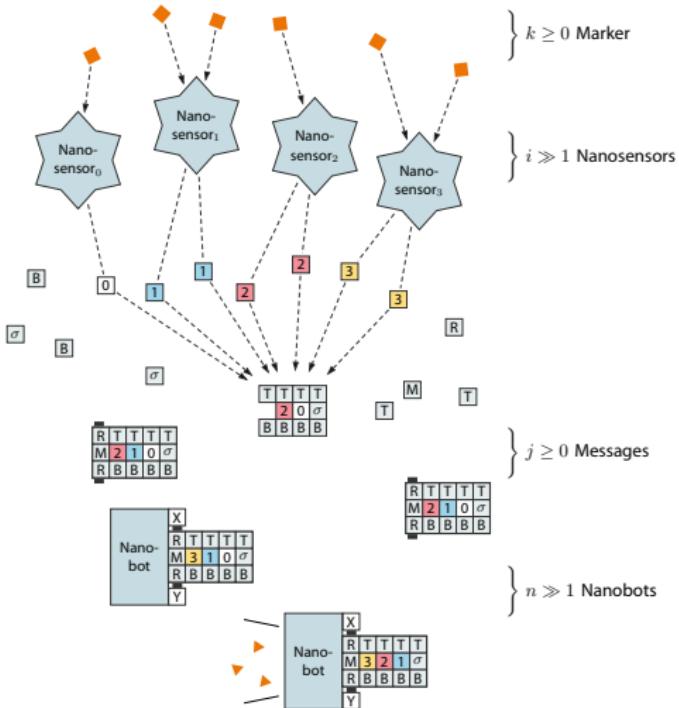
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General Procedure



Description:

1. Transformation of a *computation problem* into a *Boolean formula* Φ (if possible)
 2. Creation of a *truth table*
 3. Computation of the *disjunctive normal form* Φ
 4. Creation of a *message molecule* for each clause
- ⇒ The Boolean formula is successfully evaluated once a single message molecule is fully assembled.

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Φ -Tiles

ϕ_1	ϕ_2	...	Φ
1	1		1
1	0		1
		:	
0	1		0
0	0		1

Example truth table of
the formula Φ



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Example truth table of
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Φ -Tiles

ϕ_1	ϕ_2	...	Φ
1	1		1
1	0		1
		:	
0	1		0
0	0		1

Example truth table of
the formula Φ

- i -th row with „1“
- n -th Literal



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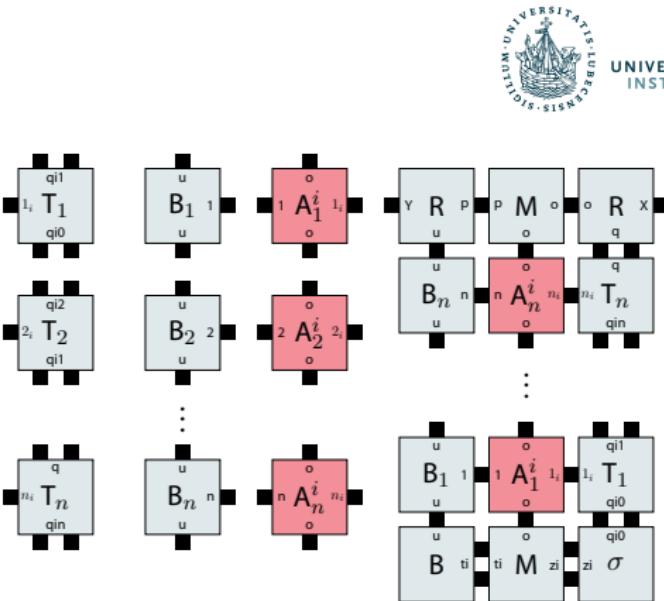
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Φ -Tileset

ϕ_1	ϕ_2	...	Φ
1	1		1
1	0		1
		:	
0	1		0
0	0		1

Example truth table of
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- i -th row with „1“
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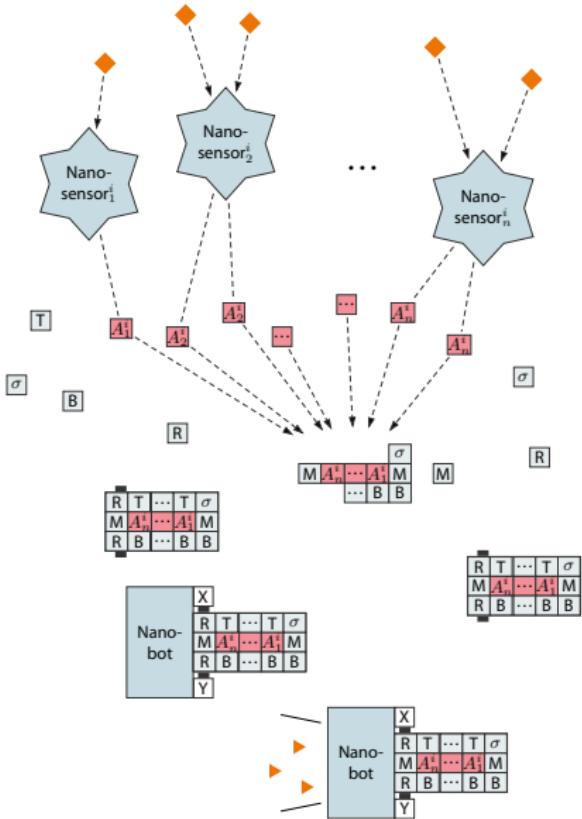
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Φ -Nanonetwork



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Turing Proof I



Proof sketch:

- ▶ Turing machine is a ***Tupel*** $M = (Q, \Sigma, \Gamma, \delta, q_0, q_{\square})$
- ▶ ***State space*** consists of ***tape, head position, state automata...***
- ▶ Simulation of a Turing Machine by a self-assembly systems
- ▶ Encoding of the machine states by ***rows from tiles***
- ▶ Creation of Tiletypes for ***transition function, tape, terminal state***
- ▶ Tile-stack of rows of Turing Machine states self-assembles
- ▶ Intuitively corresponds to a traversal of the ***Configuration graph*** of the Turing machine

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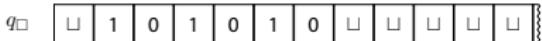
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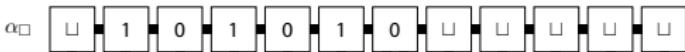
Turing Proof II



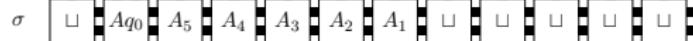
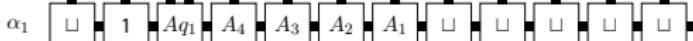
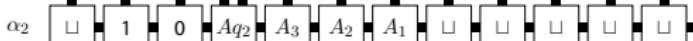
⋮



(a)



⋮



(b)

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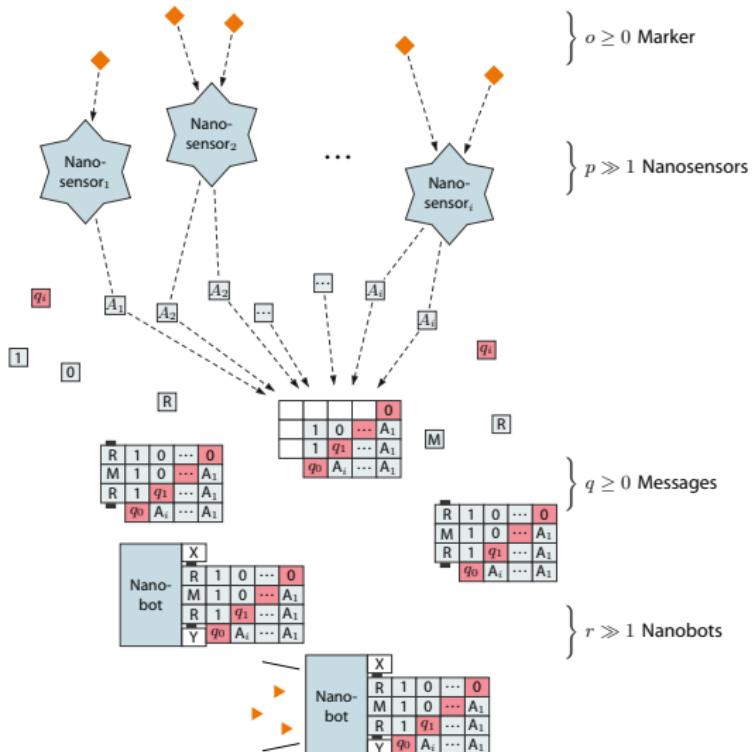
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Turing-Network



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Efficient Solvable Problems



	Medical Problems	Additional Problems	
AC ⁰ -Message:	ADD	ODD/EVEN	The Nanogroup
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	SIGN	MOD ₂	Motivation
	INC	INV	Applications
	AND/OR	LOG ₂	
NC ¹ -Message:	MULT	MIN/MAX	State of the Art
	DIV	PARITY	Prediction
	EXP	AVG	Big Problems
	MAJOR	MOD	The Nanoscale
	THRES	IT-MULT	DNA Basics
	IT-ADD ¹⁸		Message Molecules
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⇒ Less **overhead** than Turing-based tile systems, **fewer errors** and **realistic binding** at a nanobots because of **size restrictions** of the message molecules.

¹⁸Lau, Büther, and Gerlach 2017.

New Solvable Scenarios



- ▶ ***Continuous medical monitoring without quality of life limitations.*** Currently, this is only possible in a stationary environment under considerable deprivation.
- ▶ ***„Immediate treatment“ during emergence.*** So far, it almost always has to come to the outbreak of illness and associated symptoms before being intervened.
- ▶ ***Local treatment without systemic consequences.*** So far, drugs are almost always given *systemic* and thus relate to the whole organism.

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Novel Contributions



- ▶ **Fingerprinting** by detecting specific tissues via DNA markers
- ▶ Fast alternative DNA-detection mechanism compared to **PCR**
- ▶ Arbitrarily **programmable** and **error resistant**
- ▶ **Biocompatible**
- ▶ **Multi-parameter** diagnosis possible
- ▶ Can be created from **already existing** materials

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What do DNA-based nanonetworks achieve?

- ▶ DNA is a suitable material for *construction, computation* and *communication*
 - ▶ It is possible to create fully-functional nanonetworks from just DNA as a building block
 - ▶ It is possible to compute any *Boolean formula* at the nanoscale via message molecules
- ⇒ DNA-based nanonetworks only rely on already available technologies and can be used to perform *complex* and *arbitrary* computation!

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Thank you for your attention!

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