Programming biomolecular self-assembly pathways

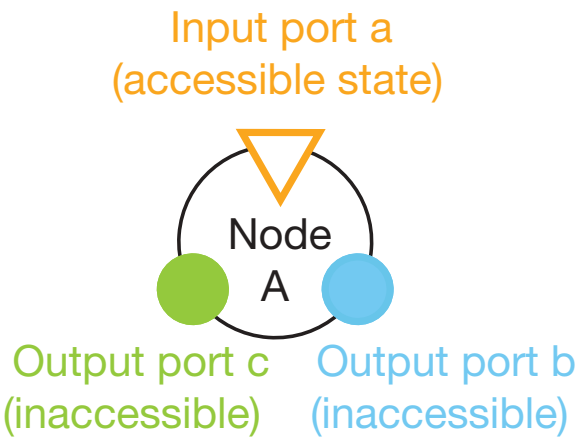
Yin, P., Choi, H. M. T., Calvert, C. R., & Pierce, N. A. (2008). Programming biomolecular self-assembly pathways. Nature, 451(7176), 318–322. doi:10.1038/nature06451

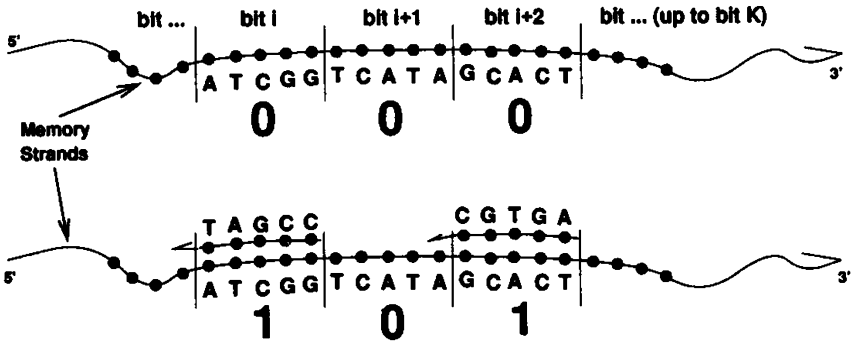
Slides by Reem Mokhtar

DNA Modeling

- Visual communication or modeling paradigms/ concepts (cartoons, states, etc)
- Graphical and Data representation (software, data structures, etc)
- Grammatical/Language representation of DNA and reactions.

Visual Communication/Models





- Purpose: ease of visual communication or modeling of a specific paradigm/concept
- May be conceptual abstractions or realistic representations of:
  - Structure
  - Reactions
- Notation used in literature
- Representation depends on needs of communication & conceptualization:
  - Tiling
  - Hybridization reactions
  - Animation of movement
  - Seesaw gates

Nodal Abstraction

Aim: diagramming reaction execution process as a “program”

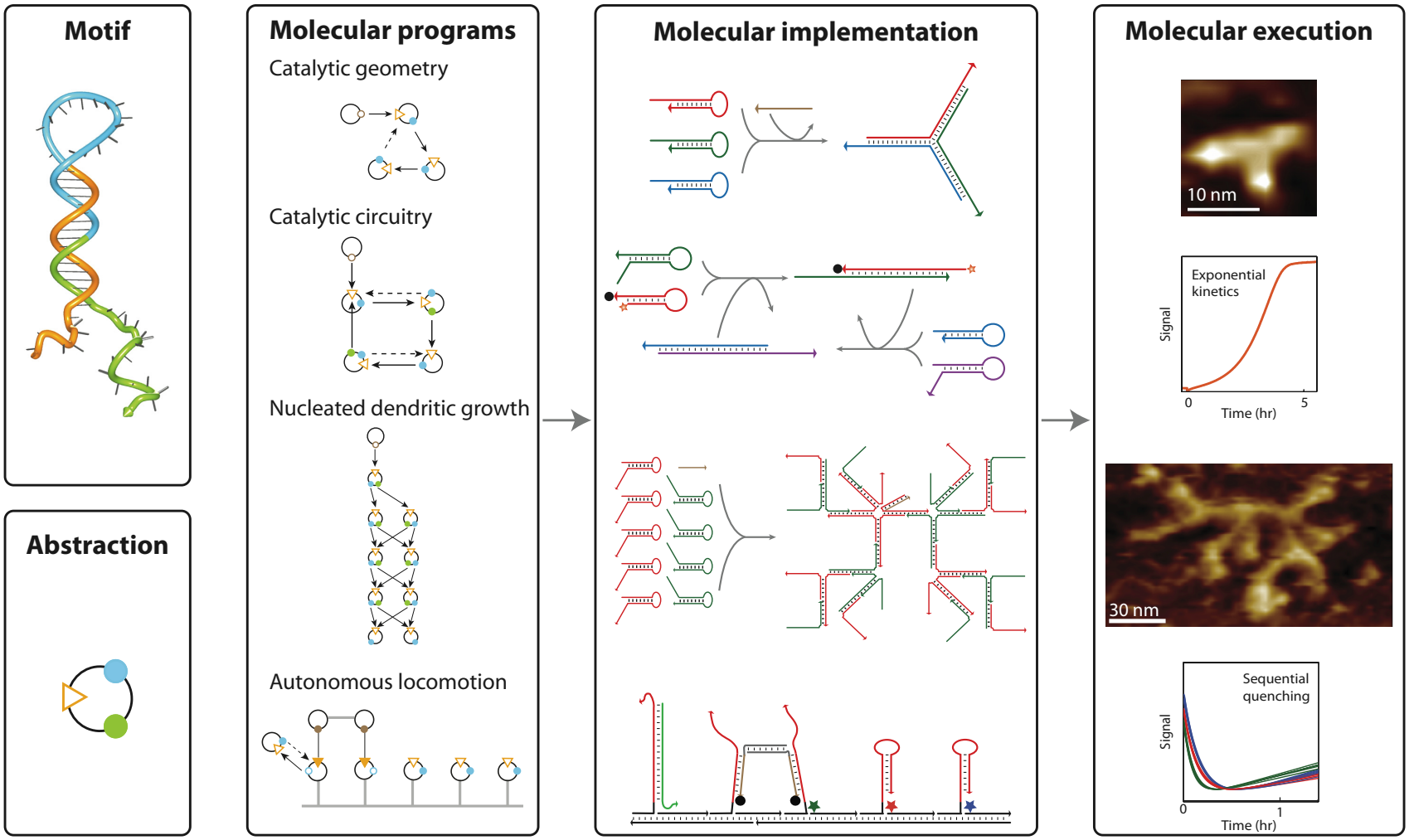


Figure S1. Summary. Diverse biomolecular self-assembly (and disassembly) pathways are programmed using an abstraction of a versatile DNA hairpin motif.

Rules

IC:

1) defined by state of each port + initial bonds

2) bond between output port/input port → reaction already took place.

Elements:

1) Static → gray line segments. inert during execution.

2) can be used to impose geometric constraints

Starting point:

1) beginning of execution → solid arrow connecting two 'accessible' ports.

2) system without 2 accessible ports + solid arrow --> no execution begins.

Rules

Assembly reaction:

1) input port → output port: solid arrow depicts assembly reaction

2) occurs when 2 ports are accessible

3) when executed, ports flip to inaccessible state → internal logic applied to output ports (example: accessible state)

4) 2+ solid arrows entering input port → parallel processes on copies of node species

Disassembly:

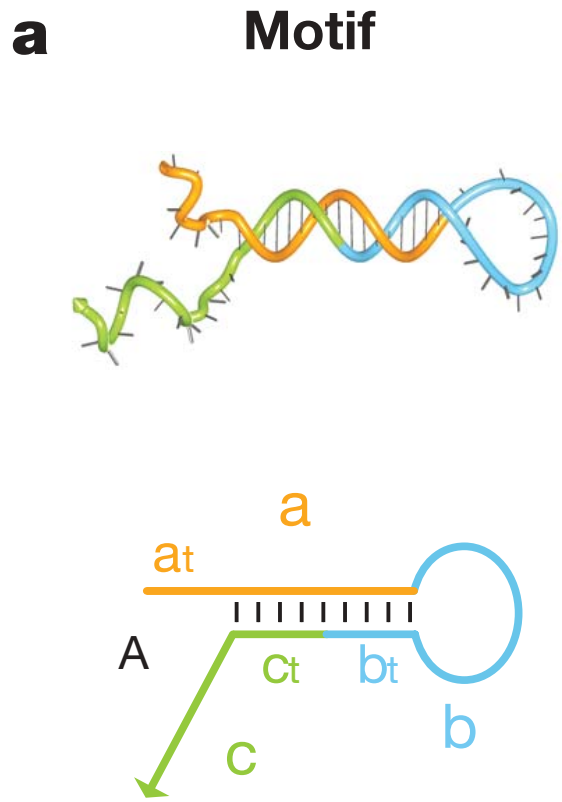
1) input port → output port: dashed arrow

2) occurs when input port inaccessible, output port accessible

3) Bond from output port to input port (both inaccessible) is replaced by displacing (inaccessible) output port. Both output port states are flipped.

Nodal Abstraction

Secondary structure of hairpin motif.



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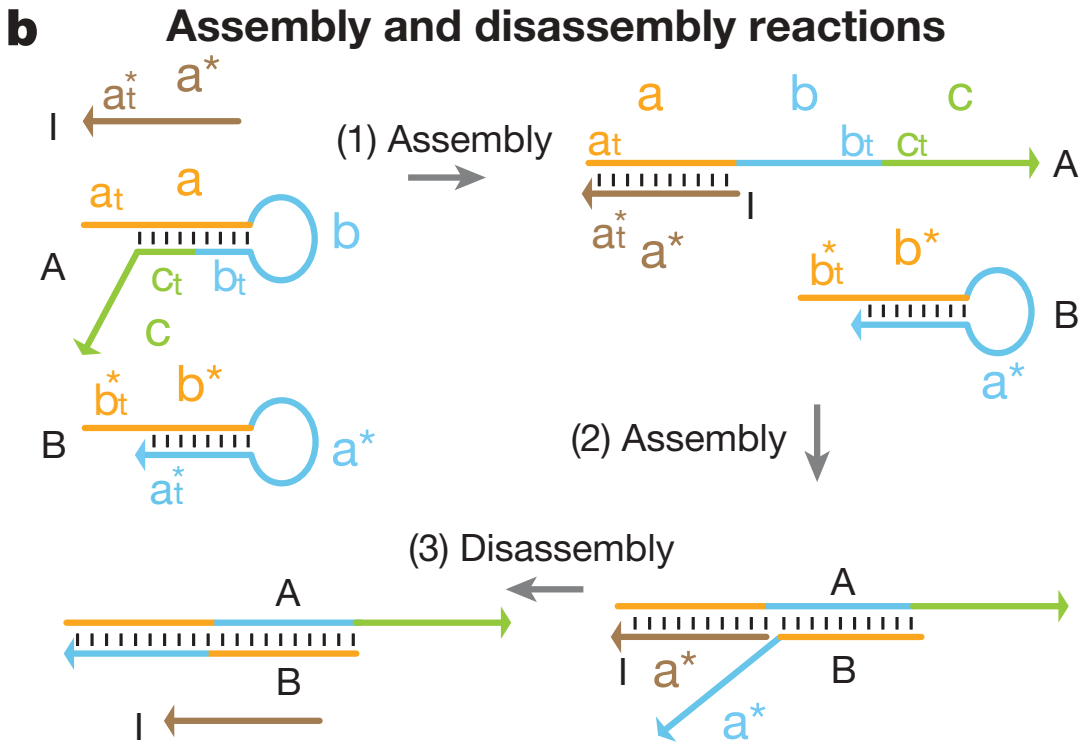
Nodal Abstraction

Secondary structure mechanism to illustrate assembly/ disassembly reactions during catalytic duplex formation



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Nodal Abstraction

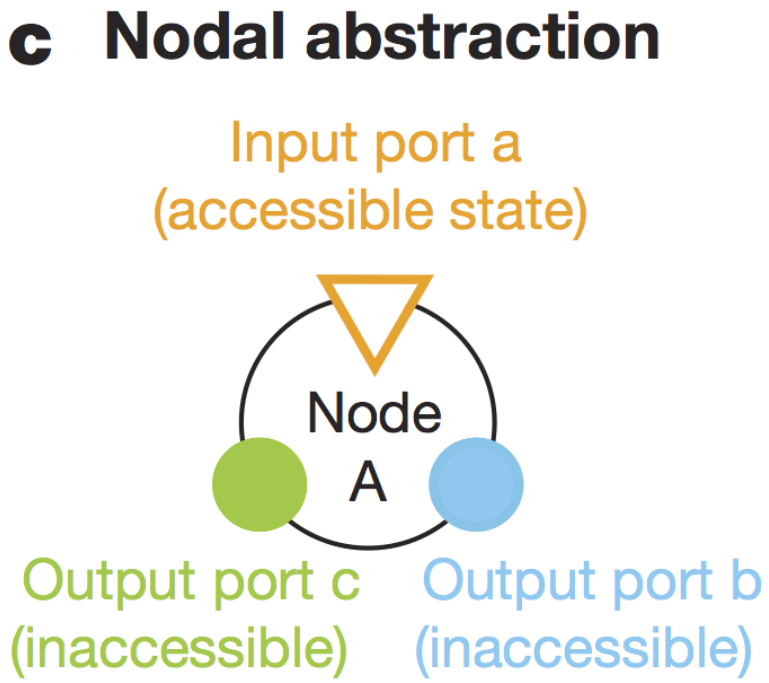
Node with 3 ports.

2 types of ports:

1. Input (circle)
2. Output (square)

State of toehold:

1. Exposed or accessible (open triangle/circle)
2. Sequestered or Inaccessible (closed triangle/circle)



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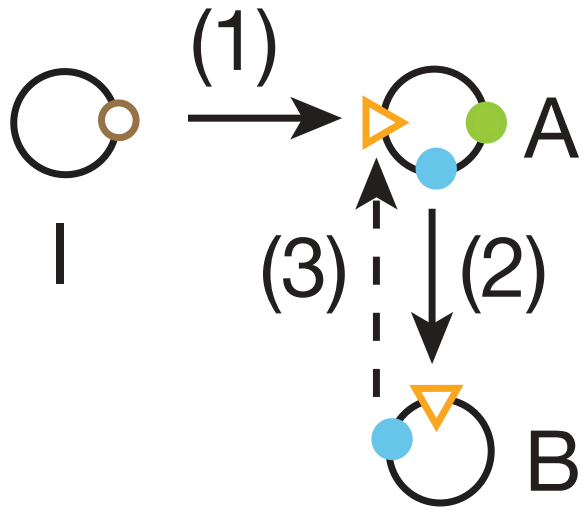
Nodal Abstraction

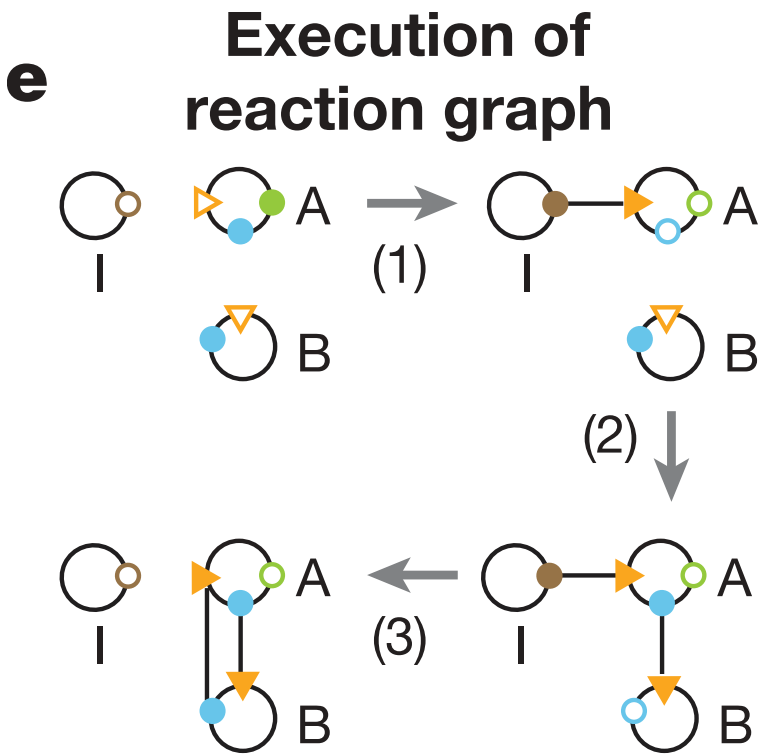
- Reaction graph
- Molecular program executed schematically in **b,e**

Reaction graph



Nodal Abstraction

Execution of reaction graph



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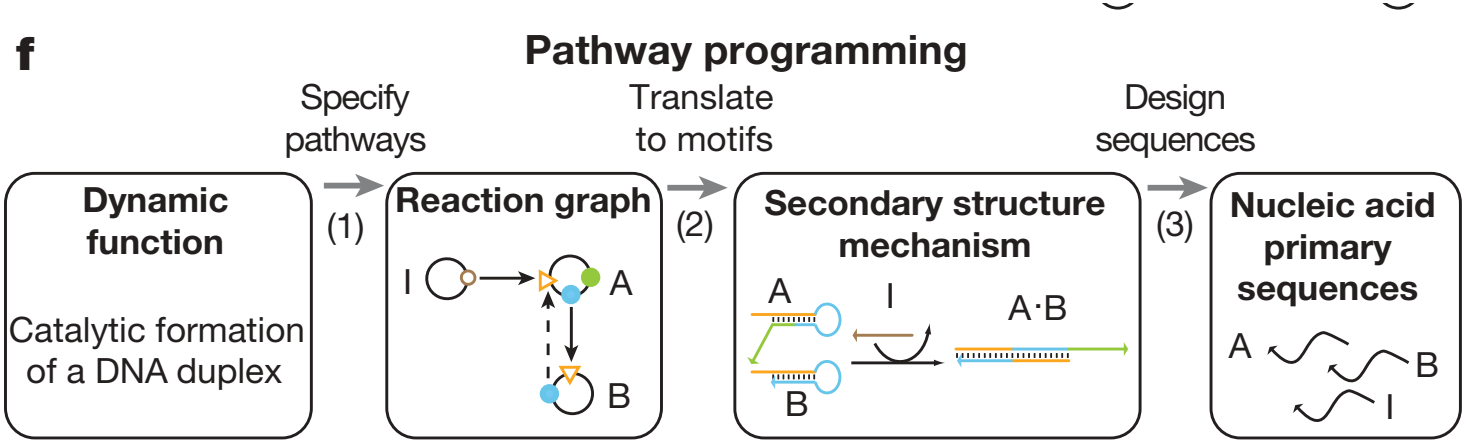
Nodal Abstraction



Hierarchical design process

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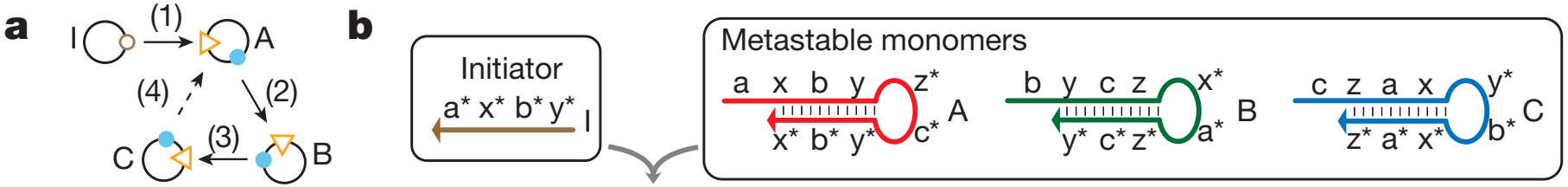

Reaction graph:

1. Only indicates sequence of reactions – not actual execution
2. Only focuses on toeholds of the species (everything else is ignored/discarded)

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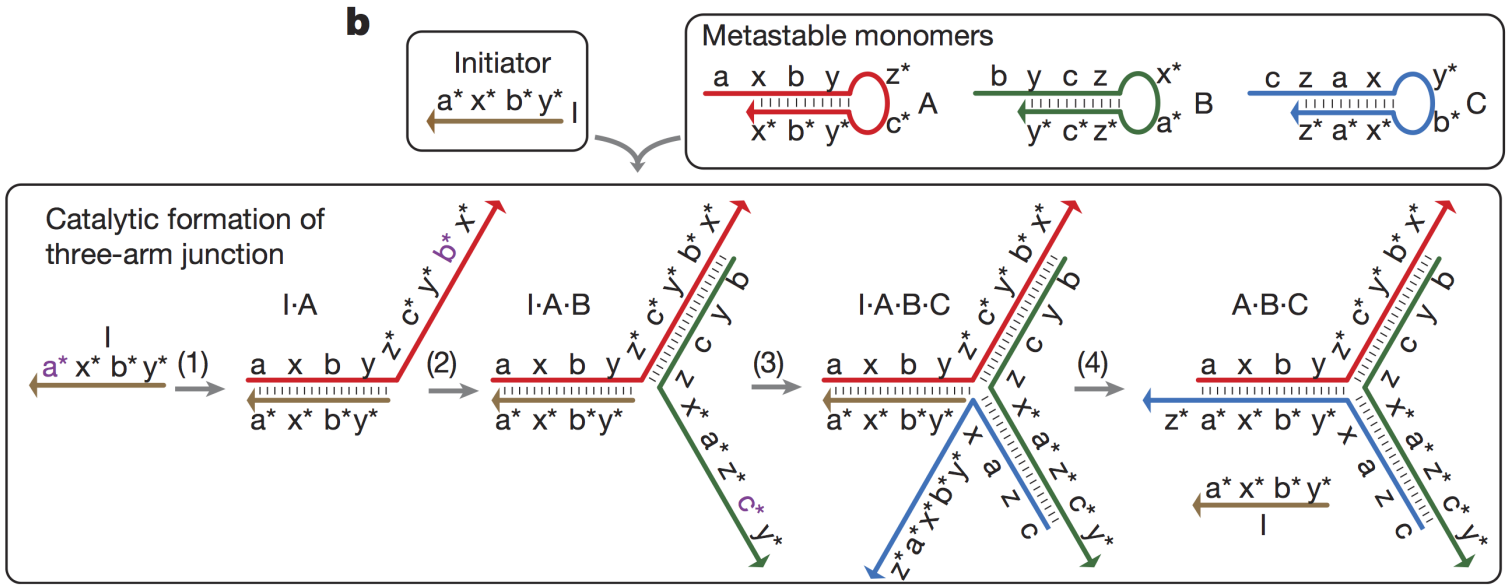
Nodal Abstraction



1. Initiator (I) + Hairpins A
2. I•A + B
3. I•A•B + C
4. A•B•C 3-arm junction + I

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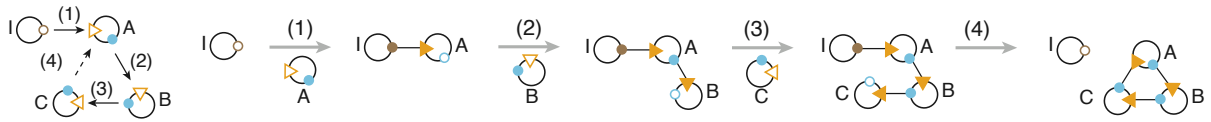

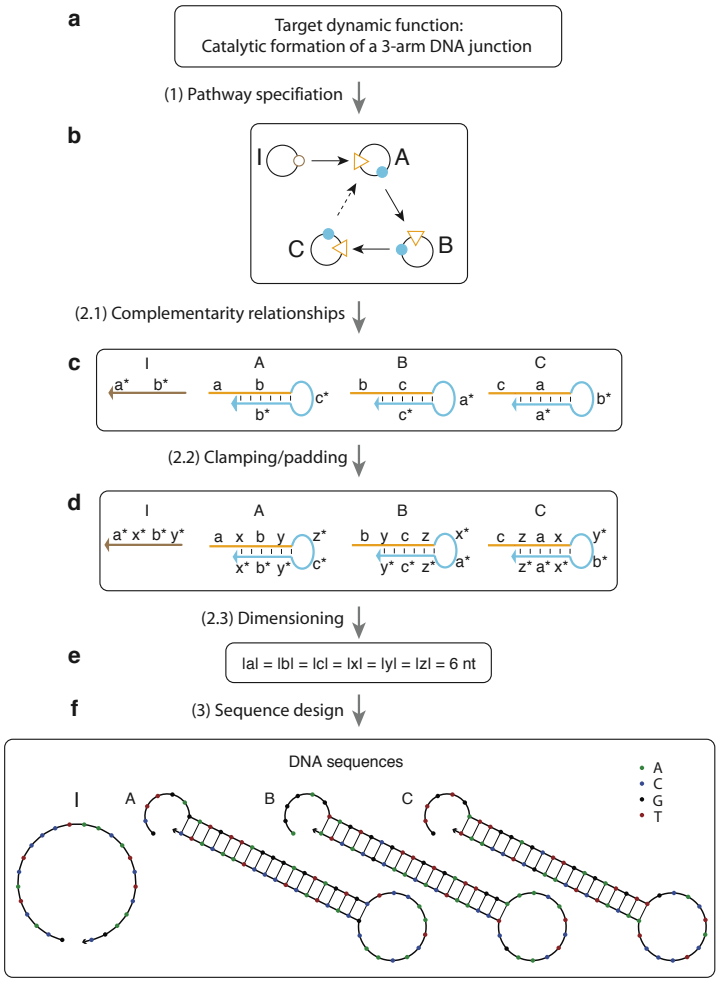

Figure S2. Procedure for designing the catalytic 3-arm junction system.

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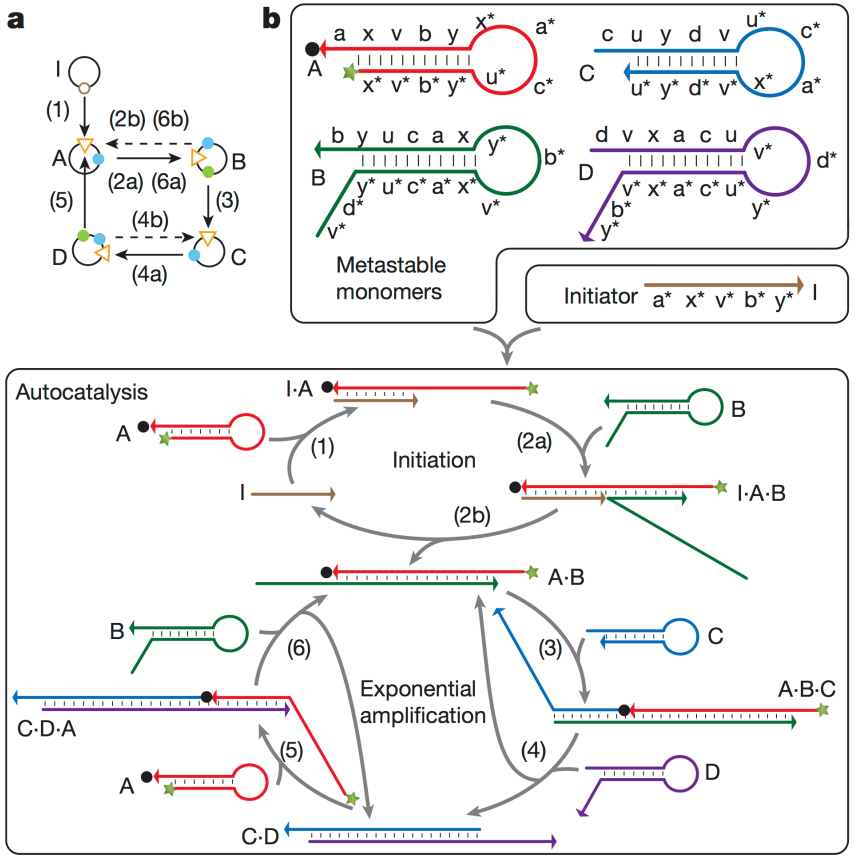

Programming catalytic circuitry: autocatalytic duplex formation by a cross-catalytic circuit with exponential kinetics.

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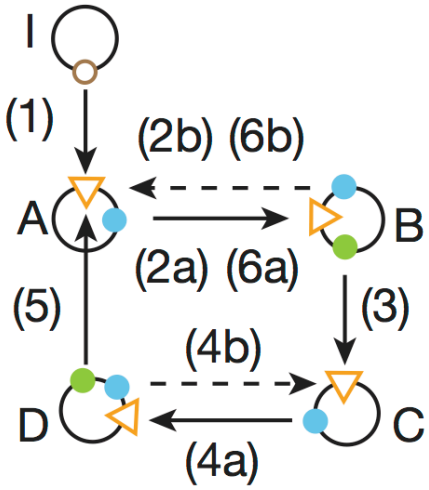

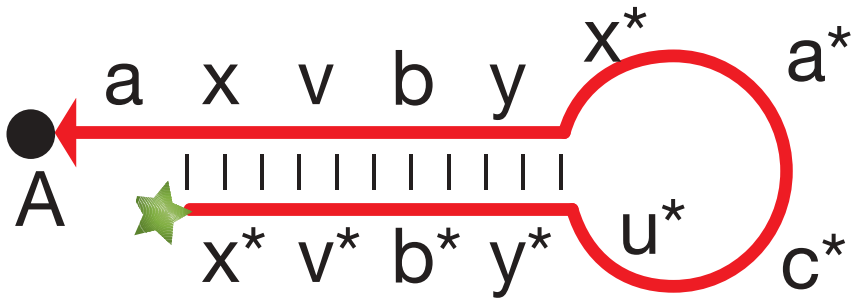

Programming catalytic circuitry: autocatalytic duplex formation by a cross-catalytic circuit with exponential kinetics.

1. Fluorophore (green star)

2. Quencher (black dot)

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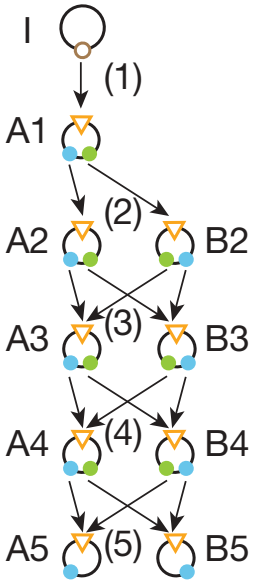

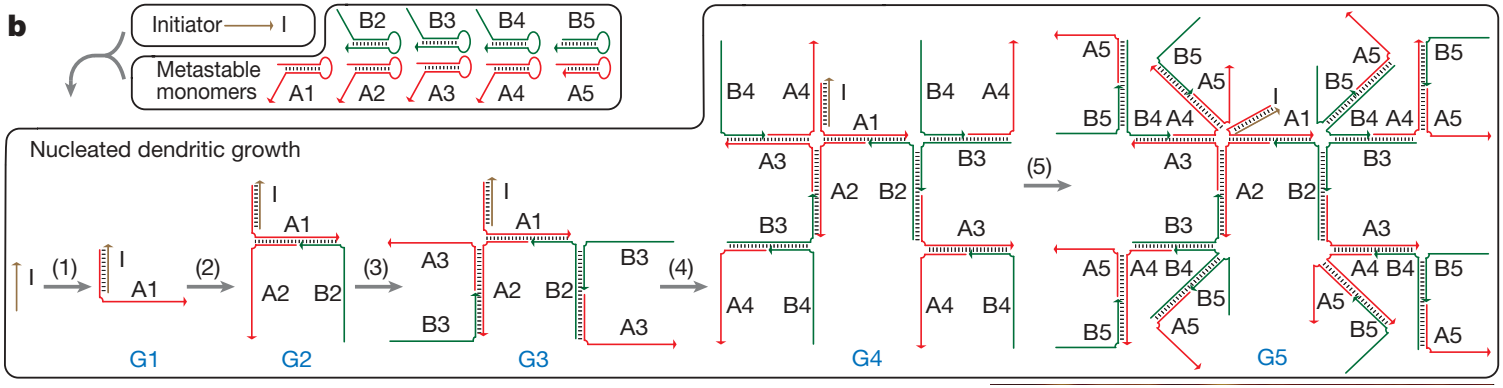

Programming nucleated dendritic growth: triggered assembly of quantized binary molecular trees

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Nodal Abstraction

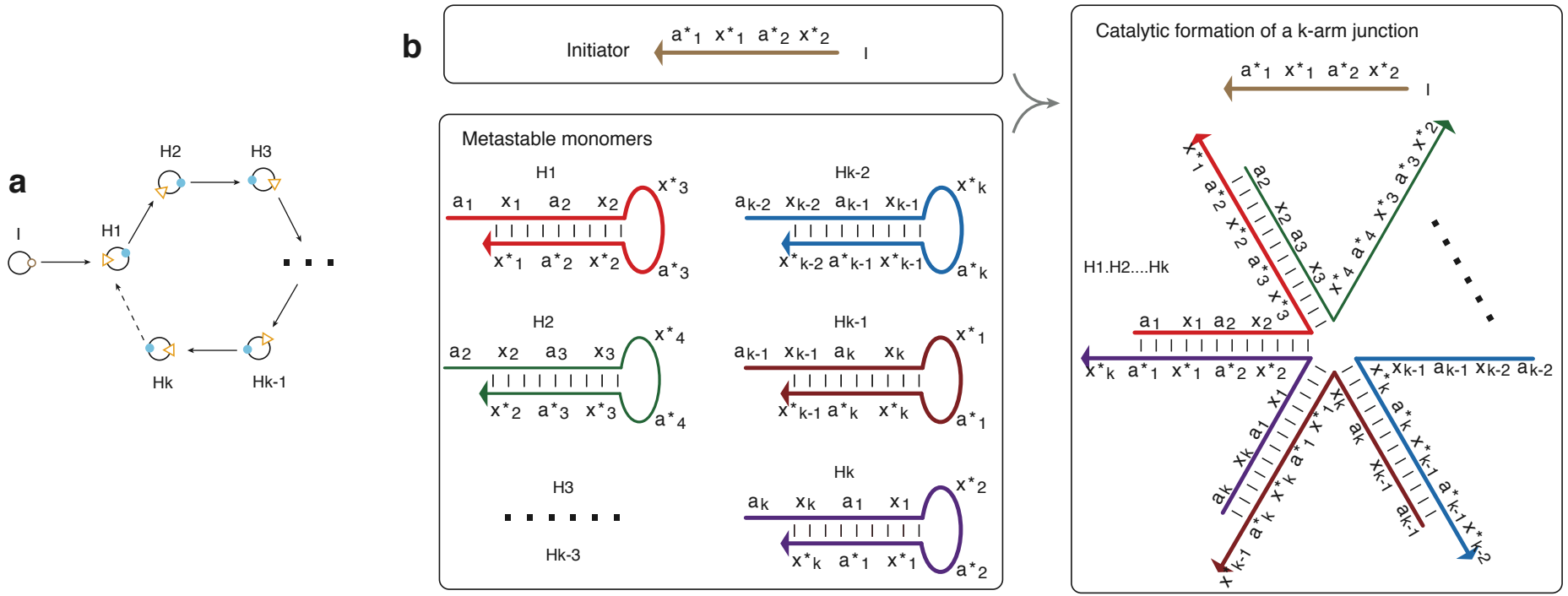

Figure S7. Catalytic formation of a k-arm junction. **a**, Reaction graph. **b**, Reaction schematics. Hairpins $H_1, H_2, \ldots, H_k$ are metastable in the absence of the initiator I. The initiator I catalyzes monomers $H_1, H_2, \ldots, H_k$ to form a k-arm DNA junction.

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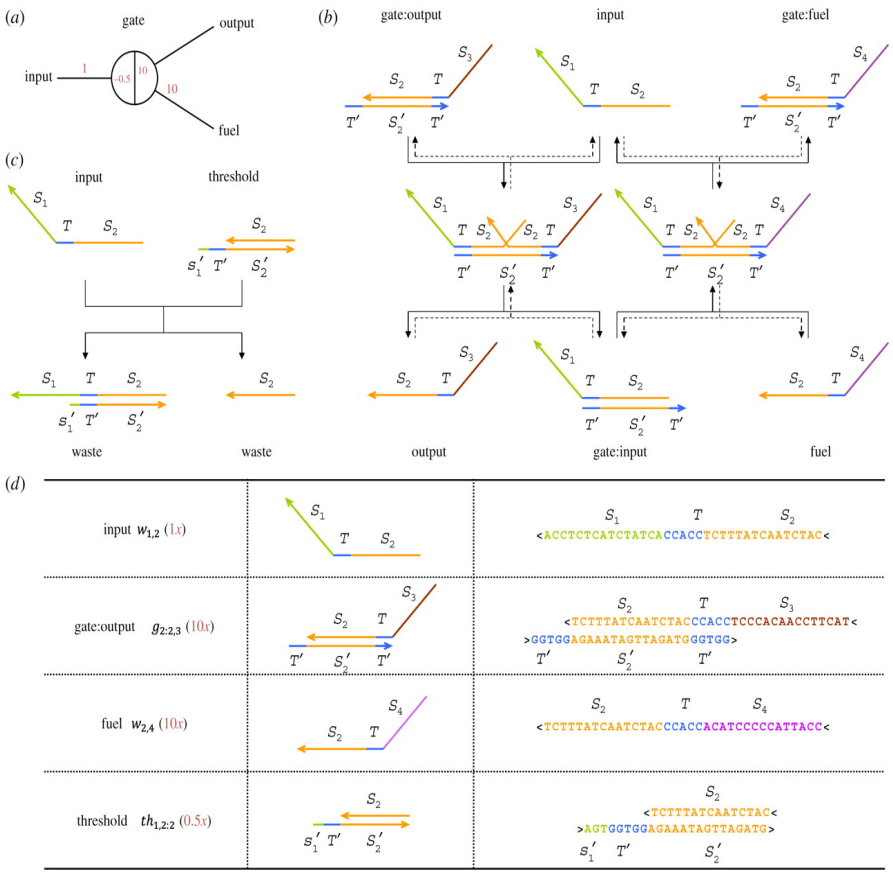
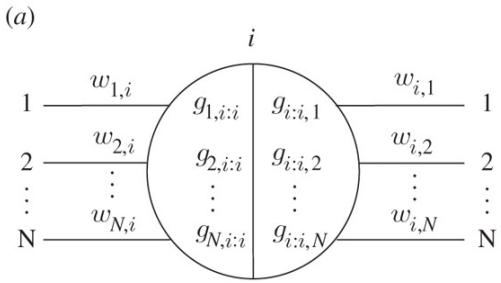
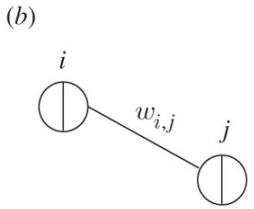
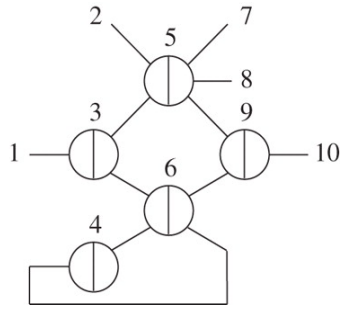
Seesaw Gates









The DNA motif for 'seesaw' gates.

Qian L , Winfree E J. R. Soc. Interface doi:10.1098/rsif. 2010.0729

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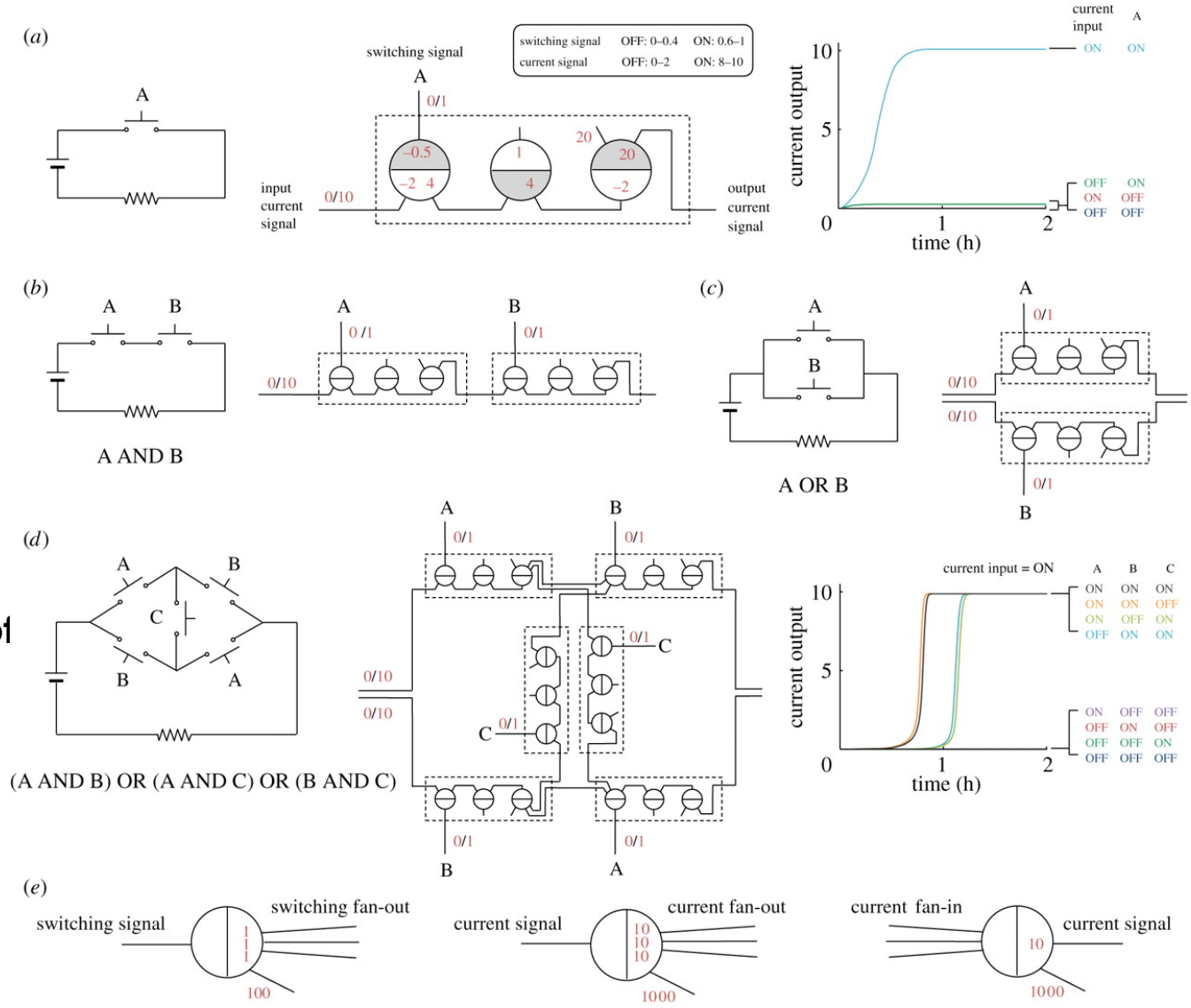
Seesaw Gates

Implementation of relay circuits.



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