

Towards the algorithmic molecular self-assembly of fractals by cotranscriptional folding

Yusei Masuda, Shinnosuke Seki, and Yuki Ubukata

University of Electro-Communications Tokyo

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Cotranscriptional folding

- Cotranscriptional folding—folding occurs during transcription

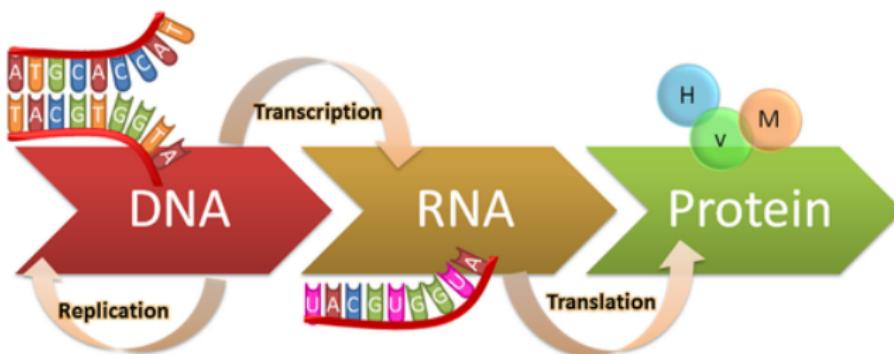


Figure: Central dogma—Information flow in biological systems.

Cotranscriptional folding

RNA polymerase

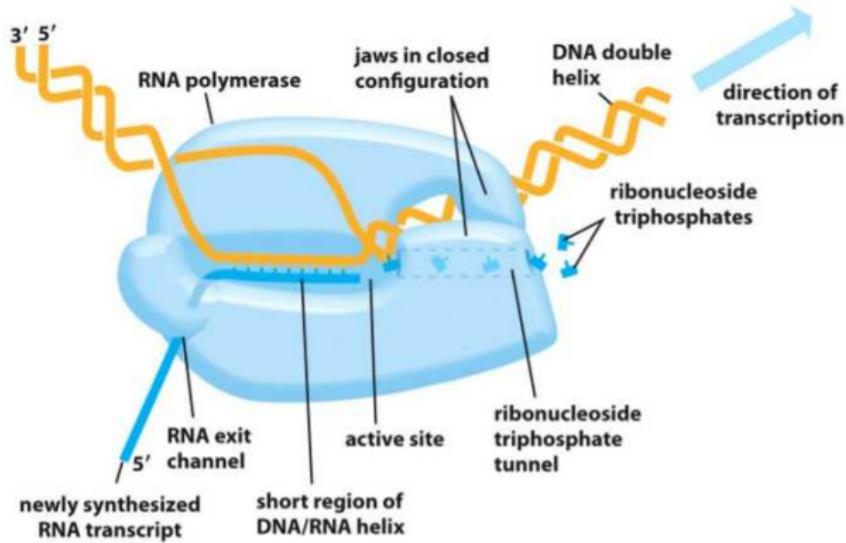


Figure 7-7 Essential Cell Biology (© Garland Science 2010)

Cotranscriptional folding

RNA Origami [Geary, Rothemund, Andersen ,*Science* 345 (2014) 799-804]

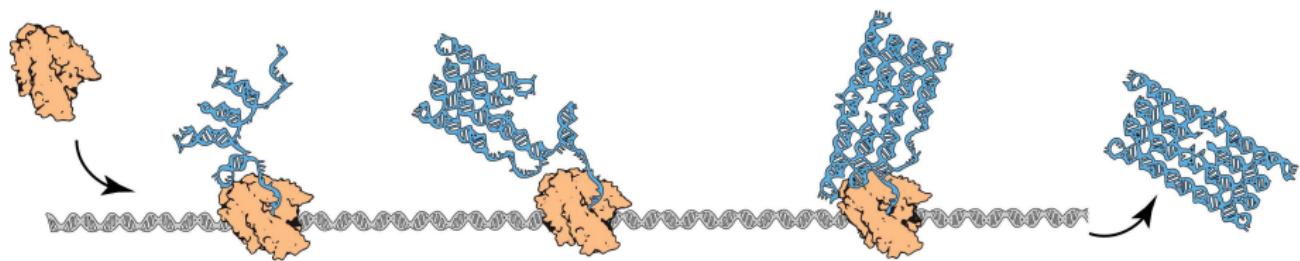


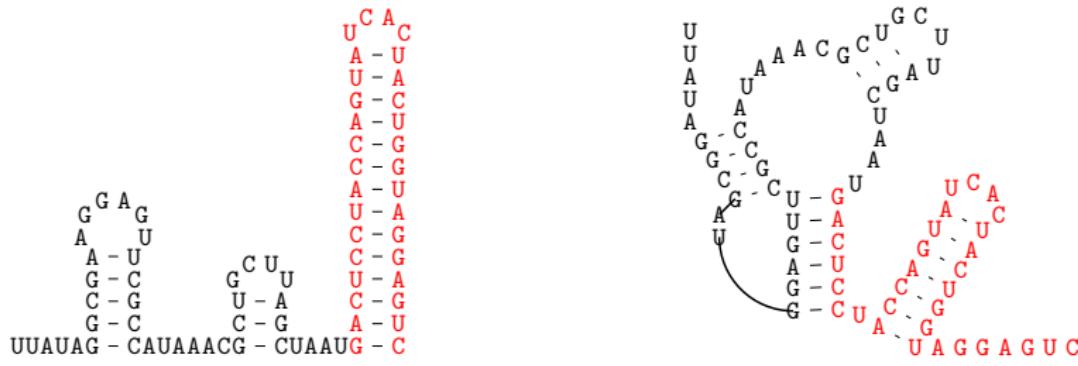
Figure: Design of ssRNA origami that self-assembles RNA tiles.

Cotranscriptional folding

Regulation in gene expression by CF [Watters et al. 2016]

Transcript: UUAUAGGCGAUGGAGUUCGCCAUAAACGCUUGCACUAGCUAAU**GACUCCUACCAGUAUCACUACUGGUAGGAGUC**

Concentration of NaF may promote or inhibit the transcript above to fold into the **terminator stem** cotranscriptionally.



Terminated (0 mM NaF)

Antiterminated (10 mM NaF)

RNA Origami [Geary, Rothemund, Andersen ,*Science* 345 (2014) 799-804]

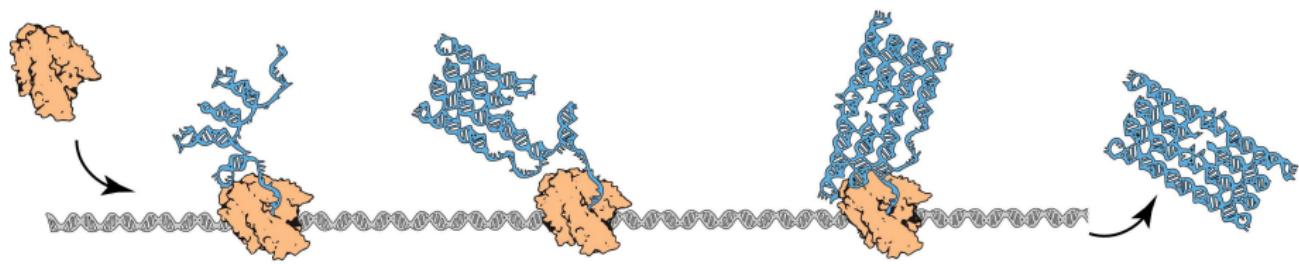
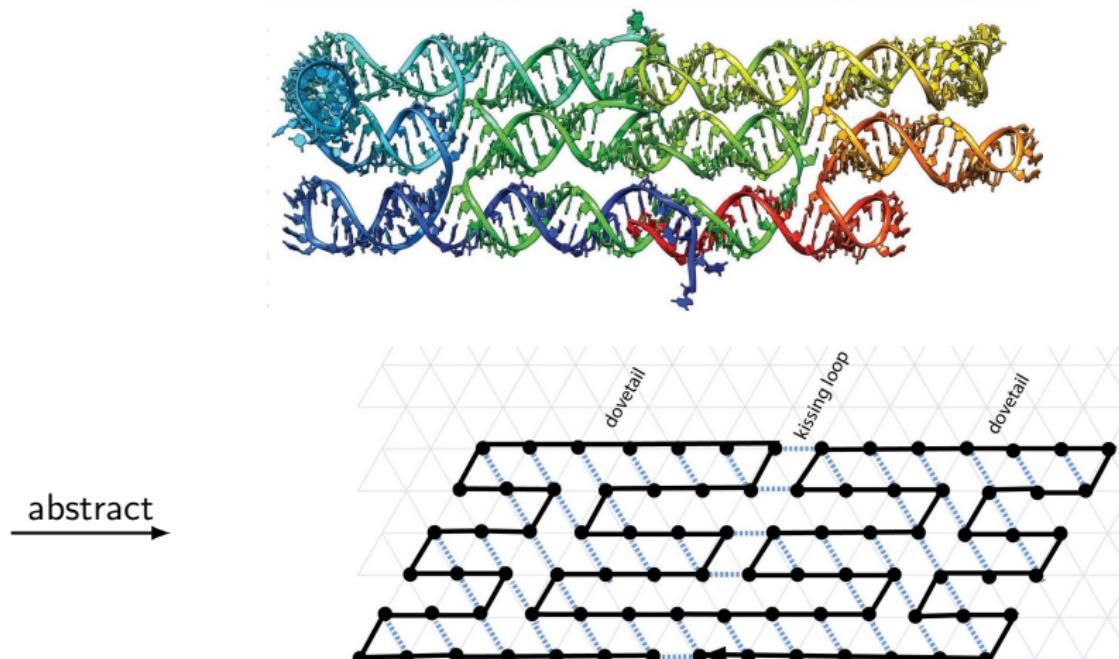


Figure: Design of ssRNA origami that self-assembles RNA tiles.

Oritatami System

- Oritatami system—a mathematical model of computation by cotranscriptional folding



Algorithmic shape self-assembly of fractal by CF

Motivations

- The initiation of algorithmic self-assembly of shape by CF
- A fractal is the benchmark of molecular self-assembly
- Traversable somehow algorithmically

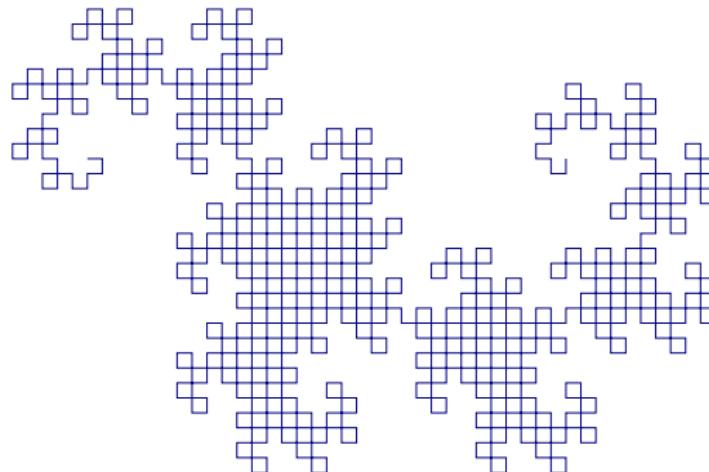


Figure: Heighway dragon.

Oritatami System

Definition

An oritatami system (OS) is a tuple $\Xi = (\Sigma, w, \mathcal{R}, \delta, \alpha)$, where

Σ finite set of bead types

$w \in \Sigma^*$ transcript, a string to be folded

$\mathcal{R} \in \Sigma \times \Sigma$ ruleset to specify which types of beads can interact

δ delay (transcription rate)

α arity, max # of interactions per bead

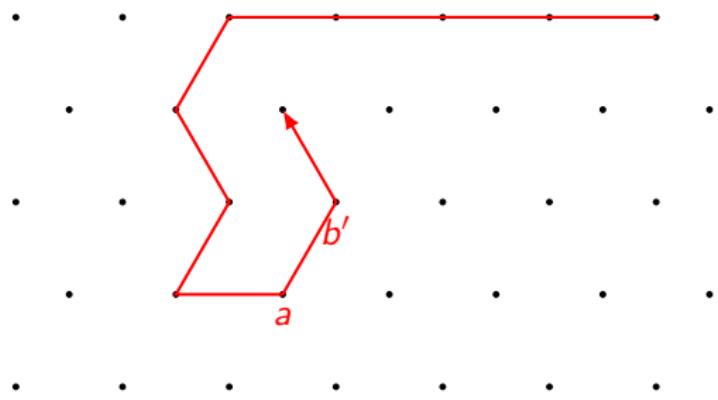
Oritatami System

Dynamics

Glider

Consider an OS with transcript $w = (bca'ac'b')^*$, rule set $R = \{(a, a'), (b, b'), (c, c')\}$, delay $\delta = 3$, and the seed below colored in red.

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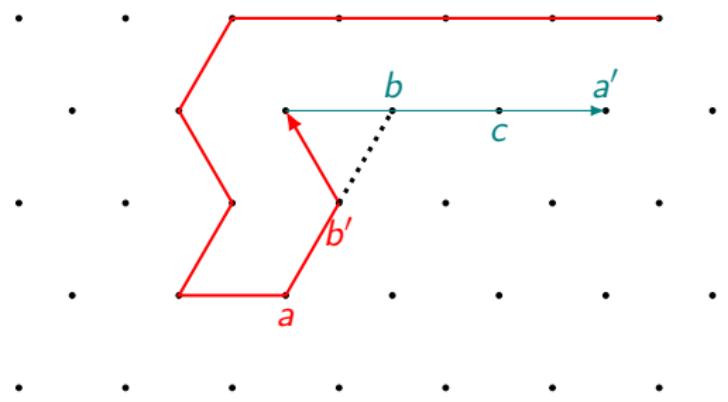
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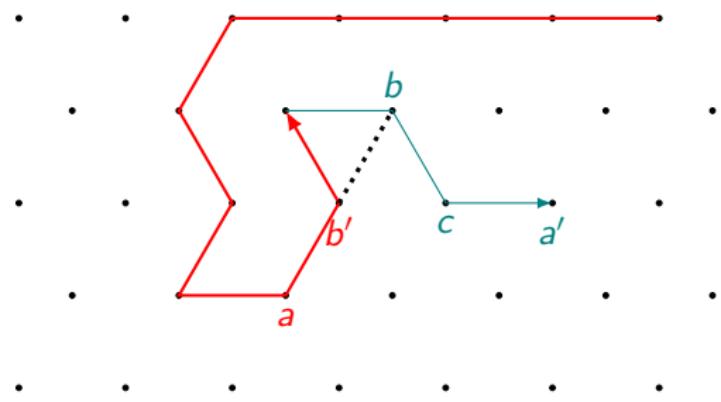
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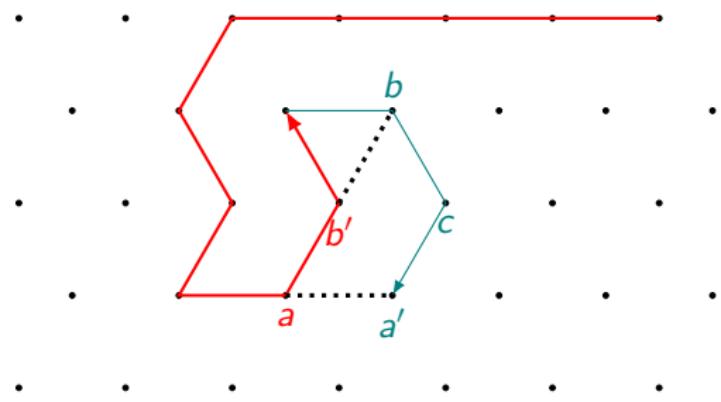
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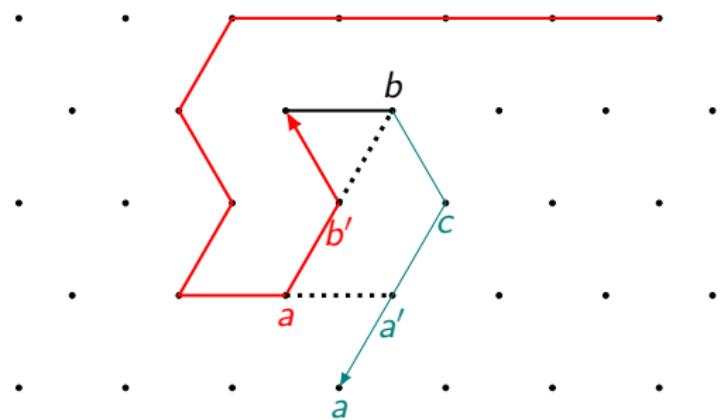
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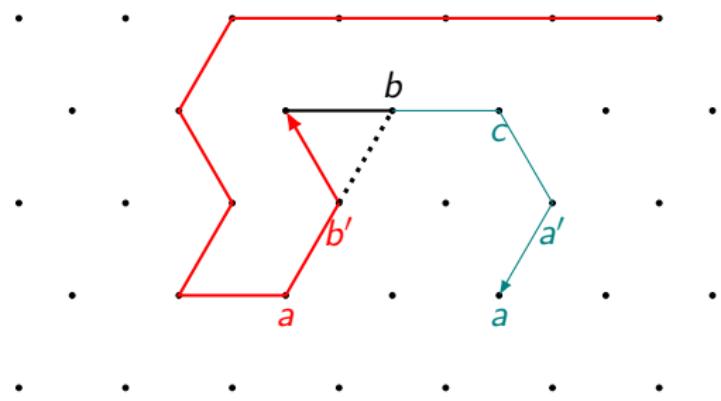
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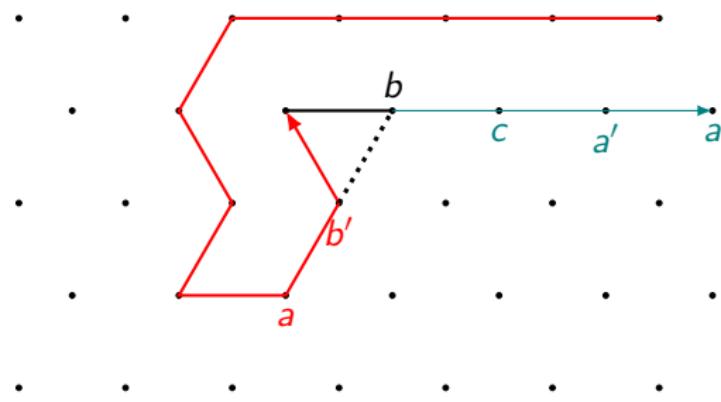
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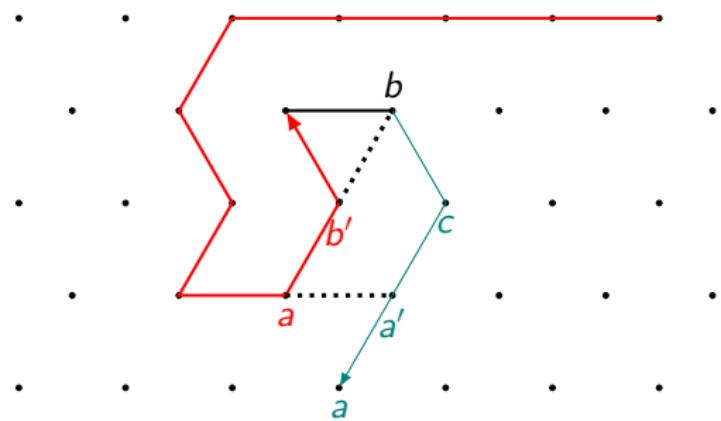
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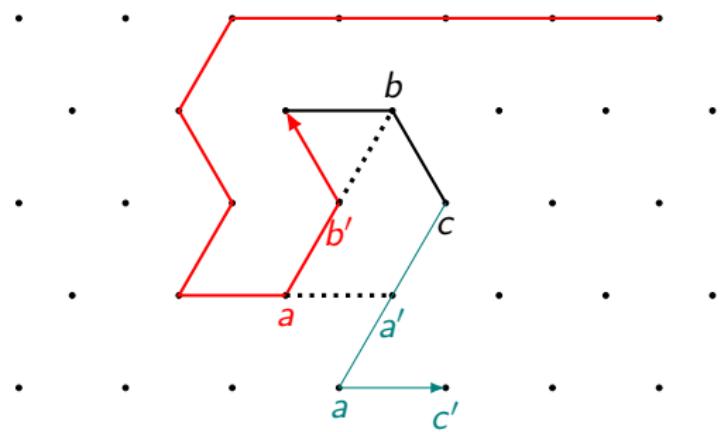
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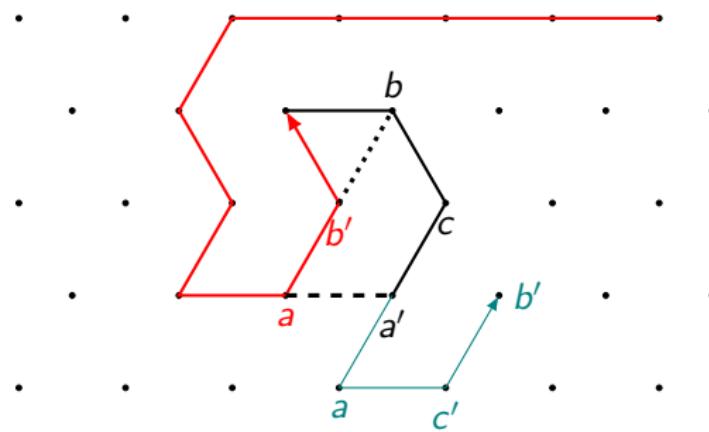
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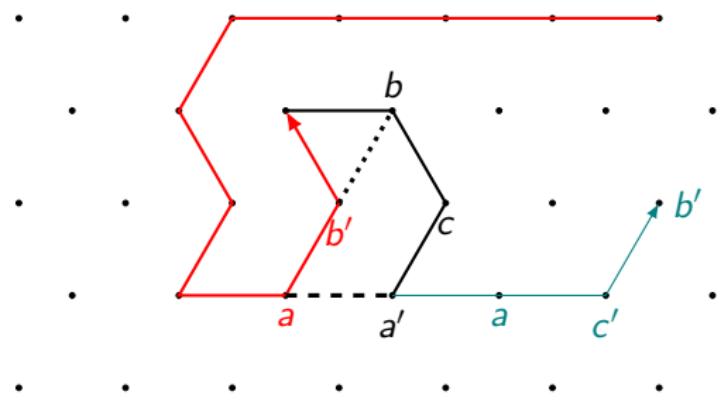
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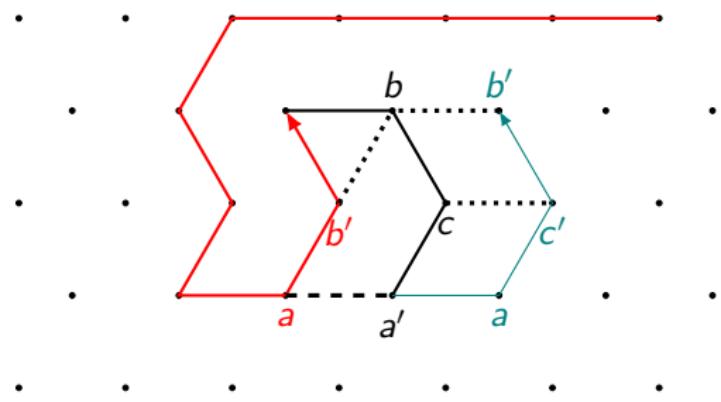
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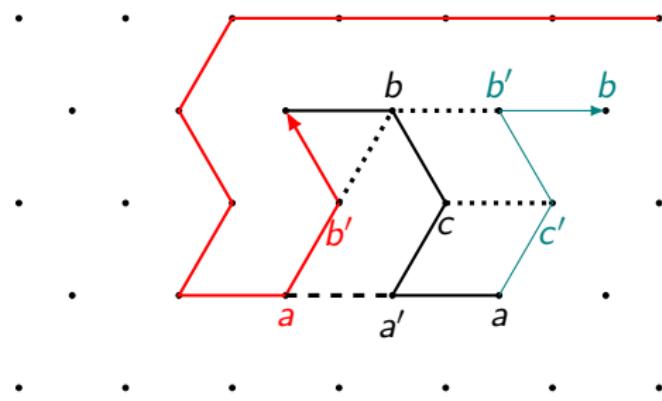
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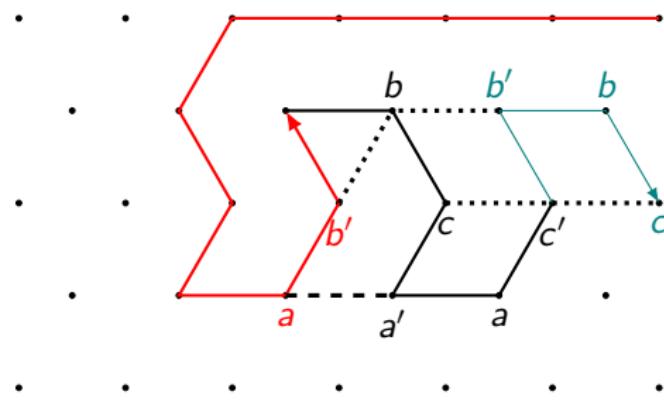
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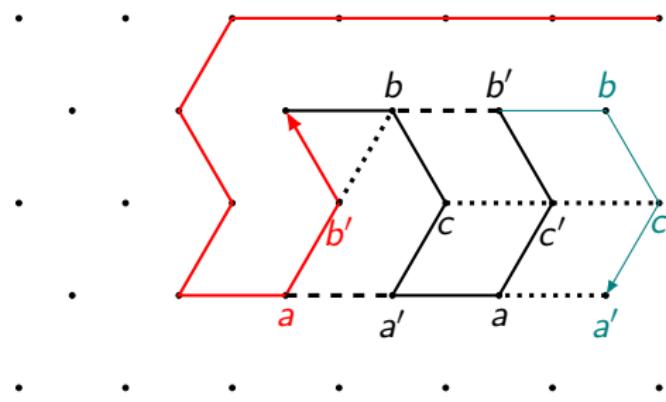
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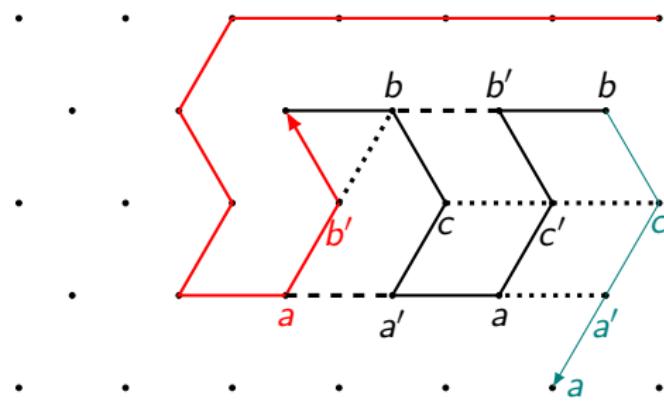
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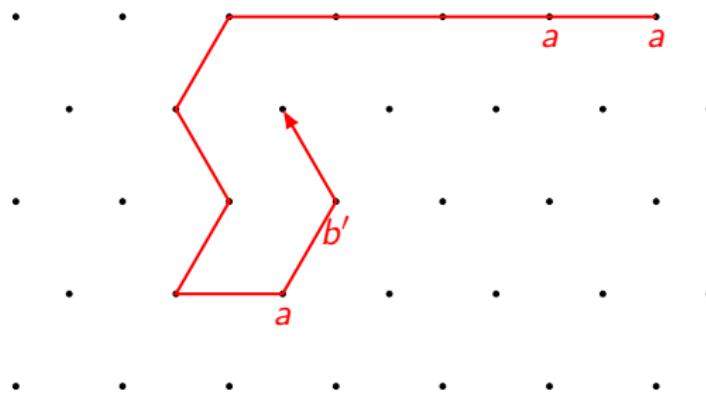
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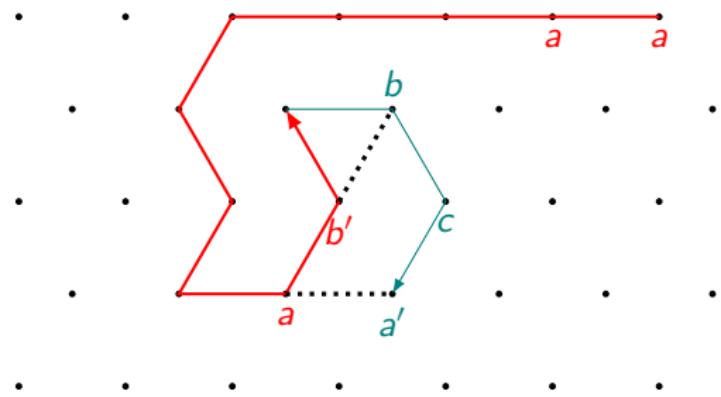
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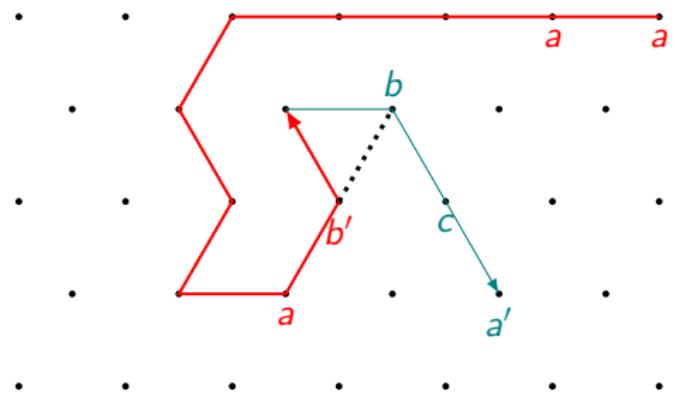
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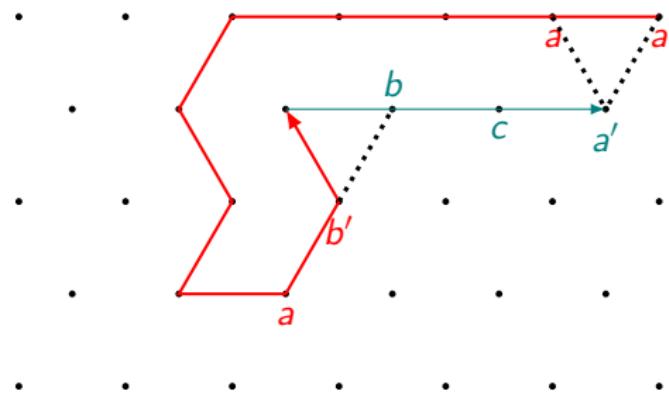
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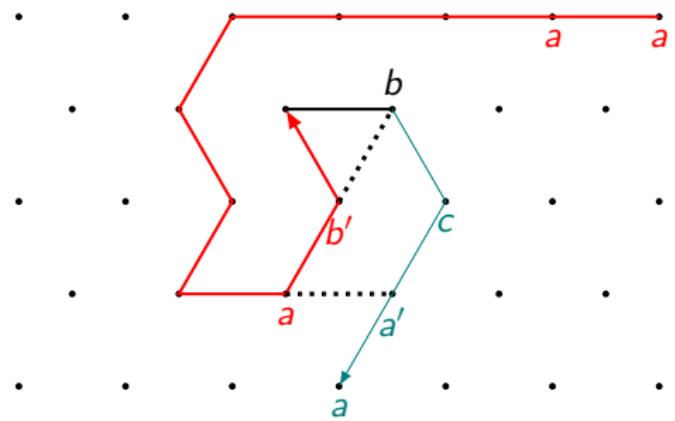
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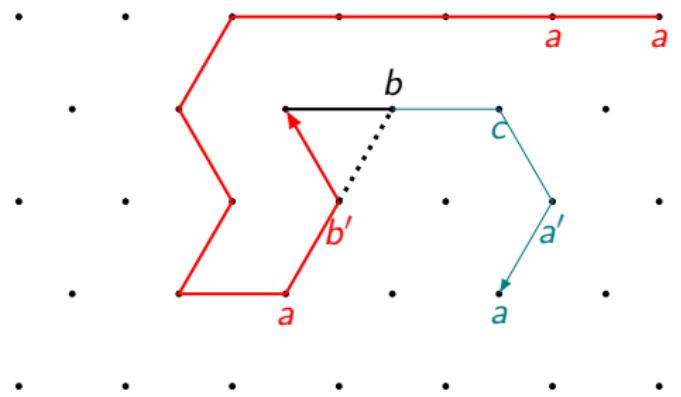
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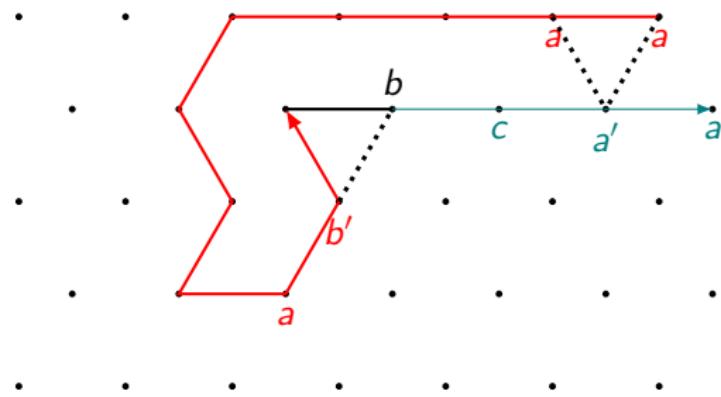
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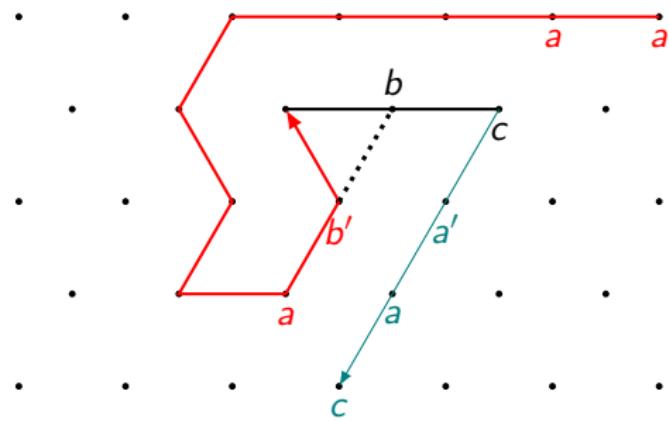
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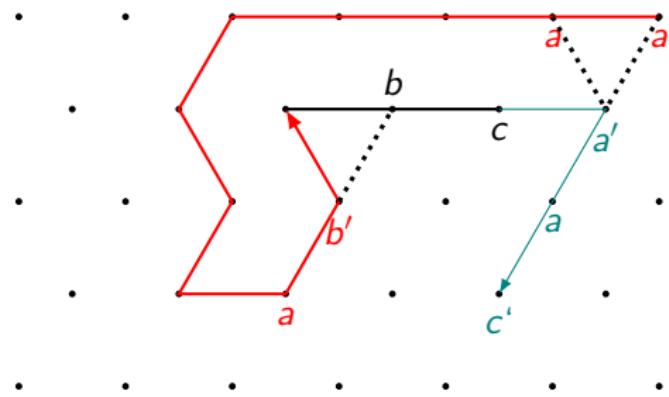
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 3. Transcribe $w[i + \delta]$ and $i = i + 1.$



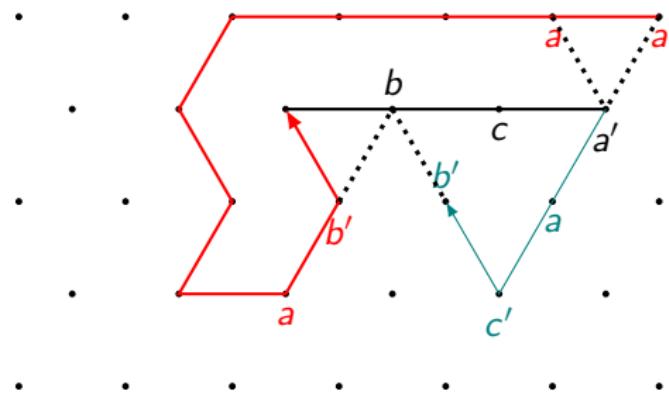
Oritatami System

Dynamics

Glider (Context-sensitive)

Consider an OS with transcript $w = (bca'ac'b')^*$, rule set $R = \{(a, a'), (b, b'), (c, c')\}$, delay $\delta = 3$, and the seed below colored in red.

- Transcribe $w[1..\delta]$ at the 3'-end of the seed.
- for ($i = 0, i \leq |w|, i = i + 1$) {
 1. Fold $w[i..i + \delta - 1]$ in all geometrically-possible manners.
 2. Stabilize $w[i]$ so as for $w[i..i + \delta - 1]$ to form as many bonds as possible.
 3. Transcribe $w[i + \delta]$ and $i = i + 1.$



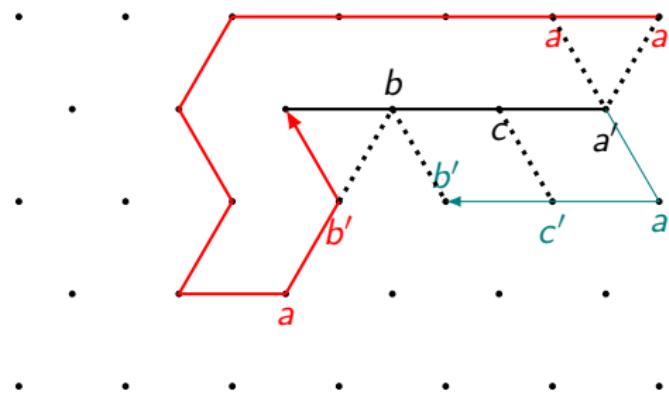
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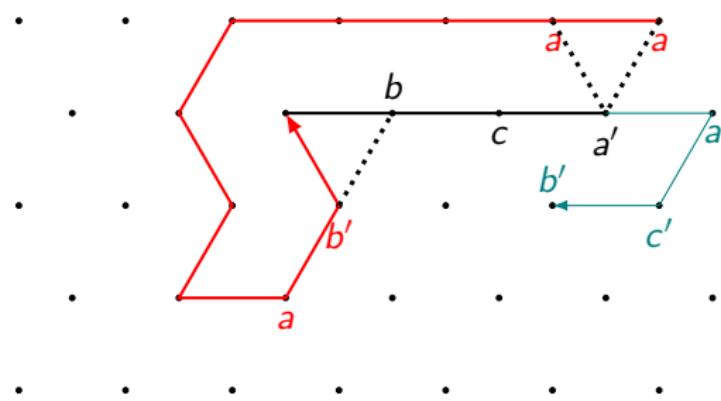
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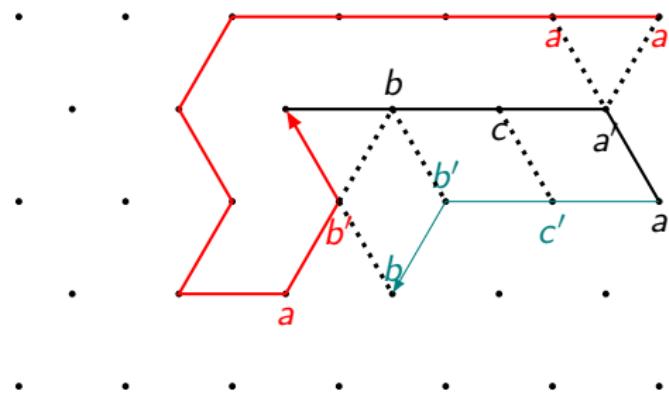
Oritatami System

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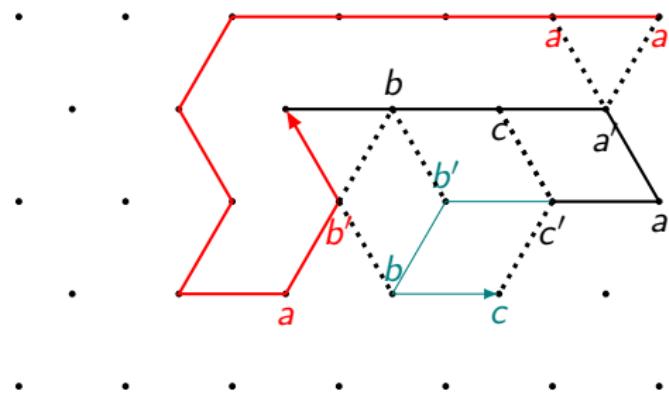
Oritatami System

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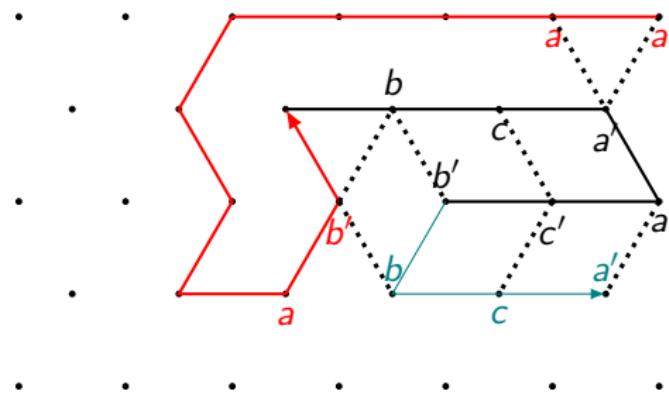
Oritatami System

Dynamics

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Module [Geary et al. 2016]

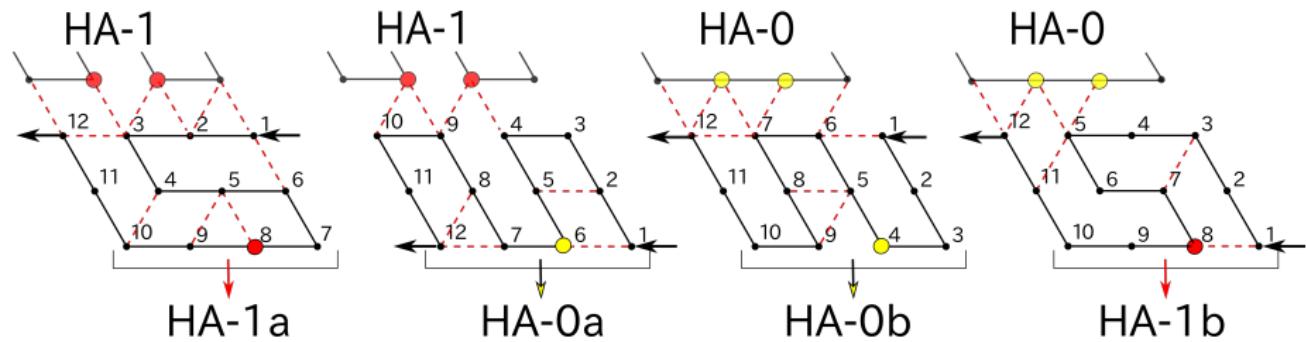
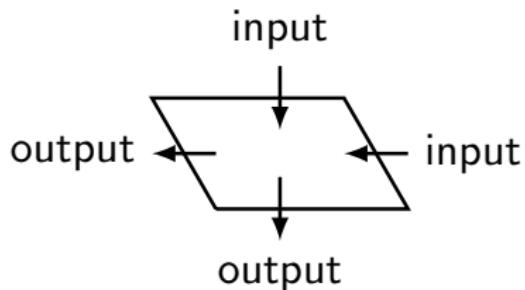


Figure: Four bricks of Half Adder *module*

Module [Geary et al. 2016]

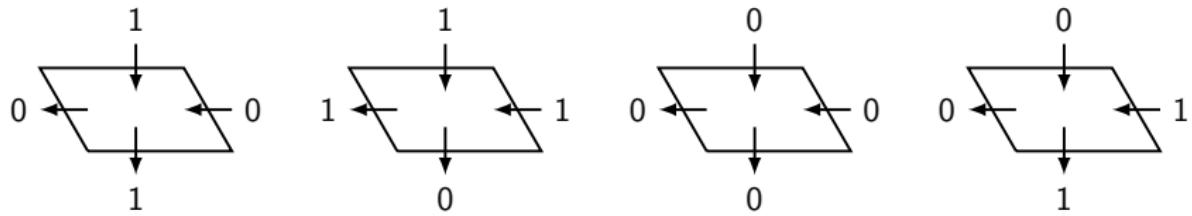
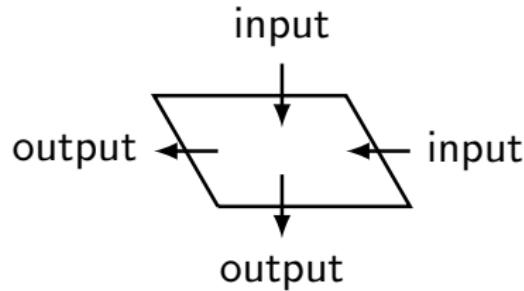
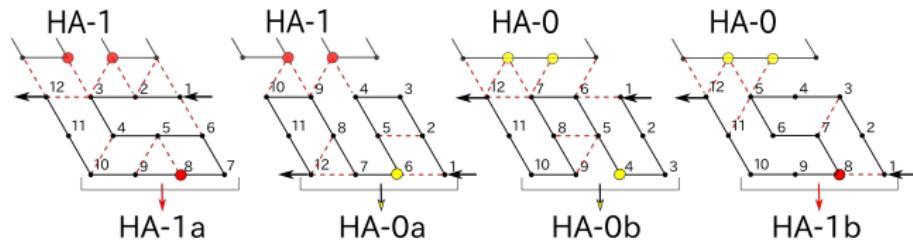


Figure: Four bricks of Half Adder module

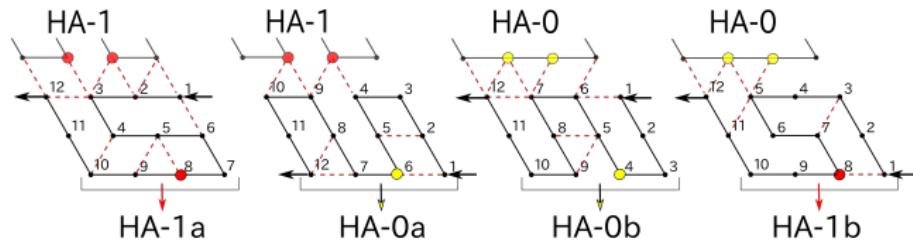
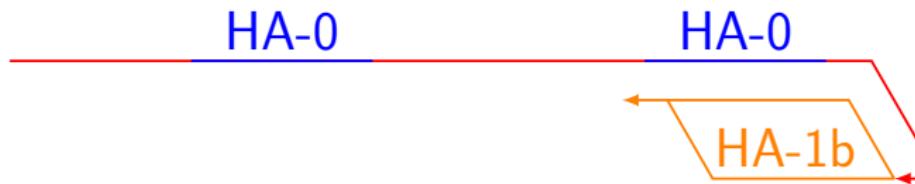
Module [Geary et al. 2016]

HA-0

HA-0

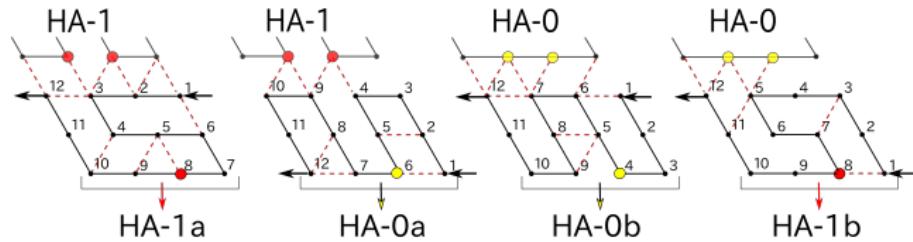
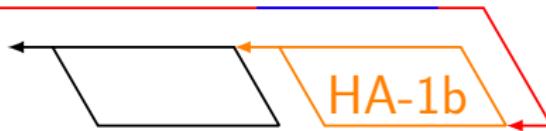


Module [Geary et al. 2016]

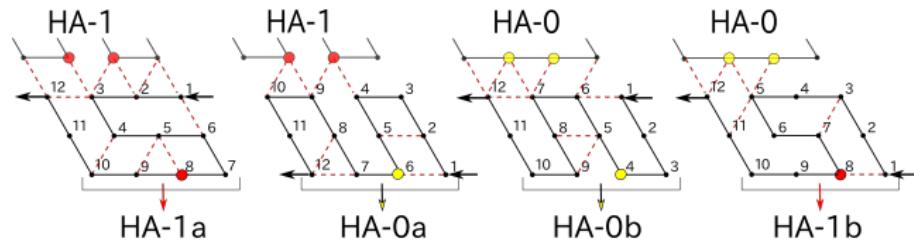
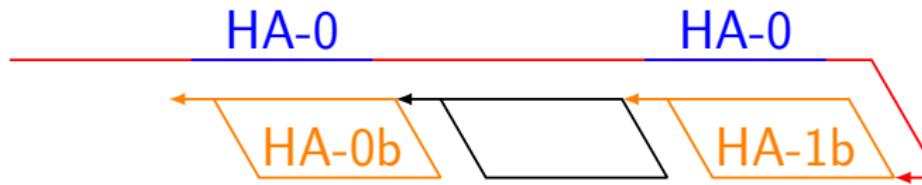


Module [Geary et al. 2016]

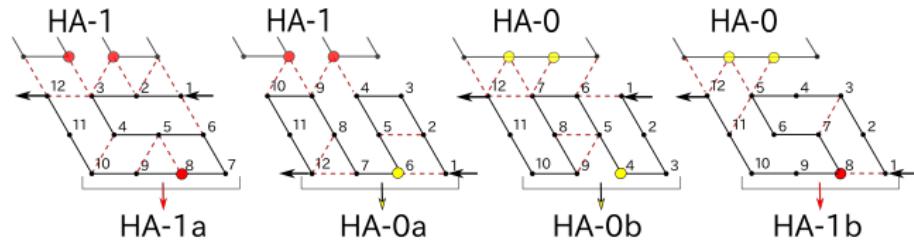
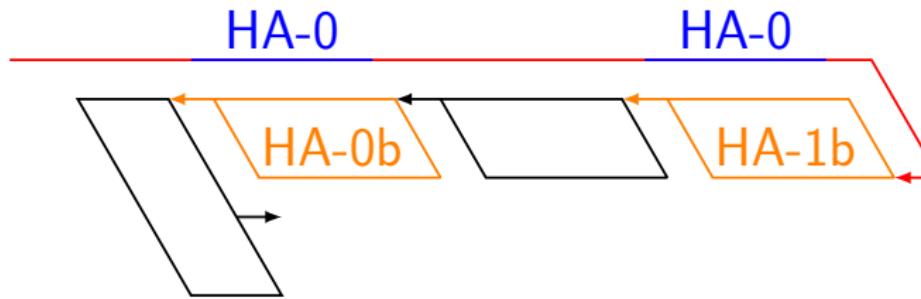
HA-0 HA-0



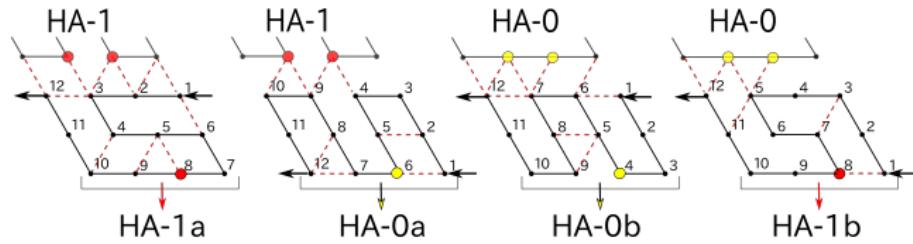
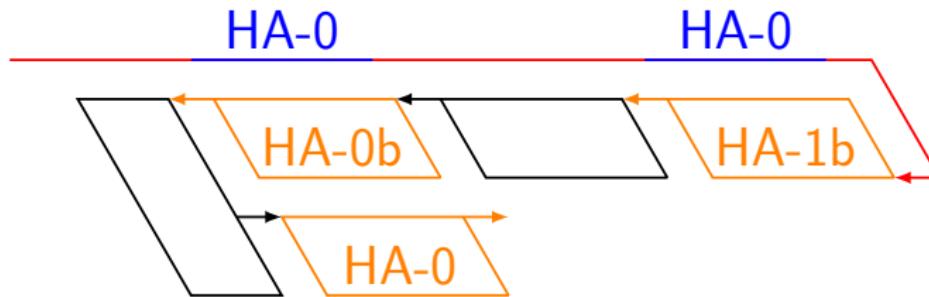
Module [Geary et al. 2016]



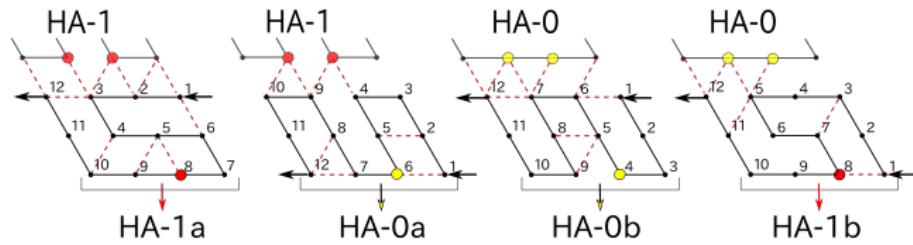
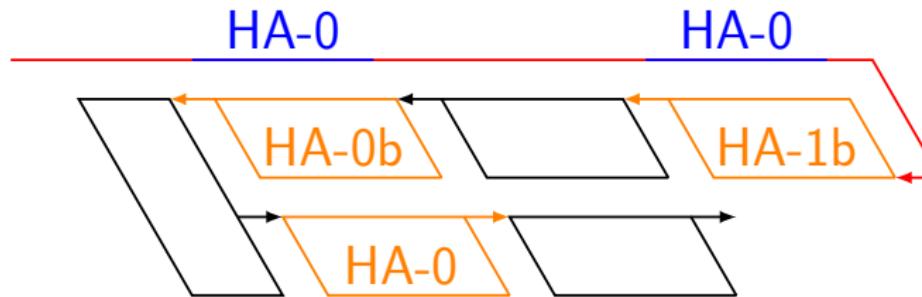
Module [Geary et al. 2016]



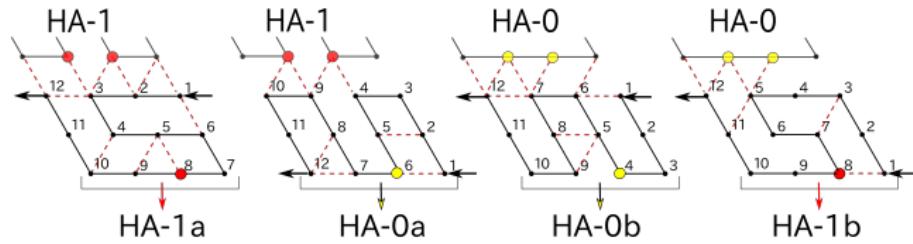
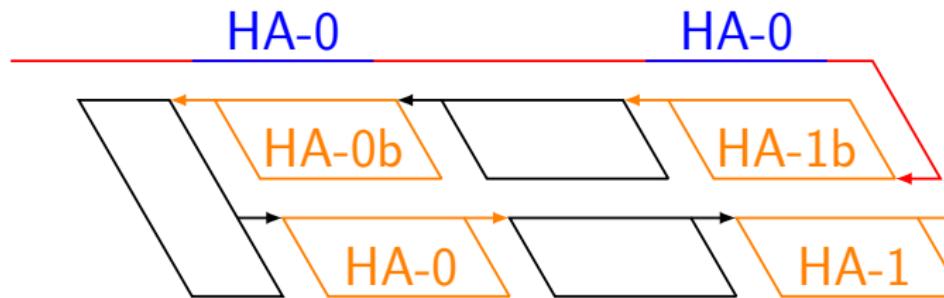
Module [Geary et al. 2016]



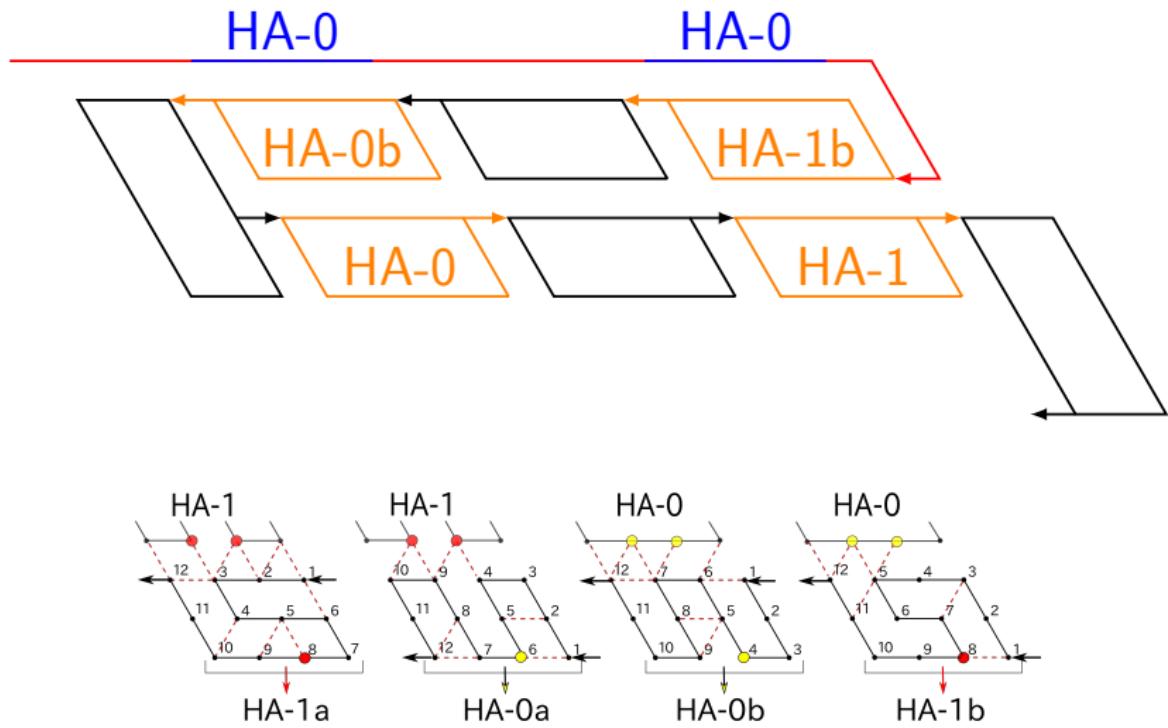
Module [Geary et al. 2016]



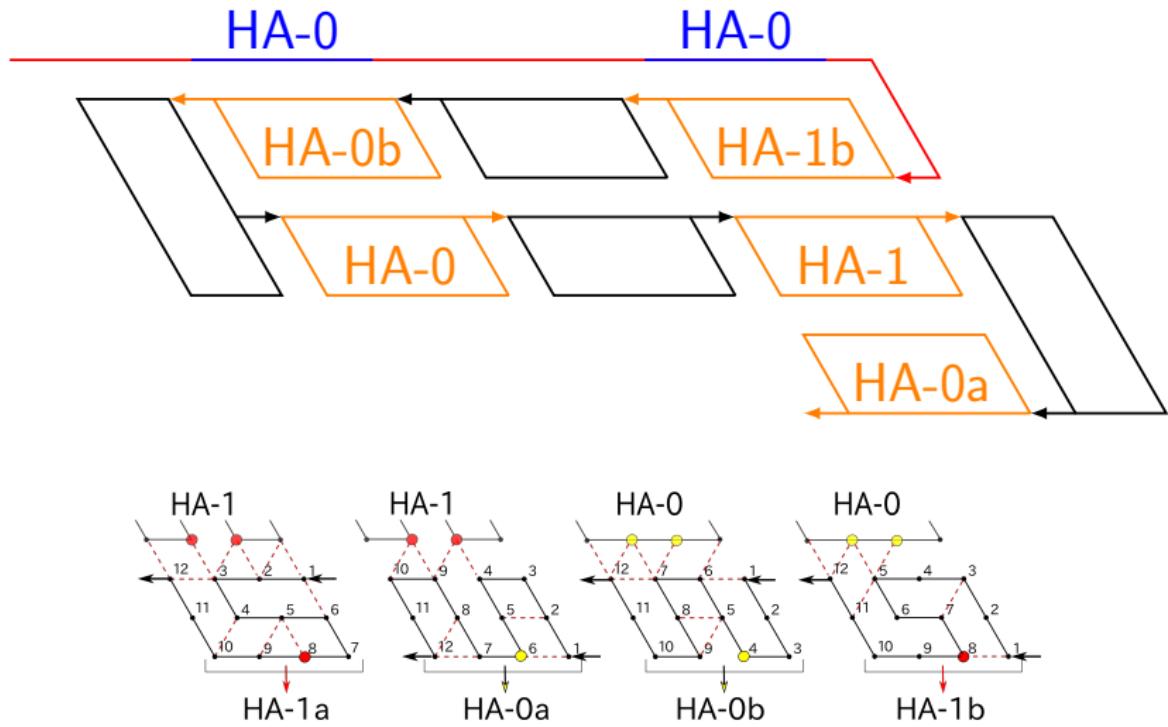
Module [Geary et al. 2016]



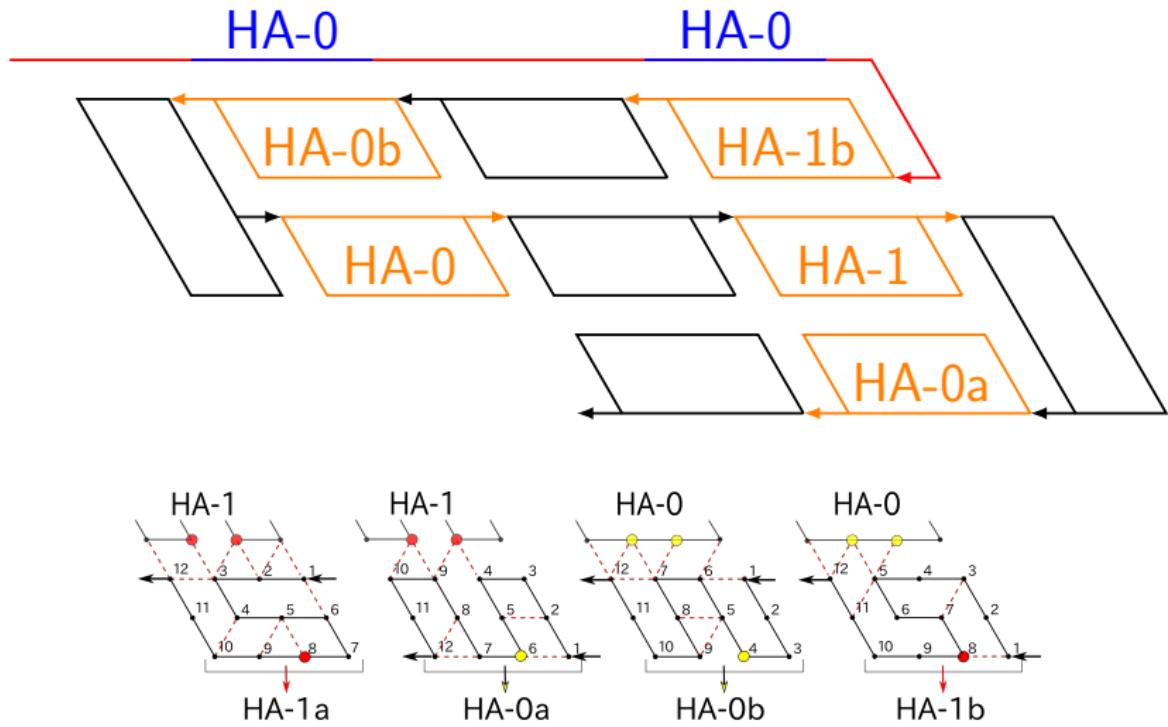
Module [Geary et al. 2016]



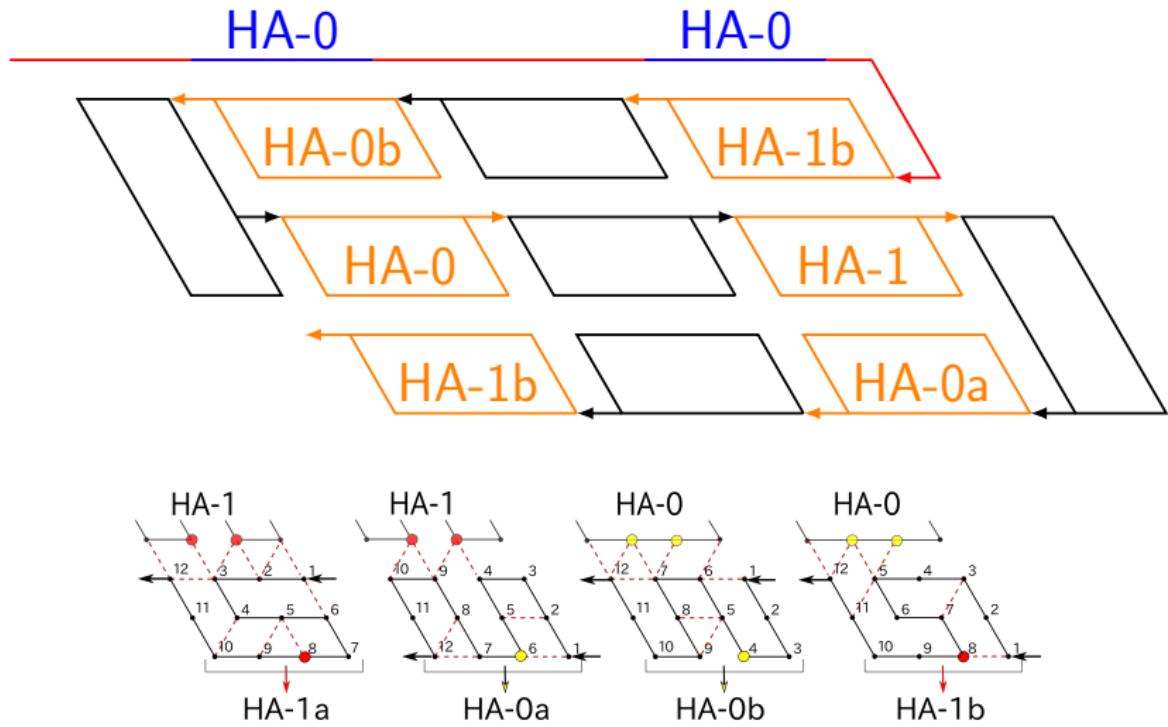
Module [Geary et al. 2016]



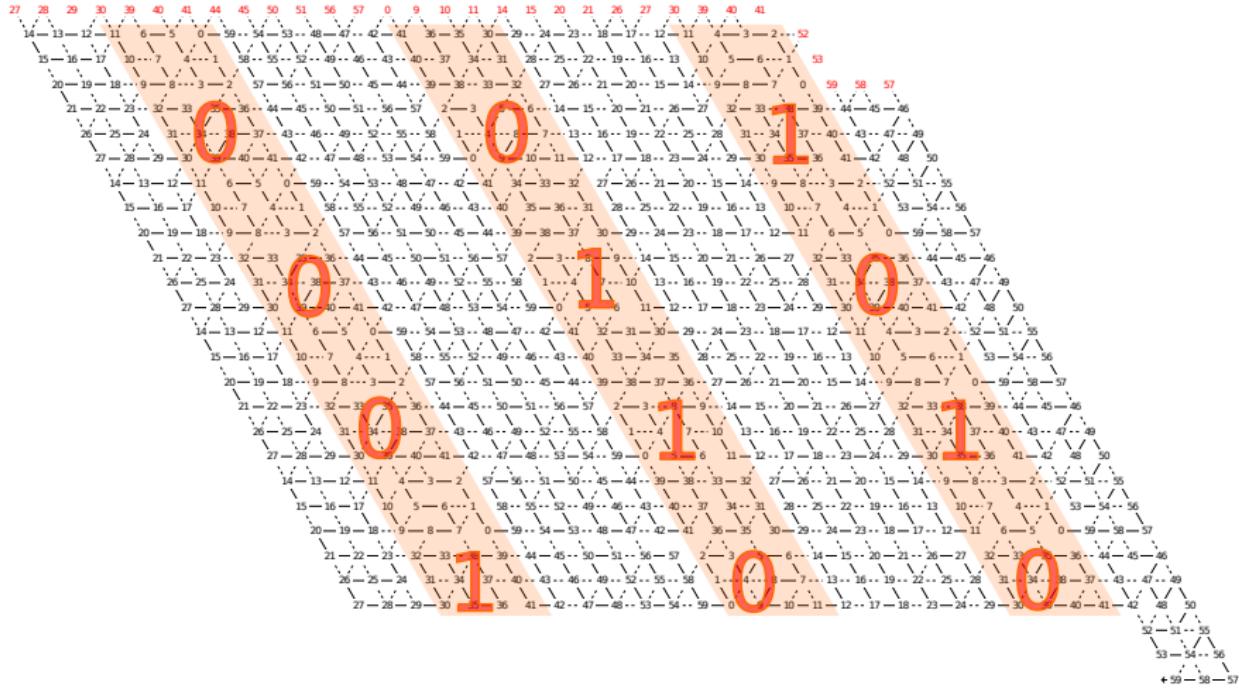
Module [Geary et al. 2016]



Module [Geary et al. 2016]



Module [Geary et al. 2016]



Implementation

- We design an oritatami system that self-assembles an n -bit fraction of the Heighway dragon.

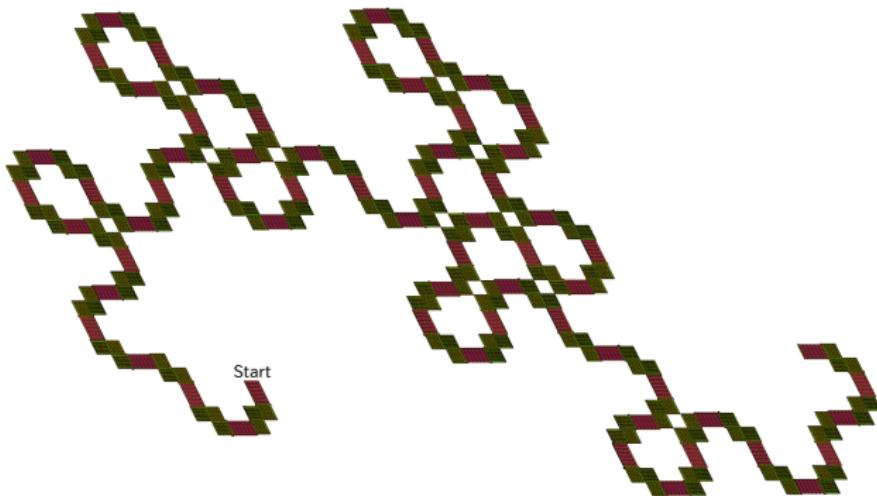


Figure: 6-bit Heighway dragon by the proposed Oritatami system.

Fractals and DFAO

Automatic sequences

Heighway dragon can be represented by the Paperfolding sequence P , which can be output by a DFAO.

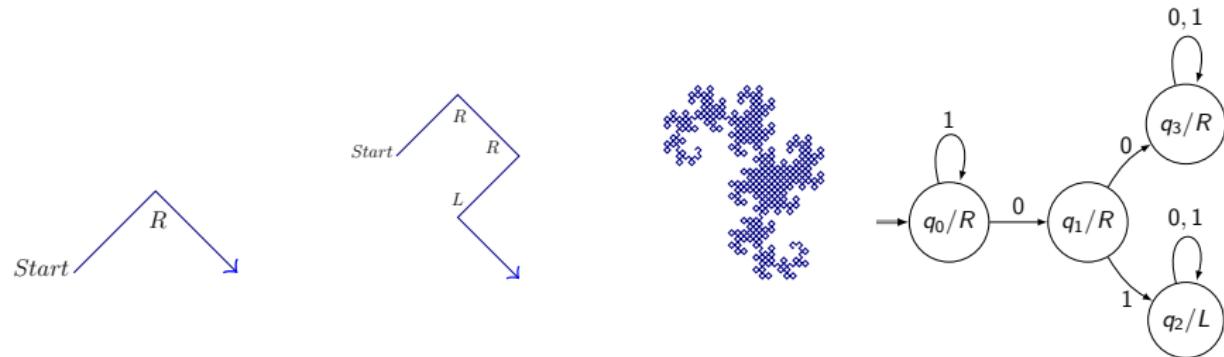


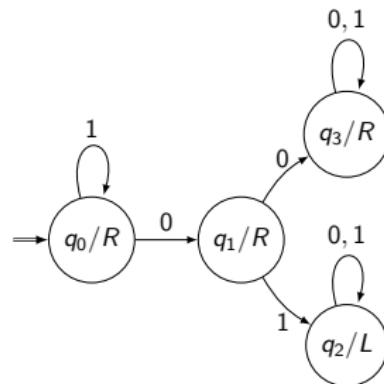
Figure: Paperfolding sequence $P = \text{RRLRRLLR}\dots$

Fractals and DFAO

- Paperfolding sequence $P = \text{RRLRRLLRRRLLRLLRRRLRRLLLRRRLRLL} \dots$

The i -th element of P ($i \geq 0$) can be computed by

- ① feeding the DFA shown right with the binary representation of i from its **LSB**, and
- ② reading R/L assigned to the reached state.



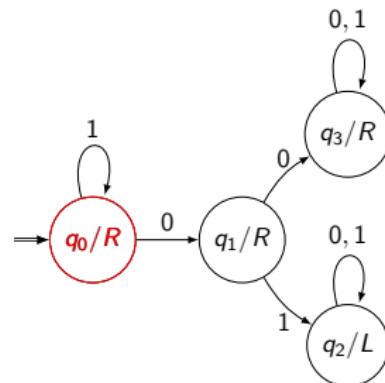
Fractals and DFAO

- Paperfolding sequence $P = \text{RRLRRLLRRRLLRLRRRLRRLLLRLRLLRL} \dots$

$i = 0$

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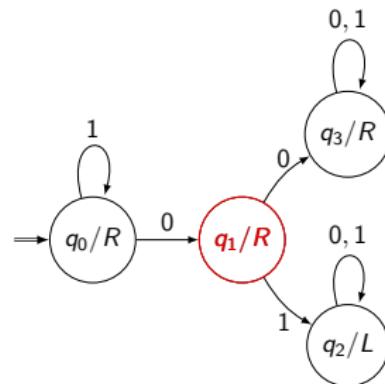
Fractals and DFAO

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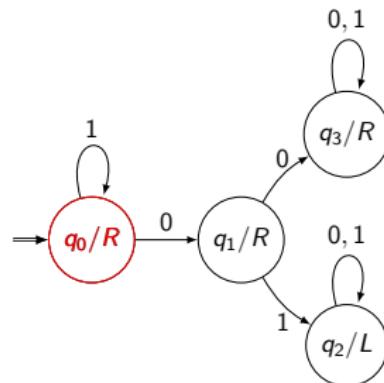
Fractals and DFAO

- Paperfolding sequence $P = \text{RRLRRLLRRRLLRLRRRLRRLLLRLRLLRL} \dots$

$i = 1$

The i -th element of P ($i \geq 0$) can be computed by

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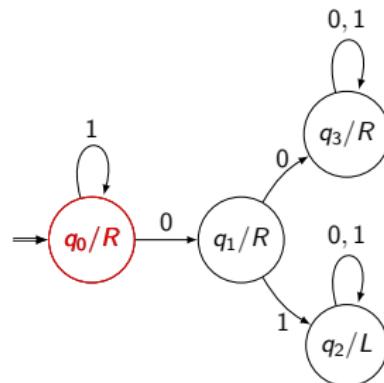
Fractals and DFAO

- Paperfolding sequence $P = \text{RRLRRLLRRRLLRLRRRLRRLLLRLRLLRL} \dots$

$$i = 2 \rightarrow 10$$

The i -th element of P ($i \geq 0$) can be computed by

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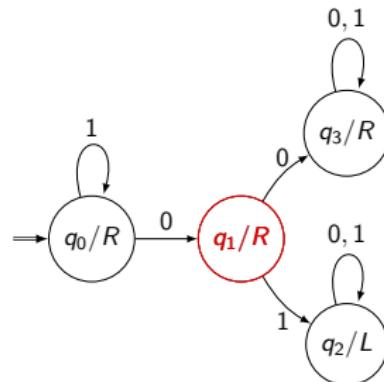
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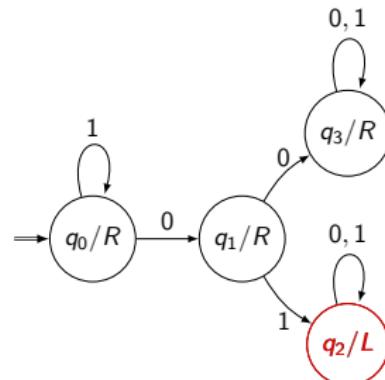
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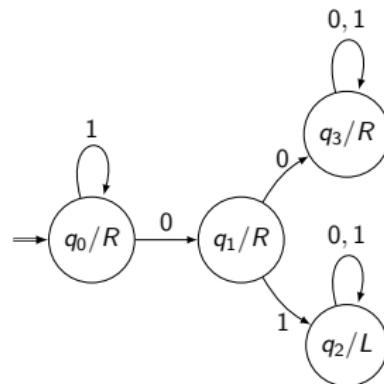


Fractals and DFAO

- Paperfolding sequence $P = \text{RRLRRLLRRRLLRLLRRRLRRLLLRRRLRLL} \dots$

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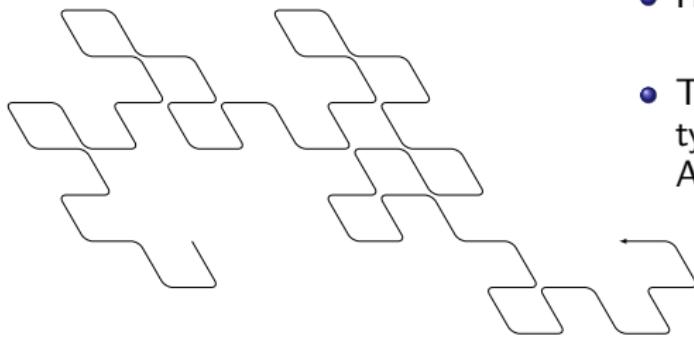
- ① feeding the DFA shown right with the binary representation of i from its **LSB**, and
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Implementation

Problems

Over the triangular grid, it is more natural to consider the slanted Heighway dragon.

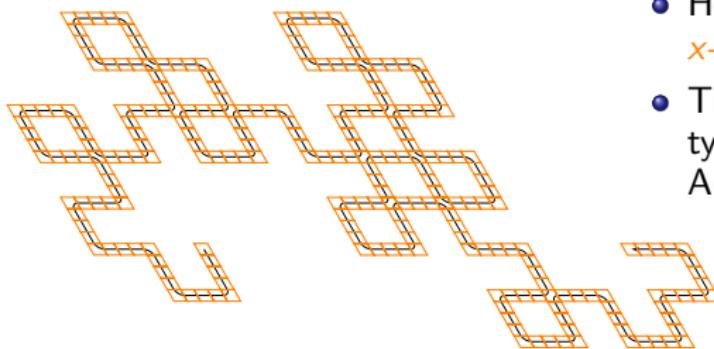


- How to avoid collisions?
- The slanted dragon involves four types of turns: L/R * A(cute)/O(btuse).
 - ▶ After the vertical line, L → O, R → A.
 - ▶ After the horizontal line, L → A, R → O.

Implementation

Problems

Over the triangular grid, it is more natural to consider the slanted Heighway dragon.



- How to avoid collisions?
x-rhombus scaling
- The slanted dragon involves four types of turns: L/R * A(cute)/O(btuse).
 - ▶ After the vertical line, L → O, R → A.
 - ▶ After the horizontal line, L → A, R → O.

Implementation

Algorithm:

- Set $i = 0$.
- Repeat the following tasks while propagating i :
 - ① Draw a vertical line segment.
 - ② Compute $P[i]$ by the DFAO and interpret it as $\underline{L \rightarrow O}, R \rightarrow A$.
 - ③ Turn accordingly and $i := i + 1$.
 - ④ Draw a horizontal line segment.
 - ⑤ Compute $P[i]$ by the DFAO and interpret it as $\underline{L \rightarrow A}, R \rightarrow O$.
 - ⑥ Turn accordingly and $i := i + 1$.

Implementation

Algorithm:

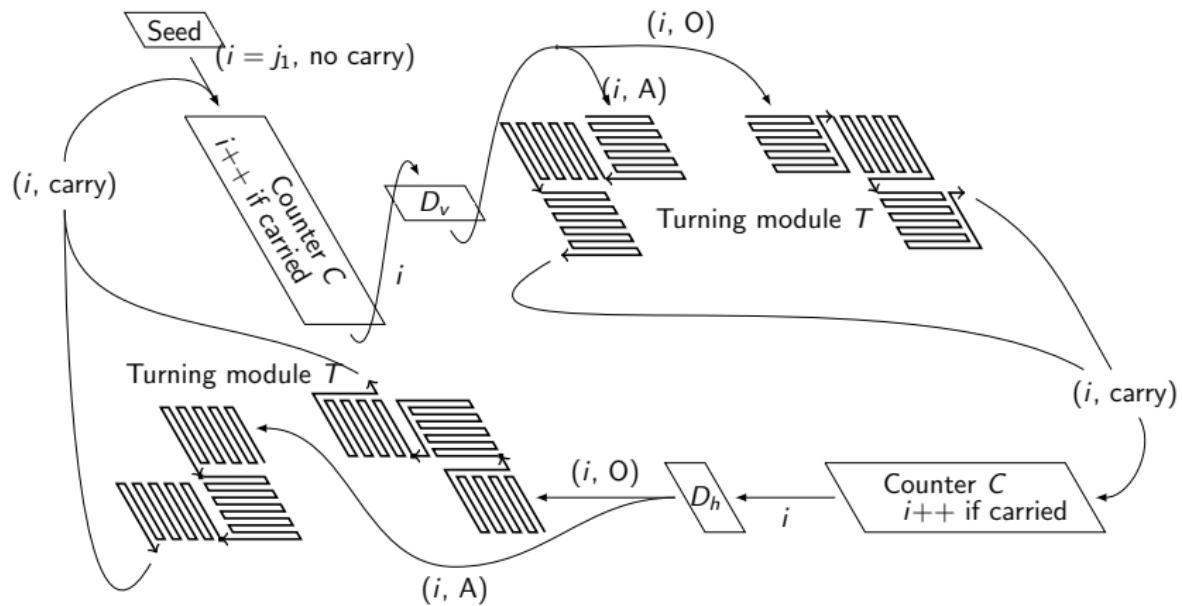
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 - ④ Draw a horizontal line segment.
 - ⑤ Compute $P[i]$ by the DFAO and interpret it as $L \rightarrow A, R \rightarrow O$.
 - ⑥ Turn accordingly and $i := i + 1$.

Transcript: $(CD_v TCD_h T)^*$, where

- C is the counter module for 1, 4 ,
- D_v, D_h are the DFAO module for 2 and 5, respectively.
- T is the turning module for 3, 6

Implementation

Module automaton



Implementation

Seed

The initial count of i is encoded on the seed. For instance $i = (100)_2$ is encode as the following sequence of bead types:

$W_{t,0} = 338 \rightarrow 339 \rightarrow 344 \rightarrow 345$ and $W_{t,1} = 346 \rightarrow 347 \rightarrow 348 \rightarrow 349$

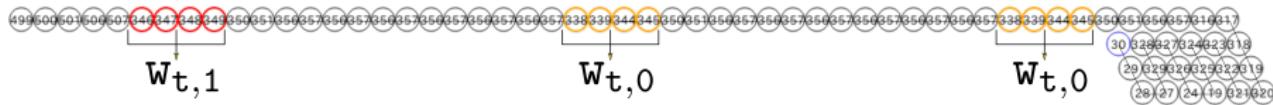
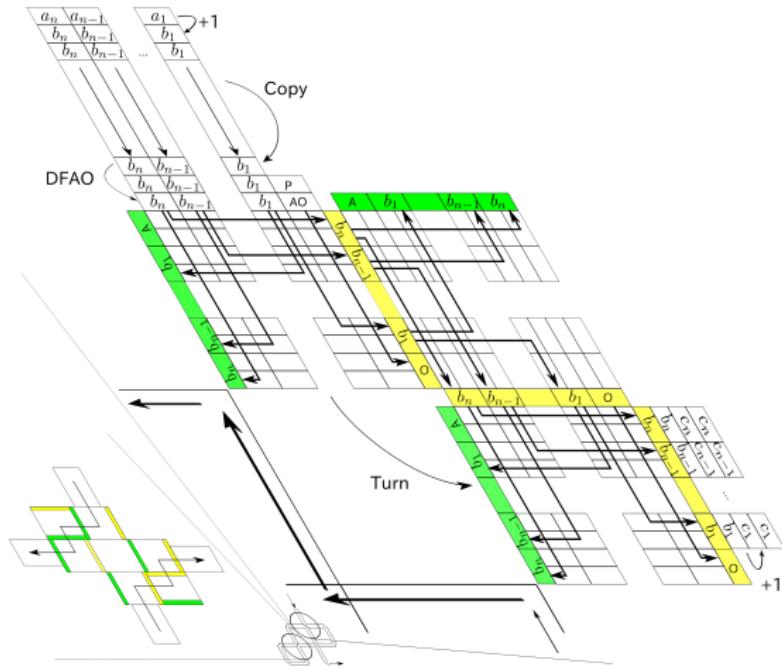


Figure: The seed for the 3-bit Highway dragon that starts at $i = 100_2$.

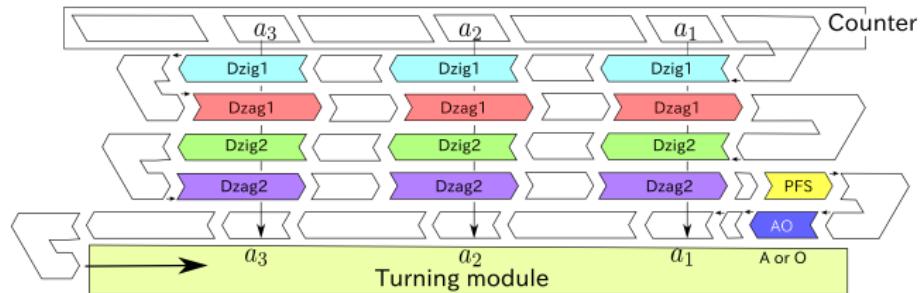
Implementation

Information flow

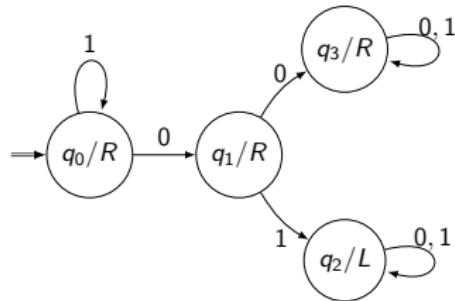


Implementation

DFAO module



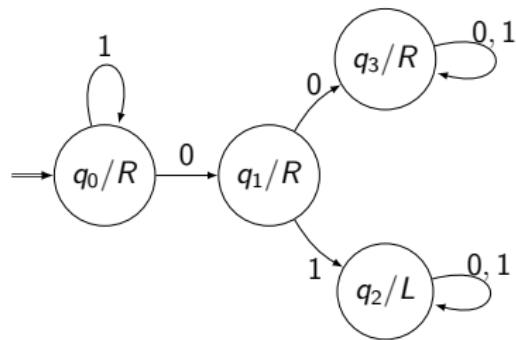
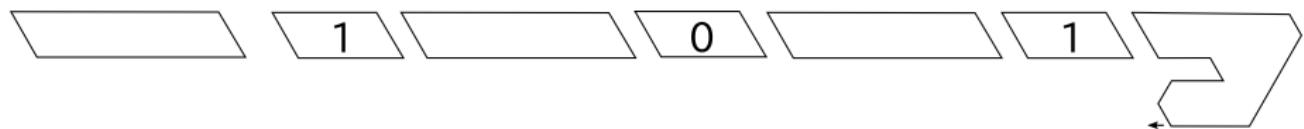
- 1st zigzag (Dzig1 & Dzag1) searches the first 0 (from LSB) and mark it as f0.
- 2nd zigzag (Dzig2 & Dzag2) checks if the f0 is followed by 0 or 1.



Implementation

DFAO module

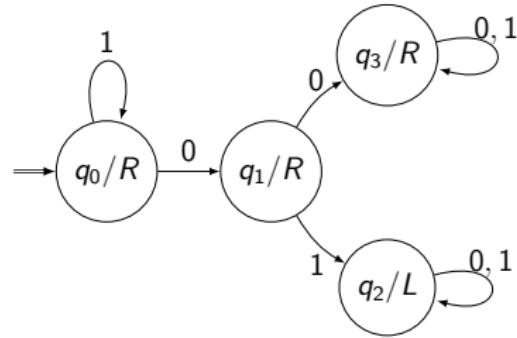
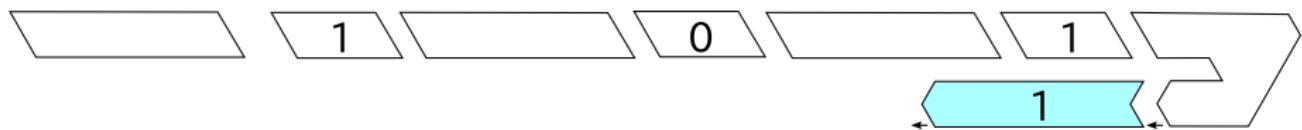
Current count = 101



Implementation

DFAO module

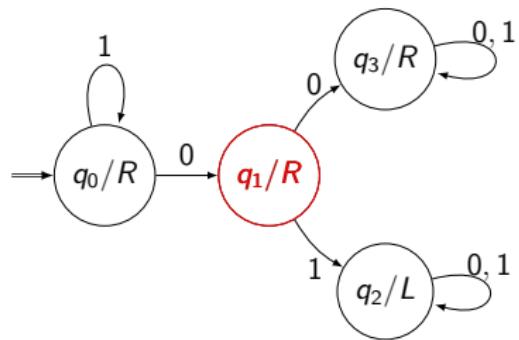
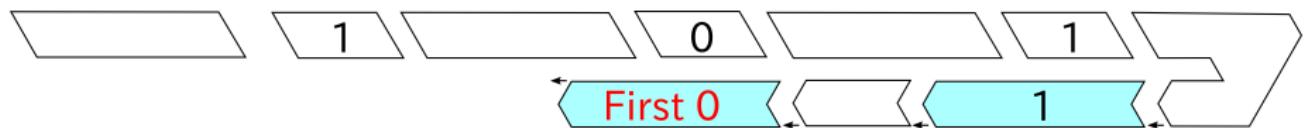
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Implementation

DFAO module

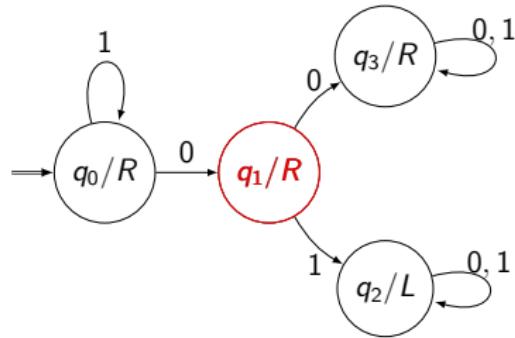
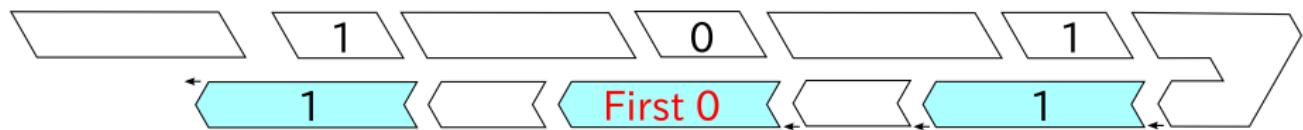
Current count = 101



Implementation

DFAO module

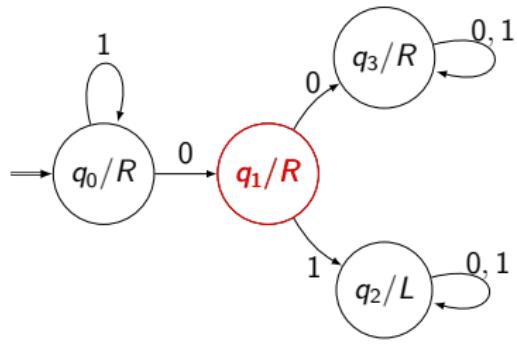
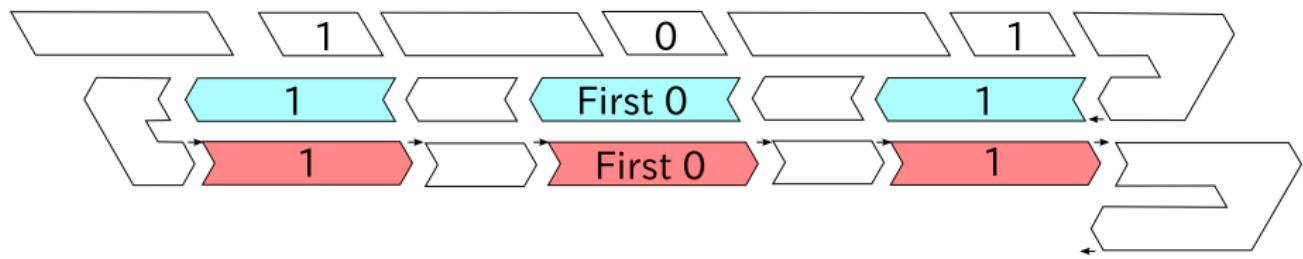
Current count = 101



Implementation

DFAO module

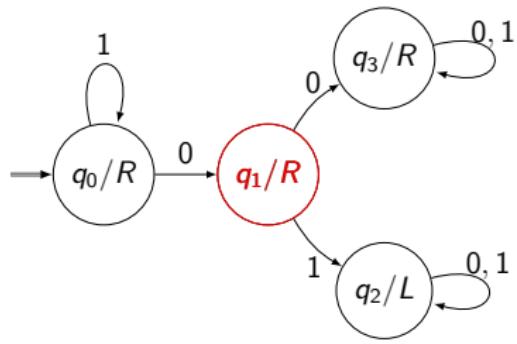
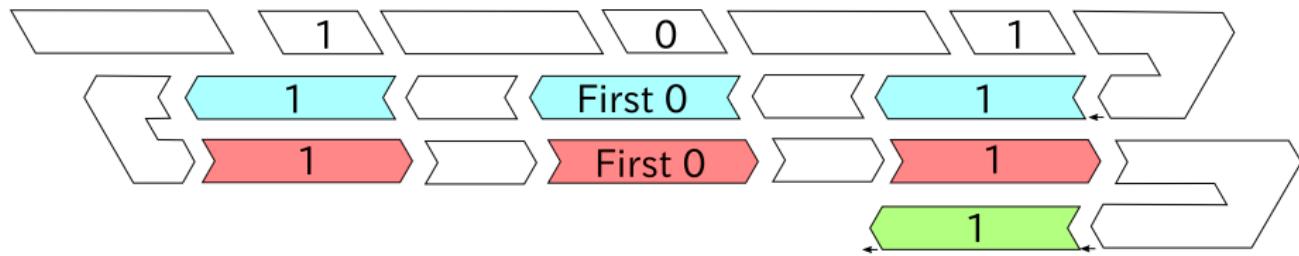
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Implementation

DFAO module

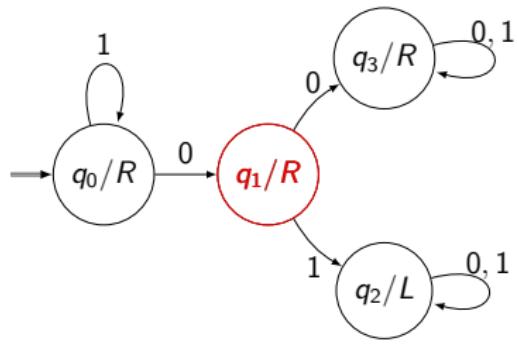
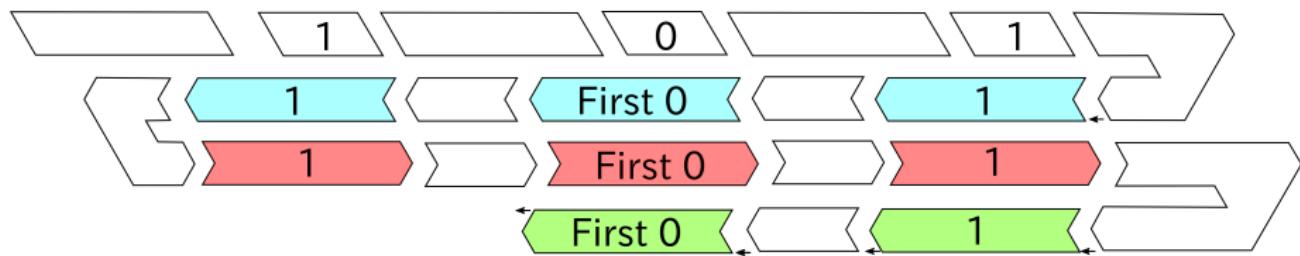
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Implementation

DFAO module

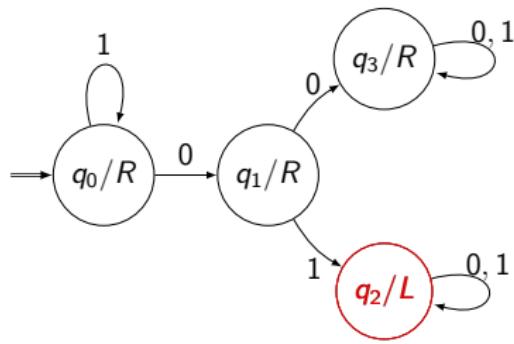
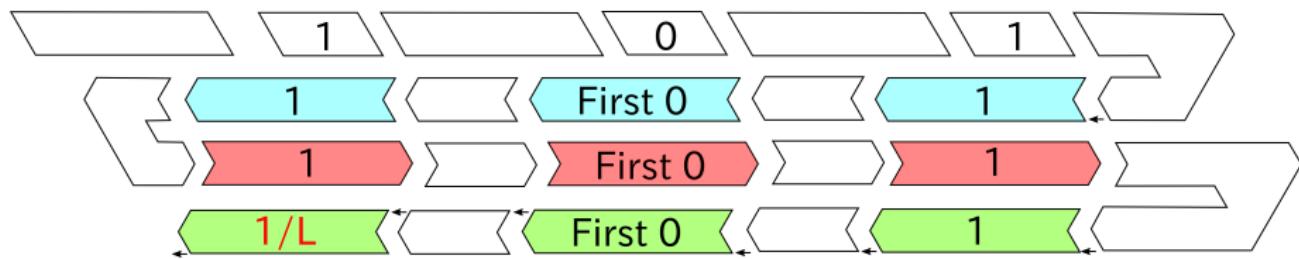
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Implementation

DFAO module

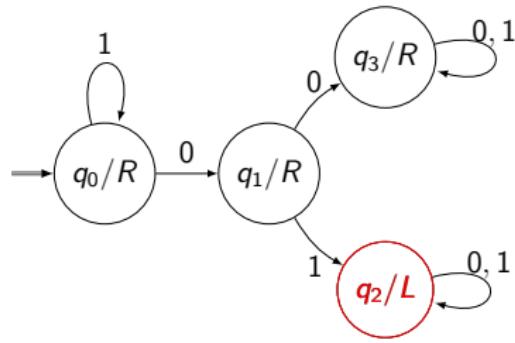
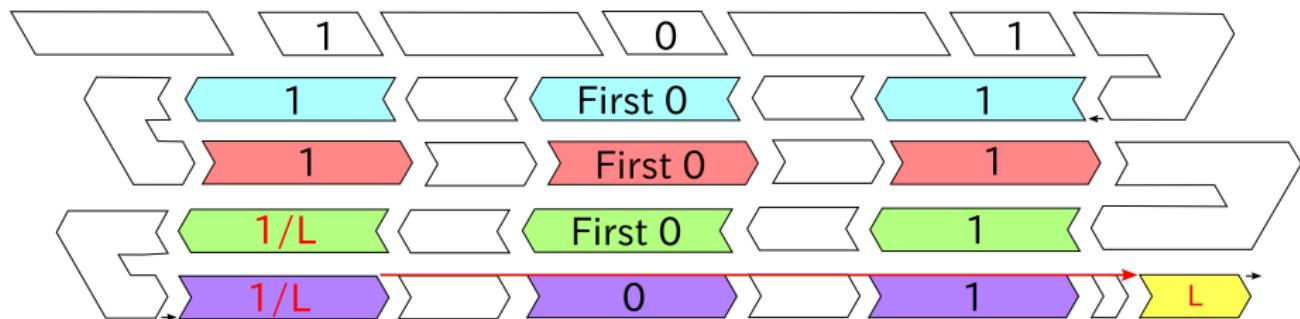
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Implementation

DFAO module

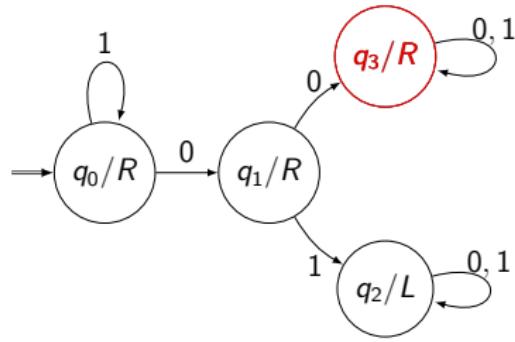
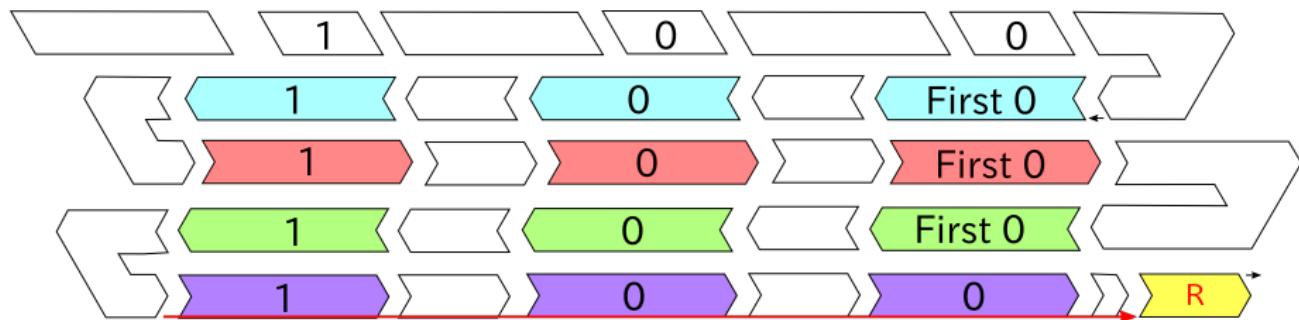
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Implementation

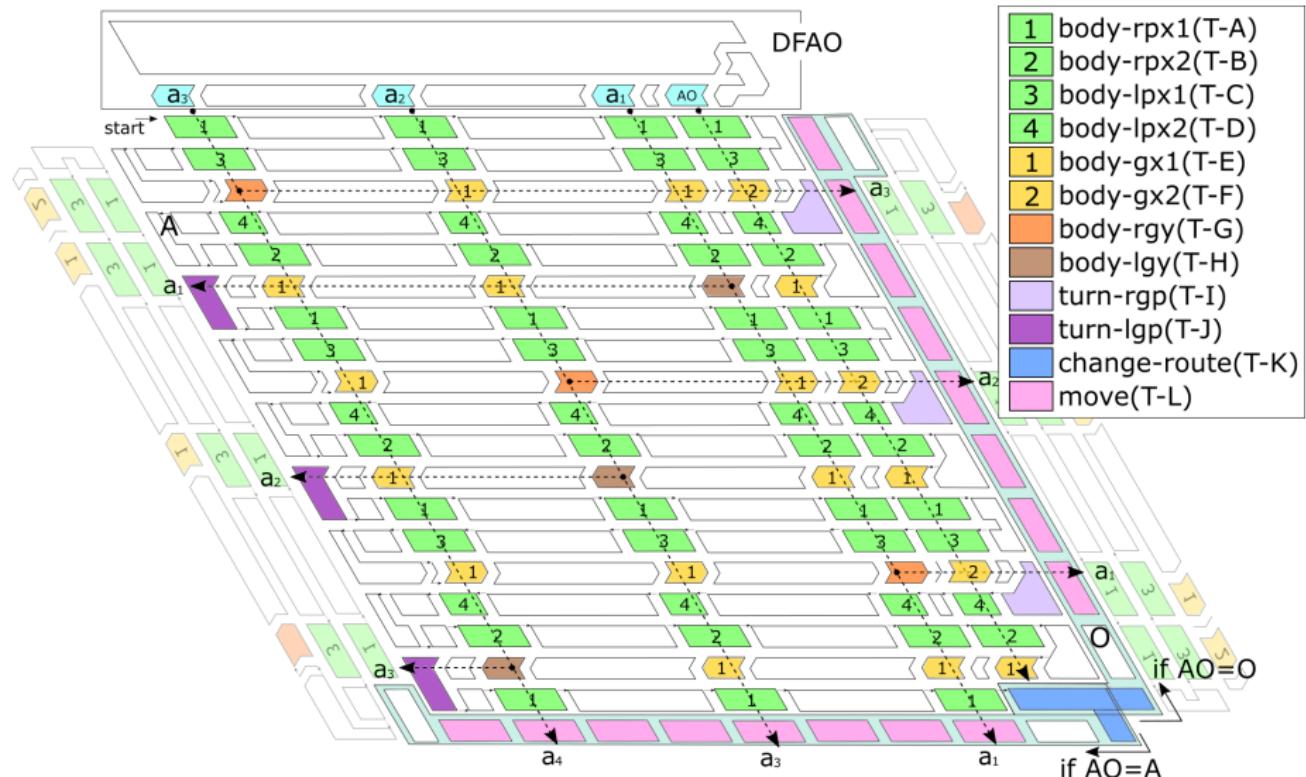
DFAO module

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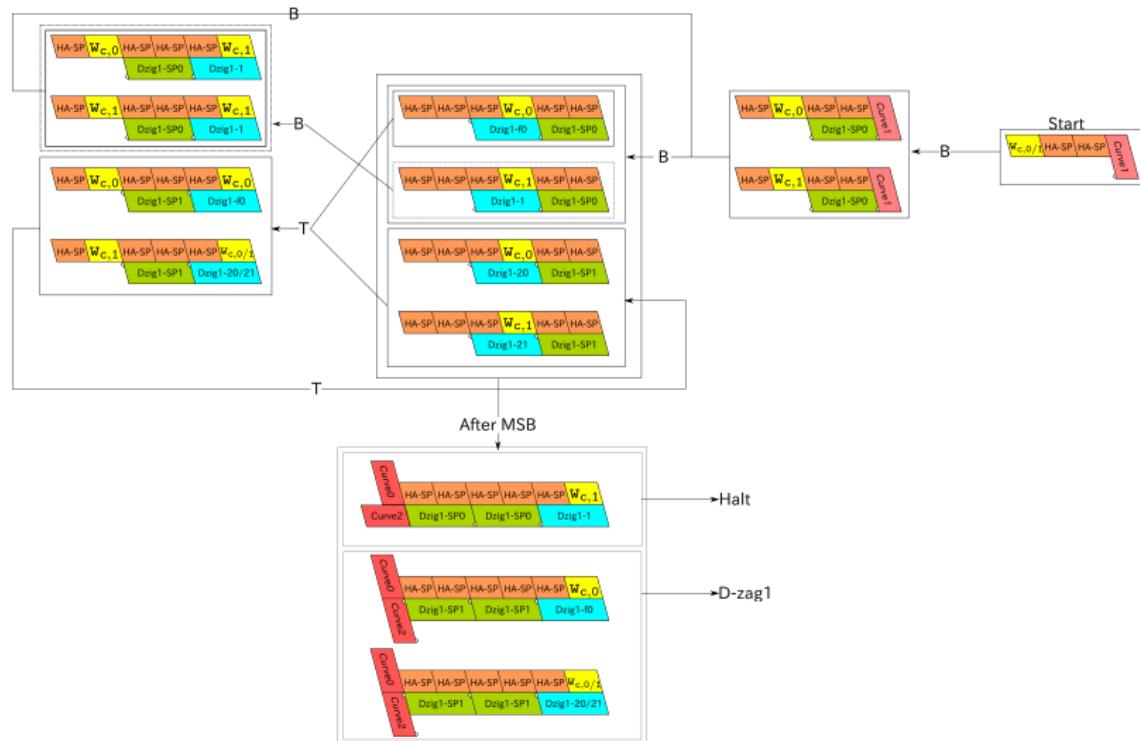
Implementation

Turning module



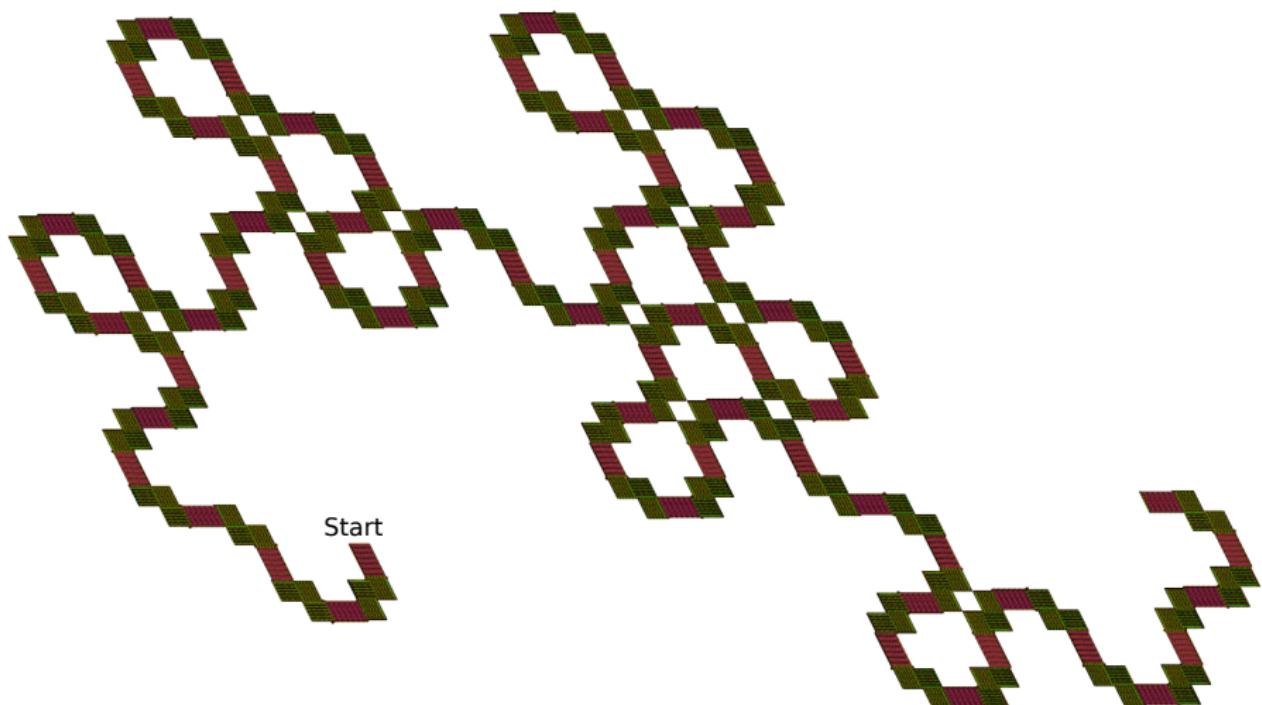
Implementation

Brick automata



Implementation

Result



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IMPORTANT DATES

Deadline for submission
April 30th, 2018 (AoE)

Notification to authors
June 1st, 2018

Camera-ready version
June 20th, 2018

INVITED SPEAKERS

Tomohiro I
Bakhadyr Khoussainov
Alexander Okhotin
Dominique Perrin
Marinella Sciortino
Andrew Winslow

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- Venue: Baltic Hall (5-6th floor at *Le Signe* in front of Fuchu station).
- Registration fee 30,000JPY.
- Pre-workshop to celebrate the birthdays of Masami Ito and Pal Dömösi will be held on September 5-7 @ Kyoto Sangyo University.