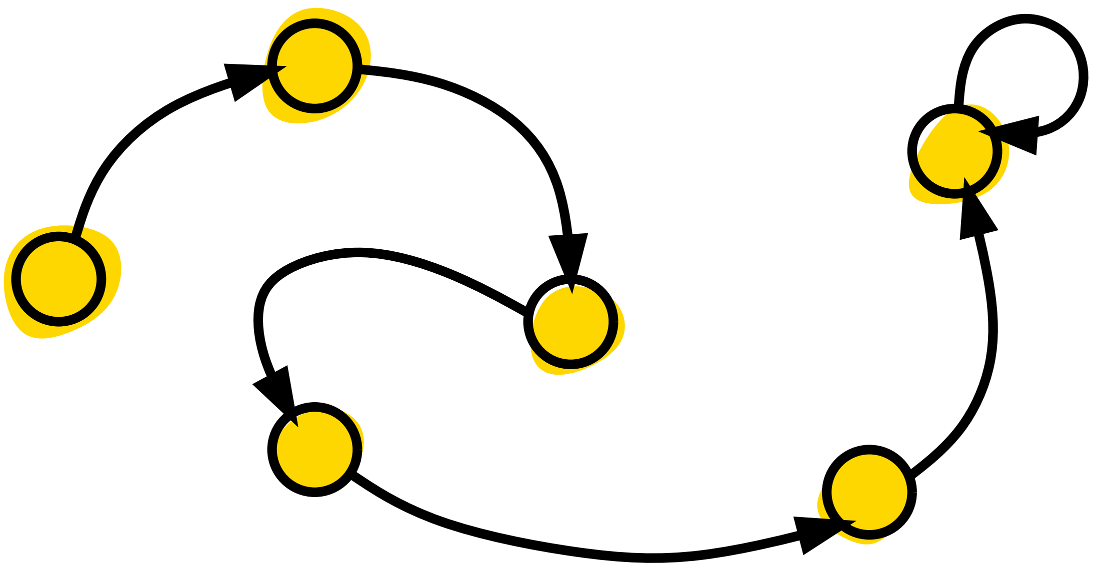
State sequences of reaction systems



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Note: in this lecture we discuss
the context-independent behaviour of RS
unless otherwise specified

Power set functions

$$f : 2^S \to 2^S$$

power set function

$$f(\varnothing) = f(S) = \varnothing$$

boundary condition

Computing (or implementing) power set functions by RS

Theorem

$$f = \mathrm{res}_{\mathcal{A}} \text{ for some } \mathcal{A}$$

$$\Updownarrow$$

$$f \text{ is a boundary power set function}$$

Proof idea

$$f(X) = Y$$

$$\Downarrow$$

$$(X, S - X, Y)$$

complement reaction

Computing power set functions by RS with restricted resources

Minimal RS

$(\{x\}, I, P)$

reactant-minimal
(only 1 reactant)

$(R, \{y\}, P)$

inhibitor-minimal
(only 1 inhibitor)

$(\{x\}, \{y\}, P)$

resource-minimal
(only 1 reactant
and 1 inhibitor)

How does minimality restrict the class of functions computed (or implemented) by RS?

Subadditive functions

union-subadditive

$$f(X \cup Y) \subseteq f(X) \cup f(Y)$$

$$f(X \cap Y) \subseteq f(X) \cup f(Y)$$

intersection-subadditive

Examples

$$(\{a, b\}, \{c, d\}, \{a, b\})$$

Not union-subadditive

$$\mathrm{res}_{\mathcal{A}}(\{a\} \cup \{b\}) = \mathrm{res}_{\mathcal{A}}(\{a, b\}) = \{a, b\}$$

$$\not\subseteq$$

$$\mathrm{res}_{\mathcal{A}}(\{a\}) \cup \mathrm{res}_{\mathcal{A}}(\{b\}) = \varnothing$$

Examples

$$(\{a, b\}, \{c, d\}, \{a, b\})$$

Not intersection-subadditive

$$\mathrm{res}_{\mathcal{A}}(\{a, b, c\} \cap \{a, b, d\}) = \mathrm{res}_{\mathcal{A}}(\{a, b\}) = \{a, b\}$$

$$\not\Cap$$

$$\mathrm{res}_{\mathcal{A}}(\{a, b, c\}) \cup \mathrm{res}_{\mathcal{A}}(\{a, b, d\}) = \varnothing$$

Theorem

f is union-subadditive

$$\Updownarrow$$

$f = \mathrm{res}_{\mathcal{A}}$ for some reactant-minimal $\mathcal{A}$

Theorem

f is intersection-subadditive

$$\Updownarrow$$

$f = \text{res}_{\mathcal{A}}$ for some inhibitor-minimal $\mathcal{A}$

Theorem

f is union- and intersection-subadditive

$$\Updownarrow$$

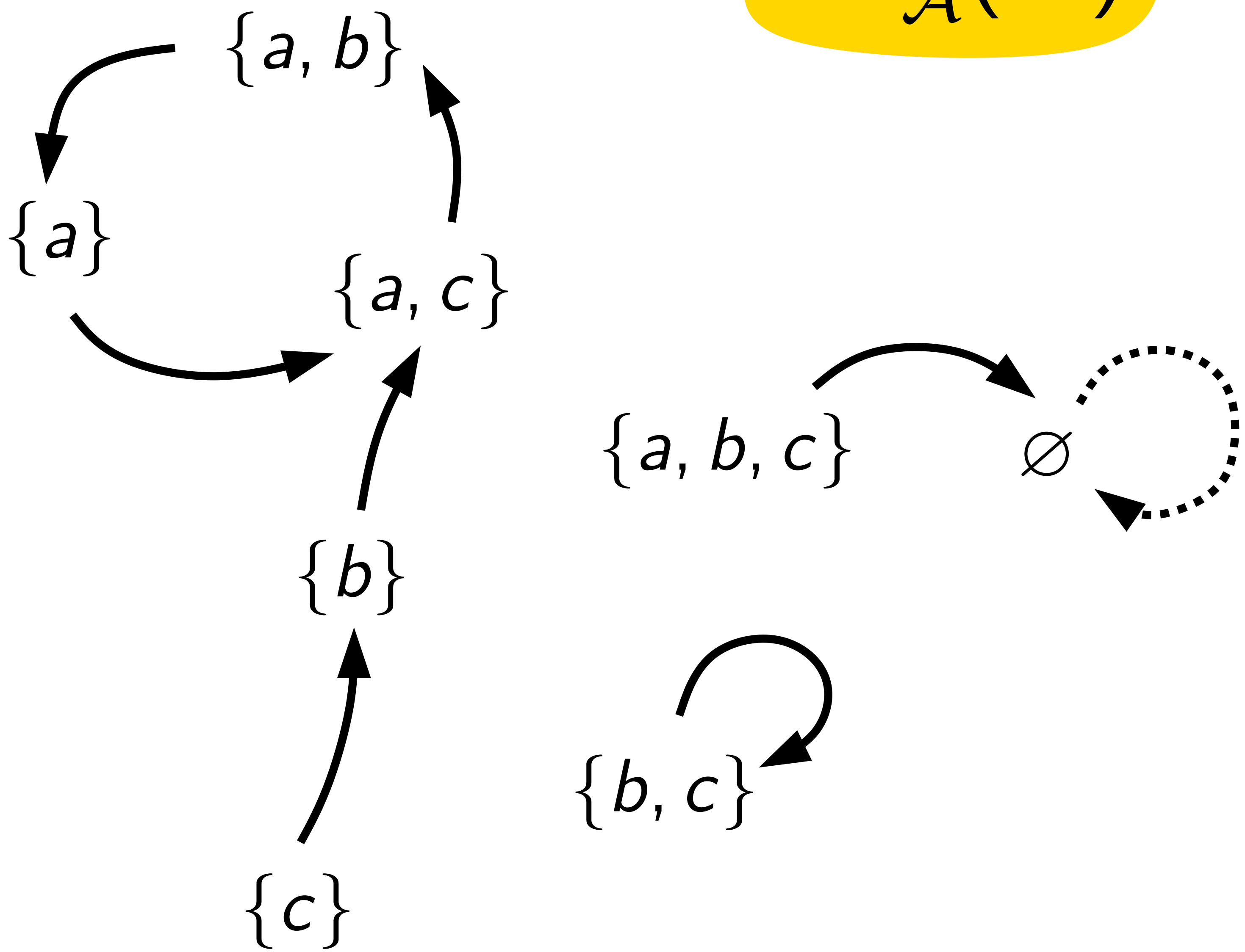
$f = \mathsf{res}_{\mathcal{A}}$ for some resource-minimal $\mathcal{A}$

Dynamics of RS:

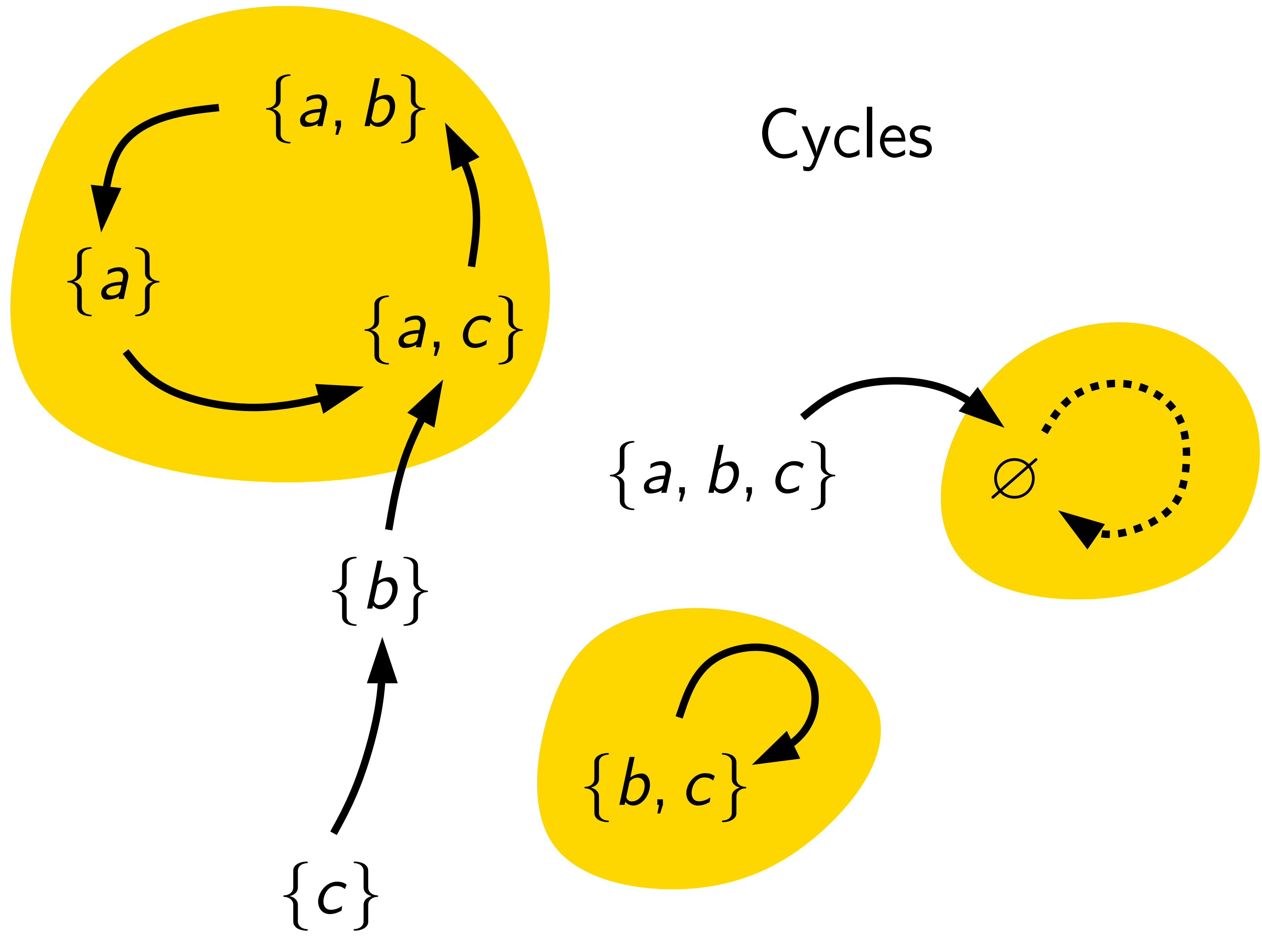
state sequences

Dynamics

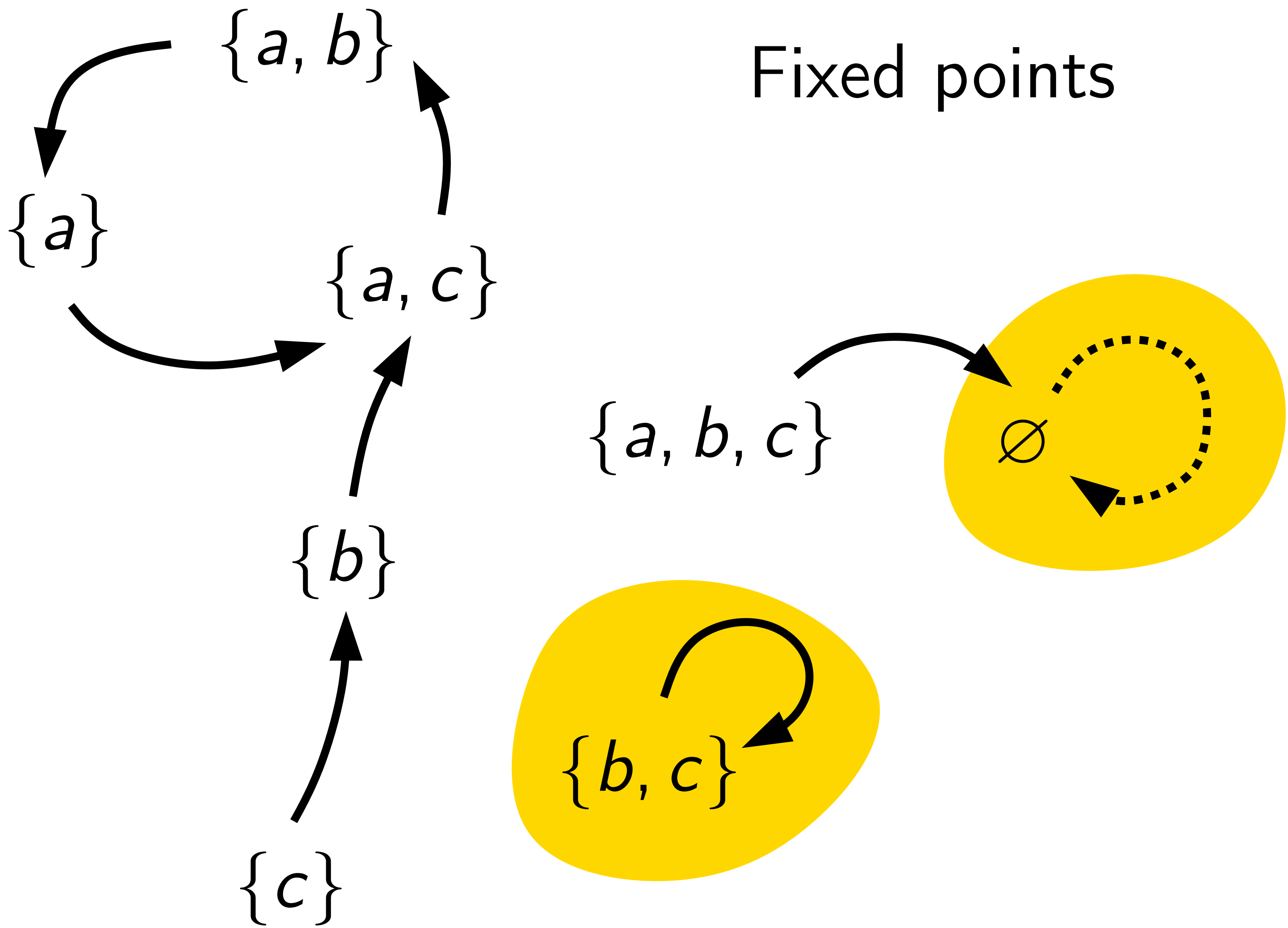
$\mathrm{res}^n_{\mathcal{A}}(T)$



Dynamics



Dynamics

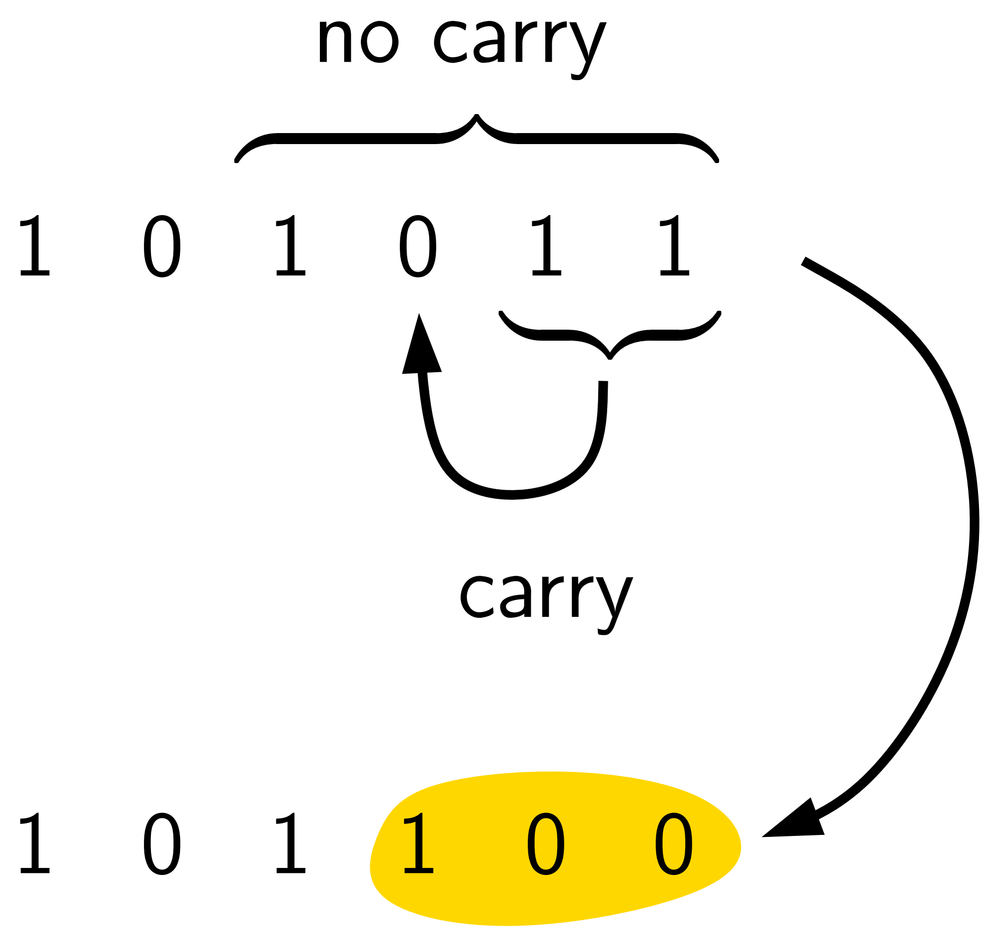


An example of interesting dynamics: implementing binary counters

Implementing binary counters

$$
\begin{array}{cccccc}
1 & 0 & 1 & 0 & 1 & 1 \\
\downarrow & & \downarrow & & \downarrow & \downarrow \\
\{\, b_5, & & b_3, & & b_1, & b_0 \,\}
\end{array}
$$

Incrementing binary counters



Reactions for incrementing binary counters

carry

$$(\{b_{i-1}, b_{i-2}, \ldots, b_0\}, \{b_i\}, \{b_i\}) \qquad \text{for } 1 \leq i \leq n$$

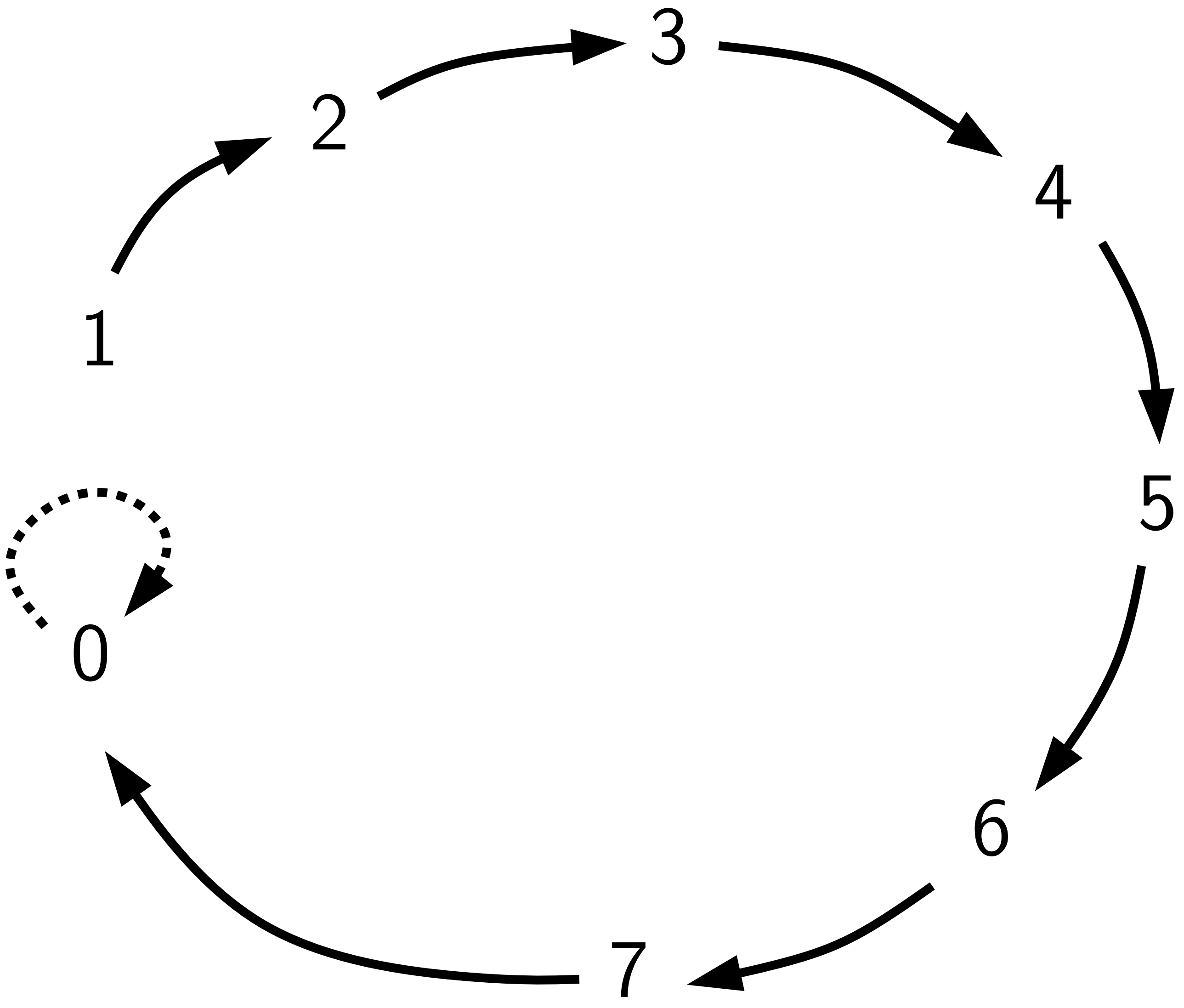
$$(\{b_i\}, \{b_0\}, \{b_0\}) \qquad \text{for } 1 \leq i \leq n$$

$$(\{b_i\}, \{b_j\}, \{b_i\}) \qquad \text{for } 0 \leq j < i \leq n$$

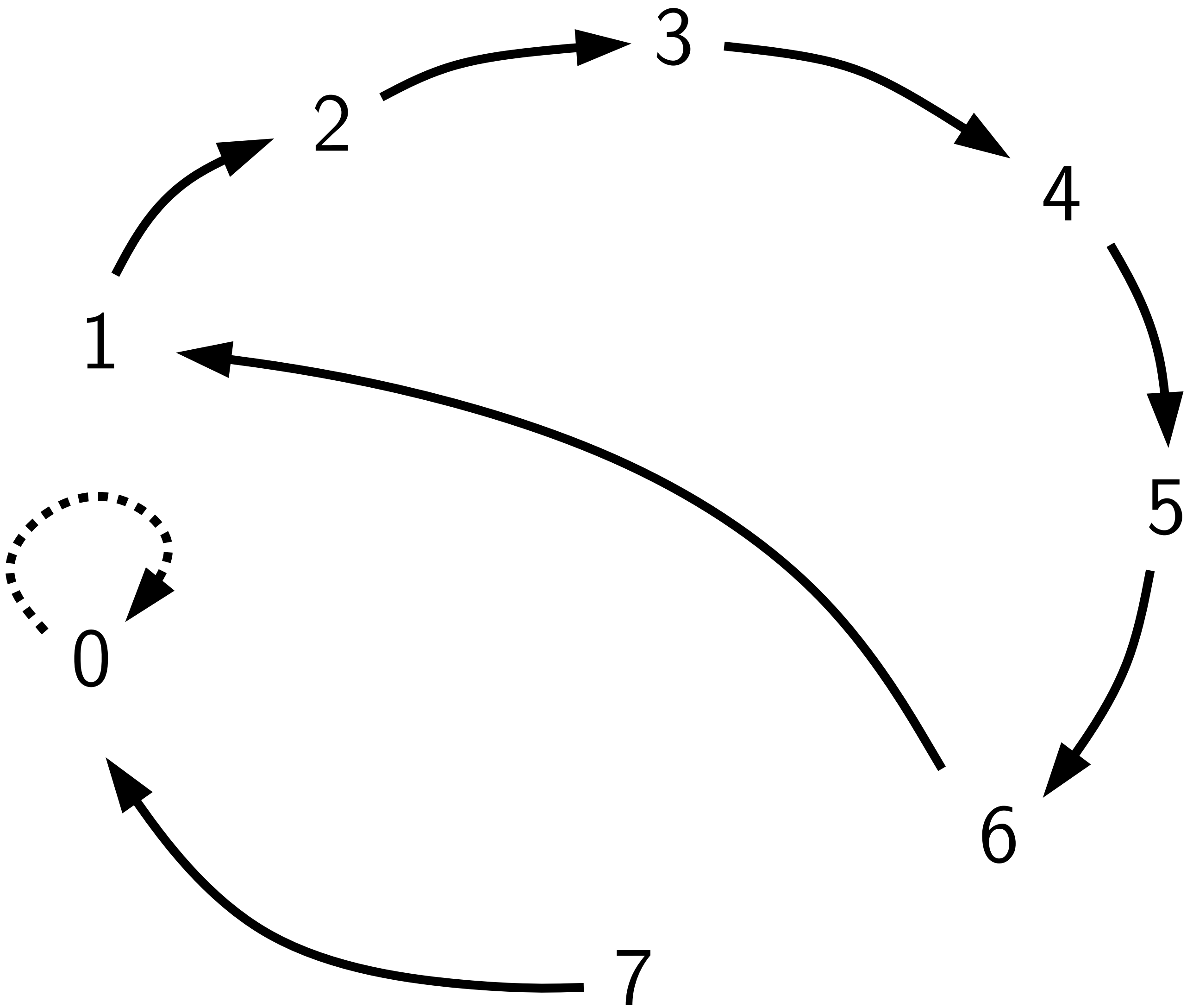
flip least significant bit

preserve 1 if no carry

Binary counters → long paths

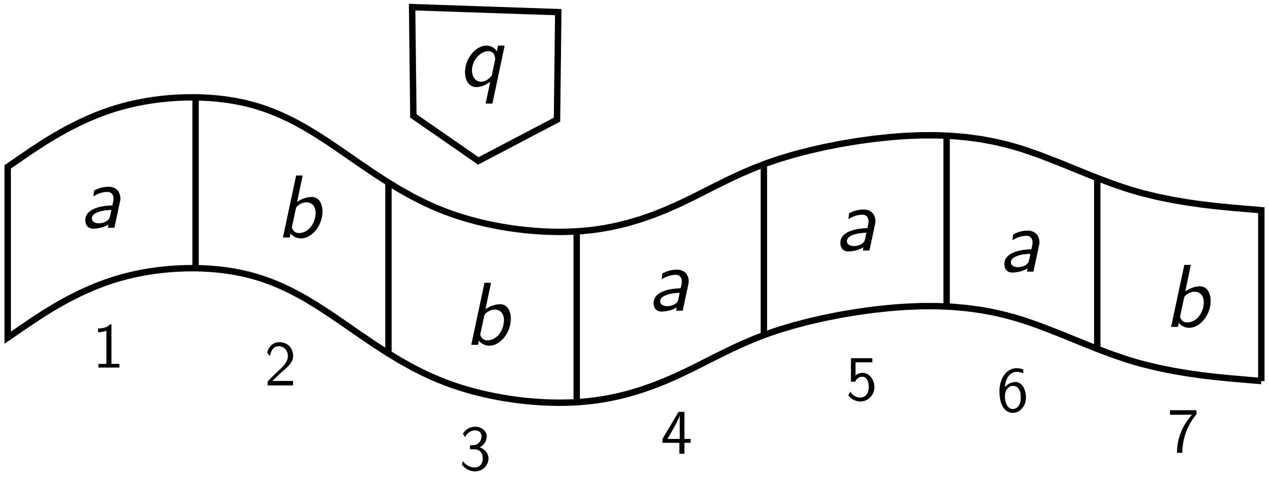


Binary counters → long cycles



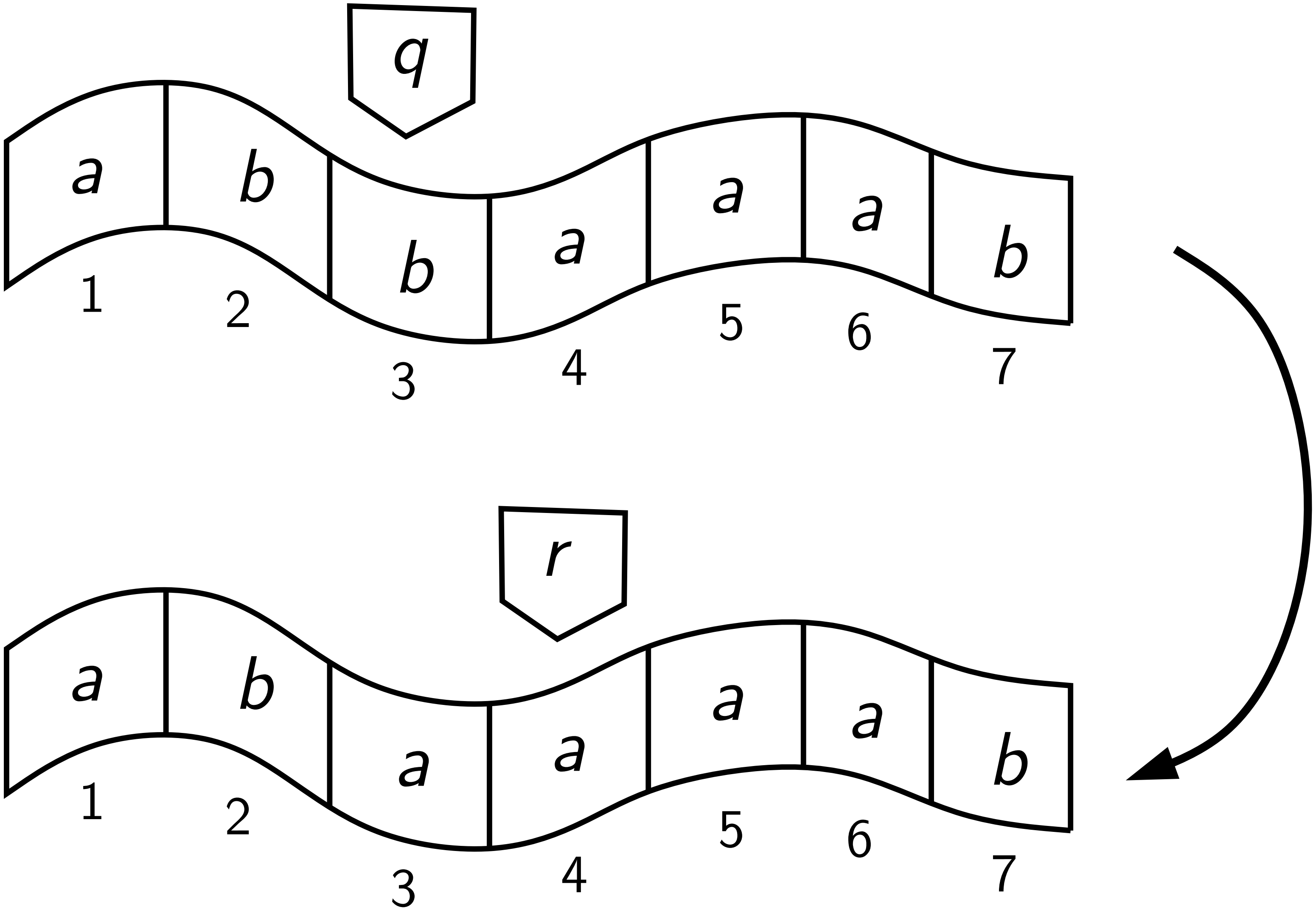
General computable dynamics: simulating Turing machines

Turing machines (with bounded tape)

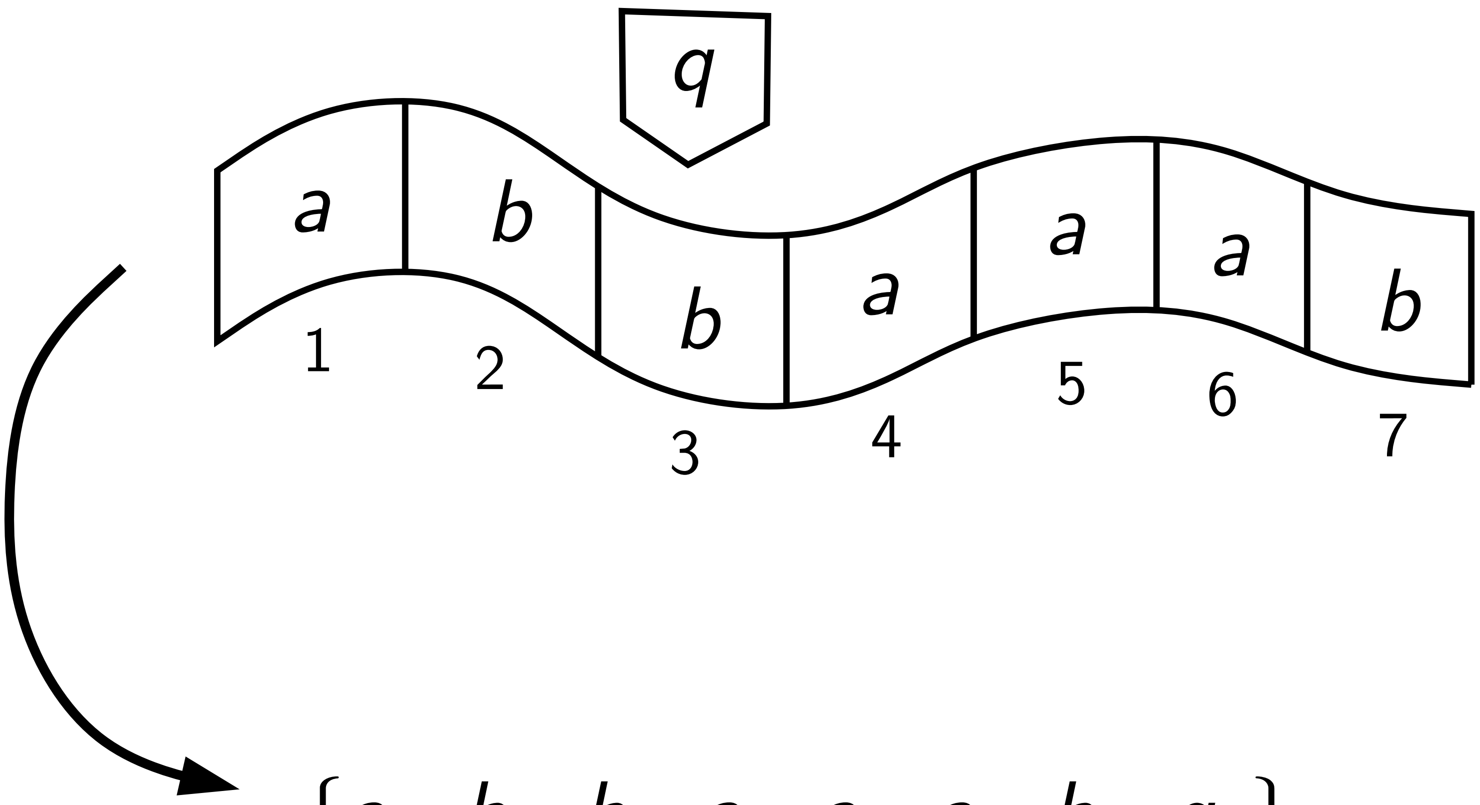


$$\begin{array}{cccccc} q & a & \longrightarrow & q & b & \triangleright \\ q & b & \longrightarrow & r & a & \triangleright \\ r & a & \longrightarrow & q & a & \triangleleft \\ r & b & \longrightarrow & r & a & \triangleright \end{array}$$

Turing machines (with bounded tape)



Encoding as reaction system



$$\{a_1, b_2, b_3, a_4, a_5, a_6, b_7, q_3\}$$

Encoding as reaction system

$$
\begin{array}{cccccc}
q & a & \rightarrow & q & b & \triangleright \\
q & b & \rightarrow & r & a & \triangleright \\
r & a & \rightarrow & q & a & \triangleleft \\
r & b & \rightarrow & r & a & \triangleright
\end{array}
$$

$$(\{q_1, a_1\}, \{\spadesuit\}, \{q_2, b_1\})$$

$$(\{q_2, a_2\}, \{\spadesuit\}, \{q_3, b_2\})$$

$$\vdots$$

$$(\{q_6, a_6\}, \{\spadesuit\}, \{q_7, b_6\})$$

Encoding as reaction system

$$\begin{array}{ccccc}
q & a & \rightarrow & q & b & \triangleright \\
q & b & \rightarrow & r & a & \triangleright \\
r & a & \rightarrow & q & a & \triangleleft \\
r & b & \rightarrow & r & a & \triangleright
\end{array}$$

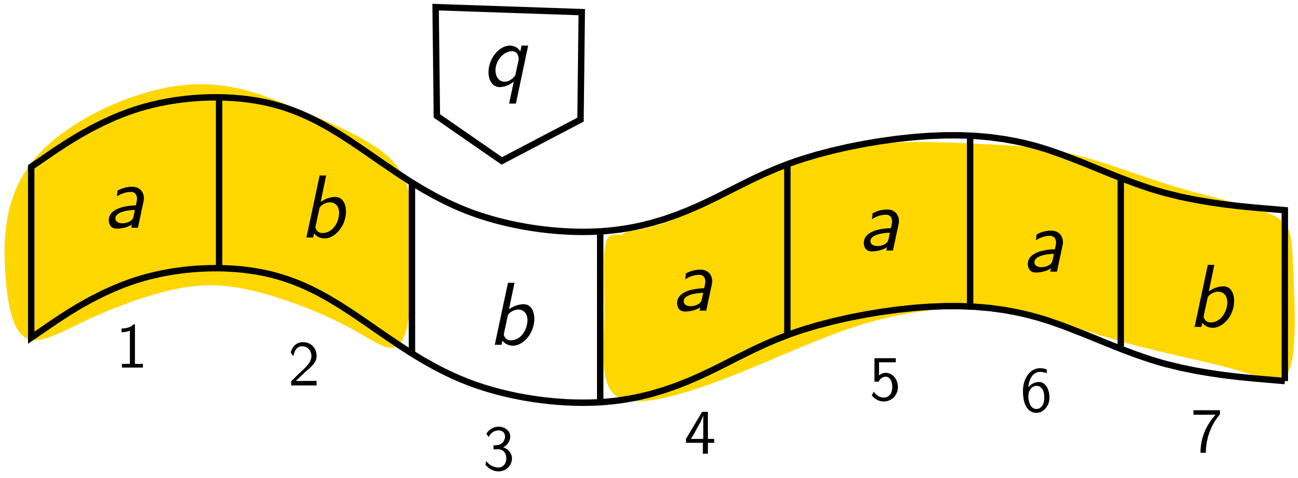
$$(\{r_2, a_2\}, \{\spadesuit\}, \{q_1, a_2\})$$

$$(\{r_3, a_3\}, \{\spadesuit\}, \{q_2, a_3\})$$

$$\vdots$$

$$(\{r_7, a_7\}, \{\spadesuit\}, \{q_6, a_7\})$$

Preserving the tape



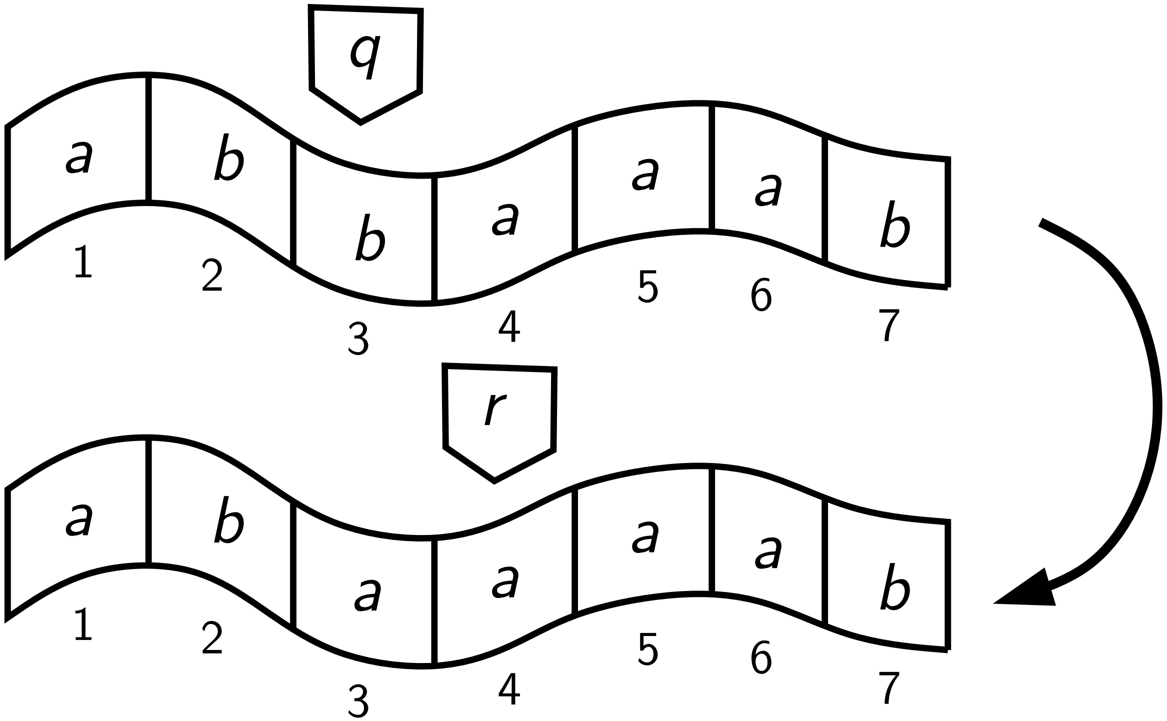
$$(\{a_1\}, \{q_1, r_1\}, \{a_1\}) \qquad (\{b_1\}, \{q_1, r_1\}, \{b_1\})$$

$$(\{a_2\}, \{q_2, r_2\}, \{a_2\}) \qquad (\{b_2\}, \{q_2, r_2\}, \{b_2\})$$

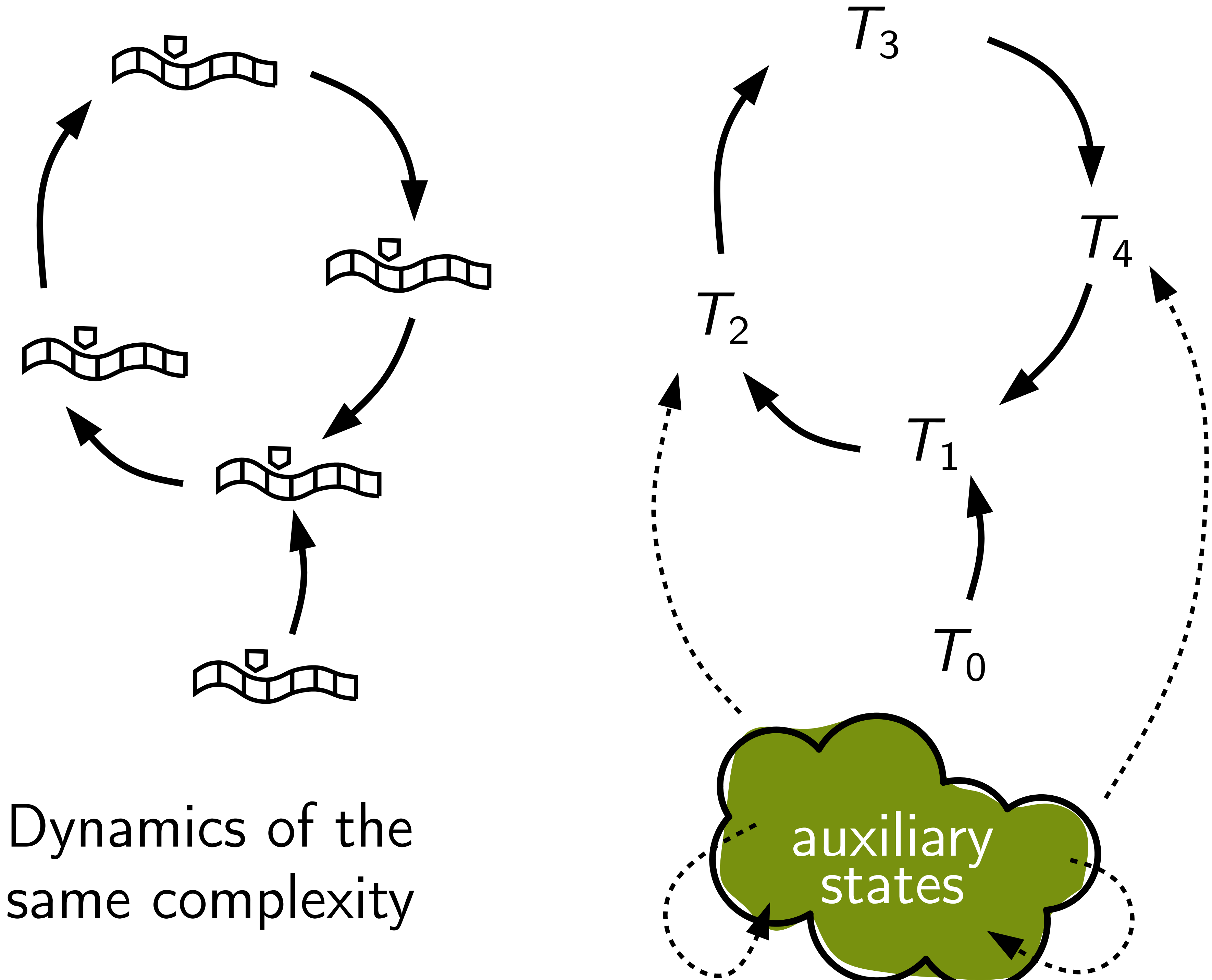
$$\vdots \qquad \vdots$$

$$(\{a_7\}, \{q_7, r_7\}, \{a_7\}) \qquad (\{b_7\}, \{q_7, r_7\}, \{b_7\})$$

Computation step



$$\{a_1, b_2, b_3, a_4, a_5, a_6, b_7, q_3\} \xrightarrow{\mathrm{res}_{\mathcal{A}}} \{a_1, b_2, a_3, a_4, a_5, a_6, b_7, r_4\}$$



Dynamics of the same complexity
T_3
T_4
T_2
T_1
T_0
auxiliary states

High-level dynamics of resource-minimal RS

Simulating power of minimal RS

It turns out that resource-minimal RS are powerful enough to simulate arbitrary RS, if we allow a less strict notion of simulation

Theorem

For each reaction system $\mathcal{A}$ there exists a resource-minimal $\mathcal{B}$ such that, for each state T and time n,

$$\mathrm{res}^{2n}_{\mathcal{B}}(T) = \mathrm{res}^{n}_{\mathcal{A}}(T)$$

Theorem

For each reaction system $\mathcal{A}$ there exists a resource-minimal $\mathcal{B}$ such that, for each state T and time n,

$$\mathrm{res}_{\mathcal{B}}^{2n}(T) = \mathrm{res}_{\mathcal{A}}^{n}(T)$$

2-to-1 simulation

Theorem

For each reaction system $\mathcal{A}$ there exists a resource-minimal $\mathcal{B}$ such that, for each state T and time n,

$$\mathrm{res}_{\mathcal{B}}^{2n}(T) = \mathrm{res}_{\mathcal{A}}^{n}(T)$$

2-to-1 simulation

$\mathcal{A}$ $\quad T_1 \longrightarrow T_2 \longrightarrow T_3 \longrightarrow T_4 \rightarrow$

$\mathcal{B}$ $\quad T_1 \to \bullet \to T_2 \to \bullet \to T_3 \to \bullet \to T_4 \to$

Proof idea

$$a = (\{x, y\}, \{z\}, \{w\}) \qquad b = (\{v\}, \{z, w\}, \{z\})$$

$$\begin{tikzcd}
\{x, y\} \arrow[d] & \{v\} \arrow[d] & \{x, z\} \arrow[d] & \{x, y, v\} \arrow[d] \\
\{\bar{b}, \heartsuit\} \arrow[d] & \{\bar{a}, \heartsuit\} \arrow[d] & \{\bar{a}, \bar{b}, \heartsuit\} \arrow[d] & \{\heartsuit\} \arrow[d] \\
\{w\} & \{z\} & \emptyset & \{w, z\}
\end{tikzcd}$$

Proof idea: given $a = (R_a, I_a, P_a)$

Reactant missing?

$(\{x\}, \{y\}, \{\bar{a}\})$ for $y \in R_a, x \in S - \{y\}$

Any inhibitor?

$(\{x\}, \{\heartsuit\}, \{\bar{a}\})$ for $x \in I_a$

If not disabled, produce P_a

$(\{\heartsuit\}, \{\bar{a}\}, P_a)$

Make $\heartsuit$ every other step

$(\{x\}, \{\heartsuit\}, \{\heartsuit\})$ for $x \in S$

Proof idea: given $a = (R_a, I_a, P_a)$

Reactant missing?

$(\{x\}, \{y\}, \{\bar{a}\})$ for $y \in R_a, x \in S - \{y\}$

Any inhibitor?

$(\{x\}, \{\heartsuit\}, \{\bar{a}\})$ for $x \in I_a$

If not disabled, produce P_a

$(\{\heartsuit\}, \{\bar{a}\}, P_a)$

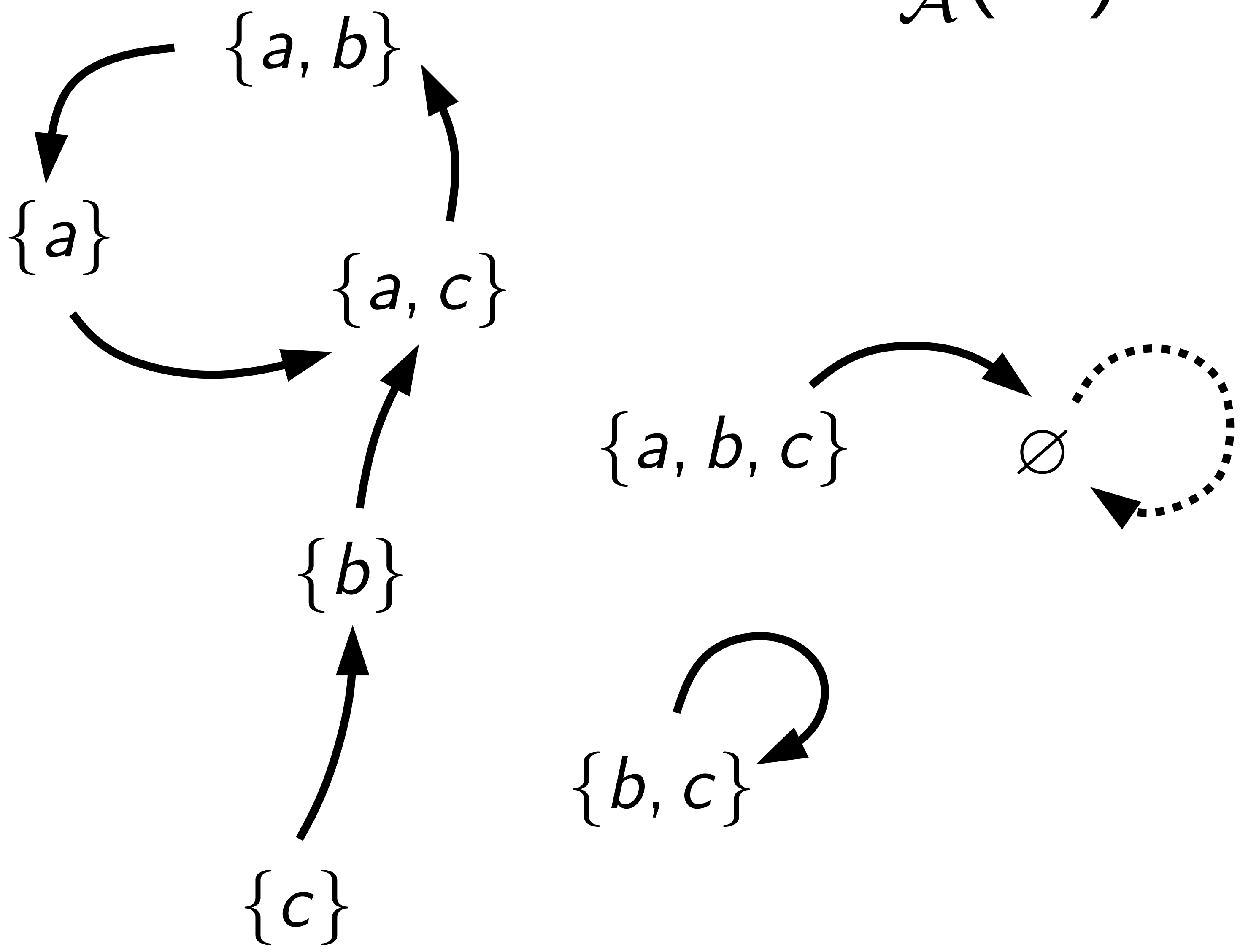
Make $\heartsuit$ every other step

$(\{x\}, \{\heartsuit\}, \{\heartsuit\})$ for $x \in S$

Minimal!

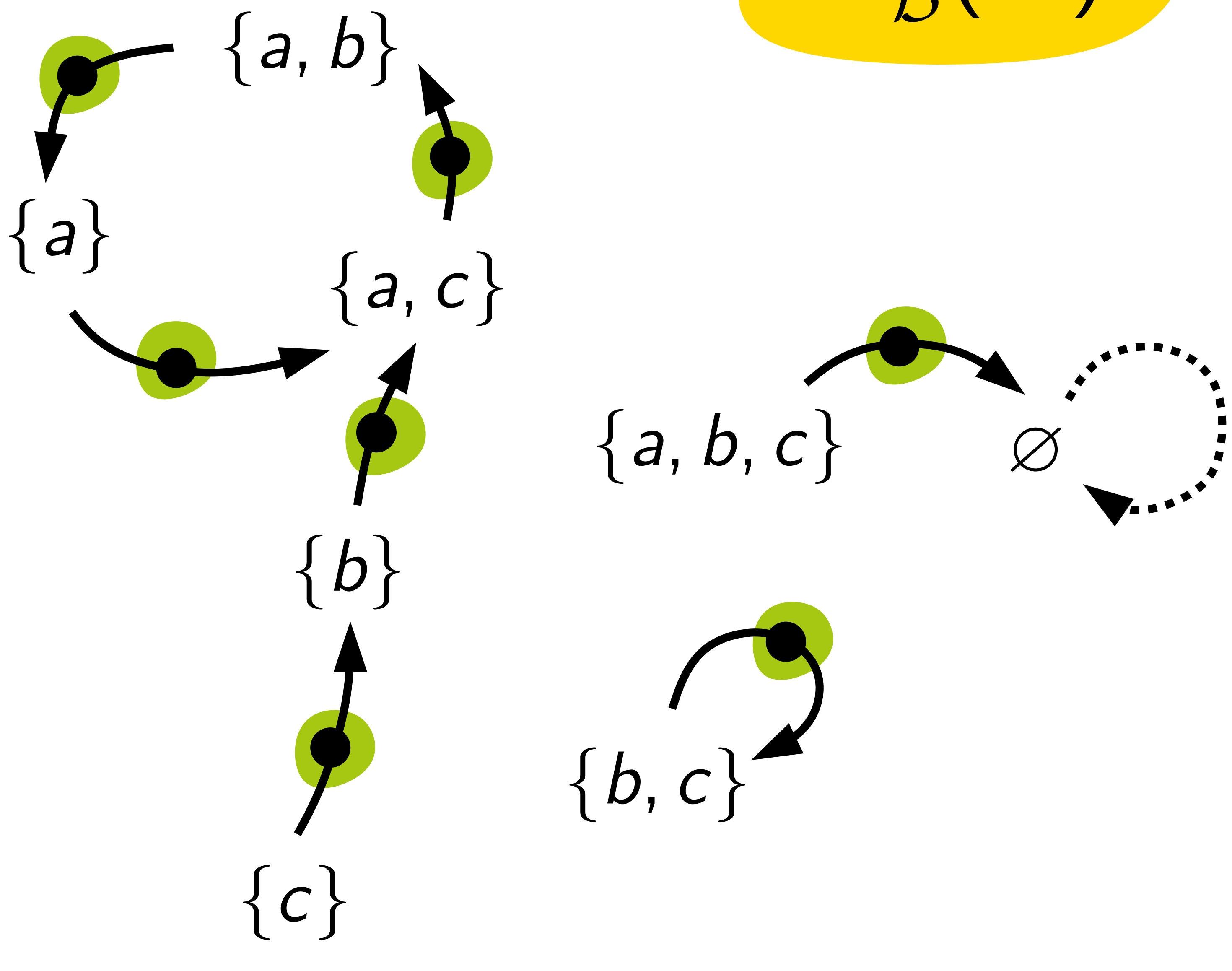
Dynamics

$$\mathrm{res}^n_{\mathcal{A}}(T)$$



Dynamics

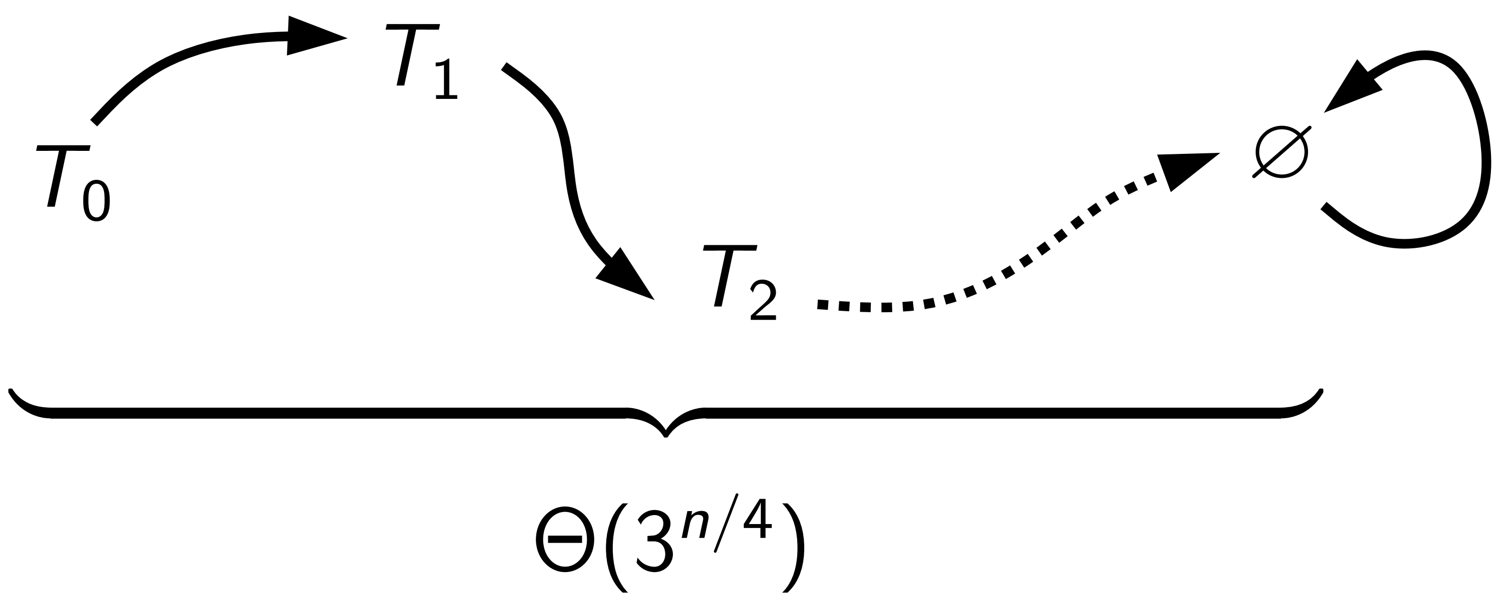
$\mathrm{res}^n_{\mathcal{B}}(T)$



Low-level (detailed) dynamics
of resource-minimal RS

Long sequences in resource-minimal reaction systems

There exists a resource-minimal reaction system with $|S| = n$ having a terminating state sequence of length $\Theta(3^{n/4})$



Almost-minimal RS

$$(R, I, P)$$

at most 2 resources

$|R| + |I| \leq 2$

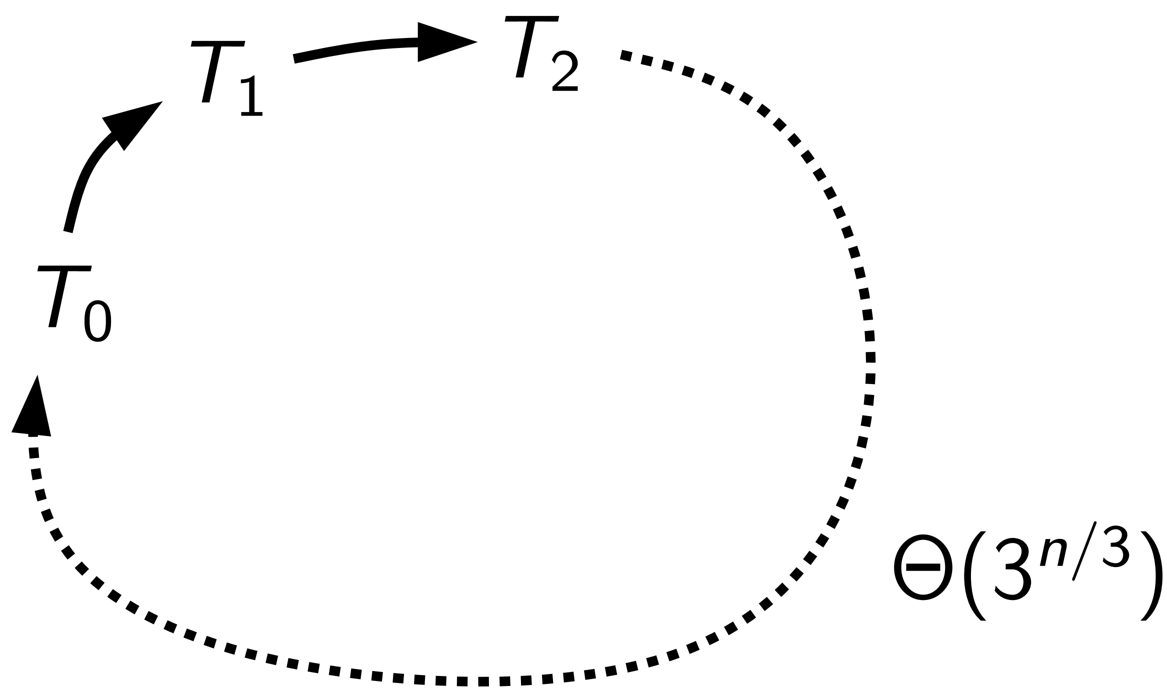
Long sequences in almost-minimal reaction systems

There exists a reaction system with at most 3 resources per reaction and $|S| = n$ having a terminating state sequence of length $\Theta(3^{n/3})$

$$\underbrace{T_0 \to T_1 \to T_2 \dashrightarrow \emptyset}_{\Theta(3^{n/3})}$$

Long cycles in almost-minimal reaction systems

There exists a reaction system with at most 3 resources per reaction and $|S| = n$ having a cycle of length $\Theta(3^{n/3})$

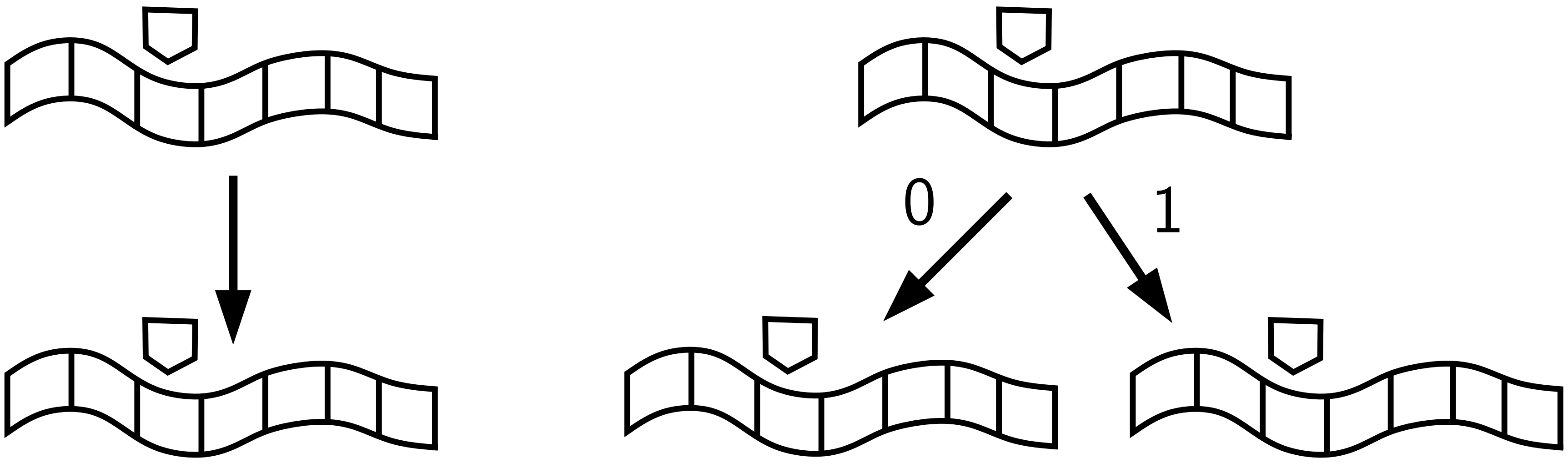


Long sequences generated by RS: known results

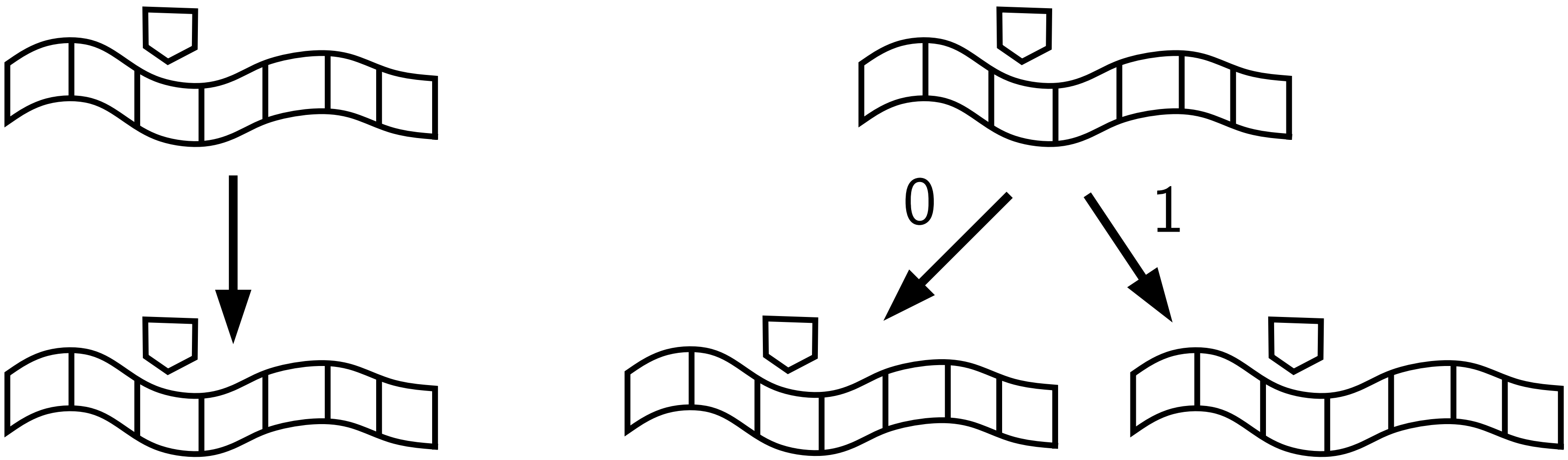
Type	Longest sequence known
Generic	$\Theta(2^n) \rightarrow$ optimal
Almost-minimal	$\Theta(3^{n/3}) \approx \Theta(1.44^n)$
Resource-minimal	$\Theta(3^{n/4}) \approx \Theta(1.32^n)$

Context-sensitivity

Context as nondeterminism

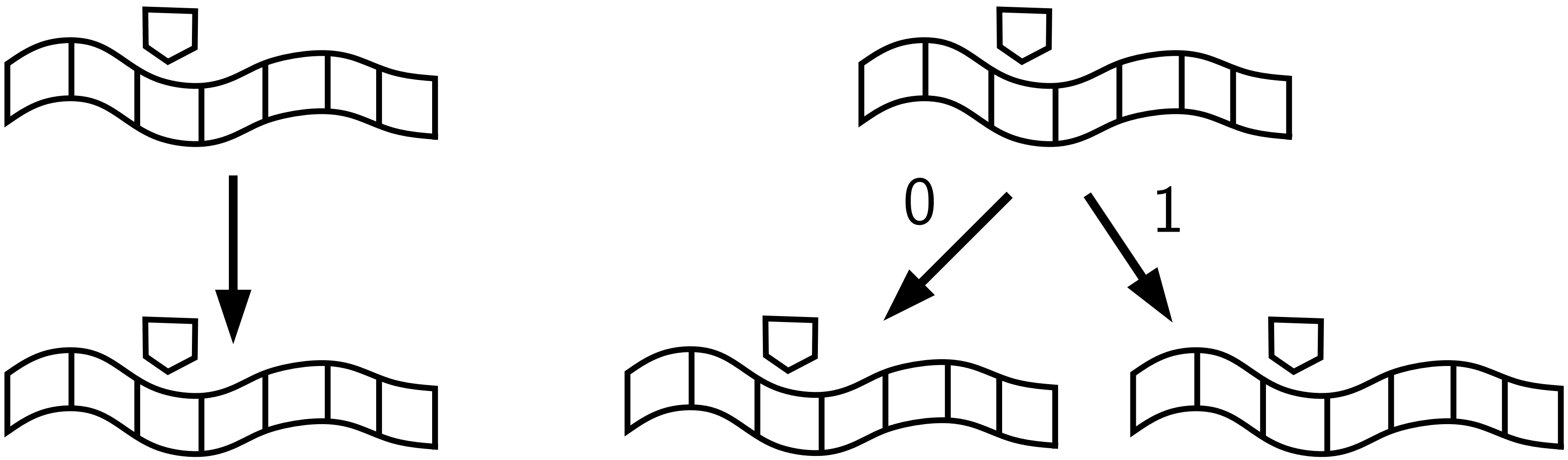


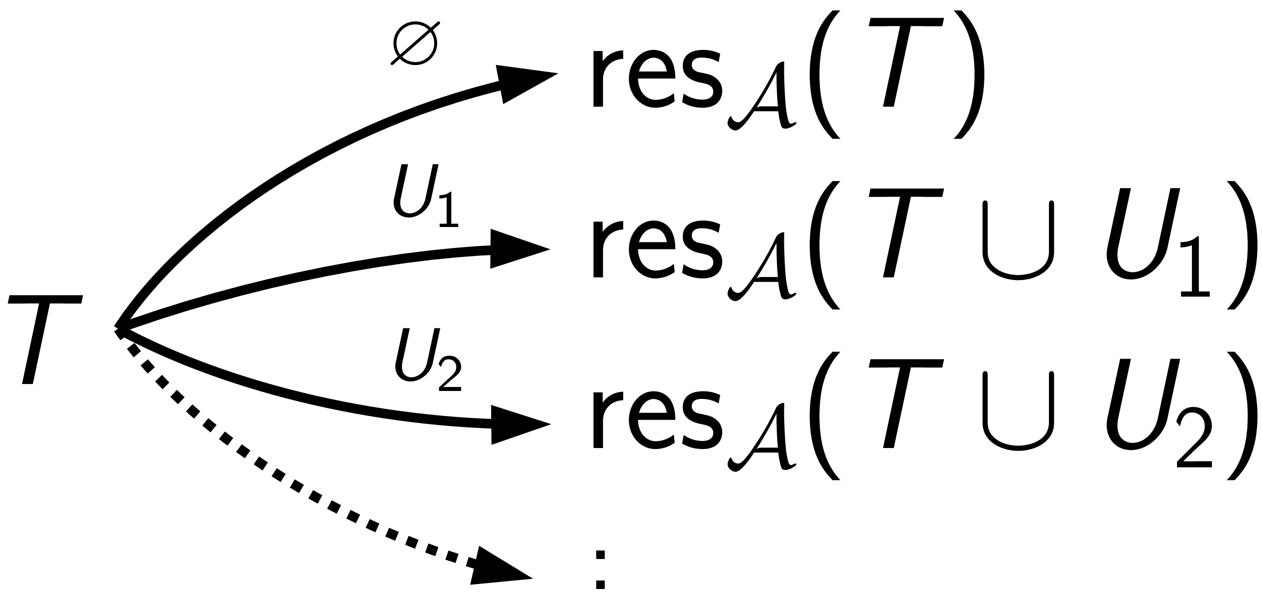
Context as nondeterminism



$$T \longrightarrow \mathsf{res}_{\mathcal{A}}(T)$$

Context as nondeterminism





Thanks for your attention!

Dziękuję za uwagę!

Any questions?