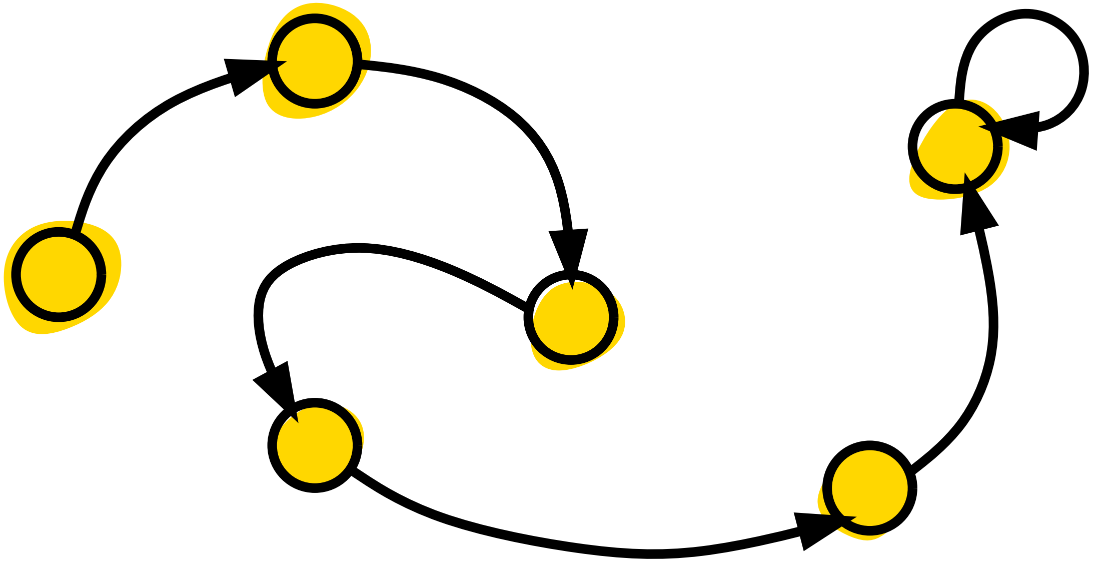
Dynamics of reaction systems



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Note: all reaction systems
in this talk are without context

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

power set function

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

boundary power set function

Theorem

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

$$\Updownarrow$$

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

Proof idea

$$f(X) = Y$$

$$\Downarrow$$

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

$(\{x\}, I, P)$ reactant-minimal (only 1 reactant)

$(R, \{y\}, P)$ inhibitor-minimal (only 1 inhibitor)

$(\{x\}, \{y\}, P)$ resource-minimal (only 1 reactant and 1 inhibitor) 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

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

$$\not\subseteq$$

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

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

$$f \text{ is union-subadditive}$$
$$\Updownarrow$$
$$f = \mathrm{res}_{\mathcal{A}} \text{ for some reactant-minimal } \mathcal{A}$$

$$f \text{ is intersection-subadditive}$$
$$\Updownarrow$$
$$f = \mathrm{res}_{\mathcal{A}} \text{ for some inhibitor-minimal } \mathcal{A}$$

Reactant-minimal $\Rightarrow$ union-subadditive

$$
\begin{tikzcd}
& a \in \mathrm{en}_{\mathcal{A}}(T \cup U) \arrow[dl] \arrow[dr] & \\
R_a = \{x\} \subseteq T \cup U \arrow[d] & & I_a \cap (T \cup U) = \varnothing \arrow[d] \\
\{x\} \subseteq T \text{ or } \{x\} \subseteq U \arrow[dr] & & I_a \cap T = \varnothing \text{ and } I_a \cap U = \varnothing \arrow[dl] \\
& a \in \mathrm{en}_{\mathcal{A}}(T) \text{ or } a \in \mathrm{en}_{\mathcal{A}}(U) \arrow[d] & \\
& \mathrm{res}_{\mathcal{A}}(T \cup U) \subseteq \mathrm{res}_{\mathcal{A}}(T) \cup \mathrm{res}_{\mathcal{A}}(U) &
\end{tikzcd}
$$

Theorem

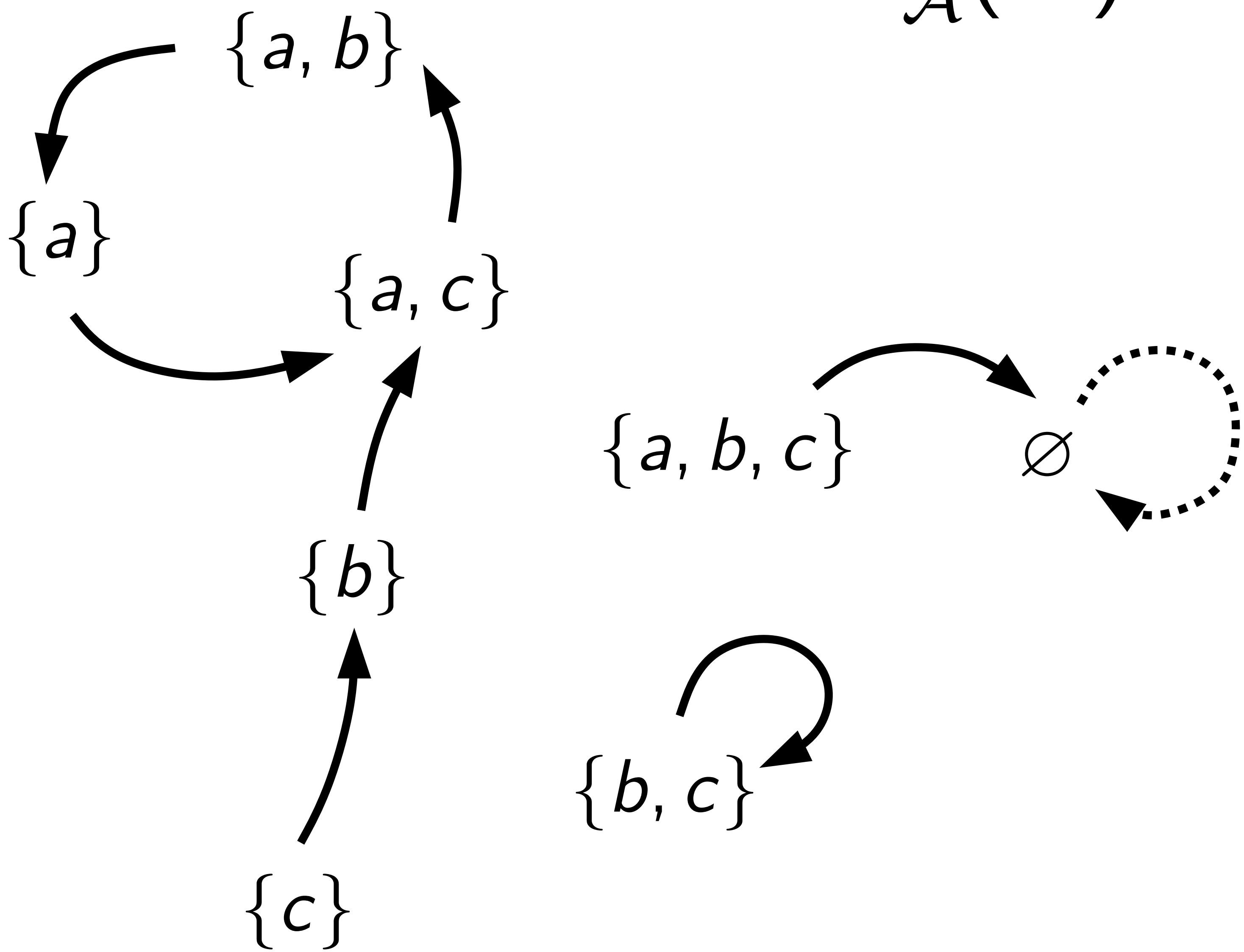
f is union- and intersection-subadditive

$$\Updownarrow$$

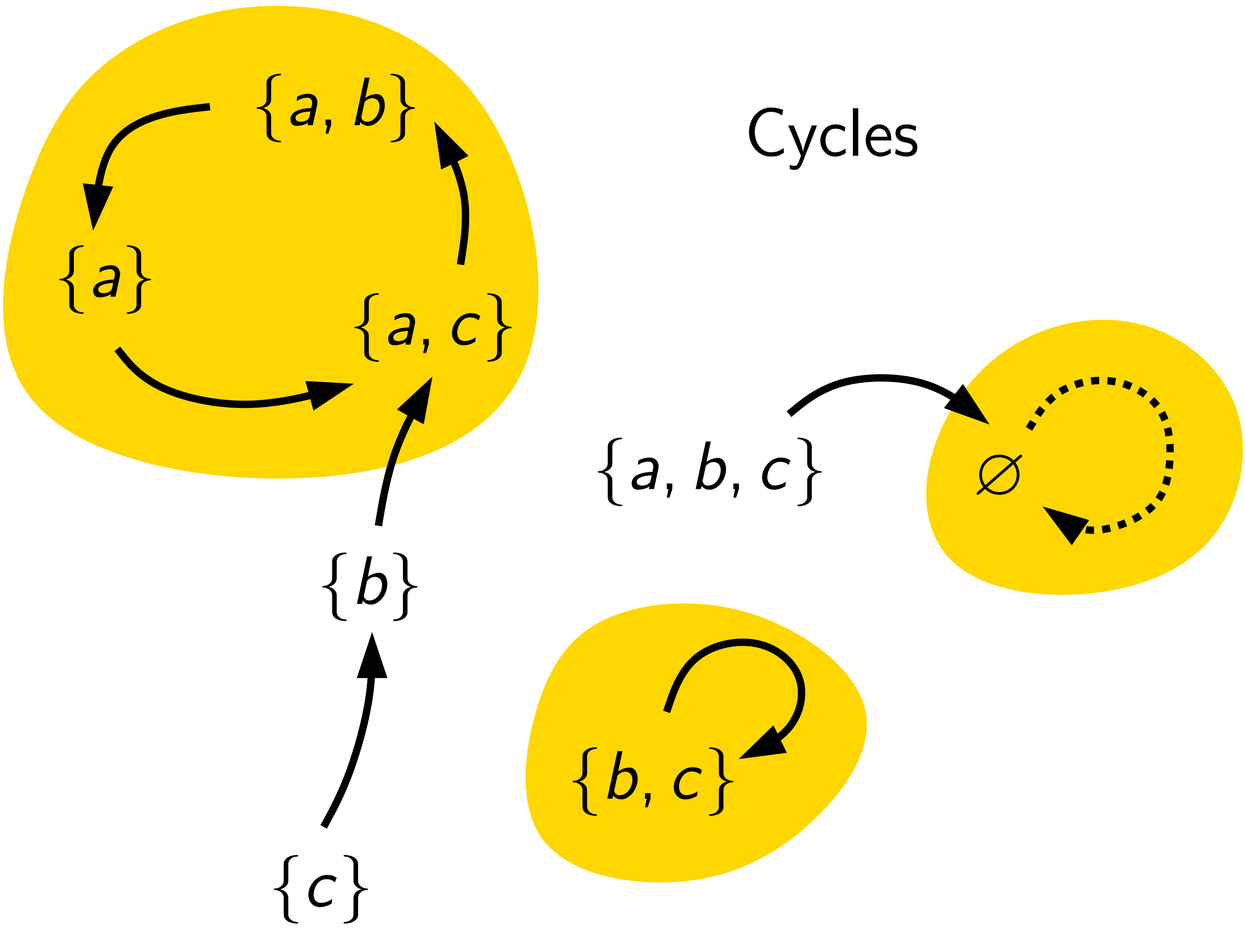
$f = \mathrm{res}_{\mathcal{A}}$ for some resource-minimal $\mathcal{A}$

Dynamics

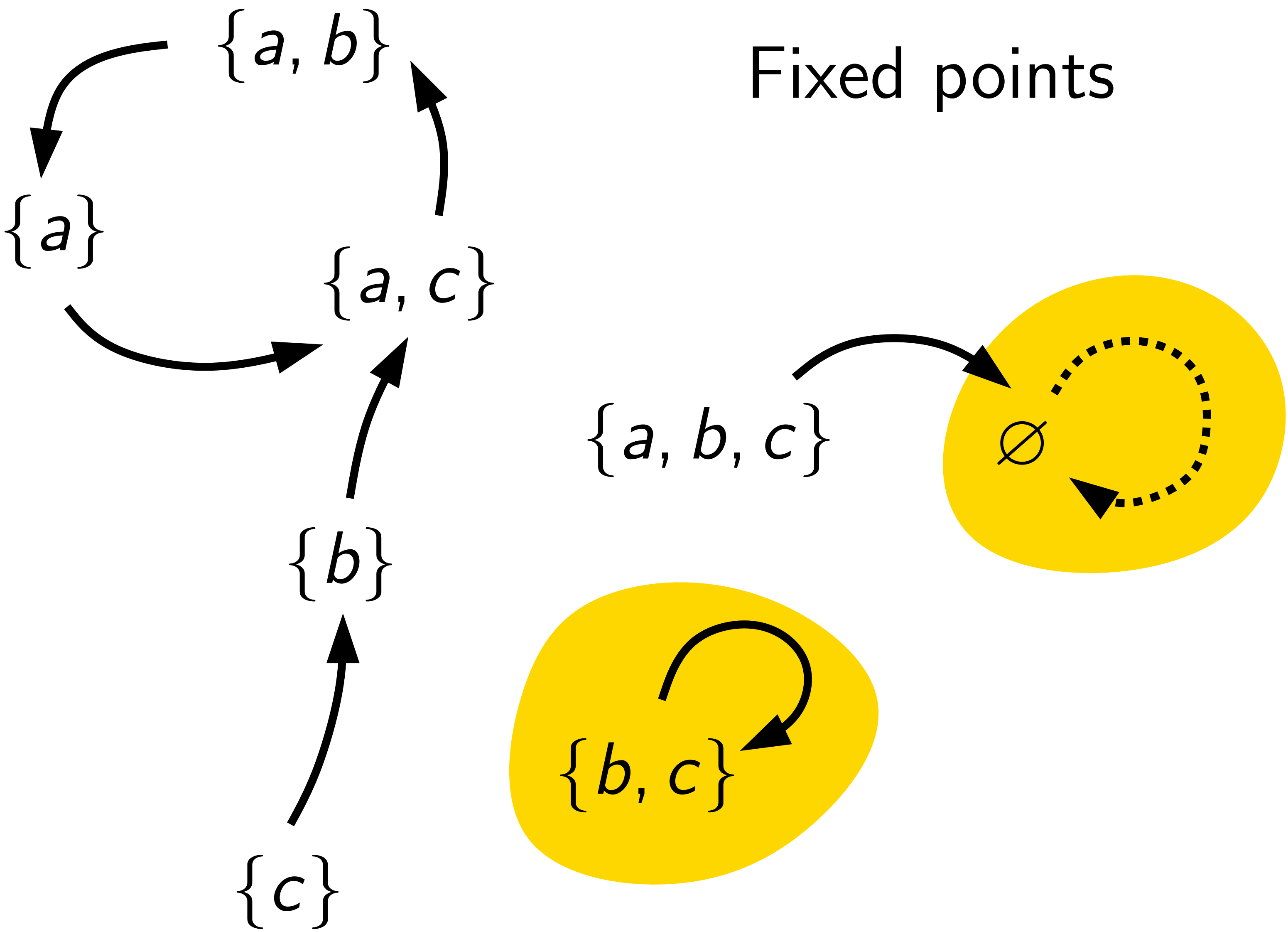
$\mathrm{res}^t_{\mathcal{A}}(T)$



Dynamics



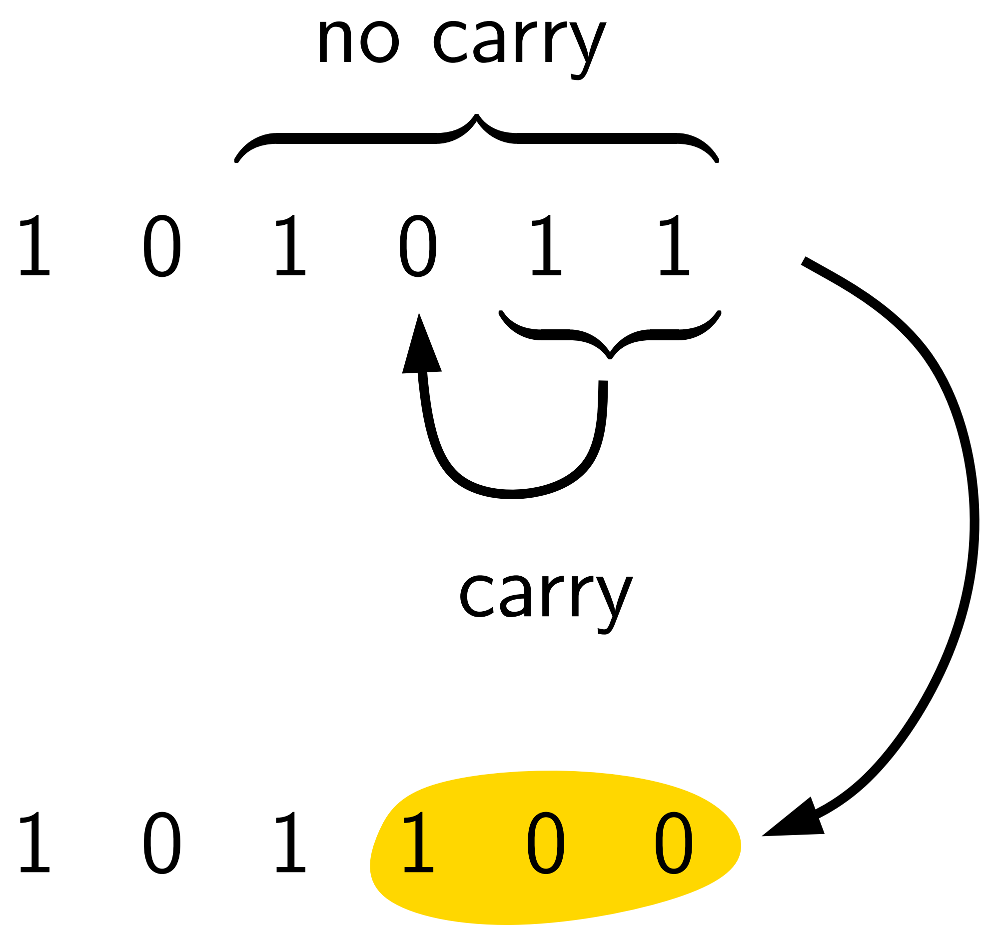
Dynamics



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

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

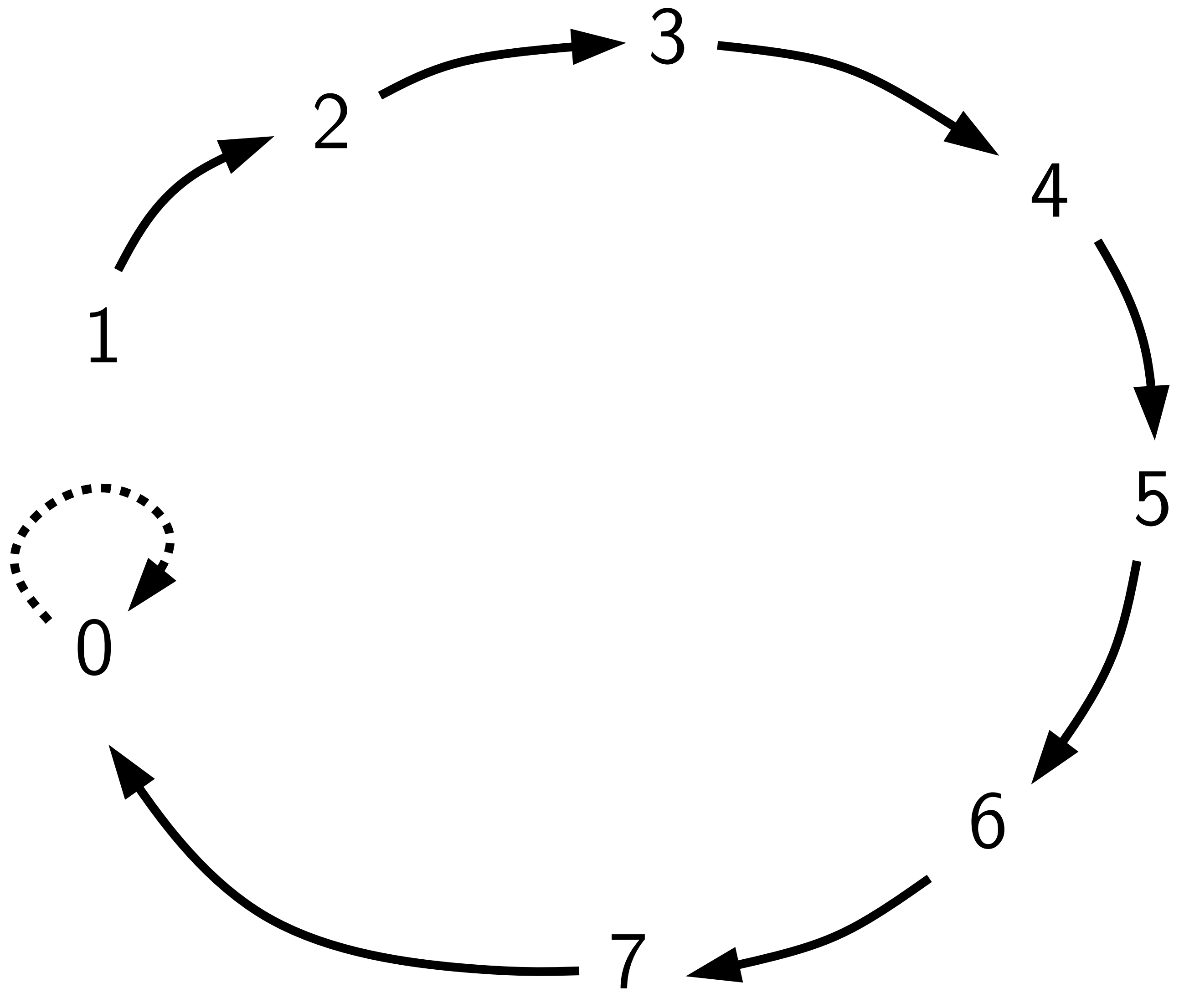
$(\{b_i\}, \{b_0\}, \{b_0\})$ for $1 \leq i \leq n$

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

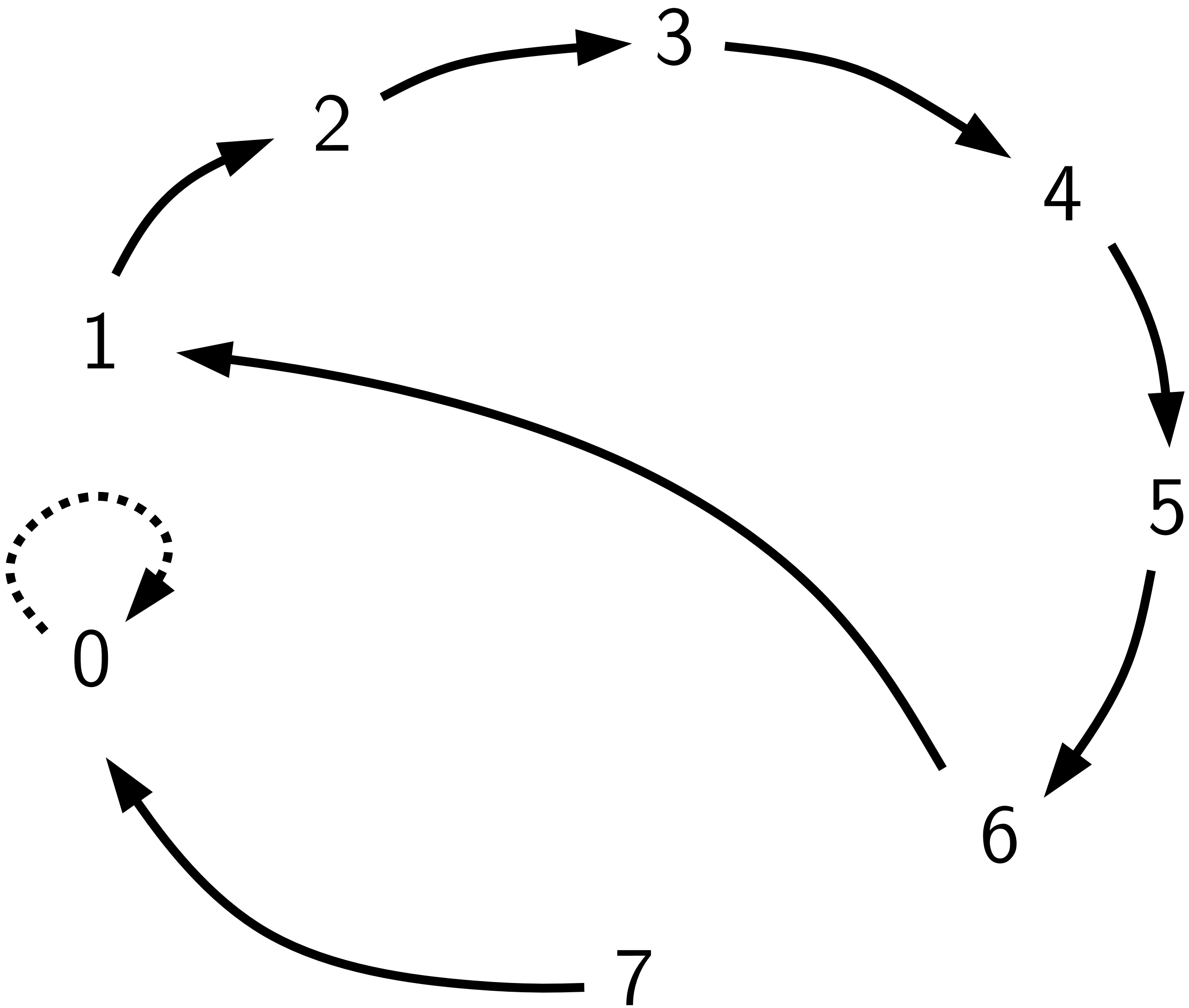
flip least significant bit

preserve 1 if no carry

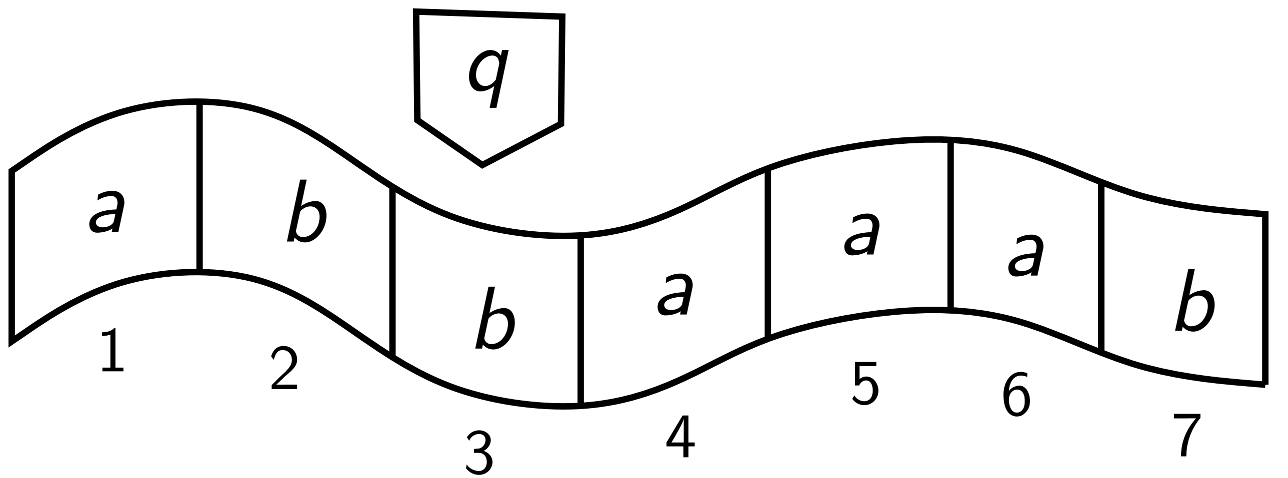
Long paths → binary counters



Long cycles $\rightarrow$ binary counters

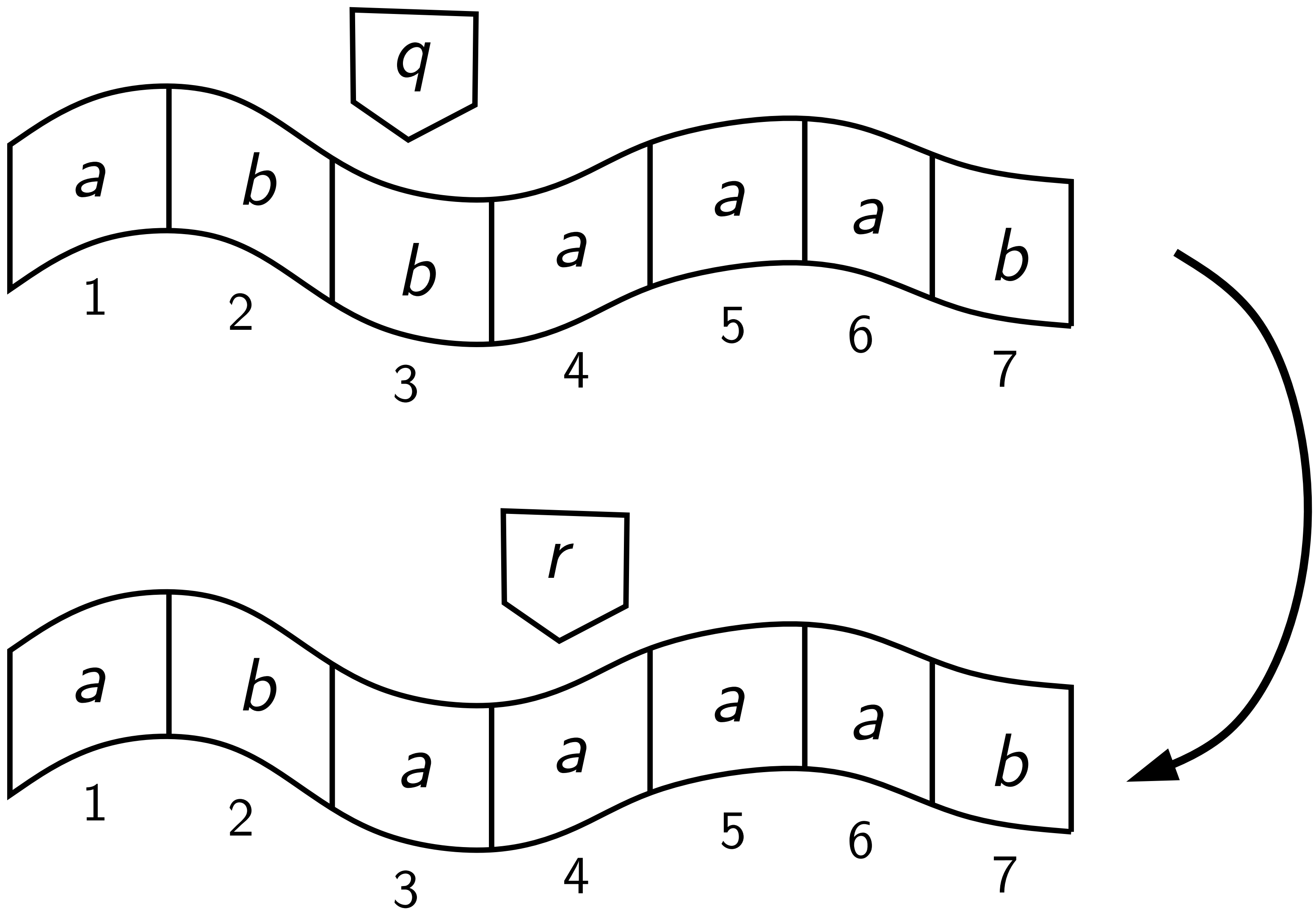


Turing machines (with bounded tape)

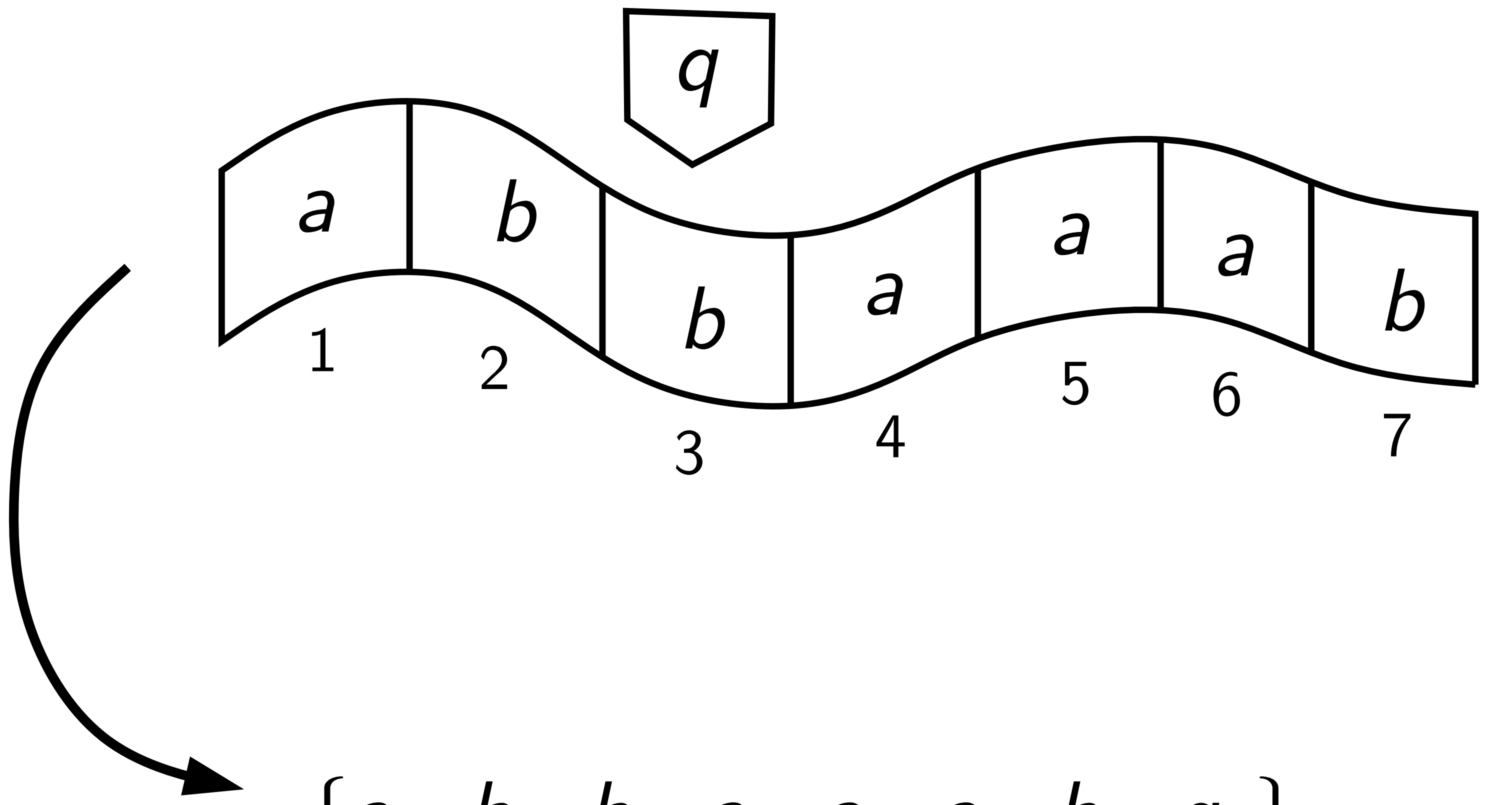


$$
\begin{array}{cccccc}
q & a & \longrightarrow & q & b & \triangleright \\
q & b & \longrightarrow & r & a & \triangleright \\
r & a & \longrightarrow & q & a & \triangleleft \\
r & b & \longrightarrow & r & a & \triangleright
\end{array}
$$

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

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

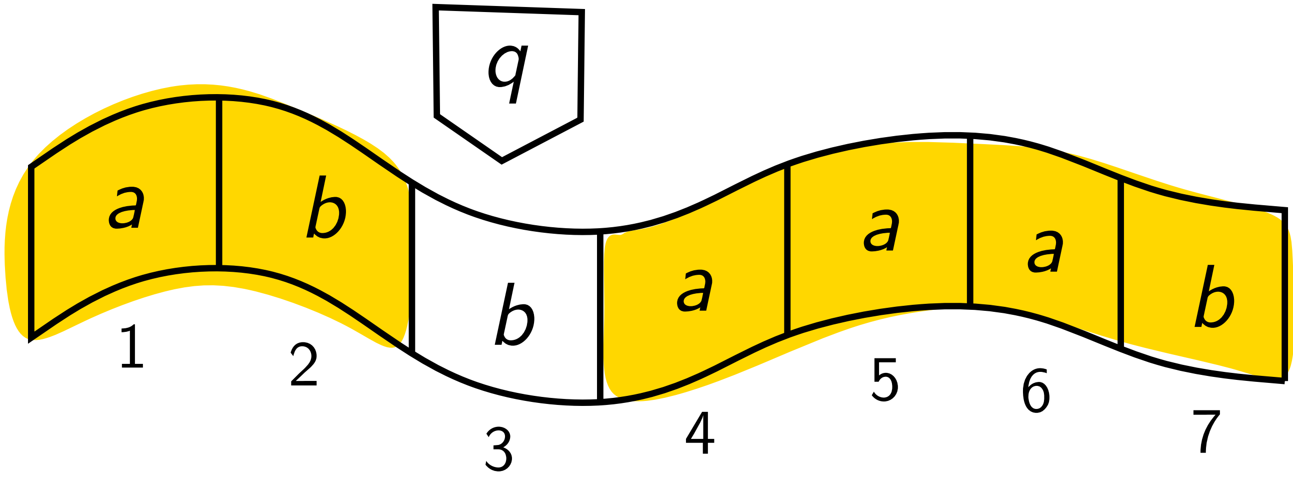
$$(\{r_2, a_2\}, \{\spadesuit\}, \{q_1, a_2\})$$

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

$$\vdots$$

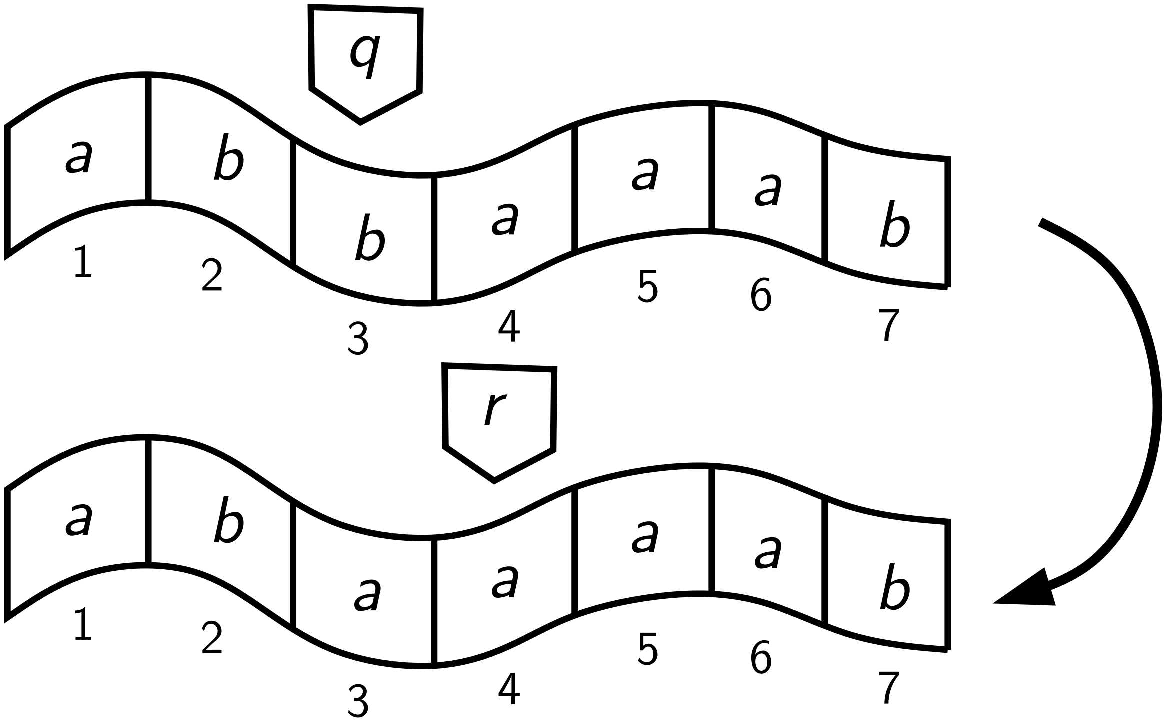
$$(\{r_7, a_7\}, \{\spadesuit\}, \{q_6, a_7\})$$

Preserving the tape



$$(\{a_1\}, \{q_1, r_1\}, \{a_1\}) \qquad (\{b_1\}, \{q_1, r_1\}, \{b_1\})$$
$$(\{a_2\}, \{q_2, r_2\}, \{a_2\}) \qquad (\{b_2\}, \{q_2, r_2\}, \{b_2\})$$
$$\vdots \qquad \vdots$$
$$(\{a_7\}, \{q_7, r_7\}, \{a_7\}) \qquad (\{b_7\}, \{q_7, r_7\}, \{b_7\})$$

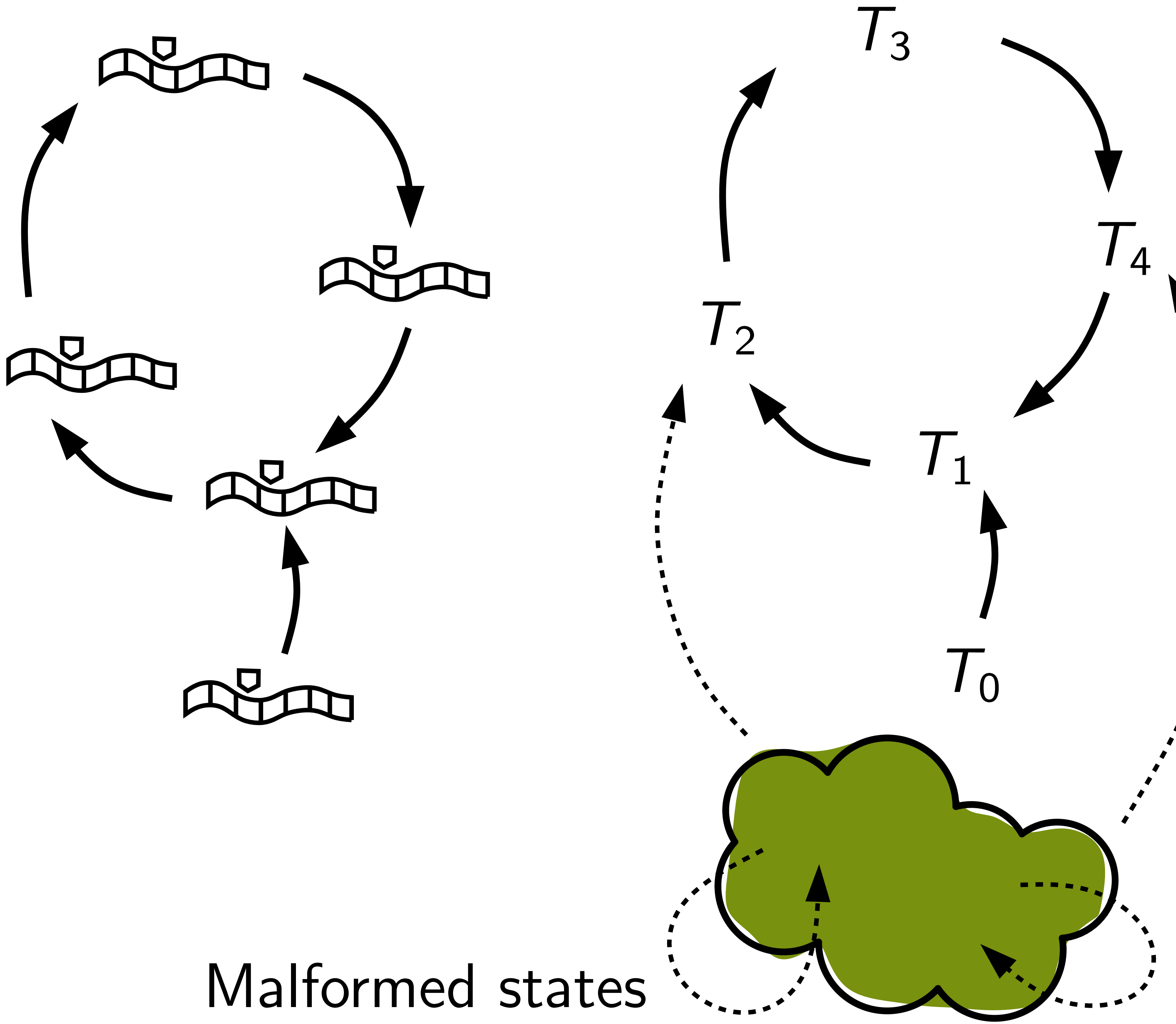
Computation step



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

$$\xrightarrow{\mathrm{res}_{\mathcal{A}}}$$

$$\{a_1, b_2, a_3, a_4, a_5, a_6, b_7, r_4\}$$



T_3
T_4
T_2
T_1
T_0
Malformed states

Complexity of the dynamics of reaction systems

Deciding if configuration C_2 is reachable from configuration C_1 is intractable (PSPACE-complete) for Turing machines with bounded tapes.

$$\Downarrow$$

Deciding if state U is reachable from state T is intractable (PSPACE-complete) for reaction systems

Does minimality make a difference?

f is union- and intersection-subadditive

$$\Updownarrow$$

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

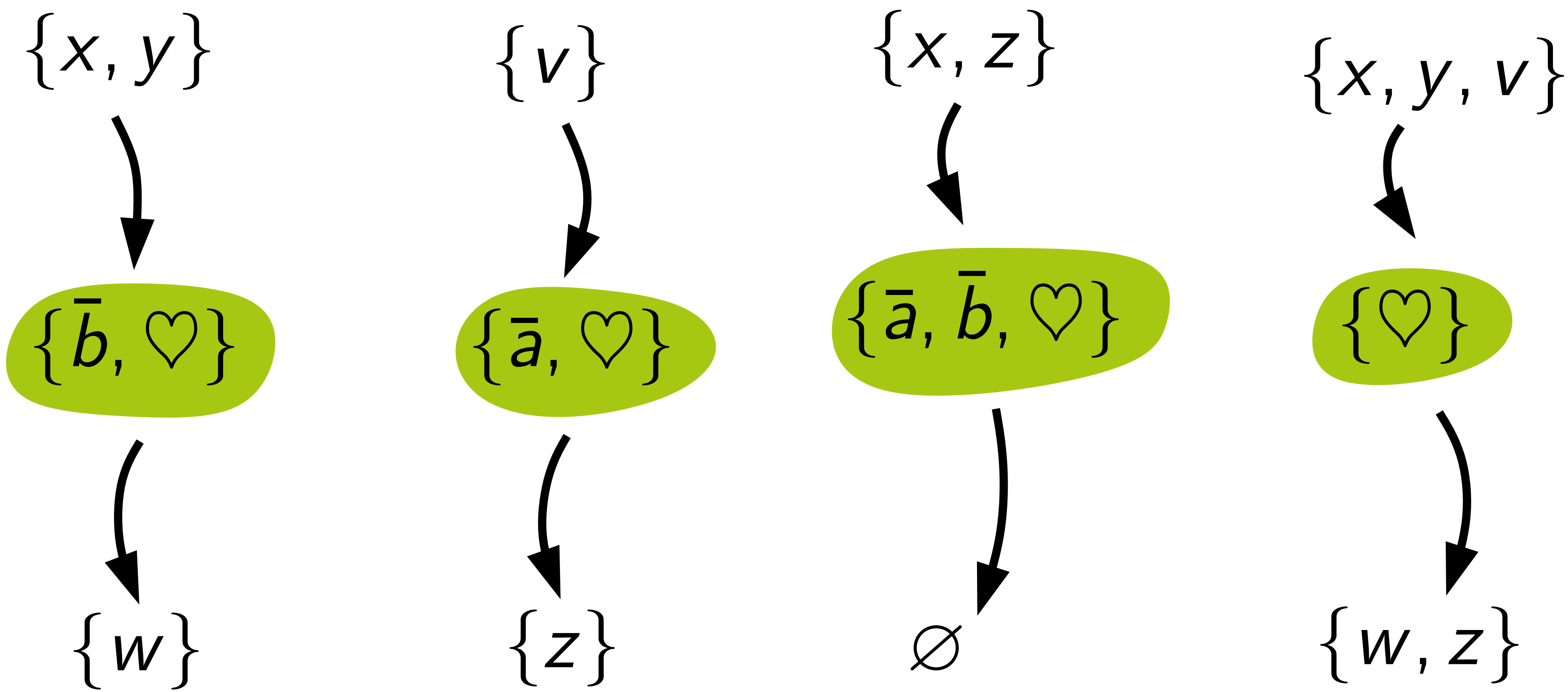
Theorem

For each reaction system $\mathcal{A}$ there exists a resource-minimal $\mathcal{B}$ such that

$$\mathrm{res}_{\mathcal{B}}^{2t}(U) = \mathrm{res}_{\mathcal{A}}^{t}(U)$$

Proof idea

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



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

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

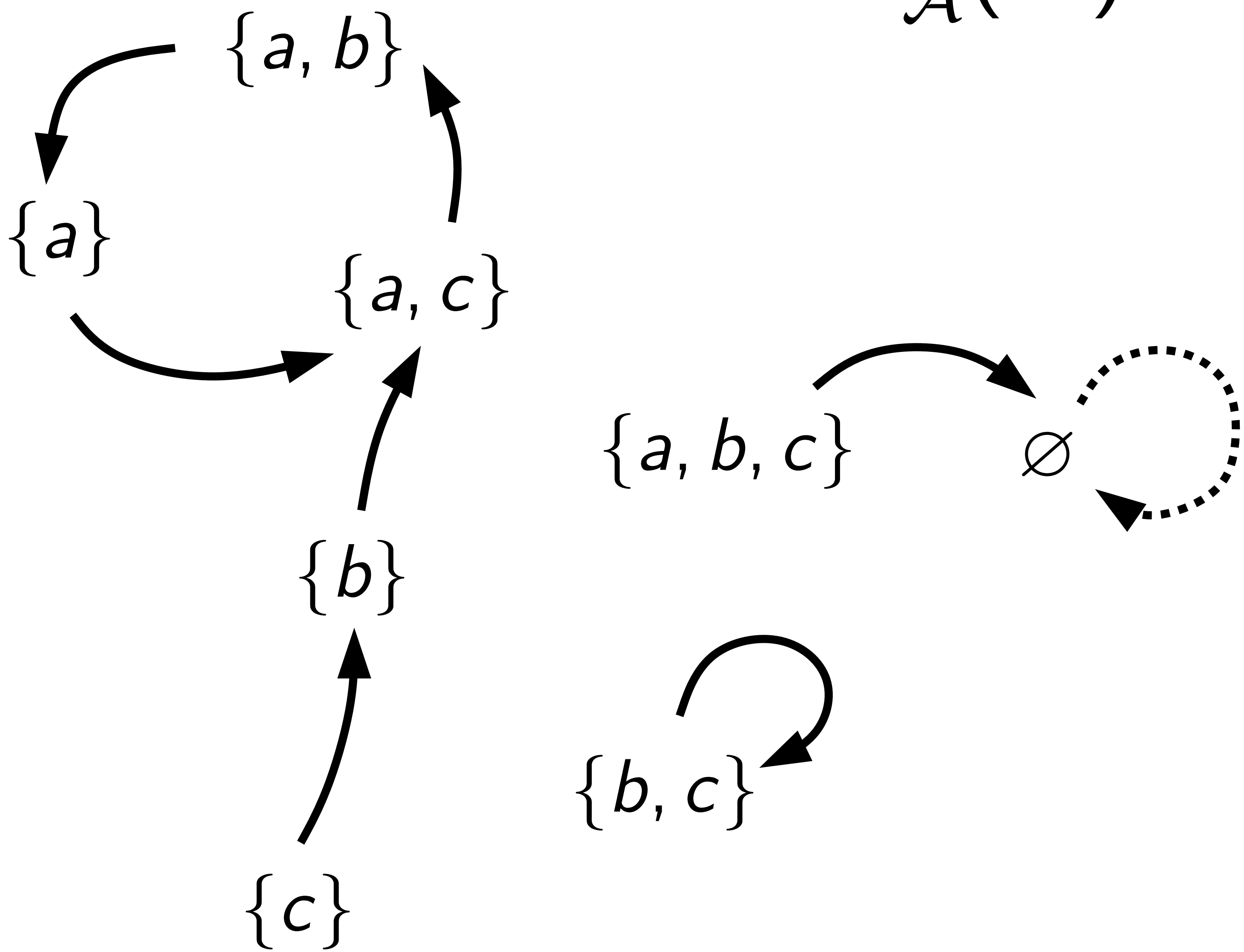
Make $\heartsuit$ every other step

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

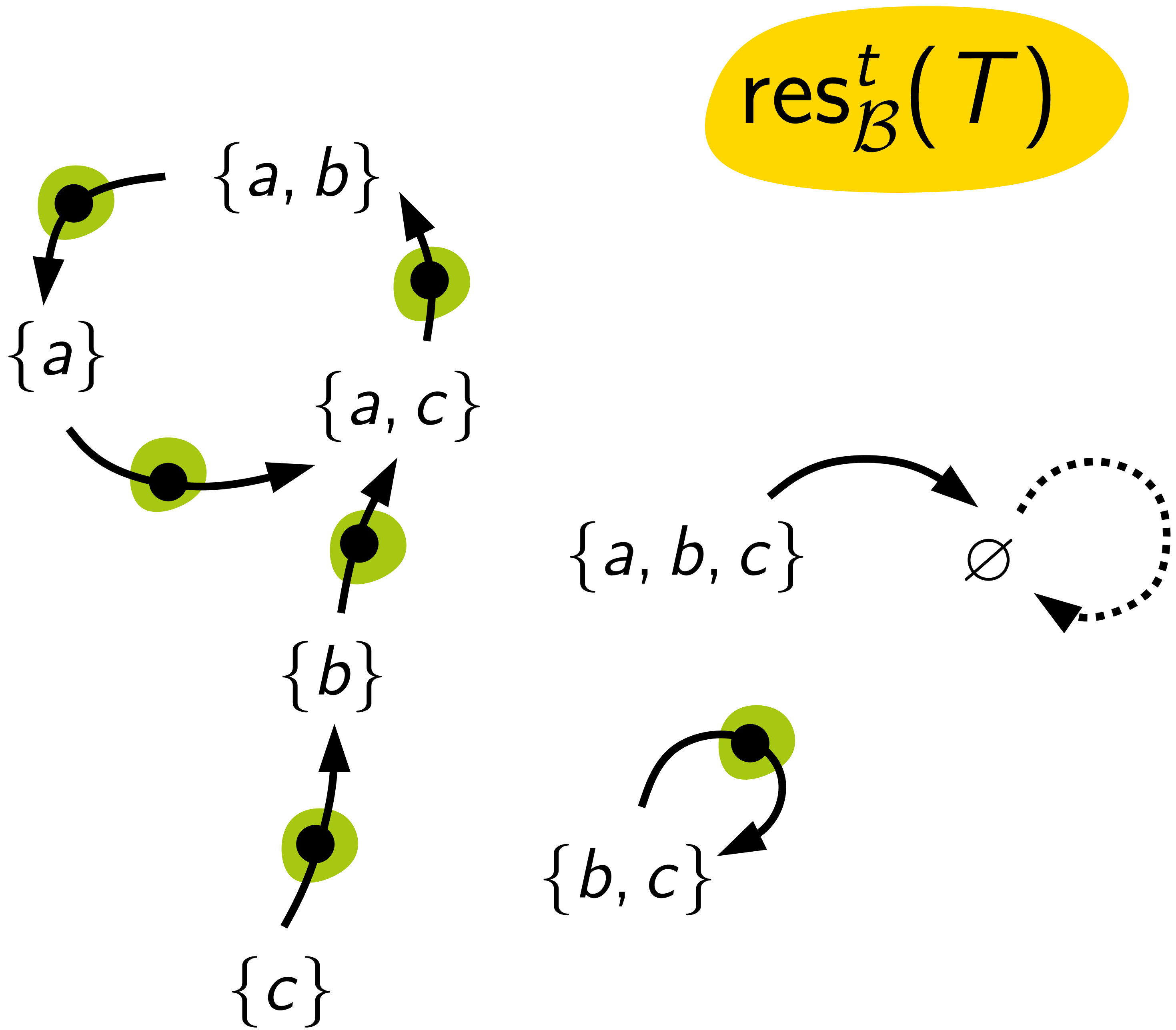
Minimal!

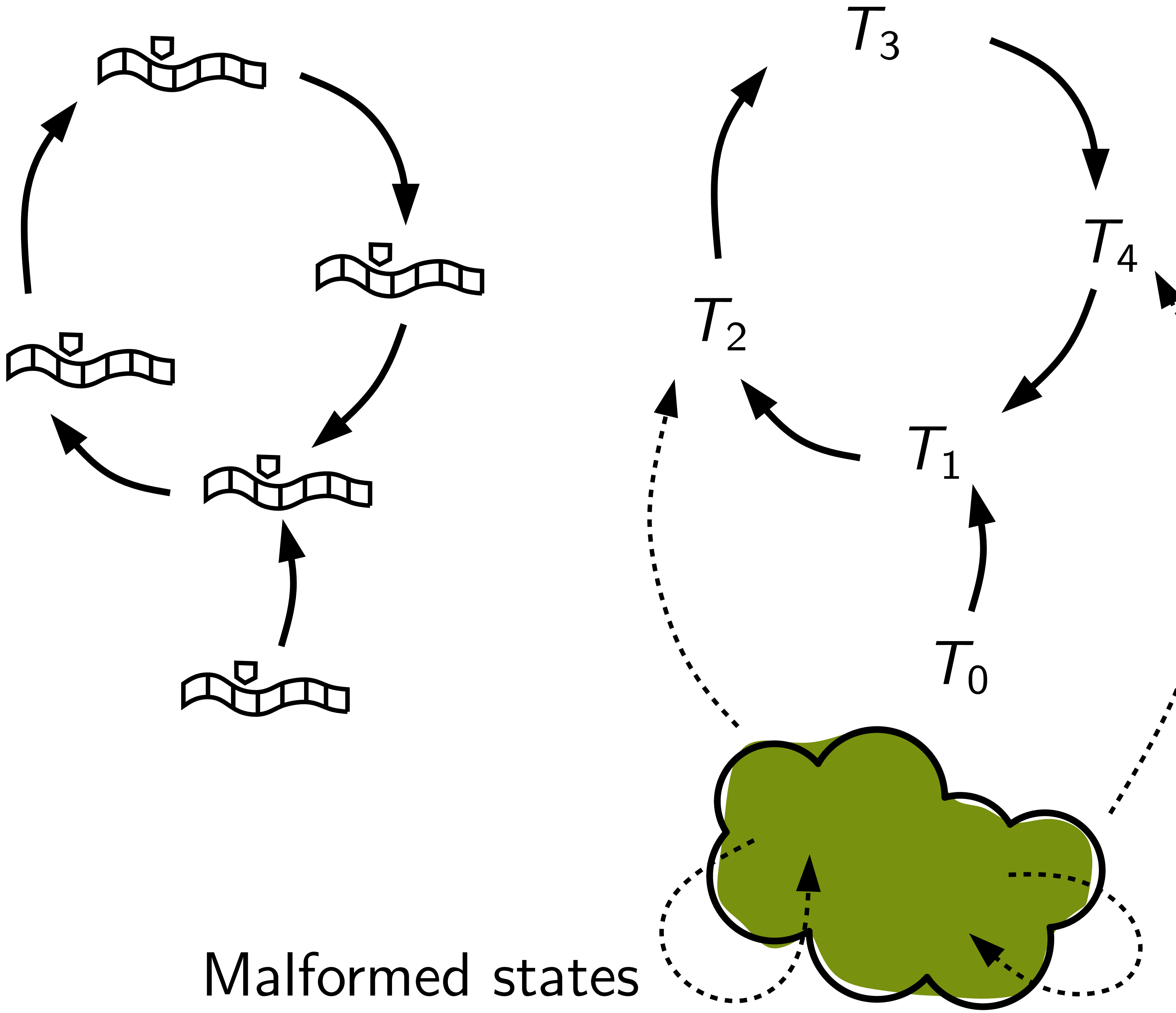
Dynamics

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

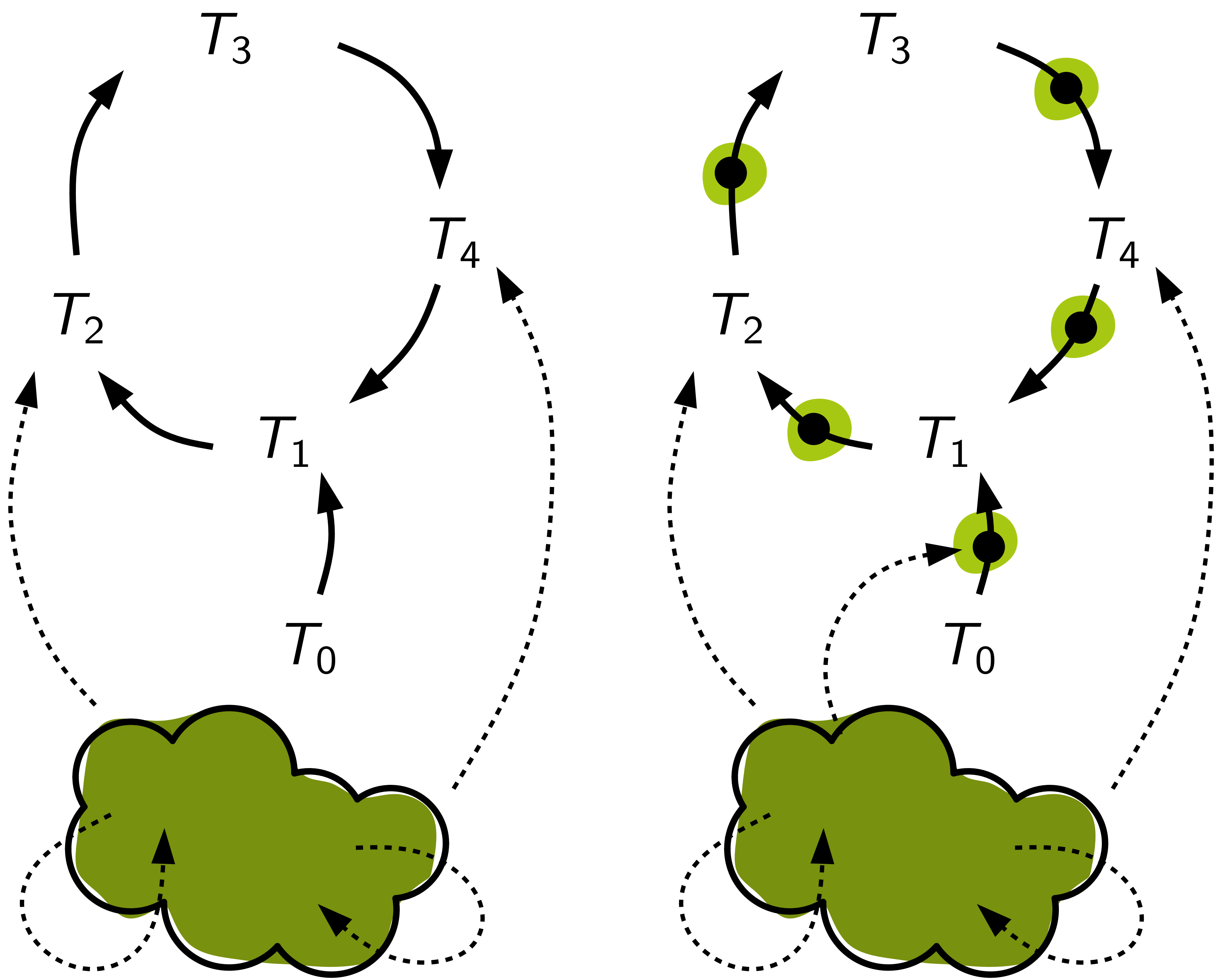


Dynamics





T_3
T_4
T_2
T_1
T_0
Malformed states


T_3
T_4
T_2
T_1
T_0
T_3
T_4
T_2
T_1
T_0

Minimality does not make things easier

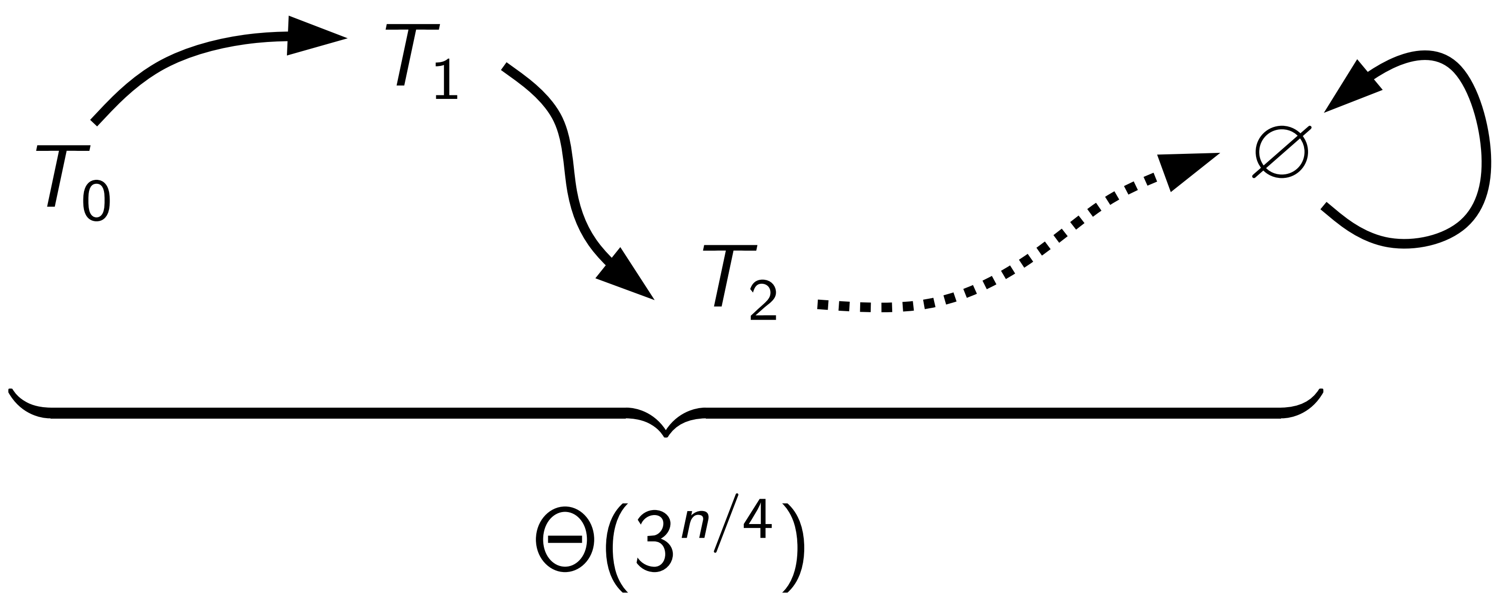
Deciding if configuration C_2 is reachable from configuration C_1 is intractable (PSPACE-complete) for Turing machines with bounded tapes.

$$\Downarrow$$

Deciding if state U is reachable from state T is intractable (PSPACE-complete) for resource-minimal reaction systems

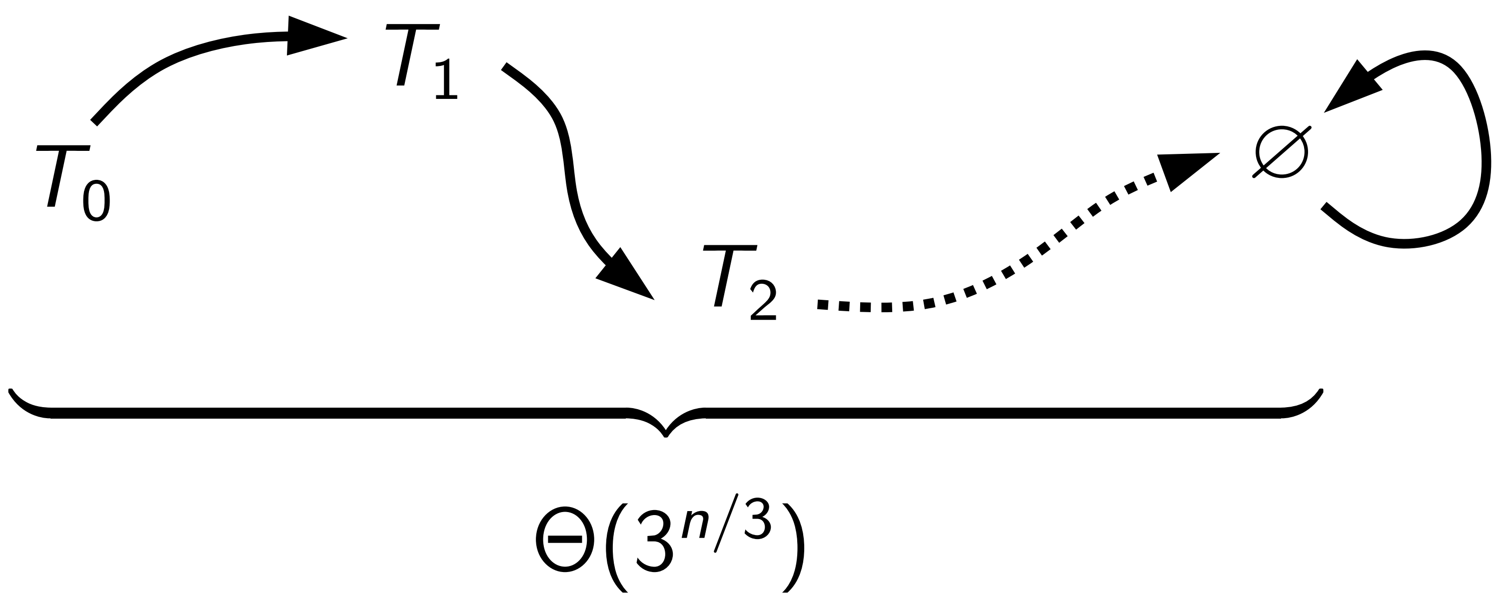
Long sequences in resource-minimal reaction systems

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



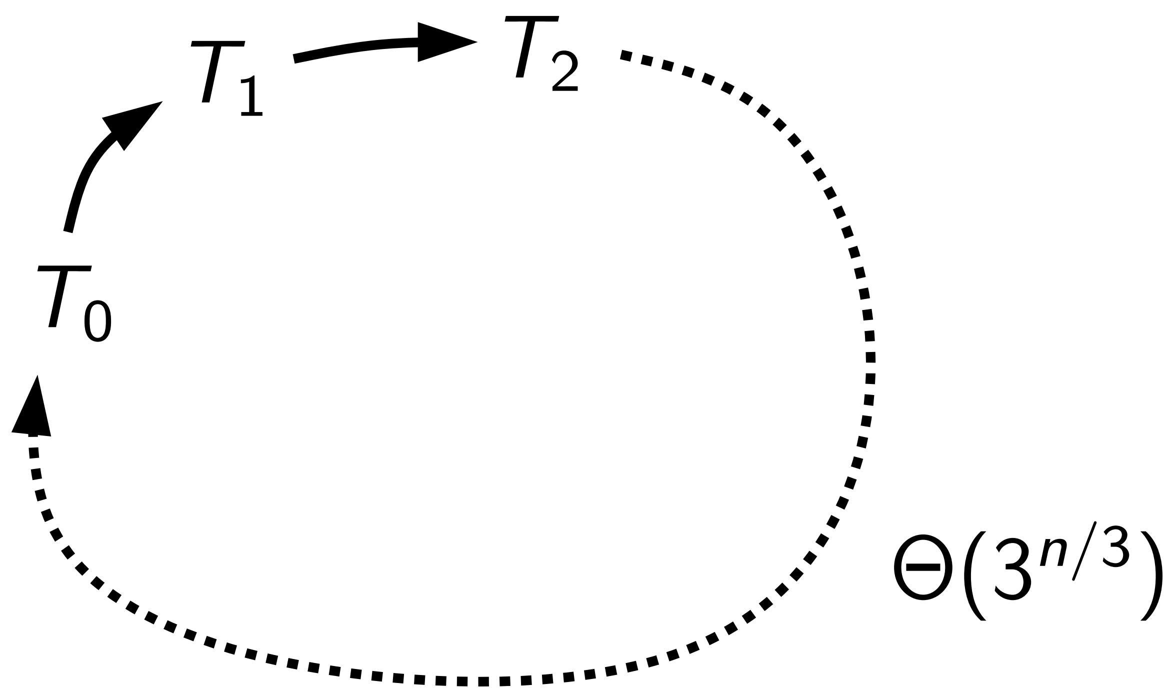
Long sequences in almost-minimal reaction systems

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



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 $\Theta(3^{n/3})$



Does minimality make a difference here?

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