Complexity of the dynamics of resource-bounded reaction systems

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Reactions

Definition

Given a finite set S, a *reaction* a over S is a triple (R, I, P) of subsets of S:

- R is the set of *reactants*,
- I is the set of *inhibitors*,
- P is the set of *products*.

Reaction Systems

Definition

A *reaction system* (RS) is a pair $\mathcal{A} = (S, A)$ where:

- S is a finite set of *symbols* or *entities*, called the *background set*;
- A is a set of reactions over S.

A *state* of $\mathcal{A}$ is a subset of S.

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A *state* of $\mathcal{A}$ is a subset of S.

Any reaction system induces a discrete dynamical system where the state set is 2^S.

Result function

A reaction $a = (R, I, P)$ is *enabled* in a state $T \subseteq S$ when:

$$R \subseteq T \quad \text{and} \quad I \cap T = \varnothing.$$

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$$\mathrm{res}_a(T) := \begin{cases} P & \text{if } a \text{ is enabled by } T \\ \varnothing & \text{otherwise.} \end{cases}$$

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Definition

The *result function* $\mathrm{res}_{\mathcal{A}}$ of a RS $\mathcal{A} = (S, A)$ is defined on any state $T \subseteq S$ as:

$$\mathrm{res}_{\mathcal{A}}(T) := \bigcup_{a \in A} \mathrm{res}_a(T).$$

Example of RS

Background set: $S = \{a, b\}$

Set of reactions: $r_1 = (\{a\}, \varnothing, \{a, b\})$

$r_2 = (\{b\}, \{a\}, \{b\})$

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Example of RS

Background set: $S = \{a, b\}$

Set of reactions: $r_1 = (\{a\}, \varnothing, \{a, b\}) \leftarrow$

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State: $T = \{b\}$

$$\{a\} \nsubseteq T \quad \Rightarrow \quad \mathrm{res}_{r_1}(T) = \varnothing$$

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$$\{b\} \subseteq T$$

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State: $T = \{b\}$

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$$\{b\} \subseteq T, \quad \{a\} \cap T = \varnothing$$

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Result function on T:

$$\mathrm{res}_{\mathcal{A}}(T) = \mathrm{res}_{r_1}(T) \cup \mathrm{res}_{r_2}(T)$$

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Result function on T:

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

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$$\begin{aligned} \{a\} \nsubseteq T \quad &\Rightarrow \quad \mathrm{res}_{r_1}(T) = \varnothing \\ \{b\} \subseteq T, \quad \{a\} \cap T = \varnothing \quad &\Rightarrow \quad \mathrm{res}_{r_2}(T) = \{b\} \end{aligned}$$

Result function on T:

$$\mathrm{res}_{\mathcal{A}}(\{b\}) = \{b\} \Rightarrow \{b\} \text{ is a fixed point}$$

Representation of the dynamic:

$$\begin{tikzcd} \{a\} \arrow[dr, bend left] & & & \\ & \{a,b\} \arrow[loop right] & \{b\} \arrow[loop right] & \varnothing \arrow[loop right] \end{tikzcd}$$

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$$\{a\} \subseteq T, \quad \varnothing \cap T = \varnothing \quad \Rightarrow \quad \mathrm{res}_{r_1}(T) = \{a, b\}$$

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State: $T = \{a\}$

$$\{a\} \subseteq T, \quad \varnothing \cap T = \varnothing \quad \Rightarrow \quad \mathrm{res}_{r_1}(T) = \{a, b\}$$
$$\{b\} \not\subseteq T, \quad \{a\} \cap T \neq \varnothing \quad \Rightarrow \quad \mathrm{res}_{r_2}(T) = \varnothing$$

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$$\begin{array}{lcl} \{a\} \subseteq T, \quad \varnothing \cap T = \varnothing & \Rightarrow & \mathrm{res}_{r_1}(T) = \{a, b\} \\ \{b\} \nsubseteq T, \ \{a\} \cap T \neq \varnothing & \Rightarrow & \mathrm{res}_{r_2}(T) = \varnothing \end{array}$$

Result function on T:

$$\mathrm{res}_{\mathcal{A}}(T) = \mathrm{res}_{r_1}(T) \cup \mathrm{res}_{r_2}(T) = \{a, b\} \cup \varnothing = \{a, b\}$$

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Representation of the dynamic:

Example of RS

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Discrete dynamical system:

$$
\begin{tikzcd}
\{a\} \arrow[dr, bend left] & & & \\
& \{a,b\} \arrow[loop right] & \{b\} \arrow[loop right] & \varnothing \arrow[loop right]
\end{tikzcd}
$$

RS vs Synchronous Boolean networks

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\{a\} \arrow[dr, bend left] & & & \\
& \{a,b\} \arrow[loop right] & \{b\} \arrow[loop right] & \varnothing \arrow[loop right]
\end{tikzcd}$$

$$x_a = \begin{cases} 1 \text{ if } a \in T \\ 0 \text{ if } a \notin T \end{cases} \qquad x_b = \begin{cases} 1 \text{ if } b \in T \\ 0 \text{ if } b \notin T \end{cases}$$

$$\begin{tikzcd}
10 \arrow[dr, bend left] & & & \\
& 11 \arrow[loop right] & 01 \arrow[loop right] & 00 \arrow[loop right]
\end{tikzcd}$$

RS vs Synchronous Boolean networks

Background set: $S = \{a, b, c\}$

Set of reactions: $(\{a, c\}, \{b\}, \{a\})$

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

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

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

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

$f : \{0, 1\}^3 \to \{0, 1\}^3$
$f(x_a, x_b, x_c) = (f_a(x_a, x_b, x_c), f_b(x_a, x_b, x_c), f_c(x_a, x_b, x_c))$

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- $f_a(x_a, x_b, x_c) = x_a \wedge x_c \wedge \neg x_b$

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- $f_a(x_a, x_b, x_c) = x_a \land x_c \land \neg x_b$
- $f_b(x_a, x_b, x_c) = (x_a \land x_b \land \neg x_c) \lor (x_c \land \neg x_a)$
- $f_c(x_a, x_b, x_c) = x_b \land \neg x_c$

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Example of RS

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Discrete dynamical system:

Example of RS: fixed points

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Discrete dynamical system:

Fixed points: $\{a, b\}, \{b\}, \varnothing$

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Fixed points: $\{a, b\}, \{b\}, \varnothing$
Fixed points attractor: $\{a, b\}$

Example of RS: fixed points

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$\qquad\qquad\qquad\quad r_2 = (\{b\}, \{a\}, \{b\})$

Discrete dynamical system:

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\end{tikzcd}$$

Fixed points: $\{a, b\}, \{b\}, \varnothing$

Fixed points attractor: $\{a, b\}$

Fixed points not attractor: $\{b\}, \varnothing$

Fixed Points: problems

Given a reaction system $\mathcal{A} = (S, A)$:

- does $\mathcal{A}$ have a fixed point?
- does $\mathcal{A}$ have a fixed point attractor?
- does $\mathcal{A}$ have a fixed point not attractor?
- ecc. . .

Fixed Points: problems

Given a reaction system $\mathcal{A} = (S, A)$:

- does $\mathcal{A}$ have a fixed point? **NP**-complete[1]
- does $\mathcal{A}$ have a fixed point attractor? **NP**-complete[1]
- and many more...

[1] Formenti, Manzoni, and Porreca 2014.

Resource-bounded systems

Class of RS
$\mathcal{RS}(\infty, \infty)$
$\mathcal{RS}(0, \infty)$
$\mathcal{RS}(\infty, 0)$
$\mathcal{RS}(1, 0)$

Resource-bounded systems: classification[2]

Class of RS	Subclass of $2^S \to 2^S$
$\mathcal{RS}(\infty, \infty)$	all
$\mathcal{RS}(0, \infty)$	antitone
$\mathcal{RS}(\infty, 0)$	monotone
$\mathcal{RS}(1, 0)$	additive

[2] Manzoni, Pocas, and Porreca 2014.

Resource-bounded systems: classification[2]

Class of RS	Subclass of $2^S \to 2^S$
$\mathcal{RS}(\infty, \infty)$	all
$\mathcal{RS}(0, \infty)$	antitone: $T \subseteq T' \Rightarrow \mathrm{res}(T) \supseteq \mathrm{res}(T')$
$\mathcal{RS}(\infty, 0)$	monotone
$\mathcal{RS}(1, 0)$	additive

[2] Manzoni, Pocas, and Porreca 2014.

Resource-bounded systems: classification[2]

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$\mathcal{RS}(1,0)$	additive

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Resource-bounded systems: classification[2]

Class of RS	Subclass of $2^S \to 2^S$
$\mathcal{RS}(\infty, \infty)$	all
$\mathcal{RS}(0, \infty)$	antitone: $T \subseteq T' \Rightarrow \mathrm{res}(T) \supseteq \mathrm{res}(T')$
$\mathcal{RS}(\infty, 0)$	monotone: $T \subseteq T' \Rightarrow \mathrm{res}(T) \subseteq \mathrm{res}(T')$
$\mathcal{RS}(1, 0)$	additive: $\mathrm{res}(T \cup T') = \mathrm{res}(T) \cup \mathrm{res}(T')$

[2] Manzoni, Pocas, and Porreca 2014.

$\exists$ fixed point for $\mathcal{RS}(\infty, 0)$

$\exists$ fixed point for $\mathcal{RS}(\infty, 0)$

Always True!
Recall that given $\mathcal{A} \in \mathcal{RS}(\infty, 0)$ then $f = \mathrm{res}_{\mathcal{A}}$ is monotone, i.e. $T_1 \subseteq T_2 \Rightarrow f(T_1) \subseteq f(T_2)$.

Theorem (Knaster Tarski)

Given $f : 2^S \to 2^S$ monotone, there exists a fixed point.

$\exists$ fixed point: summary

Problem	$\mathcal{RS}(\infty,\infty)$	$\mathcal{RS}(0,\infty)$	$\mathcal{RS}(\infty,0)$
$\exists$ fixed point	**NP**-c[1]	**NP**-c[2]	**P** [3]

[1] Formenti, Manzoni, and Porreca 2014
[2] Ascone, Bernardini, and Manzoni 2024b
[3] Knaster-Tarski Theorem

Problem	$\mathcal{RS}(\infty,\infty)$	$\mathcal{RS}(0,\infty)$	$\mathcal{RS}(\infty,0)$
A given state is a fixed point attractor	NP-c[1]	NP-c[2]	NP-c[2]
∃ fixed point	NP-c[1]	NP-c[2]	P [3]
∃ common fixed point	NP-c[1]	NP-c[2]	NP-c[2]
sharing all fixed points	coNP-c[1]	coNP-c[2]	coNP-c[2]
∃ fixed point attractor	NP-c[1]	NP-c[2]	Unknown
∃ common fixed point attractor	NP-c[1]	NP-c[2]	NP-c[2]
sharing all fixed points attractor	Π_2^{P}-c[1]	Π_2^{P}-c[2]	Π_2^{P}-c[2]
∃ fixed point not attractor	Σ_2^{P}-c[2]	Σ_2^{P}-c[2]	Σ_2^{P}-c[2]
∃ common fixed point not attractor	Σ_2^{P}-c[2]	Σ_2^{P}-c[2]	Σ_2^{P}-c[2]
sharing all fixed points not attractor	coNP-c[2]	coNP-c[2]	coNP-c[2]
$\mathrm{res}_{\mathcal{A}} = \mathrm{res}_{\mathcal{B}}$	coNP-c[2]	P [2]	P [2]

[1] Formenti, Manzoni, and Porreca 2014
[2] Ascone, Bernardini, and Manzoni 2024b
[3] Knaster-Tarski Theorem

Additive RS: $\mathcal{RS}(1,0)$

Background set: $S = \{a, b, c\}$

Reactions: $(\varnothing, \varnothing, \{a\})$ $(\{a\}, \varnothing, \{b, c\})$ $(\{c\}, \varnothing, \{c\})$

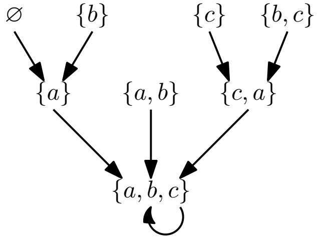

Figure: Discrete dynamical system of $\mathcal{A}$, size $\mathcal{O}(2^{|S|})$.

Background set: $S = \{a, b, c\}$
Reactions: $(\varnothing, \varnothing, \{a\})$ $(\{a\}, \varnothing, \{b, c\})$ $(\{c\}, \varnothing, \{c\})$

Influence graph $G_{\mathcal{A}} = (V_{\mathcal{A}}, E_{\mathcal{A}})$:

$\varnothing_G$

a

b c

Additive RS
Influence graph

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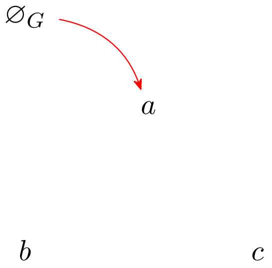
Reactions: $(\varnothing, \varnothing, \{a\})$ $(\{a\}, \varnothing, \{b, c\})$ $(\{c\}, \varnothing, \{c\})$

Influence graph $G_{\mathcal{A}} = (V_{\mathcal{A}}, E_{\mathcal{A}})$:

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



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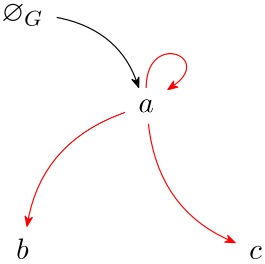
$$\mathrm{res}_{\mathcal{A}}(\{a\}) = \{a, b, c\}$$



Additive RS

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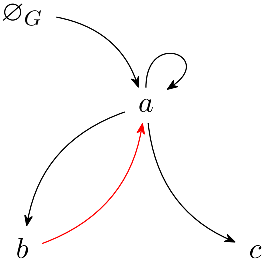
Reactions: $(\varnothing, \varnothing, \{a\})$ $(\{a\}, \varnothing, \{b, c\})$ $(\{c\}, \varnothing, \{c\})$

Influence graph $G_{\mathcal{A}} = (V_{\mathcal{A}}, E_{\mathcal{A}})$:

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



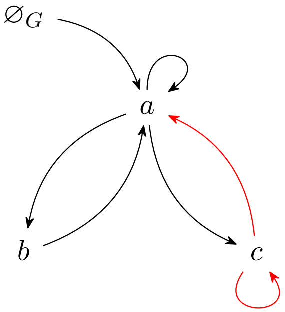
Additive RS

Influence graph

Background set: $S = \{a, b, c\}$
Reactions: $(\varnothing, \varnothing, \{a\})$ $(\{a\}, \varnothing, \{b, c\})$ $(\{c\}, \varnothing, \{c\})$

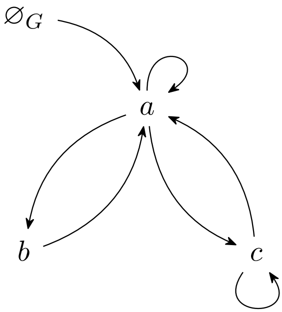
Influence graph $G_{\mathcal{A}} = (V_{\mathcal{A}}, E_{\mathcal{A}})$:

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

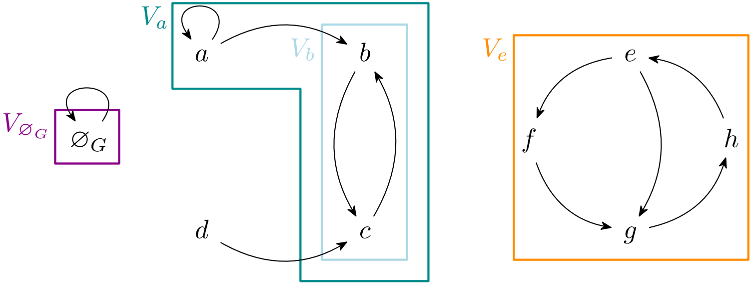


Background set: $S = \{a, b, c\}$
Reactions: $(\varnothing, \varnothing, \{a\}) \quad (\{a\}, \varnothing, \{b, c\}) \quad (\{c\}, \varnothing, \{c\})$

Influence graph $G_{\mathcal{A}} = (V_{\mathcal{A}}, E_{\mathcal{A}})$:



Fixed point *basis*



All results

Problem	$\mathcal{RS}(\infty,\infty)$	$\mathcal{RS}(0,\infty)$	$\mathcal{RS}(\infty,0)$	$\mathcal{RS}(1,0)$
A given state is a fixed point attractor	**NP**-c[1]	**NP**-c[2]	**NP**-c[2]	**P** [4]
∃ fixed point	**NP**-c[1]	**NP**-c[2]	**P** [3]	
∃ common fixed point	**NP**-c[1]	**NP**-c[2]	**NP**-c[2]	**P** [4]
sharing all fixed points	**coNP**-c[1]	**coNP**-c[2]	**coNP**-c[2]	**P** [4]
∃ fixed point attractor	**NP**-c[1]	**NP**-c[2]	Unknown	**P** [4]
∃ common fixed point attractor	**NP**-c[1]	**NP**-c[2]	**NP**-c[2]	**P** [4]
sharing all fixed points attractor	$\Pi_2^{\mathbf{P}}$-c[1]	$\Pi_2^{\mathbf{P}}$-c[2]	$\Pi_2^{\mathbf{P}}$-c[2]	**P** [4]
∃ fixed point not attractor	$\Sigma_2^{\mathbf{P}}$-c[2]	$\Sigma_2^{\mathbf{P}}$-c[2]	$\Sigma_2^{\mathbf{P}}$-c[2]	**P** [4]
∃ common fixed point not attractor	$\Sigma_2^{\mathbf{P}}$-c[2]	$\Sigma_2^{\mathbf{P}}$-c[2]	$\Sigma_2^{\mathbf{P}}$-c[2]	**P** [4]
sharing all fixed points not attractor	**coNP**-c[2]	**coNP**-c[2]	**coNP**-c[2]	**P** [4]
$\mathrm{res}_{\mathcal{A}} = \mathrm{res}_{\mathcal{B}}$	**coNP**-c[2]	**P** [2]	**P** [2]	

[1] Formenti, Manzoni, and Porreca 2014

[2] Ascone, Bernardini, and Manzoni 2024b

[3] Knaster-Tarski Theorem

[4] Ascone, Bernardini, and Manzoni 2024a

Open problems

- Is $\exists$ *fixed point attractor* for $\mathcal{RS}(\infty, 0)$ **NP**-complete?

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Problem	$\mathcal{RS}(\infty, \infty)$	$\mathcal{RS}(0, \infty)$	$\mathcal{RS}(\infty, 0)$	$\mathcal{RS}(1, 0)$
Reachability[3]	**PSPACE**-c	**PSPACE**-c	**PSPACE**-c	**NP**-c?

[3] Dennunzio et al. 2016.

Future directions

- Study similar problems related to cycles and global attractors (almost completed).

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- Study similar problems related to cycles and global attractors (almost completed).
- Study what happens for $\mathcal{RS}(2,0), \mathcal{RS}(3,0), \ldots$

How could resource bounded $\mathcal{RS}$ be of any interests for the P system community?

Consider the inhibitorless $\mathcal{RS}(\infty, 0)$ case.

[4] Ascone, Bernardini, Formenti, et al. 2024; Ascone, Bernardini, Leiter, et al. 2025.

How could resource bounded $\mathcal{RS}$ be of any interests for the P system community?

Consider the inhibitorless $\mathcal{RS}(\infty, 0)$ case. Changes:

- sets $\rightarrow$ multisets
- allow inputs
- choose a manner to select reactions (e.g. *maximally parallel manner*).

We get a non deterministic automaton pretty close to a 1-membrane P system, called *Chemical Pure Reaction Automata*.[4]

[4] Ascone, Bernardini, Formenti, et al. 2024; Ascone, Bernardini, Leiter, et al. 2025.

Results for CPRA

Theorem

CPRA in mp are Turing complete.

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Deterministic CPRA in mp are not Turing complete.

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Deterministic CPRA in mp are not Turing complete.

Ingredients:

- Commutative algebra result: Dickson's Lemma.
- Generalize results in the dynamics of $\mathcal{RS}(\infty, 0)$.

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