State sequences of interactive processes of reaction systems

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Note: all reaction systems in this talk are without context
$f : 2^S \rightarrow 2^S$

$f(\emptyset) = f(S) = \emptyset$
Theorem

\[ f = \text{res}_\mathcal{A} \text{ for some } \mathcal{A} \]

\[ \iff \]

\[ f \text{ is a boundary power set function} \]
Proof idea

\[ f(X) = Y \]

\[ (X, S - X, Y) \]
(\{x\}, I, P) \quad \text{reactant-minimal (only 1 reactant)}

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

(\{x\}, \{y\}, P) \quad \text{resource-minimal (only 1 reactant and 1 inhibitor)}
\[ f(X \cup Y) \subseteq f(X) \cup f(Y) \]

\[ f(X \cap Y) \subseteq f(X) \cup f(Y) \]
Examples

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

Not union-subadditive

$$\text{res}_A(\{a\} \cup \{b\}) = \text{res}_A(\{a, b\}) = \{a, b\}$$

$$\uparrow$$

$$\text{res}_A(\{a\}) \cup \text{res}_A(\{b\}) = \emptyset$$
Examples

\[(\{a, b\}, \{c, d\}, \{a, b\})\]

Not intersection-subadditive

\[\text{res}_A(\{a, b, c\} \cap \{a, b, d\}) = \text{res}_A(\{a, b\}) = \{a, b\} \quad \uparrow \]

\[\text{res}_A(\{a, b, c\}) \cup \text{res}_A(\{a, b, d\}) = \emptyset\]
Theorem

\[ f \text{ is union-subadditive} \]
\[ \iff \]
\[ f = \text{res}_A \text{ for some reactant-minimal } A \]

\[ f \text{ is intersection-subadditive} \]
\[ \iff \]
\[ f = \text{res}_A \text{ for some inhibitor-minimal } A \]
Theorem

\[ f \text{ is union- and intersection-subadditive} \]

\[ f = \text{res}_A \text{ for some resource-minimal } A \]
Dynamics

\[ \text{res}_A^t(T) \]
Dynamics

Cycles
Dynamics

Fixed points

\{a, b\} \rightarrow \{a, c\} \rightarrow \{a\} \rightarrow \{b\} \rightarrow \{c\} \rightarrow \{a, b, c\} \rightarrow \emptyset \rightarrow \{b, c\} \rightarrow \{a, b, c\}
Implementing binary counters

\[
\begin{array}{cccccc}
1 & 0 & 1 & 0 & 1 & 1 \\
\end{array}
\]

\[
\downarrow \quad \downarrow \quad \downarrow \quad \downarrow \\
\{ b_5, \quad b_3, \quad b_1, b_0 \} 
\]
Incrementing binary counters

1 0 1 0 1 1 1

no carry

1 0 1 1 0 0

carry
Reactions for incrementing binary counters

- \( \{b_{i-1}, b_{i-2}, \ldots, b_0\}, \{b_i\}, \{b_i\} \) 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 \( 0 \leq j < i \leq n \)

- Preserve 1 if no carry

- Carry

- Flip least significant bit

- Preserve 1 if no carry

- For 1 ≤ i ≤ n

- For 0 ≤ j < i ≤ n

- For 1 ≤ i ≤ n
Long paths → binary counters
Long cycles $\rightarrow$ binary counters
Turing machines (with bounded tape)

\[
\begin{align*}
q \ a & \rightarrow \ q \ b \ \uparrow \\
q \ b & \rightarrow \ r \ a \ \uparrow \\
r \ a & \rightarrow \ q \ a \ \uparrow \\
r \ b & \rightarrow \ r \ a \ \uparrow
\end{align*}
\]
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

\[
\begin{align*}
q & \quad a & \rightarrow & \quad q & \quad b & \quad \triangleright \\
q & \quad b & \rightarrow & \quad r & \quad a & \quad \triangleright \\
r & \quad a & \rightarrow & \quad q & \quad a & \quad \triangleleft \\
r & \quad b & \rightarrow & \quad r & \quad a & \quad \triangleright \\
(\{q_1, a_1\}, \{\spadesuit\}, \{q_2, b_1\}) & \quad , \\
(\{q_2, a_2\}, \{\spadesuit\}, \{q_3, b_2\}) & \quad , \\
\vdots & \quad , \\
(\{q_6, a_6\}, \{\spadesuit\}, \{q_7, b_6\}) & \quad .
\end{align*}
\]
Encoding as reaction system

\[
\begin{align*}
q \ a & \rightarrow q \ b \ \triangleright \\
q \ b & \rightarrow r \ a \ \triangleright \\
r \ a & \rightarrow q \ a \ \triangleleft \\
r \ b & \rightarrow r \ a \ \triangleright
\end{align*}
\]

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

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

\[
\vdots
\]

\((\{r_7, a_7\}, \{\spadesuit\}, \{q_6, a_7\})\)
Preserving the tape

\[
\begin{align*}
&\left(\{a_1\}, \{q_1, r_1\}, \{a_1\}\right) & \left(\{b_1\}, \{q_1, r_1\}, \{b_1\}\right) \\
&\left(\{a_2\}, \{q_2, r_2\}, \{a_2\}\right) & \left(\{b_2\}, \{q_2, r_2\}, \{b_2\}\right) \\
&\vdots & \vdots \\
&\left(\{a_7\}, \{q_7, r_7\}, \{a_7\}\right) & \left(\{b_7\}, \{q_7, r_7\}, \{b_7\}\right)
\end{align*}
\]
Computation step

\[
\begin{align*}
\{a_1, b_2, b_3, a_4, a_5, a_6, b_7, q_3\} \\
\{a_1, b_2, a_3, a_4, a_5, a_6, b_7, r_4\}
\end{align*}
\]
Dynamics of the same complexity
Does minimality make a difference?

\[ f \text{ is union- and intersection-subadditive} \]

\[ f = \text{res}_A \text{ for some resource-minimal } A \]
Theorem

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

$$\text{res}_B^{2^t}(U) = \text{res}_A^t(U)$$
Proof idea

\[ a = (\{x, y\}, \{z\}, \{w\}) \quad b = (\{v\}, \{z, w\}, \{z\}) \]
Proof idea: given \( a = (R_a, I_a, P_a) \)

Reactant missing?
\[
(\{x\}, \{y\}, \{\overline{a}\}) \quad \text{for } y \in R_a, x \in S - \{y\}
\]

Any inhibitor?
\[
(\{x\}, \{\spadesuit\}, \{\overline{a}\}) \quad \text{for } x \in I_a
\]

If not disabled, produce \( P_a \)
\[
(\{\spadesuit\}, \{\overline{a}\}, P_a)
\]

Make \( \spadesuit \) every other step
\[
(\{x\}, \{\spadesuit\}, \{\spadesuit\}) \quad \text{for } x \in S
\]
Proof idea: given \( a = (R_a, I_a, P_a) \)

Reactant missing?
\[
(\{x\}, \{y\}, \{\bar{a}\}) \quad \text{for } y \in R_a, x \in S - \{y\}
\]

Any inhibitor?
\[
(\{x\}, \{\heartsuit\}, \{\bar{a}\}) \quad \text{for } x \in I_a
\]

If not disabled, produce \( P_a \)
\[
(\{\heartsuit\}, \{\bar{a}\}, P_a)
\]

Make \( \heartsuit \) every other step
\[
(\{x\}, \{\heartsuit\}, \{\heartsuit\}) \quad \text{for } x \in S
\]

Minimal!
Dynamics

\[ \text{res}_A^t(T) \]

\{a\} \rightarrow \{a, b\} \rightarrow \{a, c\} \rightarrow \{b\} \rightarrow \{c\} \rightarrow \{a, b, c\} \rightarrow \emptyset \rightarrow \{b, c\} \rightarrow \{a, b, c\} \rightarrow \text{res}_A^t(T)
Dynamics

\[ \text{res}^t_B(T) \]
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?

<table>
<thead>
<tr>
<th>Type</th>
<th>Longest sequence known</th>
</tr>
</thead>
<tbody>
<tr>
<td>Generic</td>
<td>$\Theta(2^n) \rightarrow$ optimal</td>
</tr>
<tr>
<td>Almost-minimal</td>
<td>$\Theta(3^{n/3}) \approx \Theta(1.44^n)$</td>
</tr>
<tr>
<td>Resource-minimal</td>
<td>$\Theta(3^{n/4}) \approx \Theta(1.32^n)$</td>
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</tbody>
</table>
Context as nondeterminism
Context as nondeterminism

\[ \text{res}_{\mathcal{A}}(T) \]
Context as nondeterminism

\[ \text{res}_A(T) \]
\[ \text{res}_A(T \cup U_1) \]
\[ \text{res}_A(T \cup U_2) \]
\[ \ldots \]
Thanks for your attention!
Grazie per la vostra attenzione!

Any questions?