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SIMPLE REACTION SYSTEMS AND THEIR CLASSIFICATION*

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Reaction systems are a model of computation inspired by biochemical reactions involving reactants, inhibitors and products from a finite background set. We define a notion of multi-step simulation among reaction systems and derive a classification with respect to the amount of resources (reactants and inhibitors) involved in each reaction. We prove that "simple" reaction systems, having at most one reactant and one inhibitor per reaction, suffice in order to simulate arbitrary systems. Finally, we show that the equivalence relation of mutual simulation induces exactly five linearly ordered classes of reaction systems characterizing well-known subclasses of the functions over Boolean lattices, such as the constant, additive (join-semilattice endomorphisms), monotone, and antitone functions.

Keywords: Natural computing; reaction systems.

1. Introduction

Reaction systems, introduced by Ehrenfeucht and Rozenberg [4,5], are a formalized abstraction of biochemical processes in which the dynamics are discrete, in both space and time, and are described in terms of *reactions*. A reaction is modeled as a

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set of *reactants*, necessary for the reaction to take place, a set of *inhibitors*, whose presence blocks the reaction from occurring, and a set of *products*.

Reaction systems may be considered a qualitative model, as opposed to a quantitative one, as we only focus on the presence or absence of chemical species, and not on the precise amounts. In particular, multiple reactions having common reactants do not interfere; indeed, *all* reactions that are enabled at a certain time step happen simultaneously. Another feature of reaction systems which differentiates them from other biologically inspired computational models is the lack of permanency: the state of the system only consists of the products of the reactions that took place in the last time step, without preserving the entities that were not involved in any reaction.

Mathematically, a reaction systems defines a transition function (the *result* function) between states, i.e., sets of entities (chemical species), which completely describes the dynamics of the system. In many cases, the study of the properties of reaction systems involves the comparison of the result functions of different systems or classes of systems. A natural way to understand the modeling power of reaction systems is to consider their behavior when the amount of resources (reactants and inhibitors per reactions) is limited. It was proved [3,7] that there exist infinite proper hierarchies of classes of result functions: by allowing more resources, more functions become definable by reaction systems. The idea of studying reaction systems with a minimal number of resources was also carried on in [2], where the properties and the functions defined by minimal reaction systems were studied.

While the analysis of result functions is a direct way to compare reaction systems, the classification it provides has a very high granularity. Requiring the equality of the whole dynamics can be restrictive for certain applications where we are interested in a higher-level view of the behavior of the systems. As an analogy, consider a simulation between Turing machines: we are often not interested in a step-by-step correspondence of configurations, and we allow the simulation to be slower than the original machine. In a similar fashion, in this paper we define a notion of simulation in which the simulating system is allowed to use several steps to simulate a single step of the other system; auxiliary entities (analogous to an alphabet extension) may also be involved in the simulation.

The resulting equivalence relation of mutual simulability is coarser than equality of result functions, but still captures the intuitive idea of "having the same behavior". This relation induces exactly five equivalence classes of reaction systems. Interestingly, these classes correspond to well-defined properties of the result functions as functions over finite Boolean lattices; indeed, they correspond to the constant, additive (join-semilattice endomorphisms), monotone, antitone, and the totality of functions. These equivalence classes are ordered linearly by the simulation preorder. We also give exact lower bounds to the number of steps required to perform the simulations, and prove that auxiliary entities are, in general, necessary if we want to preserve the five equivalence classes.

Differently from the original paper that introduced the notion of multi-step simu-

lation for reaction systems [6], this extended version provides in many cases a better construction and proves in all cases the minimality of the resulting simulation and the necessity of using additional entities, solving most of the problems originally left open. Furthermore, the characterization of equivalence classes in terms of functions, which was barely sketched in the original paper, is here expanded and completed.

This paper is structured as follows. In Section 2 we recall the definitions and notation related to reaction systems. In Section 3 we introduce the notion of k-simulation and prove that any reaction system can be k-simulated by a system in "normal form" using only one reactant and one inhibitor per reaction. Then we turn our attention to limited variants of reaction systems. In Section 4 we consider reaction systems using only inhibitors, characterizing the antitone functions; we prove that one inhibitor suffices to simulate them, and that they are weaker than reaction systems using both reactants and inhibitors. In Section 5 we analyze reaction systems using only reactants, characterizing the monotone functions; we prove that two reactants suffice to simulate them (while single-reactant reaction systems are weaker and characterize the additive functions), and that they are weaker than inhibitor-only reaction systems. In Section 6 we finalize the classification by proving that reaction systems without reactants and inhibitors characterize the constant functions, and thus are the weakest variant. Section 7 contains our conclusions and suggestion for further research.

2. Basic Notions

In this paper we denote sets by upper-case letters, reactions and atomic elements by lower-case letters, and reaction systems and families of sets by calligraphic letters. Given a set X, we denote by 2^X the power set of X. Recall that 2^X is a Boolean lattice with respect to set inclusion, having $\cup$ and $\cap$ as join and meet operations.

A reaction is formally defined as follows.

Definition 1. *Given a finite set S (the* background set*), a* reaction over S *is a triple of sets $a = (R_a, I_a, P_a) \in 2^S \times 2^S \times 2^S$. We call R_a the set of* reactants*, I_a the set of* inhibitors*, and P_a the set of* products*.*

Since we will show that one reactant and one inhibitor suffice to simulate any reaction system (see Theorem 11), in this paper we also admit empty reactant and inhibitor sets, as in the original definition [5], in order to investigate the expressivity of the resulting reactions and to prove that they are strictly weaker than reactions involving both kinds of resources.

Definition 2. *A* reaction system *is a pair $\mathcal{A} = (S, A)$ where S is a finite set and A a set of reactions over S.*

A *state* of a reaction system $\mathcal{A} = (S, A)$ is any subset of S. The dynamics of a reaction systems are defined as follows.

Definition 3. *Let $\mathcal{A} = (S, A)$ be a reaction system, $a = (R_a, I_a, P_a) \in A$, and $T \subseteq S$. We say that a is* enabled by T *if and only if $R_a \subseteq T$ and $I_a \cap T = \varnothing$.*

The result of a on T *is defined as*

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

The result of $\mathcal{A}$ on T *is defined as* $\mathrm{res}_{\mathcal{A}}(T) = \bigcup_{a \in A} \mathrm{res}_a(T)$.

The *state sequence* of a reaction system $\mathcal{A}$ with initial state T is given by successive iterations of the result function:

$$\left(\mathrm{res}^n_{\mathcal{A}}(T)\right)_{n \in \mathbb{N}} = \left(T, \mathrm{res}_{\mathcal{A}}(T), \mathrm{res}^2_{\mathcal{A}}(T), \dots\right).$$

Since the background set of a reaction system is finite, the state space is also finite; hence, every state sequence is ultimately periodic.

3. Simulation between Reaction Systems

In order to compare reaction systems with respect to their ability to generate state sequences, we define a notion of simulation less restrictive than equality of result functions: here, the simulating system may use several steps to simulate a single step of the original system. This is consistent with notions of simulation employed for many computational models (e.g., Turing machines), when we are not interested in the strict correspondence of every pair of configurations, but only in the overall behavior of the two systems.

Definition 4 (*k*-simulation) *Let $\mathcal{A} = (S, A)$ and $\mathcal{A}' = (S', A')$, with $S \subseteq S'$, be reaction systems, and let $k \in \mathbb{N}$. We say that $\mathcal{A}'$ k-simulates $\mathcal{A}$ if and only if, for all $T \subseteq S$ and all $n \in \mathbb{N}$, we have*

$$\mathrm{res}^n_{\mathcal{A}}(T) = \mathrm{res}^{kn}_{\mathcal{A}'}(T) \cap S.$$

In other words, when considering the sequences of states of $\mathcal{A}$ and $\mathcal{A}'$ starting from T, the n-th state of $\mathcal{A}$ coincides with the (kn)-th state of $\mathcal{A}'$ with respect to the elements of S (some auxiliary elements of $S' - S$ may also occur). We use the notion of k-simulation to define a relation on classes of reaction system.

Definition 5. *Let X and Y be classes of reaction systems, and let $k \in \mathbb{N}$. We define the binary relation $\preceq_k$ as follows: $X \preceq_k Y$ if and only if for all $\mathcal{A} \in X$ there exists a reaction system in Y that ℓ-simulates $\mathcal{A}$ for some $\ell \leq k$.*

We say that $X \preceq Y$ if and only if $X \preceq_k Y$ for some $k \in \mathbb{N}$. We write $X \approx_k Y$ if $X \preceq_k Y$ and $Y \preceq_k X$, and $X \approx Y$ for $X \preceq Y \wedge Y \preceq X$. Finally, the notation $X \prec Y$ is shorthand for $X \preceq Y \wedge Y \not\preceq X$.

Notice that $X \subseteq Y$ always implies $X \preceq_1 Y$, i.e., the set inclusion relation is coarser than k-simulation, since any reaction system is trivially 1-simulated by itself.

A k-simulation and an ℓ-simulation can be composed into a $(k\ell)$-simulation.

Lemma 6. *$X \preceq_k Y$ and $Y \preceq_\ell Z$ implies $X \preceq_{k\ell} Z$.*

Proof. For all $\mathcal{A} = (S, A) \in X$ there exist $\mathcal{B} = (S', A') \in Y$ with $S \subseteq S'$ and $h \leq k$ such that

$$\operatorname{res}_{\mathcal{B}}^{hn}(T) \cap S = \operatorname{res}_{\mathcal{A}}^{n}(T)$$

for all $n \in \mathbb{N}$ and $T \subseteq S$. Furthermore, there exist $\mathcal{C} = (S'', A'') \in Z$ and $m \leq \ell$ such that

$$\operatorname{res}_{\mathcal{C}}^{mn}(T) \cap S' = \operatorname{res}_{\mathcal{B}}^{n}(T)$$

for all $n \in \mathbb{N}$ and $T \subseteq S \subseteq S'$. By combining the previous statements and intersecting with S, we get

$$\left(\operatorname{res}_{\mathcal{C}}^{mhn}(T) \cap S'\right) \cap S = \operatorname{res}_{\mathcal{C}}^{mhn}(T) \cap S = \operatorname{res}_{\mathcal{B}}^{hn}(T) \cap S = \operatorname{res}_{\mathcal{A}}^{n}(T)$$

for all $T \subseteq S$ and $n \in \mathbb{N}$. In other words, the reaction system $\mathcal{C}$ (mh)-simulates $\mathcal{A}$. Since $mh \leq k\ell$, we obtain $X \preceq_{k\ell} Z$. □

From this lemma, we immediately get the following result:

Proposition 7. *The relation $\preceq$ is a preorder. Hence, the relation $\approx$ is an equivalence relation.*

We classify reaction systems according to the maximum amount of reactants and inhibitors appearing in their reactions.

Definition 8. *For all $r, i \in \mathbb{N}$, we denote by $\mathcal{RS}(r, i)$ the class of reaction systems $\mathcal{A} = (S, A)$ such that, for all $(R, I, P) \in A$, we have $|R| \leq r$ and $|I| \leq i$. We also define the classes $\mathcal{RS}(\infty, i) = \bigcup_{r \in \mathbb{N}} \mathcal{RS}(r, i)$, $\mathcal{RS}(r, \infty) = \bigcup_{i \in \mathbb{N}} \mathcal{RS}(r, i)$, and $\mathcal{RS}(\infty, \infty) = \bigcup_{r,i \in \mathbb{N}} \mathcal{RS}(r, i)$.*

Notice that $\mathcal{RS}(\infty, \infty)$ is the class of all reaction systems. In this classification the maximum number of products is not mentioned, because every reaction with p products can be replaced by p reactions having a single product [1].

Proposition 9. *For each reaction system $\mathcal{A} = (S, A)$ there exists a reaction system $\mathcal{A}' = (S, A')$ over the same background set having at most one product per reaction and such that $\operatorname{res}_{\mathcal{A}}(T) = \operatorname{res}_{\mathcal{A}'}(T)$ for all $T \subseteq S$.*

Every function over finite power sets is the result function of a reaction system in $\mathcal{RS}(\infty, \infty)$, that is, with an unbounded number of reactants and inhibitors. A similar result was proved by Ehrenfeucht et al. [2].

Proposition 10. *Let $f \colon 2^S \to 2^S$ be a function with $|S| = n$. Then $f = \operatorname{res}_{\mathcal{A}}$ for some $\mathcal{A} = (S, A) \in \mathcal{RS}(n, n)$.*

Proof. Let $\mathcal{A} = (S, A) \in \mathcal{RS}(n, n)$ with the following reactions:

$$(T, S - T, f(T)) \qquad \text{for all } T \subseteq S.$$

Let $T \subseteq S$. Then, the only reaction enabled by T is $a = (T, S - T, f(T))$, since for each $U \neq T$ we have either $U \subsetneq T$, or $U \not\subseteq T$ and then $(S - U) \cap T \neq \varnothing$. Hence $\mathrm{res}_{\mathcal{A}}(T) = \mathrm{res}_a(T) = f(T)$ as required. □

However, reactants and inhibitors can be both reduced to one with a 2-step simulation. This provides a minimal normal form for reaction systems computing arbitrary functions.

Theorem 11 (Normal form) $\mathcal{RS}(\infty, \infty) \approx_2 \mathcal{RS}(1, 1)$.

Proof. By definition we have $\mathcal{RS}(1, 1) \preceq_1 \mathcal{RS}(\infty, \infty)$, implying the weaker statement $\mathcal{RS}(1, 1) \preceq_2 \mathcal{RS}(\infty, \infty)$. Thus, we only need to prove $\mathcal{RS}(\infty, \infty) \preceq_2 \mathcal{RS}(1, 1)$.

Let $\mathcal{A} = (S, A) \in \mathcal{RS}(r, i)$. Let $\mathcal{A}' = (S', A')$ be a reaction system having $S' = S \cup A$, that is, we enlarge the background set S with an element for each reaction in A (which is represented by the reaction itself). The set A' contains, for each reaction $a = (R_a, I_a, P_a) \in A$, the following reactions:

$$(\varnothing, \{x\}, \{a\}) \qquad \text{for each } x \in R_a \tag{1}$$

$$(\{y\}, \varnothing, \{a\}) \qquad \text{for each } y \in I_a \tag{2}$$

$$(\varnothing, \{a\}, P_a). \tag{3}$$

Hence $\mathcal{A}' \in \mathcal{RS}(1, 1)$. In order to prove that $\mathcal{A}'$ 2-simulates $\mathcal{A}$, it suffices to show that, for all $n \in \mathbb{N}$, if n is even, then

$$\mathrm{res}^n_{\mathcal{A}'}(T) \cap S = \mathrm{res}^{n/2}_{\mathcal{A}}(T) \tag{4}$$

and if n is odd, then

$$\mathrm{res}^n_{\mathcal{A}'}(T) \cap A = \left\{a : a \text{ is not enabled by } \mathrm{res}^{(n-1)/2}_{\mathcal{A}}(T)\right\}. \tag{5}$$

By induction on n: if $n = 0$, then (4) holds by definition.

If $n > 0$ is odd, then by induction hypothesis we have

$$\mathrm{res}^{n-1}_{\mathcal{A}'}(T) \cap S = \mathrm{res}^{(n-1)/2}_{\mathcal{A}}(T).$$

Notice that the only reactions producing elements of A are those in (1) and (2); furthermore, for every $a \in A$, the element a is produced if and only if there exists some $x \in R_a$ such that $x \notin \mathrm{res}^{n-1}_{\mathcal{A}'}(T)$ or there exists some $y \in I_a$ such that $y \in \mathrm{res}^{n-1}_{\mathcal{A}'}(T)$. Thus, by induction hypothesis, the element $a \in S'$ is produced in $\mathcal{A}'$ at time n if and only if the reaction $a \in A$ is not enabled in $\mathcal{A}$ at time $\frac{n-1}{2}$. As a consequence, statement (5) holds.

If $n > 0$ is even, then by induction hypothesis we have

$$\mathrm{res}^{n-1}_{\mathcal{A}'}(T) \cap A = \left\{a : a \text{ is not enabled by } \mathrm{res}^{(n-2)/2}_{\mathcal{A}}(T)\right\}.$$

The only reactions having elements of S as products are those in (3): for every such reaction $(\varnothing, \{a\}, P_a)$, the set P_a is produced if and only if $a \notin \mathrm{res}^{n-1}_{\mathcal{A}'}(T)$. Thus, for every reaction $a = (R_a, I_a, P_a) \in A$, the corresponding reaction $(\varnothing, \{a\}, P_a)$ is enabled in $\mathcal{A}'$ at time $n-1$ if and only if a is enabled in $\mathcal{A}$ at time $\frac{n-2}{2}$. Hence, statement (4) holds, i.e., $\mathcal{A}'$ 2-simulates $\mathcal{A}$. □

The number of steps required by the simulation cannot be reduced to one; this generally holds whenever we are reducing the amount of resources of the reaction system.

Proposition 12. *$\mathcal{RS}(r,i) \not\leq_1 \mathcal{RS}(r',i')$ whenever $r'+i' < r+i$.*

Proof. Let $\mathcal{A} = (S, A) \in \mathcal{RS}(r,i)$ be a reaction system with $|S| = r+i$ and a single reaction $a = (R, I, P)$ with $R \cup I = S$, $R \cap I = \varnothing$, and $P \neq \varnothing$.

Suppose $\mathcal{A}$ is 1-simulated by $\mathcal{A}' = (S', A') \in \mathcal{RS}(r', i')$ with $r'+i' < r+i$. Then, there exists $b = (R', I', P') \in A'$ with $R' \cap I' = \varnothing$ and $P' \cap S \neq \varnothing$, otherwise we would have

$$\mathrm{res}^1_{\mathcal{A}'}(R) \cap S = \varnothing \neq P = \mathrm{res}^1_{\mathcal{A}}(R).$$

Since $|R' \cup I'| = r'+i' < r+i = |S|$, there exists $x \in S - (R' \cup I')$. If $x \in R$ then R' enables b but not a:

$$\mathrm{res}^1_{\mathcal{A}'}(R') \cap S \supseteq \mathrm{res}_b(R') \cap S = P' \cap S \neq \varnothing = \mathrm{res}^1_{\mathcal{A}}(R'),$$

while if $x \in S - R = I$ then $R' \cup \{x\}$ inhibits a but not b:

$$\mathrm{res}^1_{\mathcal{A}'}(R' \cup \{x\}) \cap S \supseteq \mathrm{res}_b(R' \cup \{x\}) \cap S = P' \cap S \neq \varnothing = \mathrm{res}^1_{\mathcal{A}}(R' \cup \{x\}).$$

In both cases the value of $\mathrm{res}^1_{\mathcal{A}'}$ restricted to S differs from $\mathrm{res}^1_{\mathcal{A}}$ in at least one point, contradicting the fact that $\mathcal{A}'$ 1-simulates $\mathcal{A}$. □

Furthermore, increasing the size of the background set by adding auxiliary entities is generally necessary.

Proposition 13. *There exist reaction systems $\mathcal{A} = (S, A)$ with $|S| \geq 3$ that cannot be k-simulated (for any $k \in \mathbb{N}$) by reaction systems $\mathcal{A}' = (S, A') \in \mathcal{RS}(1,1)$, i.e., having the same background set.*

Proof. Let S be a finite set with $|S| = n \geq 3$, and let $T_1, T_2, \ldots, T_{2^n}$ be an enumeration of 2^S. Let $f\colon 2^S \to 2^S$ be defined as

$$f(T_i) = \begin{cases} T_{i+1} & \text{if } i < 2^n \\ T_{2^n} & \text{if } i = 2^n \end{cases}$$

By Proposition 10 we have $f = \mathrm{res}_{\mathcal{A}}$ for some $\mathcal{A} = (S, A) \in \mathcal{RS}(n,n)$. We prove that no $\mathcal{A}' = (S, A')$ k-simulates $\mathcal{A}$ for any $k > 1$. Suppose otherwise; then $\mathcal{A}'$ generates the state sequence

$$(T_1, \mathrm{res}^1_{\mathcal{A}'}(T_1), \mathrm{res}^2_{\mathcal{A}'}(T_1), \ldots, \mathrm{res}^k_{\mathcal{A}'}(T_1) = T_2).$$

Notice that T_2 can be either part of a cycle in $\mathcal{A}'$, or outside any cycle. In the first case, the state T_2 appears infinitely often in the state sequence starting at T_1, including at positions that are multiple of k and correspond to the state sequence of $\mathcal{A}$ starting at T_1, while it should only appear once. In the second case, in particular we have $\mathrm{res}_{\mathcal{A}'}(T_1) \neq T_2$, and $\mathrm{res}_{\mathcal{A}'}(T_1)$ is also outside any cycle (as it would imply T_2 in a cycle). Hence, $\mathrm{res}_{\mathcal{A}'}(T_1)$ will never appear again; but we have $\mathrm{res}_{\mathcal{A}'}(T_1) = T_i$ for some $i > 1$, and a k-simulation requires $\mathrm{res}_{\mathcal{A}'}^{k(i-1)}(T_1) = \mathrm{res}_{\mathcal{A}}^{i-1}(T_1) = T_i$. Hence, $\mathcal{A}'$ does not k-simulate $\mathcal{A}$ for any $k > 1$.

Now we identify a subset of enumerations of 2^S that are not the result functions of any $\mathcal{A}' = (S, A') \in \mathcal{RS}(1, 1)$, thus proving that some of the reaction systems $\mathcal{A}$ described above cannot be 1-simulated either. Let $x, y, z \in S$ be distinct elements, and fix $f(\{x\}) = S$, $f(\{x, y\}) = \varnothing$, and $f(\varnothing) = \varnothing$ (i.e., $T_{2^n} = \varnothing$). Suppose $\mathcal{A}'$ 1-simulates $\mathcal{A}$ with $f = \mathrm{res}_{\mathcal{A}}$. Since S is the image of some state, for each $w \in S$ there exists a reaction $(R, I, P) \in A'$ with $w \in P$. Since $f(\varnothing) = \varnothing$, we must have $R \neq \varnothing$. Since $f(\{x\}) = S$, one of these reactions has $R = \{x\}$. But this requires $I = \{y\}$, since $f(\{x, y\}) = \varnothing$. Hence, for each $w \in S$ we have a reaction $(\{x\}, \{y\}, P)$ with $w \in P$. As a consequence $\mathrm{res}_{\mathcal{A}'}(\{x, z\}) = S$; but $f(\{x, z\}) \neq S$ since $S \neq T_{2^n}$ has only one preimage. □

4. Reactantless Reaction Systems

Having established a minimum amount of resources needed to simulate general reaction systems, we are interested in analyzing the behavior of weaker systems. Let us begin by considering reaction systems without reactants and using only inhibitors. These can be simulated in 3 steps with only one inhibitor.

Lemma 14. $\mathcal{RS}(0, \infty) \approx_3 \mathcal{RS}(0, 1)$.

Proof. Trivially, $\mathcal{RS}(0, 1) \preceq_3 \mathcal{RS}(0, \infty)$ holds.

Let $\mathcal{A} = (S, A) \in \mathcal{RS}(0, \infty)$, and let $\mathcal{A}' = (S', A') \in \mathcal{RS}(0, 1)$ with background set $S' = S \cup \bar{S} \cup 2^S$, where $\bar{S} = \{\bar{x} : x \in S\}$ is disjoint from $S \cup 2^S$. For each $x \in S$, A' contains the reaction

$$(\varnothing, \{x\}, \{\bar{x}\}) \tag{6}$$

and, for each $a = (\varnothing, I_a, P_a) \in A$, the reactions

$$(\varnothing, \{\bar{x}\}, \{I_a\}) \qquad \text{for each } x \in I_a \tag{7}$$

$$(\varnothing, \{I_a\}, P_a). \tag{8}$$

We prove, by induction on n, that for all $T \subseteq S$ we have

$$\mathrm{res}_{\mathcal{A}'}^n(T) \cap S = \mathrm{res}_{\mathcal{A}}^{n/3}(T) \qquad \text{if } n = 3m; \tag{9}$$

$$\bar{x} \in \mathrm{res}_{\mathcal{A}'}^n(T) \iff x \notin \mathrm{res}_{\mathcal{A}}^{(n-1)/3}(T) \qquad \text{if } n = 3m + 1; \tag{10}$$

$$I_a \in \mathrm{res}_{\mathcal{A}'}^n(T) \cap 2^S \iff I_a \cap \mathrm{res}_{\mathcal{A}}^{(n-2)/3}(T) \neq \varnothing \qquad \text{if } n = 3m + 2. \tag{11}$$

For $n = 0$, we have $\mathrm{res}^0_{\mathcal{A}'}(T) \cap S = T = \mathrm{res}^0_{\mathcal{A}}(T)$.

If $n > 0$ is a multiple of 3, then by induction hypothesis

$$I_a \in \mathrm{res}^{n-1}_{\mathcal{A}'}(T) \cap 2^S \iff I_a \cap \mathrm{res}^{(n-3)/3}_{\mathcal{A}}(T) \neq \varnothing.$$

Notice that, if $X \in \mathrm{res}^{n-1}_{\mathcal{A}'}(T) \cap 2^S$, then necessarily $X = I_a$ for some $a \in A$, as the only reactions producing elements of 2^S have the form (7). For each reaction $a \in A$ we have a corresponding reaction a' of type (8), and a is inhibited at time $\frac{n-3}{3}$ in $\mathcal{A}$ if and only if a' is inhibited at time $n-1$ in $\mathcal{A}'$: statement (9) follows.

If $n > 0$ with $n = 3m + 1$, by induction hypothesis we have

$$\mathrm{res}^{n-1}_{\mathcal{A}'}(T) \cap S = \mathrm{res}^{(n-1)/3}_{\mathcal{A}}(T).$$

We have $\bar{x} \in \mathrm{res}^n_{\mathcal{A}'}(T)$ if and only if the reaction $(\varnothing, \{x\}, \{\bar{x}\})$ was enabled at time $n-1$, that is $x \notin \mathrm{res}^{n-1}_{\mathcal{A}'}(T) \cap S = \mathrm{res}^{(n-1)/3}_{\mathcal{A}}(T)$ as required.

Finally, if $n > 0$ with $n = 3m + 2$, by induction hypothesis

$$\bar{x} \in \mathrm{res}^{n-1}_{\mathcal{A}'}(T) \iff x \notin \mathrm{res}^{(n-2)/3}_{\mathcal{A}}(T).$$

Let $a \in A$. We have $I_a \in \mathrm{res}^n_{\mathcal{A}'}(T) \cap 2^S$ if and only if at least one of the reactions of the form (7) was enabled at time $n-1$. This means that there exists $x \in I_a$ such that $\bar{x} \notin \mathrm{res}^{n-1}_{\mathcal{A}'}(T)$ and $x \in \mathrm{res}^{(n-2)/3}_{\mathcal{A}}(T)$. Equivalently, $I_a \cap \mathrm{res}^{(n-2)/3}_{\mathcal{A}}(T) \neq \varnothing$. This proves (11).

The statement of the proposition immediately follows from (9). □

The result functions of reaction systems using only inhibitors coincide with the functions $f\colon 2^S \to 2^S$ for which $X \subseteq Y$ implies $f(X) \supseteq f(Y)$, i.e., the antitone functions.

Proposition 15. *A function $f\colon 2^S \to 2^S$ with $|S| = i$ is antitone if and only if $f = \mathrm{res}_{\mathcal{A}}$ for some $\mathcal{A} \in \mathcal{RS}(0, i)$.*

Proof. Let $\mathcal{A} = (S, A) \in \mathcal{RS}(0, i)$, and let $T_1 \subseteq T_2 \subseteq S$. Since the reactions of $\mathcal{A}$ have no reagents, every $a \in A$ that is enabled by T_2 is also enabled by T_1, hence $\mathrm{res}_a(T_2) \subseteq \mathrm{res}_a(T_1)$. As a consequence, the function $\mathrm{res}_{\mathcal{A}}$ is antitone:

$$\mathrm{res}_{\mathcal{A}}(T_2) = \bigcup_{a \in A} \mathrm{res}_a(T_2) \subseteq \bigcup_{a \in A} \mathrm{res}_a(T_1) = \mathrm{res}_{\mathcal{A}}(T_1).$$

Conversely, let $f\colon 2^S \to 2^S$ with $|S| = i$ be antitone. Then, by Proposition 10, we have $f = \mathrm{res}_{\mathcal{A}}$ for some $\mathcal{A} = (S, A) \in \mathcal{RS}(i, i)$. Let $\mathcal{A}' = (S, A') \in \mathcal{RS}(0, i)$ be the reaction system obtained by erasing all reactants from the reactions of $\mathcal{A}$ which can actually be enabled, i.e.,

$$A' = \{(\varnothing, I, P) : (R, I, P) \in A \text{ for some } R \subseteq S \text{ with } R \cap I = \varnothing\}.$$

Then $\mathrm{res}_{\mathcal{A}'} = \mathrm{res}_{\mathcal{A}}$. Indeed, for all $T \subseteq S$ we have $\mathrm{res}_{\mathcal{A}}(T) \subseteq \mathrm{res}_{\mathcal{A}'}(T)$, since reaction $(\varnothing, I, P) \in A$ is enabled by T whenever $(R, I, P) \in A'$ with $R \cap I = \varnothing$ is. In order to show the converse inclusion $\mathrm{res}_{\mathcal{A}'}(T) \subseteq \mathrm{res}_{\mathcal{A}}(T)$, let $x \in \mathrm{res}_{\mathcal{A}'}(T)$.

Then $x \in P$ for some $(\varnothing, I, P) \in A'$ with $I \cap T = \varnothing$, and we have $a = (R, I, P) \in A$ for some $R \subseteq S$ with $R \cap I = \varnothing$. Since a is enabled by $S - I$, we have $x \in \mathrm{res}_{\mathcal{A}}(S - I)$, and, since $T \subseteq S - I$ and $\mathrm{res}_{\mathcal{A}}$ is antitone, we have $\mathrm{res}_{\mathcal{A}}(S - I) \subseteq \mathrm{res}_{\mathcal{A}}(T)$, i.e., $x \in \mathrm{res}_{\mathcal{A}}(T)$ as required. □

This result also implies that the 3-simulation above is minimal.

Proposition 16. *$\mathcal{RS}(0, \infty) \not\preceq_k \mathcal{RS}(0, 1)$ for $k < 3$.*

Proof. By Proposition 12 we have $\mathcal{RS}(0, \infty) \not\preceq_1 \mathcal{RS}(0, 1)$.

Let $\mathcal{A} = (S, A) \in \mathcal{RS}(0, \infty)$ with $S \neq \varnothing$ and $(\varnothing, S, S)$ as its only reaction. Suppose $\mathcal{A}' \in \mathcal{RS}(0, 1)$ 2-simulates $\mathcal{A}$. Then $\mathrm{res}^2_{\mathcal{A}'}(\varnothing) \cap S = \mathrm{res}_{\mathcal{A}}(\varnothing) = S$. By Proposition 15, $\mathrm{res}_{\mathcal{A}'}$ is antitone, hence $\mathrm{res}^2_{\mathcal{A}'}$ is monotone. Thus $\mathrm{res}^2_{\mathcal{A}'}(\varnothing) \cap S$ is a subset of $\mathrm{res}^2_{\mathcal{A}'}(S) \cap S$, that is, $\mathrm{res}^2_{\mathcal{A}'}(S) \cap S = S \neq \varnothing = \mathrm{res}_{\mathcal{A}}(S)$, a contradiction. □

Since an arbitrary function can be neither monotone nor antitone, reaction systems using only inhibitors are weaker than general ones.

Lemma 17. *$\mathcal{RS}(0, \infty) \prec \mathcal{RS}(1, 1)$.*

Proof. Let $\mathcal{A} = (S, A) \in \mathcal{RS}(1, 1)$ be a reaction system with $|S| \geq 2$ and $(\{x\}, \{y\}, \{x, y\})$ as its only reaction. Suppose that $\mathcal{A}' \in \mathcal{RS}(0, \infty)$ k-simulates $\mathcal{A}$. If k is even, then $\mathrm{res}^k_{\mathcal{A}'}$ is monotone, which is a contradiction since

$$\mathrm{res}_{\mathcal{A}}(\{x\}) = \mathrm{res}^k_{\mathcal{A}'}(\{x\}) \cap S \subseteq \mathrm{res}^k_{\mathcal{A}'}(\{x, y\}) \cap S = \mathrm{res}_{\mathcal{A}}(\{x, y\}) = \varnothing.$$

On the other hand, if k is odd, then $\mathrm{res}^k_{\mathcal{A}'}$ is antitone, and we obtain

$$\mathrm{res}_{\mathcal{A}}(\varnothing) = \mathrm{res}^k_{\mathcal{A}'}(\varnothing) \cap S \supseteq \mathrm{res}^k_{\mathcal{A}'}(\{x\}) \cap S = \mathrm{res}_{\mathcal{A}}(\{x\}) = \{x, y\},$$

another contradiction. □

The key results on reaction systems without reactants can be summarized as follows.

Theorem 18. *$\mathcal{RS}(0, 1) \approx \mathcal{RS}(0, \infty) \prec \mathcal{RS}(1, 1)$.*

5. Inhibitorless Reaction System

Another way of limiting reaction systems is by avoiding inhibitors. Reaction systems using only reactants can always be simulated by using two reactants per reactions.

Lemma 19. *$\mathcal{RS}(r, 0) \preceq_{\lceil \log_2 r \rceil} \mathcal{RS}(2, 0)$ for all $r \geq 2$.*

Proof. Given $\mathcal{A} = (S, A) \in \mathcal{RS}(r, 0)$, we define a reaction system $\mathcal{A}' = (S', A')$ in $\mathcal{RS}(2, 0)$ that $\lceil \log_2 r \rceil$-simulates $\mathcal{A}$.

First of all, we need a way to describe a set by a collection of its subsets of bounded cardinality. A k-covering of a finite set Y is a family $\mathcal{X} = \{X_1, \ldots, X_m\}$

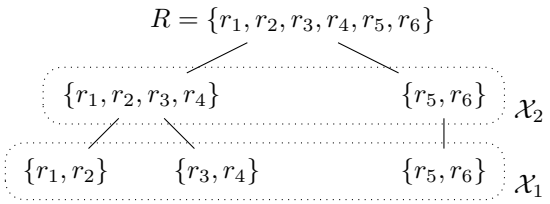

Fig. 1. A possible sequence $\mathcal{X}_1, \mathcal{X}_2$ of coverings of the set $R = \{r_1, \ldots, r_6\}$. Notice that $\mathcal{X}_1$ and $\mathcal{X}_2$ contain the same set $\{r_5, r_6\}$. The entities associated with R in S' are then $r_1, \ldots, r_6$ from R, together with $\{r_1, r_2\}_1, \{r_3, r_4\}_1, \{r_5, r_6\}_1$ from $\mathcal{X}_1$, and $\{r_1, r_2, r_3, r_4\}_2, \{r_5, r_6\}_2$ from $\mathcal{X}_2$.

of subsets of Y such that $\bigcup \mathcal{X} = Y$ and, for all $X_i \in \mathcal{X}$, we have $|X_i| \leq k$. Observe that, if $|Y| = n$, there exists a k-covering of Y with at most $\lceil \frac{n}{k} \rceil$ elements. Furthermore, if $\mathcal{X} = \{X_1, \ldots, X_m\}$ is a k-covering of Y, then a $2k$-covering of Y with $\lceil \frac{m}{2} \rceil$ elements can be defined as $\mathcal{X}' = \{X_1 \cup X_2, X_3 \cup X_4, \ldots, X_{m-1} \cup X_m\}$.

Let $(R, \varnothing, P) \in A$ with $R \neq \varnothing$ and let $\mathcal{X}_1$ be a 2-covering of R with $|\mathcal{X}_1| \leq \lceil r/2 \rceil$; given $\mathcal{X}_i$ with $i < \ell = \lceil \log_2 r \rceil - 1$, let $\mathcal{X}_{i+1}$ with $|\mathcal{X}_{i+1}| \leq \lceil r/2^{i+1} \rceil$ be a 2^{i+1}-covering of R such that, for each $Q \in \mathcal{X}_{i+1}$, there exist $M, N \in \mathcal{X}_i$ with $M \cup N = Q$. Then A' contains the following reactions, where the elements of a covering $\mathcal{X}_i$ are subscripted by i:

$$(Q, \varnothing, \{Q_1\}) \qquad \text{if } Q \in \mathcal{X}_1 \tag{12}$$

$$(\{M_i, N_i\}, \varnothing, \{Q_{i+1}\}) \qquad \text{if } M, N \in \mathcal{X}_i,\ Q = M \cup N \in \mathcal{X}_{i+1},\ 1 \leq i < \ell \tag{13}$$

$$(\{M_\ell, N_\ell\}, \varnothing, P) \qquad \text{if } R = M \cup N \text{ and } M, N \in \mathcal{X}_\ell \tag{14}$$

The set A' contains reactions (12)–(14) for each $a \in A$ having at least one reactant, and furthermore it contains, unchanged, all the reactions of A with no reactants. Notice that each reaction in A' has at most two reactants, i.e., $\mathcal{A}' \in \mathcal{RS}(2, 0)$.

An example of a sequence of k-coverings for a set of reactants is given in Fig. 1. Notice how they can be visualized as the different levels of a binary tree, where the children of a node are a $\lceil \frac{k}{2} \rceil$-covering of the parent.

Let $a = (R, \varnothing, P) \in A$ with $R \neq \varnothing$, $T \subseteq S$, let $A'_a \subseteq A'$ be the set of reactions of type (12)–(14) simulating a, and let $\mathcal{X}_1, \ldots, \mathcal{X}_\ell$ the coverings for a described above. By construction, A'_a "preserves" the reactants of a in subscripted sets, in the following sense:

$$R \subseteq T \iff R \subseteq \bigcup \{M \in \mathcal{X}_t : M_t \in \mathrm{res}^t_{A'_a}(T)\} \qquad \text{for } 1 \leq t \leq \ell. \tag{15}$$

In particular, at step ℓ, the two sets M_ℓ, N_ℓ of reaction (14) belong to $\mathrm{res}^\ell_{A'_a}(T)$ if and only if $R \subseteq T$, and at the next step we have $\mathrm{res}^{\lceil \log_2 r \rceil}_{A'_a}(T) = \mathrm{res}_a(T)$.

We also have $\mathrm{res}_a(T) = \mathrm{res}^{\lceil \log_2 r \rceil}_{A'_a}(T)$, with $A'_a = \{a\}$, for reactions with no reactants. Since all the reactions involve no inhibitors, we have

$$\mathrm{res}_{\mathcal{A}}(T) = \bigcup_{a \in A} \mathrm{res}_a(T) = \bigcup_{a \in A} \mathrm{res}^{\lceil \log_2 r \rceil}_{A'_a}(T) \subseteq \mathrm{res}^{\lceil \log_2 r \rceil}_{\mathcal{A}'}(T) \cap S.$$

Now let $x \in \mathrm{res}_{\mathcal{A}'}^{\lceil \log_2 r \rceil}(T) \cap S$. Then, x is either a product of a reaction $(\varnothing, \varnothing, P)$ belonging to both A and A', or of a reaction of type (14). In the first case, it immediately follows that $x \in \mathrm{res}_{\mathcal{A}}(T)$.

In the second case, the reaction of type (14) simulates a reaction $a \in A$ having reactants $R = M \cup N$ with $M_\ell, N_\ell \in \mathrm{res}_{\mathcal{A}'}^{\ell}(T)$. The two sets M_ℓ, N_ℓ are, in turn, products of reactions of type (12) or (13) belonging to A'_a; hence, $M_\ell, N_\ell \in \mathrm{res}_{A'_a}^{\ell}(T)$. By (15) we have $R \subseteq T$, hence $x \in \mathrm{res}_a(T) \subseteq \mathrm{res}_{\mathcal{A}}(T)$.

This proves that the reaction system $\mathcal{A}'$ $\lceil \log_2 r \rceil$-simulates $\mathcal{A}$. □

The result functions of this subclass of reaction system are exactly the monotone functions.

Proposition 20. *A function $f\colon 2^S \to 2^S$ with $|S| = r$ is monotone if and only if $f = \mathrm{res}_{\mathcal{A}}$ for some $\mathcal{A} \in \mathcal{RS}(r, 0)$.*

Proof. Let $\mathcal{A} = (S, A) \in \mathcal{RS}(r, 0)$, and let $T_1 \subseteq T_2 \subseteq S$. Since the reactions of $\mathcal{A}$ have no inhibitors, every $a \in A$ that is enabled by T_1 is also enabled by T_2, hence $\mathrm{res}_a(T_1) \subseteq \mathrm{res}_a(T_2)$. As a consequence, the function $\mathrm{res}_{\mathcal{A}}$ is monotone:

$$\mathrm{res}_{\mathcal{A}}(T_1) = \bigcup_{a \in A} \mathrm{res}_a(T_1) \subseteq \bigcup_{a \in A} \mathrm{res}_a(T_2) = \mathrm{res}_{\mathcal{A}}(T_2).$$

Conversely, let $f\colon 2^S \to 2^S$ with $|S| = r$ be monotone. Then, by Proposition 10, we have $f = \mathrm{res}_{\mathcal{A}}$ for some $\mathcal{A} = (S, A) \in \mathcal{RS}(r, r)$. Let $\mathcal{A}' = (S, A') \in \mathcal{RS}(r, 0)$ be the reaction system obtained by erasing all inhibitors from the reactions of $\mathcal{A}$ which can actually be enabled, i.e.,

$$A' = \{(R, \varnothing, P) : (R, I, P) \in A \text{ for some } I \subseteq S \text{ with } R \cap I = \varnothing\}.$$

Then $\mathrm{res}_{\mathcal{A}'} = \mathrm{res}_{\mathcal{A}}$. Indeed, for all $T \subseteq S$ we have $\mathrm{res}_{\mathcal{A}}(T) \subseteq \mathrm{res}_{\mathcal{A}'}(T)$, since reaction $(R, \varnothing, P) \in A'$ is enabled by T whenever $(R, I, P) \in A$ is. In order to show the converse inclusion $\mathrm{res}_{\mathcal{A}'}(T) \subseteq \mathrm{res}_{\mathcal{A}}(T)$, let $x \in \mathrm{res}_{\mathcal{A}'}(T)$. Then $x \in P$ for some $(R, \varnothing, P) \in A'$ with $R \subseteq T$, and there exists $a = (R, I, P) \in A$ for some $I \subseteq S$ with $R \cap I = \varnothing$. Since a is enabled by R, we have $x \in \mathrm{res}_{\mathcal{A}}(R)$ and, since $\mathrm{res}_{\mathcal{A}}$ is monotone, we have $\mathrm{res}_{\mathcal{A}}(R) \subseteq \mathrm{res}_{\mathcal{A}}(T)$, i.e., $x \in \mathrm{res}_{\mathcal{A}}(T)$ as required. □

Another property of reaction systems using r reactants per reaction and no inhibitors is that every entity generated in n steps is also generated by a state with at most r^n entities.

Lemma 21. *Let $\mathcal{A} = (S, A) \in \mathcal{RS}(r, 0)$. Then, for all $T \subseteq S$ and $n \in \mathbb{N}$, if $x \in \mathrm{res}_{\mathcal{A}}^n(T)$ then there exists $T' \subseteq T$ with $|T'| \leq r^n$ such that $x \in \mathrm{res}_{\mathcal{A}}^n(T')$.*

Proof. By induction on n. If $n = 0$, then $\mathrm{res}_{\mathcal{A}}^n(T) = T$, hence $x \in \mathrm{res}_{\mathcal{A}}^n(T)$ means $x \in T$; by letting $T' = \{x\}$ we have $T' \subseteq T$, $|T'| = 1 \leq r^n$, and $x \in \mathrm{res}_{\mathcal{A}}^n(T')$.

Now suppose $n > 0$. If $x \in \mathrm{res}_{\mathcal{A}}^n(T)$, then x is the product of some reaction $a = (R, \varnothing, P) \in A$ with $|R| \leq r$ and $x \in P$, and furthermore we have $R \subseteq \mathrm{res}_{\mathcal{A}}^{n-1}(T)$.

By applying $|R|$ times the induction hypothesis, we know that for each $y \in R$ there exists $T'_y \subseteq T$ with $|T'_y| \leq r^{n-1}$ such that $y \in \mathrm{res}^{n-1}_{\mathcal{A}}(T'_y)$. Let $T' = \bigcup_{y \in R} T'_y \subseteq T$; since the function $\mathrm{res}_{\mathcal{A}}$ is monotone (Proposition 20), we have $y \in \mathrm{res}^{n-1}_{\mathcal{A}}(T')$ for all $y \in R$, that is, $R \subseteq \mathrm{res}^{n-1}_{\mathcal{A}}(T')$. Hence a is enabled by $\mathrm{res}^{n-1}_{\mathcal{A}}(T')$, giving $x \in P \subseteq \mathrm{res}^{n}_{\mathcal{A}}(T')$. Since $|T'| \leq \sum_{y \in R} |T'_y| \leq r \times r^{n-1}$, the thesis follows. □

Lemma 21 implies that the $\lceil \log_2 r \rceil$-simulation we employed when reducing the number of reactants to 2, which is the only k-simulation in this paper where k depends on the size of the simulated reaction system, cannot be improved.

Proposition 22. *$\mathcal{RS}(r, 0) \not\preceq_k \mathcal{RS}(2, 0)$ for every $k < \lceil \log_2 r \rceil$.*

Proof. Let $\mathcal{A} = (S, A)$ with $|S| = r$ and $(S, \varnothing, S)$ as its only reaction. Then $\mathcal{A} \in \mathcal{RS}(r, 0)$, and

$$\mathrm{res}_{\mathcal{A}}(T) = \begin{cases} S & \text{if } T = S \\ \varnothing & \text{if } T \subsetneq S \end{cases}$$

Suppose $\mathcal{A}' \in \mathcal{RS}(2, 0)$ k-simulates $\mathcal{A}$ for some $k < \lceil \log_2 r \rceil$, and let $x \in \mathrm{res}_{\mathcal{A}}(S)$. Then $x \in \mathrm{res}^{k}_{\mathcal{A}'}(S) \cap S$, and in particular $x \in \mathrm{res}^{k}_{\mathcal{A}'}(S)$. By Lemma 21, there exists a $T' \subseteq S$ such that $x \in \mathrm{res}^{k}_{\mathcal{A}'}(T')$ and $|T'| \leq 2^k$. Since k is integer, $k < \lceil \log_2 r \rceil$ implies $k < \log_2 r$, hence $|T'| \leq 2^k < 2^{\log_2 r} = r = |S|$, that is, $T' \subsetneq S$. However, since $x \in S$, we have $x \in \mathrm{res}^{k}_{\mathcal{A}'}(T') \cap S = \mathrm{res}_{\mathcal{A}}(T') = \varnothing$, a contradiction. □

When only *one* reactant per reaction is used, we characterize the subset of the monotone functions consisting of all the additive ones, i.e., the endomorphisms of the join-semilattice $(2^S, \cup)$. A function $f \colon 2^S \to 2^S$ is an endomorphism if and only if $f(X \cup Y) = f(X) \cup f(Y)$ for all $X, Y \subseteq S$.

Proposition 23. *A function $f \colon 2^S \to 2^S$ is a join-semilattice endomorphism if and only if $f = \mathrm{res}_{\mathcal{A}}$ for some $\mathcal{A} \in \mathcal{RS}(1, 0)$.*

Proof. Let $\mathcal{A} = (S, A) \in \mathcal{RS}(1, 0)$, and let $T_1, T_2 \subseteq S$. Since the reactions of $\mathcal{A}$ have no inhibitors, a reaction enabled by $T \subseteq S$ is also enabled by all its supersets; hence $\mathrm{res}_{\mathcal{A}}(T_1) \cup \mathrm{res}_{\mathcal{A}}(T_2) \subseteq \mathrm{res}_{\mathcal{A}}(T_1 \cup T_2)$. Conversely, let $x \in \mathrm{res}_{\mathcal{A}}(T_1 \cup T_2)$; then, there exists $(R, \varnothing, P) \in A$ with $x \in P$ and $R \subseteq T_1 \cup T_2$. Since $|R| \leq 1$, we have either $R \subseteq T_1$ or $R \subseteq T_2$. Hence $x \in \mathrm{res}_{\mathcal{A}}(T_1)$ or $x \in \mathrm{res}_{\mathcal{A}}(T_2)$; therefore we obtain $\mathrm{res}_{\mathcal{A}}(T_1 \cup T_2) \subseteq \mathrm{res}_{\mathcal{A}}(T_1) \cup \mathrm{res}_{\mathcal{A}}(T_2)$.

Now let $f \colon 2^S \to 2^S$, with $|S| = r$, be a join-semilattice endomorphism. Then f is monotone, and by Proposition 20 we have $f = \mathrm{res}_{\mathcal{A}}$ for some $\mathcal{A} = (S, A) \in \mathcal{RS}(r, 0)$. Let $\mathcal{A}' = (S, A') \in \mathcal{RS}(1, 0)$ be the reaction system obtained from $\mathcal{A}$ by deleting the reactions having more that one reactant, i.e.,

$$A' = \{(R, \varnothing, P) : (R, \varnothing, P) \in A \text{ and } |R| \leq 1\}.$$

Then $\mathrm{res}_{\mathcal{A}'} = \mathrm{res}_{\mathcal{A}}$. Indeed, let $T \subseteq S$; since $\mathrm{res}_{\mathcal{A}}$ is a homomorphism, we have

$$\mathrm{res}_{\mathcal{A}}(T) = \mathrm{res}_{\mathcal{A}}\left(\varnothing \cup \bigcup_{y\in T}\{y\}\right) = \mathrm{res}_{\mathcal{A}}(\varnothing) \cup \bigcup_{y\in T}\mathrm{res}_{\mathcal{A}}(\{y\}).$$

Only reactions with at most one reactant (those in A') are enabled by $\{y\}$, hence we have

$$\mathrm{res}_{\mathcal{A}}(T) = \mathrm{res}_{\mathcal{A}'}(\varnothing) \cup \bigcup_{y\in T}\mathrm{res}_{\mathcal{A}'}(\{y\}) = \mathrm{res}_{\mathcal{A}'}\left(\varnothing \cup \bigcup_{y\in T}\{y\}\right) = \mathrm{res}_{\mathcal{A}'}(T)$$

since $\mathrm{res}_{\mathcal{A}'}$ is a homomorphism, as proved above. □

Even when iterated, join-semilattice endomorphisms do not characterize all monotone functions; hence, one reactant is weaker than two.

Lemma 24. $\mathcal{RS}(1,0) \prec \mathcal{RS}(2,0)$.

Proof. The iterated composition of a join-semilattice endomorphism is also a join-semilattice endomorphism:

$$f^k(T_1 \cup T_2) = f^{k-1}(f(T_1) \cup f(T_2)) = \cdots = f^k(T_1) \cup f^k(T_2).$$

Let $S = \{x, y\}$ and $g\colon 2^S \to 2^S$ be defined by $g(S) = S$ and $g(T) = \varnothing$ for $T \neq S$. Notice that g is monotone but not a join-semilattice endomorphism. Then, for every $S' \supseteq S$, every join-semilattice endomorphism $f\colon 2^{S'} \to 2^{S'}$, and every $k \in \mathbb{N}$, if $f^k(T) \cap S = g(T)$ for all $T \subseteq S$, we have

$$g(S) = f^k(\{x\} \cup \{y\}) \cap S = \big(f^k(\{x\}) \cap S\big) \cup \big(f^k(\{y\}) \cap S\big) = g(\{x\}) \cup g(\{y\}) = \varnothing.$$

However, $g(S) = S$, a contradiction. □

Perhaps surprisingly, a single inhibitor simulates arbitrarily many reactants.

Lemma 25. $\mathcal{RS}(\infty,0) \preceq_2 \mathcal{RS}(0,1)$.

Proof. Let $\mathcal{A} = (S, A) \in \mathcal{RS}(\infty, 0)$. Let $\mathcal{A}' = (S', A') \in \mathcal{RS}(0,1)$ with $S' = S \cup 2^S$ and having, for each reaction $a = (R_a, \varnothing, P_a) \in A$, the following set of reactions:

$$(\varnothing, \{x\}, \{R_a\}) \qquad \text{for each } x \in R_a \tag{16}$$

$$(\varnothing, \{R_a\}, P_a). \tag{17}$$

Let $T \subseteq S$. We prove, by induction on n, that

$$\mathrm{res}^n_{\mathcal{A}'}(T) \cap S = \mathrm{res}^{n/2}_{\mathcal{A}}(T) \qquad \text{if } n \text{ is even} \tag{18}$$

$$R_a \in \mathrm{res}^n_{\mathcal{A}'}(T) \iff R_a \nsubseteq \mathrm{res}^{(n-1)/2}_{\mathcal{A}}(T) \qquad \text{if } n \text{ is odd.} \tag{19}$$

For $n = 0$ we have $\mathrm{res}^0_{\mathcal{A}'}(T) \cap S = T = \mathrm{res}^0_{\mathcal{A}}(T)$.

For even $n > 0$ we have, by induction hypothesis,

$$R_a \in \mathrm{res}^{n-1}_{\mathcal{A}'}(T) \iff R_a \nsubseteq \mathrm{res}^{(n-2)/2}_{\mathcal{A}}(T).$$

Notice that the only reactions in A' with products in S have the form (17), and they are enabled at time $n-1$ if and only if $R_a \subseteq \mathrm{res}_{\mathcal{A}}^{(n-2)/2}(T)$, i.e., if and only if reaction a is enabled in $\mathcal{A}$ at time $\frac{n-2}{2}$. Condition (18) follows.

For odd $n > 0$, by induction hypothesis we have

$$\mathrm{res}_{\mathcal{A}'}^{n-1}(T) \cap S = \mathrm{res}_{\mathcal{A}}^{(n-1)/2}(T)$$

The only reactions of $\mathcal{A}'$ having products in 2^S have the form (16). The element R_a is produced if and only if there exists $x \in R_a$ with $x \notin \mathrm{res}_{\mathcal{A}'}^{n-1}(T) \cap S$, i.e., if and only if reaction a is *not* enabled in $\mathcal{A}$ at time $\frac{n-1}{2}$, as in (19).

The statement of the lemma follows from (18). □

On the other hand, reactants alone cannot simulate even a single inhibitor.

Lemma 26. $\mathcal{RS}(2,0) \prec \mathcal{RS}(0,1)$.

Proof. By Lemma 25 we have $\mathcal{RS}(2,0) \preceq_2 \mathcal{RS}(0,1)$.

Let $\mathcal{A} = (S, A) \in \mathcal{RS}(0,1)$ be defined by $S = \{x\}$ and $(\varnothing, \{x\}, \{x\})$ as the only reaction. By Proposition 15, the function $\mathrm{res}_{\mathcal{A}}$ is antitone; furthermore, it is not monotone, as it is not a constant function. By Proposition 20, for any $\mathcal{A}' \in \mathcal{RS}(2,0)$ the function $\mathrm{res}_{\mathcal{A}'}^{k}$ is monotone for all $k \in \mathbb{N}$. Therefore, $\mathcal{A}'$ cannot k-simulate $\mathcal{A}$. □

The following theorem summarizes the key results on reactant-only reaction systems.

Theorem 27. $\mathcal{RS}(1,0) \prec \mathcal{RS}(2,0) \approx \mathcal{RS}(\infty,0) \prec \mathcal{RS}(0,1)$.

6. Classification of Reaction Systems

Only one class of reaction systems is missing: those which do not use reactants nor inhibitors. They characterize the constant functions.

Proposition 28. *A function $f\colon 2^S \to 2^S$ is constant if and only if $f = \mathrm{res}_{\mathcal{A}}$ for some $\mathcal{A} \in \mathcal{RS}(0,0)$.*

Proof. Let $\mathcal{A} = (S, A) \in \mathcal{RS}(0,0)$. Then, every reaction $a \in A$ has the form $(\varnothing, \varnothing, P_a)$, and is always enabled, since $\varnothing \subseteq T$ and $\varnothing \cap T = \varnothing$ for each $T \subseteq S$. Hence

$$\mathrm{res}_{\mathcal{A}}(T) = \bigcup_{a \in A} P_a \qquad \text{for each } T \subseteq S$$

i.e., $\mathrm{res}_{\mathcal{A}}$ is a constant function.

Conversely, let $f\colon 2^S \to 2^S$ be a constant function. Let $\mathcal{A} = (S, A) \in \mathcal{RS}(0,0)$ be the reaction system having $(\varnothing, \varnothing, f(\varnothing))$ as its only reaction. Then, for each $T \subseteq S$, we have $\mathrm{res}_{\mathcal{A}}(T) = f(\varnothing) = f(T)$ as required. □

Clearly, this variant of reaction systems is weaker than all the others.

Lemma 29. $\mathcal{RS}(0,0) \prec \mathcal{RS}(1,0)$.

Proof. Let $\mathcal{A} = (S, A) \in \mathcal{RS}(1,0)$ be a reaction system having $(\{x\}, \varnothing, \{x\})$ as its only reaction, and suppose $\mathcal{A}' \in \mathcal{RS}(0,0)$ k-simulates $\mathcal{A}$. Then $\mathrm{res}^k_{\mathcal{A}'}$ is a constant function, and we have a contradiction:

$$\varnothing = \mathrm{res}_{\mathcal{A}}(\varnothing) = \mathrm{res}^k_{\mathcal{A}'}(\varnothing) \cap S = \mathrm{res}^k_{\mathcal{A}'}(\{x\}) \cap S = \mathrm{res}_{\mathcal{A}}(\{x\}) = \{x\}. \qquad \square$$

The classification of reaction systems with respect to the number of reactants and inhibitors can thus be summarized as follows.

Theorem 30. *The relation $\preceq$ is a total preorder on the set of classes of reaction systems of the form $\mathcal{RS}(r,i)$. The classes are comparable according to the following diagram for all $r_1 \geq 1$, $r_2 \geq 2$ and $i \geq 1$:*

$$\begin{array}{ccccccc}
\mathcal{RS}(0,0) & \prec & \mathcal{RS}(1,0) & \prec & \mathcal{RS}(2,0) & \prec & \mathcal{RS}(0,1) & \prec & \mathcal{RS}(1,1) \\
 & & & & \wr & & \wr & & \wr \\
 & & & & \mathcal{RS}(r_2,0) & \prec & \mathcal{RS}(0,i) & \prec & \mathcal{RS}(r_1,i) \\
 & & & & \wr & & \wr & & \wr \\
 & & & & \mathcal{RS}(\infty,0) & \prec & \mathcal{RS}(0,\infty) & \prec & \mathcal{RS}(\infty,\infty)
\end{array}$$

In particular, the relation $\approx$ induces exactly five equivalence classes.

7. Conclusions

In this paper a new notion of multi-step simulation between reaction systems, called k-simulation, has been defined. This definition allows a reaction system to use both additional time and additional entities to simulate another system. We have proved that the class of reaction systems with only one reactant and one inhibitor is sufficient to simulate any other reaction system using only two time steps per step of the original system.

We have investigated reaction systems without reactants, i.e., having only inhibitors, and we have proved that they characterize exactly the antitone functions between Boolean lattices and that every system of that kind can be simulated by a system having reactions with only one inhibitor. The situation when only reactants are present is not symmetrical. In fact, these systems represent every monotone function between Boolean lattices, and to simulate them it is necessary to use two reactants. The case of reaction systems having reactions with only one reactant and zero inhibitors is strictly weaker, as they characterize only additive functions. Finally, reaction systems without both reactants and inhibitors are the weakest ones and characterize the constant functions.

All the proposed constructions are provably optimal in time, i.e., the number of time steps employed to simulate a step of the original system is minimal. Furthermore, all constructions require a number of additional entities and reactions that is

polynomial with respect to the sum of the cardinalities of the background and the reaction sets of the original system.

Summarizing, each reaction system belongs to one of five classes, linearly ordered by the relation of k-simulability and characterizing well-known classes of functions between Boolean lattices.

Since auxiliary entities are sometimes necessary when reducing the amount of resources in each reaction, it would be interesting to establish which equivalence classes are induced by a stronger form of k-simulation with auxiliary entities only appearing in the intermediate steps, i.e., satisfying $\mathrm{res}^n_{\mathcal{A}}(T) = \mathrm{res}^{kn}_{\mathcal{A}'}(T)$.

While the characterization of the classes of functions corresponding to the five equivalence classes described in this paper is completed, it would be interesting to characterize the functions defined by other classes of reaction systems. Conversely, it would be interesting to start with a class of functions and investigate if it corresponds to some restriction on the resources used by reaction systems.

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