Relevance of Entities in Reaction Systems

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Abstract. Reaction systems are a model for the investigation of processes carried out by biochemical reactions in living cells. A reaction system consists of a set of reactions which transform a current system's state (a set of entities) into the successor state. In this paper we investigate which entities are actually relevant from the point of view of generating dynamic processes through such state transformations.

Keywords: reaction system, living cell, natural computing.

1 Introduction

The investigation of the computational nature of biochemical reactions is a research theme of Natural Computing. One of the goals of this research is to contribute to a computational understanding of the functioning of the living cell.

Reaction systems [1–7] are a formal framework for the investigation of processes carried out by biochemical reactions in living cells. The central idea of this framework is that the functioning of a living cell is based on interactions between (a large number of) individual reactions, and moreover these interactions are regulated by two main mechanisms: facilitation/acceleration and inhibition/retardation. These interactions determine the dynamic processes taking place in living cells, and reaction systems are an abstract model of these processes. This model is based on principles remarkably different from those underlying other *models of computation* in computer science. This is a consequence of the fact that on the one hand the model takes into account the basic bioenergetics of the living cell while on the other hand its (high) degree of abstraction allows it to be a qualitative rather than quantitative model.

In a nutshell, a reaction system consists of a finite set of reactions which can be applied to subsets (*states*) of a given set of entities, determining in this way the transformations of states. The specific question we address in this paper is which entities can be considered as relevant in the sense that state changes are "sensitive" to them.

H. Bordihn, M. Kutrib, and B. Truthe (Eds.): Dassow Festschrift 2012, LNCS 7300, pp. 44–55, 2012.

We provide a characterisation of relevant elements in terms of resources of reactions. In our considerations we use a specific "natural" notion of relevance, but we also discuss its relationship to other possible "natural" definitions of relevance.

The paper is organised in the following way. After setting up in Section 2 some mathematical notation used in the paper, we describe basic notions concerning reactions in Section 3, and basic notions concerning reaction systems in Section 4. In Section 5, we introduce the central notions of this paper: relevant/irrelevant sets and entities, and prove their basic properties. In Section 6, we demonstrate that for a reduced reaction system the set of relevant entities coincides with the resources used by the system's reactions. Then, in Section 7, we discuss two alternative formalisations of the notion of relevance. The last section contains a brief discussion of our results.

2 Preliminaries

Throughout the paper we use mostly standard mathematical notation. We use $X \div Y$ to denote the symmetric difference $(X \setminus Y) \cup (Y \setminus X)$ of two sets X and Y.

3 Reactions

In this section, we recall some key definitions concerning reactions and sets of reactions (see, e.g., [1, 5]).

Let Z be a finite nonempty set. A *reaction* over Z is a triplet of the form $a = (R, I, P)$, where $R, I, P \subseteq Z$ are nonempty sets such that $R \cap I = \varnothing$. The three component sets of reaction a are denoted by R_a, I_a and P_a, respectively, and called the *reactants*, *inhibitors* and *products* (of a). We denote by $rac(Z)$ the set of all possible reactions over Z.

Let $C \subseteq Z$. A reaction $a \in rac(Z)$ is *enabled* by C if $R_a \subseteq C$ and $I_a \cap C = \varnothing$. We denote this by $en_a(C)$. The *result* of a reaction $a \in rac(Z)$ on C is defined by

$$res_a(C) = \begin{cases} P_a & \text{if } a \text{ is enabled by } C \\ \varnothing & \text{otherwise .} \end{cases}$$

Moreover, the *result* of a set of reactions $B \subseteq rac(Z)$ on C, denoted by $res_B(C)$, is the union of the products of all the reactions from B, that is

$$res_B(C) = \bigcup_{b \in B} res_b(C) \ .$$

Note that $res_B(\varnothing) = \varnothing$ as the set of reactants of any reaction is nonempty and so no reaction is enabled by $C = \varnothing$. Also, $res_B(Z) = \varnothing$ as the set of inhibitors of any reaction is nonempty and so no reaction is enabled by Z.

Let $a, b \in rac(Z)$. Then b *covers* a if $res_b(C) = res_{\{a,b\}}(C)$, for all $C \subseteq Z$. We denote this by $b \geq a$; thus what a does (produces) is already covered (produced) by b. We also say that b *strictly covers* a if $b \geq a$ and $a \neq b$. Note that $\geq$ is a partial order.

As a matter of fact (see [5]), $b \geq a$ iff $R_b \subseteq R_a$, $I_b \subseteq I_a$ and $P_b \supseteq P_a$. Thus $b \geq a$ if b requires a subset of reactants of a and a subset of inhibitors of a but still produces at least all the products of a. Note that if $b \geq a$ then, for each $C \subseteq Z$, $en_a(C)$ implies $en_b(C)$.

4 Reaction Systems

A *reaction system* is a pair $\mathcal{A} = (S, A)$, where S is a finite nonempty *background* set comprising the *entities* of $\mathcal{A}$, and A is the set of reactions over S. To capture the *dynamic* behaviour of $\mathcal{A}$, we now describe all possible transitions between its states, where a *state* of $\mathcal{A}$ is any set C of its entities. Thus a reaction system with a background set S has exactly $2^{|S|}$ states.

Let $C \subseteq S$ be a state of a reaction system $\mathcal{A} = (S, A)$. Then $res_{\mathcal{A}}(C) = res_A(C)$ is the *result* of all the reactions of $\mathcal{A}$ enabled by C.

The state transformations captured by the above definition are deterministic. Thus, indeed, a reaction system $\mathcal{A} = (S, A)$ defines (specifies, implements) a function $res_{\mathcal{A}} : 2^S \rightarrow 2^S$, called the *result function* of $\mathcal{A}$. In the general model of reaction systems, processes of $\mathcal{A}$ are also influenced by the "environment" which reflects the fact that the living cell is an open system; it communicates and interacts with its environment. However, for the notions that we study in this paper it suffices to consider context-independent processes, i.e., processes determined by the system $\mathcal{A}$ only (without influence of its environment). In this way the successor state for a given state is determined solely by the result function $res_{\mathcal{A}}$.

Note that in this case, the successor $res_{\mathcal{A}}(C)$ of a current state C consists only of entities from the product sets of reactions of $\mathcal{A}$ enabled by C. This means that there is no *permanency* for entities $\mathcal{A}$: an entity from a current state will be present in (will carry over to) the successor state only if it is produced by at least one reaction enabled by the current state. This way of defining state transitions in reaction systems is motivated by the basic bioenergetics of the living cell, and it constitutes a fundamental difference with models of computations considered in computer science.

Since in this paper we are interested in state transitions in reaction systems, it is convenient to convey the subsequent discussion in terms of functions specified by reaction systems.

Proposition 1. *Let $\mathcal{A} = (S, A)$ be a reaction system. Then*

$$\bigcup_{C \in 2^S} res_{\mathcal{A}}(C) = \bigcup_{a \in A} P_a \ .$$

Proof. Follows from the fact that each reaction $a \in A$ is enabled by the state R_a. □

In other words, the entities occurring in the sets of the codomain of the result function of a reaction system are all the entities which occur in the products of the reactions of the system.

Let $\mathcal{A} = (S, A)$ be a reaction system and $b \in rac(S)$. Then b is *consistent* with $\mathcal{A}$ if $res_b(C) \subseteq res_{\mathcal{A}}(C)$, for all $C \subseteq S$; thus adding b to A yields a reaction system with the same result function.

A reaction system $\mathcal{A} = (S, A)$ is *reduced* if, for all $a \in A$,

(i) $res_{\mathcal{A}} \neq res_{A \setminus \{a\}}$.
(ii) there is no $b \in rac(S)$ which is consistent with $\mathcal{A}$ and strictly covers a.

Intuitively, (i) excludes reactions which do not add anything new to the results produced by other reactions in $\mathcal{A}$. As to the second condition, note that if b is consistent with $\mathcal{A}$ and b strictly covers a then b is (from the point of view of $\mathcal{A}$) a more 'efficient' version of a. Therefore, condition (ii) requires that all the reactions in $\mathcal{A}$ are in their most efficient version.

The two conditions in the definition of a reduced reaction system are independent. Consider, for example, the reaction system $\mathcal{A}_1 = (S, \{a, b\})$, where

$$S = \{1, 2\} \qquad a = (\{1\}, \{2\}, \{1\}) \qquad b = (\{1\}, \{2\}, \{2\})\,.$$

Then both reactions are necessary to specify $res_{\mathcal{A}_1}$. On the other hand, a and b are covered by $c = (\{1\}, \{2\}, \{1, 2\})$ which is consistent with $res_{\mathcal{A}_1}$ and can be used to define a more efficient $\mathcal{A}_1' = (S, \{c\})$ specifying the same function as $\mathcal{A}_1$.

Conversely, let us consider the reaction system $\mathcal{A}_2 = (S, \{a, b, c\})$, where

$$S = \{1, 2, 3\} \quad a = (\{1, 2\}, \{3\}, \{1, 2\}) \quad b = (\{1\}, \{3\}, \{1\}) \quad c = (\{2\}, \{3\}, \{2\})\,.$$

In this case, the first condition is not satisfied because reaction a is redundant (its enabledness implies enabledness of both b and c which together also produce $\{1, 2\}$). However, the second condition is satisfied as all reactions over $\{1, 2, 3\}$ strictly covering a or b or c are inconsistent with $res_{\mathcal{A}_2}$.

We close this section by demonstrating that considering only reduced reaction systems is not a restriction as far as result functions of reaction systems are concerned.

Theorem 1. *For every reaction system $\mathcal{A}$ there exists an* equivalent *reduced reaction system $\mathcal{A}'$, i.e., the two systems have the same background sets and the same result function.*

Proof. Let $\mathcal{A} = (S, A)$. Consider the set $con(\mathcal{A})$ of all the reactions from $rac(S)$ consistent with $\mathcal{A}$. Note that $(S, con(\mathcal{A}))$ is equivalent with $\mathcal{A}$ — as a matter of fact, it is the largest implementation of $res_{\mathcal{A}}$.

Let D be the set of all reactions in $con(\mathcal{A})$ which are $\geq$-maximal in $con(\mathcal{A})$.

Now we replace, in any order, each $a \in A$ which is not maximal in $con(\mathcal{A})$ by a reaction $b \in D$ such that $b \geq a$, Let A'' be the resulting set of reactions. Clearly, $\mathcal{A}'' = (S, A'')$ is equivalent with $\mathcal{A}$, and $\mathcal{A}''$ satisfies condition (ii) from the definition of a reduced system.

Next, in order to ensure that also (i) is satisfied, we inspect one by one all reactions, in any order, beginning with A'' and remove those reactions from the current set of reactions which can be removed without changing the result function. Let A' be the final outcome of this procedure. Clearly, $\mathcal{A}' = (S, A')$ still satisfies (ii), but it also satisfies (i). Thus $\mathcal{A}'$ is reduced, and moreover $\mathcal{A}'$ is equivalent to $\mathcal{A}$. Hence the theorem holds. □

5 Relevance in Reaction Systems

A central problem in the investigation of result functions of reaction systems is to understand when and why (for a given reaction system $\mathcal{A}$) $res_{\mathcal{A}}$ does not distinguish between two different states T and U, i.e., $res_{\mathcal{A}}(T) = res_{\mathcal{A}}(U)$. Intuitively, this means that the difference between T and U is irrelevant from the point of view of $res_{\mathcal{A}}$. In this paper, we define irrelevant sets of entities as the sets such that *whenever* two sets differ by an irrelevant set, then they will not be distinguishable by $res_{\mathcal{A}}$. Since the operation of symmetric difference is a mathematically natural way to define the difference between two sets, we use this operation in our definition of relevance. With this idea in mind, we say that:

– $X \subseteq S$ is *relevant* in $\mathcal{A}$ if

$$(\exists T, U \subseteq S) \ \ [T \div U = X \ \text{ and } res_{\mathcal{A}}(T) \neq res_{\mathcal{A}}(U)] \,. \tag{i}$$

– $x \in S$ is *relevant* in $\mathcal{A}$ if $\{x\}$ is relevant in $\mathcal{A}$, i.e.,

$$(\exists T \subseteq S) \ \ [\, res_{\mathcal{A}}(T \setminus \{x\}) \neq res_{\mathcal{A}}(T \cup \{x\})\,] \,. \tag{ii}$$

Intuitively, a set of entities X is *irrelevant* if any two sets of entities which 'differ' exactly by X are transformed to the same state, hence X is irrelevant from the $res_{\mathcal{A}}$ point of view. Thus, as expressed by (i), X is relevant if we can find two sets of entities which 'differ' exactly by X and for which $res_{\mathcal{A}}$ yields different results. What we are really interested in is whether *entities* are relevant or irrelevant, as expressed by part (ii) of the above definition. However, defining the relevance of sets through the relevance of their elements does not work, as shown in Section 6 (see the comments after Proposition 3). Thus we had to define (i) first.

Now, for a reaction system $\mathcal{A} = (S, A)$, we define:

– the *relevant domain* of $\mathcal{A}$ as $rdom(\mathcal{A}) = \{x \in S : x \text{ is relevant in } \mathcal{A}\}$.
– the *irrelevant domain* of $\mathcal{A}$ as $irdom(\mathcal{A}) = \{x \in S : x \text{ is irrelevant in } \mathcal{A}\}$.

Intuitively, $rdom(\mathcal{A})$ comprises those entities to which $res_{\mathcal{A}}$ is 'sensitive', and $irdom(\mathcal{A})$ those to which $res_{\mathcal{A}}$ is 'insensitive'.

It turns out that by combining irrelevant entities we never obtain a relevant set of entities. In other words, irrelevance is persistent, as shown next.

Proposition 2. *Let $\mathcal{A}$ be a reaction system. Then each $X \subseteq irdom(\mathcal{A})$ is irrelevant in $\mathcal{A}$.*

Proof. Let $\mathcal{A} = (S, A)$, and let X be a nonempty subset of $irdom(\mathcal{A})$. Let $T, U \subseteq S$ be such that $T \div U = X$. Let $T \setminus U = Y$ and $U \setminus T = Z$; thus $X = Y \cup Z$. Since $X \neq \emptyset$, at least one of Y, Z is nonempty.

Without loss of generality, assume that $Y \neq \varnothing$, thus $Y = \{y_1, y_2, \ldots, y_n\}$ for some $n \geq 1$. Let $T_0 = T$, $T_1 = T_0 \setminus \{y_1\}$, $T_2 = T_1 \setminus \{y_2\}$, $\ldots$, $T_n = T_{n-1} \setminus \{y_n\} = T \cap U$. Since, for each $i \in \{1, \ldots, n\}$, $y_i \in Y$ is irrelevant, we get

$$res_{\mathcal{A}}(T) = res_{\mathcal{A}}(T_0) = \ldots = res_{\mathcal{A}}(T_n) = res_{\mathcal{A}}(T \cap U) \; . \qquad (*)$$

Similarly, one proves that

$$res_{\mathcal{A}}(T \cap U) = res_{\mathcal{A}}(U) \; . \qquad (**)$$

It follows from $(*)$ and $(**)$ that

$$res_{\mathcal{A}}(T) = res_{\mathcal{A}}(T \cap U) = res_{\mathcal{A}}(U) \; .$$

This implies that, for all $T, U \subseteq S$ with $T \div U = X$, we have $res_{\mathcal{A}}(T) = res_{\mathcal{A}}(U)$. Therefore X is irrelevant. □

As a corollary of Proposition 2 we get the following property of the sets of reactants of reactions in a reaction system.

Lemma 1. *Let $\mathcal{A}$ be a reaction system. For each reaction $a \in A$, $R_a \not\subseteq irdom(\mathcal{A})$.*

Proof. Let $a \in A$. Assume to the contrary that $R_a \subseteq irdom(\mathcal{A})$. Then, by Proposition 2, R_a is irrelevant. Since $R_a \div \varnothing = R_a$ and $res_{\mathcal{A}}(\varnothing) = \varnothing$, this means that

$$res_{\mathcal{A}}(R_a) = \varnothing \; . \qquad (*)$$

On the other hand, $en_a(R_a)$ and therefore

$$res_{\mathcal{A}}(R_a) = P_a \; . \qquad (**)$$

But $(*)$ and $(**)$ imply that $P_a = \varnothing$, a contradiction with the definition of a reaction. Therefore $R_a \not\subseteq irdom(\mathcal{A})$. □

6 Characterising Relevant Domains

When it comes to sets of relevant entities, one should expect a relationship with resources used by the reaction system. Here by the *resources* of a single reaction a we mean $M_a = R_a \cup I_a$. The essence of the next result is that relevant entities must be resources.

Theorem 2. *Let $\mathcal{A} = (S, A)$ be a reaction system. Then*

$$rdom(\mathcal{A}) \subseteq \bigcup_{a \in A} M_a \; .$$

Proof. Let $x \in S$. If $x \notin \bigcup_{a \in A} M_a$, then it follows directly from the definition of $res_{\mathcal{A}}$ that, for each $T \subseteq S$, $res_{\mathcal{A}}(T \setminus \{x\}) = res_{\mathcal{A}}(T \cup \{x\})$. Hence x is irrelevant and so $x \notin rdom(\mathcal{A})$. □

The inclusion in the formulation of the above theorem can be replaced by equality in case of a reaction system with a single reaction.

Proposition 3. *Let* $\mathcal{A} = (S, \{a\})$ *be a reaction system. Then*

$$rdom(\mathcal{A}) = M_a \ .$$

Moreover, every nonempty set $X \subseteq R_a \cup I_a$ *is relevant.*

Proof. To show the second part of the statement of the theorem, let $X \subseteq R_a \cup I_a$ be such that $X \neq \varnothing$. Let $X' = X \cap R_a$ and $X'' = X \cap I_a$. To observe that X is relevant it then suffices (see (i) in Section 5) to take $T = R_a$ and $U = (R_a \setminus X') \cup X''$. We have then $T \div U = X$, but $res_a(T) \neq res_a(U)$. Hence all resources are relevant, and so from Theorem 2 it follows immediately that $rdom(\mathcal{A}) = M_a$. □

Thus we also obtained a counterpart of Proposition 2 for sets of relevant entities in case of a system with a single reaction. However, any attempt to extend this to reaction systems with more reactions is bound to fail, as illustrated by the following example. Consider the reaction system $\mathcal{A}_3 = (S, \{a, b\})$, where

$$S = \{1,2\} \qquad a = (\{1\},\{2\},\{1\}) \qquad b = (\{2\},\{1\},\{1\}) \ .$$

Then 1 is relevant because $\{1,2\} \div \{2\} = \{1\}$ and $res_{\mathcal{A}_3}(\{1,2\}) = \varnothing \neq \{1\} = res_{\mathcal{A}_3}(\{2\})$, and 2 is relevant because $\{1,2\} \div \{1\} = \{2\}$ and $res_{\mathcal{A}_3}(\{1,2\}) = \varnothing \neq \{1\} = res_{\mathcal{A}_3}(\{1\})$. However, $X = \{1,2\}$ is not a relevant set of entities which is seen as follows. If $T, U \subseteq S$ are such that $T \div U = X$, then either $\{T, U\} = \{\{1\},\{2\}\}$ or $\{T, U\} = \{\varnothing, S\}$. In the former case we obtain $res_{\mathcal{A}_3}(T) = \{1\} = res_{\mathcal{A}_3}(U)$, and in the latter $res_{\mathcal{A}_3}(T) = \varnothing = res_{\mathcal{A}_3}(U)$.

In general, not all resources are relevant. Consider, for example, the reaction system $\mathcal{A}_4 = (S, \{a, b\})$, where

$$S = \{1,2,3\} \qquad a = (\{1\},\{2\},\{1\}) \qquad b = (\{1,3\},\{2\},\{1\}) \ .$$

Then entity 3 is not relevant since 3 is a resource only in the presence of entity 1 and then it has no additional influence on the result.

To strengthen the general results obtained so far, we turn our attention to reduced reaction systems which, intuitively, contain neither redundant nor inefficient reactions. Moreover, by Theorem 1, any reaction system is equivalent to a reduced reaction system, and so we still deal with all possible result functions of reaction systems.

It is easy to see that every reaction system with a single reaction is reduced. In the following main result of this paper which strengthens Theorem 2 we show that in the case of any reduced reaction system the relevant entities are precisely the resources used by the system.

Theorem 3. *Let* $\mathcal{A} = (S, A)$ *be a reduced reaction system. Then*

$$rdom(\mathcal{A}) = \bigcup_{a \in A} M_a \ .$$

Proof (Theorem 3). By Theorem 2 it suffices to prove that $\bigcup_{a\in A} M_a \subseteq rdom(\mathcal{A})$. We do this by showing that:

$$(\forall x \in S) \;\; [\, x \notin rdom(\mathcal{A}) \implies x \notin \textstyle\bigcup_{a\in A} M_a \,] \; . \tag{\$}$$

To this aim we will now present two lemmas: the first demonstrates that all the reactants are relevant, and the second one demonstrates the same for inhibitors.

Lemma 2. *For each reaction $a \in A$, $R_a \cap irdom(\mathcal{A}) = \varnothing$.*

Proof (Lemma 2). Assume to the contrary that there exists $a \in A$ such that

$$R_a \cap irdom(\mathcal{A}) \neq \varnothing \; .$$

Let $b = (R_a \setminus irdom(\mathcal{A}), I_a, P_a)$. By Lemma 1, $R_b = R_a \setminus irdom(\mathcal{A}) \neq \varnothing$, and so $b \in rac(S)$. Clearly, b strictly covers a, and so, because $\mathcal{A}$ is reduced, b is *not* consistent with $res_{\mathcal{A}}$. Hence, there exists $T \subseteq S$ such that $en_b(T)$ and $res_b(T) = P_b \nsubseteq res_{\mathcal{A}}(T)$. Since $P_b = P_a$, we get

$$P_a \nsubseteq res_{\mathcal{A}}(T) \; . \tag{$*$}$$

Let $U = T \cup (R_a \cap irdom(\mathcal{A}))$. Since $en_b(T)$, we have (1) $R_b \subseteq T$ and (2) $I_b \cap T = \varnothing$. Since $R_a \setminus R_b = R_a \cap irdom(\mathcal{A})$, (1) implies that $R_a \subseteq U$. Since $I_b = I_a$ (and $I_a \cap R_a = \varnothing$), $I_a \cap U = \varnothing$. Therefore $en_a(U)$ and, consequently,

$$P_a \subseteq res_{\mathcal{A}}(U) \; . \tag{$**$}$$

Thus by $(*)$ and $(**)$ we get that

$$P_a \nsubseteq res_{\mathcal{A}}(T) \;\; \text{and} \;\; P_a \subseteq res_{\mathcal{A}}(T \cup (R_a \cap irdom(\mathcal{A}))) \; .$$

This implies that the set $U \div T$ is relevant, which contradicts Proposition 2 (as $U \div T \subseteq R_a \cap irdom(\mathcal{A})$ and so, by Proposition 2, $U \div T$ must be irrelevant). Therefore Lemma 2 holds. *(Lemma 2)* □

Lemma 3. *For each reaction $a \in A$, $I_a \cap irdom(\mathcal{A}) = \varnothing$.*

Proof (Lemma 3). Assume to the contrary that there exists $a \in A$ such that $I_a \cap irdom(\mathcal{A}) \neq \varnothing$. Clearly, for each $T \subseteq S$, $res_{A\setminus\{a\}}(T) \subseteq res_{\mathcal{A}}(T)$. Moreover, because $\mathcal{A}$ is reduced, there exists $T_a \subseteq S$ such that $res_{A\setminus\{a\}}(T_a) \neq res_{\mathcal{A}}(T_a)$. Thus

$$res_{A\setminus\{a\}}(T_a) \subset res_{\mathcal{A}}(T_a) \; . \tag{$*$}$$

Clearly, $en_a(T_a)$, as otherwise $res_{A\setminus\{a\}}(T_a) = res_{\mathcal{A}}(T_a)$ which contradicts $(*)$.

Let $U = T_a \cup irdom(\mathcal{A})$. By Lemma 2, for each $b \in A$, if $R_b \subseteq U$ then $R_b \subseteq T_a$. Consequently, if $b \in A$ is enabled by U, then it is also enabled by T_a, implying that

$$(\forall B \subseteq A) \;\; [res_B(U) \subseteq res_B(T_a)] \; . \tag{$**$}$$

Since we assumed that $I_a \cap irdom(\mathcal{A}) \neq \varnothing$, reaction a is not enabled by U and so $res_{\mathcal{A}}(U) \subseteq res_{A\setminus\{a\}}(U)$. Since, by (∗∗), $res_{A\setminus\{a\}}(U) \subseteq res_{A\setminus\{a\}}(T_a)$, we get that $res_{\mathcal{A}}(U) \subseteq res_{A\setminus\{a\}}(T_a)$. Consequently, by (∗), we obtain $res_{\mathcal{A}}(U) \subset res_{\mathcal{A}}(T_a)$. Since $U = T_a \cup irdom(\mathcal{A})$, this implies that the set $U \div T_a$ is relevant, which contradicts Proposition 2 (as $U \div T_a \subseteq irdom(\mathcal{A})$ and so, by Proposition 2, $U \div T_a$ must be irrelevant).

Hence it must be that $I_a \cap irdom(\mathcal{A}) = \varnothing$, and consequently Lemma 3 holds. *(Lemma 3)* □

By Lemma 2 and Lemma 3, $irdom(\mathcal{A}) \cap \bigcup_{a\in A} M_a = \varnothing$, which implies that ($) holds and, consequently, the theorem holds. *(Theorem 3)* □

Our definition of a reduced reaction system $\mathcal{A}$ requires that $\mathcal{A}$ does not have *redundant* reactions, and moreover each reaction is in its most "efficient" form (as far as $\mathcal{A}$ is concerned). A redundant reaction is a reaction that can be removed without influencing the result function $res_{\mathcal{A}}$. Another sort of redundancy is the presence of resources which are not relevant: such entities influence the enabling of (some) reactions but do not influence state transitions! Theorem 3 says that also this kind of redundancy cannot happen in reduced reaction systems.

7 Alternative Notions of Relevance

In defining irrelevant/relevant sets of entities we relied on the operation of symmetric difference. In our view, this is just one of three natural choices to capture the notion of irrelevance/relevance. In this section, we analyse the relationships between them.

Let $X \subseteq S$ be a set of entities of a reaction system $\mathcal{A} = (S, A)$.

– X is *1-irrelevant* in $\mathcal{A}$ if:

$$(\forall T, U \subseteq S)\ \ [\, T \div U = X \implies res_{\mathcal{A}}(T) = res_{\mathcal{A}}(U)\,]\,.$$

– X is *2-irrelevant* in $\mathcal{A}$ if:

$$(\forall T, U \subseteq S)\ \ [\, U \subseteq T \text{ and } T \setminus U = X \implies res_{\mathcal{A}}(T) = res_{\mathcal{A}}(U)\,]\,.$$

– X is *3-irrelevant* in $\mathcal{A}$ if:

$$(\forall T \subseteq S)\ \ [\, res_{\mathcal{A}}(T \setminus X) = res_{\mathcal{A}}(T \cup X)\,]\,.$$

We will use the notations $irr1_{\mathcal{A}}(X)$, $irr2_{\mathcal{A}}(X)$ and $irr3_{\mathcal{A}}(X)$, respectively.

The first of the above three notions of irrelevance is the one investigated until now in this paper. The second considers X irrelevant if removing its elements from any set of entities does not change the result. The third notion of irrelevance considers X irrelevant if, as far as the result function is concerned, removing X from any set of entities has the same effect as adding X to this set of entities.

We now demonstrate relationships between these three notions of relevance.

Lemma 4. *For every $X \subseteq S$, $irr1_{\mathcal{A}}(X)$ implies $irr2_{\mathcal{A}}(X)$.*

Proof. Let $X \subseteq S$ and assume $irr1_{\mathcal{A}}(X)$. Let $T, U \subseteq S$ with $U \subseteq T$ be such that $T \setminus U = X$. Then $T \div U = T \setminus U = X$, and since $irr1_{\mathcal{A}}(X)$, we get $res_{\mathcal{A}}(T) = res_{\mathcal{A}}(U)$. Hence $irr2_{\mathcal{A}}(X)$ and consequently the result holds. □

Lemma 5. *For every $X \subseteq S$, $irr2_{\mathcal{A}}(X)$ implies $irr3_{\mathcal{A}}(X)$.*

Proof. Let $X \subseteq S$ and assume $irr2_{\mathcal{A}}(X)$, hence

$$(\forall T, U \subseteq S) \ \ [U \subseteq T \text{ and } T \setminus U = X \implies res_{\mathcal{A}}(T) = res_{\mathcal{A}}(U)] \, .$$

Consider arbitrary $T' \subseteq S$. Let $T' \setminus X = U$ and $T' \cup X = T$. Thus $T \setminus U = X$ and $U \subseteq T$. Hence, by $irr2_{\mathcal{A}}(X)$, we get

$$res_{\mathcal{A}}(T) = res_{\mathcal{A}}(U) \, . \tag{$*$}$$

We note that

$$res_{\mathcal{A}}(T' \cup X) = res_{\mathcal{A}}(T) \text{ and } res_{\mathcal{A}}(T' \setminus X) = res_{\mathcal{A}}(U) \, . \tag{$**$}$$

By $(*)$ and $(**)$ we get $res_{\mathcal{A}}(T' \cup X) = res_{\mathcal{A}}(T' \setminus X)$. Therefore $irr3_{\mathcal{A}}(X)$ and so the result holds. □

Lemma 6. *For every $X \subseteq S$, $irr3_{\mathcal{A}}(X)$ implies $irr2_{\mathcal{A}}(X)$.*

Proof. Let $X \subseteq S$ and assume $irr3_{\mathcal{A}}(X)$, hence

$$(\forall T \subseteq S) \ \ [\, res_{\mathcal{A}}(T \setminus X) = res_{\mathcal{A}}(T \cup X)\,] \, .$$

Consider then arbitrary $T, U \subseteq S$ such that $U \subseteq T$ and $T \setminus U = X$. We note that, by $X \subseteq T$, we have

$$T \cup X = T \, . \tag{$\dagger$}$$

Moreover, by $irr3_{\mathcal{A}}(X)$, we have

$$res_{\mathcal{A}}(T \cup X) = res_{\mathcal{A}}(T \setminus X) \, . \tag{$\ddagger$}$$

Hence, by $(\dagger)$ and $(\ddagger)$, $res_{\mathcal{A}}(T) = res_{\mathcal{A}}(T \setminus X)$. Since $U = T \setminus X$, we get $res_{\mathcal{A}}(T) = res_{\mathcal{A}}(U)$. Therefore $irr2_{\mathcal{A}}(X)$ and so the result holds. □

We can therefore conclude that

Theorem 4. *1-irrelevance implies 2-irrelevance which in turn is equivalent to 3-irrelevance.*

Proof. The theorem follows directly from Lemma 4, Lemma 5 and Lemma 6. □

Hence the notion of relevant sets of entities as defined in Section 5 turns out to be the strongest among those discussed in this section, and therefore a reasonable choice for formalising the intuitive notion of relevance (from the point of view of result functions of reaction systems).

Finally, note that for singleton sets X the three notions of irrelevance coincide. This is no longer the case if X has two or more elements. Consider, for example, the reaction system $\mathcal{A}_5 = (S, \{a\})$, where

$$S = \{1, 2, 3\} \qquad a = (\{1, 2\}, \{3\}, \{1\})\,.$$

Then the set $X = \{1, 3\}$ is not 1-irrelevant but it is 3-irrelevant. Hence the implication in the above theorem cannot be reversed.

8 Conclusions

In this paper, we presented an investigation of sets of entities of reaction systems which are relevant from the point of view of result functions. In particular, we proved that for the reduced reaction systems relevant entities are precisely those which are used as resources by the reactions. We have also discussed the relationship between the notion of relevance investigated in this paper and two alternative notions of relevance.

In our future work we intend to investigate derived notions of relevance where one is interested in establishing which entities become irrelevant ‘sooner or later’. For example, one might say that a set of entities $X \subseteq S$ is *eventually irrelevant* in a reaction system $\mathcal{A}$ if

$$(\forall T, U \subseteq S)(\exists n \geq 1)\ \ [\, T \div U = X \quad \Longrightarrow \quad res^n_{\mathcal{A}}(T) = res^n_{\mathcal{A}}(U)\,]\,,$$

where $res^n_{\mathcal{A}}$ is the n-fold iteration of $res_{\mathcal{A}}$. In other words, eventual irrelevance implies that the initial distinction between states T and U will eventually disappear with the iteration of $res_{\mathcal{A}}$ whenever the two states differ by the set of entities X.

Acknowledgement. This research was supported by the Pascal Chair award from the Leiden Institute of Advanced Computer Science (LIACS) of Leiden University. The authors are indebted to the referees for useful comments; in particular, the detailed comments by one of the referees were very valuable in the production of the current version of this paper.

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