

Properties of Communicating Reaction Systems

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Abstract: Communicating reaction systems are new variants of networks of reaction systems where the components communicate with each other by sending products or reactions. Reaction system, a mathematical formalism inspired by the biochemistry of the living cell, focuses on an abstract set-based representation of chemical reactions via facilitation and inhibition. In this paper we examine bio-inspired properties of communicating reaction systems such as steady state and mass conservation.

Keywords: reaction system, communicating reaction systems, steady state, conserved set

1 Introduction

The concept of a reaction system (an R system) was introduced by A. Ehrenfeucht and G. Rozenberg as a formal model of interactions between biochemical reactions. The interested reader is referred to [9] for the original motivation. The main idea of the authors was to model the behavior of biological systems in which a large number of individual reactions interact with each other.

A reaction system consists of a finite set of objects that represent chemicals and a finite set of triplets that represent chemical reactions. Each reaction consists of three nonempty finite sets: the set of reactants, the set of inhibitors, and the set of products. The set of reactants and the set of inhibitors are disjoint. Let T be a set of reactants. A reaction is enabled for T and it can be performed if all of its reactants are present in T and none of its inhibitors are in T . When the reaction is performed, then the set of its reactants is replaced by the set of its products. All enabled reactions are applied in parallel. The set of products obtained by the reactions performed in parallel is the union of the sets of products that were obtained by the reactions that were enabled for T . For further details on reaction systems consult [7].

Reaction systems are qualitative models, opposed to membrane systems (P systems) that are quantitative ones. The model of reaction systems focuses only on the presence or absence of the chemical species, and does not consider their amounts. Multiple reactions that have common reactants do not interfere. All of the reactions that are enabled at a certain step are performed simultaneously. An-

other feature of reaction systems which makes them different from other bio-inspired computational models, as for example, P systems, is the lack of permanency: the state of the system consists of the products of those reactions that were performed in the last step. Those reactants that were not involved in any reaction disappear from the system. This property is widely used in the theory of R systems.

R systems have been studied in detail over the last sixteen years. One interesting topic of their study is the theory of networks of reaction systems [4]. Such a construct is a virtual graph with a reaction system in each node. These reaction systems are defined over the same background set and work in a synchronized manner, governed by the same clock. After performing the reactions enabled for the current set of reactants at a node, certain products from other nodes can be added to the node's product set. The nodes, thus the reaction systems interact with each other using distribution and communication protocols. The set of products of each reaction system in the network forms a part of the environment of the network. Important ideas and results on these constructs can be found in [5, 4]. A recent development in the area is the concept of communicating reaction systems with direct communication (cdcR systems), introduced in [6]. A cdcR system consists of a finite number of components. Each component consists of a finite number of extended reactions, and these extended reactions are of the same type. Components of a cdcR system are defined over the same background set. The components, in addition to performing standard reactions, communicate products or reactions to certain predefined target components.

There are various research topics in the domain of reactions systems. One type of investigations focuses on the mathematical properties of reaction systems, for example functions defined by reaction systems, state sequences, effect of limited resources, cycles and connections to propositional logic. For details consult [8, 11, 12]. One other research direction focuses on the capabilities of reaction systems as a modeling framework. In [1, 2, 3] a series of such biologically inspired properties are defined and studied.

In this paper we examine some of these biologically inspired properties like steady state, conserved sets in the frame of communicating reaction systems with direct communication. A system is said to be in a steady state if it does not experience any changes over time. Studying steady states is a relevant topic in many fields of science.

Similarly, also mass conservation plays important role in many scientific areas.

The paper is organized as follows. In Section 2 we introduce basic notions and notations concerning reactions and reaction systems. In Section 3 we recall communicating reaction systems with direct communication and in Section 4 we define different properties of cdcR systems which communicate products. Finally, we provide conclusions and few suggestions for further research in Section 5.

2 Reaction Systems

For basic notions of formal languages and computation theory the reader is encouraged to consult [10].

In this section we recall the basic notions concerning reaction systems, following [9, 7]. For technical reasons, some notations are presented in a form that slightly deviates from the original one.

Let S be a finite nonempty set; S is called the background set. A reaction ρ over S is a triplet (R, I, P) where R, I, P are nonempty subsets of S such that $R \cap I = \emptyset$. Sets R, I, P are called the set of reactants, the set of inhibitors, and the set of products of ρ , respectively; they can also be denoted by R_ρ, I_ρ , and P_ρ . In this case the reaction is denoted by $\rho : (R_\rho, I_\rho, P_\rho)$.

A finite nonempty set of reactions over the same background set is a reaction system. Thus, a reaction system is an ordered pair $\mathcal{A} = (S, A)$, where S is a background set and A is a finite nonempty set of reactions over S .

Now we recall how reaction systems operate over a set of reactants.

Let S be a background set, $T \subseteq S$, $\rho : (R_\rho, I_\rho, P_\rho)$ be a reaction over S , and let A be a finite set of reactions over S . Then

1. ρ is enabled for T iff $R_\rho \subseteq T$ and $I_\rho \cap T = \emptyset$;
2. the result of applying ρ to T , denoted by $res_\rho(T)$, equals P_ρ if ρ is enabled for T and is equal to the emptyset, \emptyset , otherwise;
3. the result of applying A to T , denoted by $res_A(T)$, is $\bigcup_{\rho \in A} res_\rho(T)$.

That is, a reaction ρ is enabled for a set of reactants T if T contains all reactants of ρ and none of its inhibitors. If ρ is enabled for T , then its products contribute to the successor state of the reaction system. For $T \subseteq S$, $en_A(T)$ denotes the set of reactions in A that are enabled for T . It is easy to see that res_A defines a function on 2^S , called the result function.

The state sequence of a reaction system \mathcal{A} with initial state T is given by successive iterations of the result function: $(res_{\mathcal{A}}^n(T))_{n \in \mathbb{N}} = (T, res_{\mathcal{A}}(T), res_{\mathcal{A}}^2(T), \dots)$.

3 Communicating Reaction Systems

In this section we briefly recall the most important concepts concerning a variant of communicating reaction systems (cdcR(p) systems, for short), where the reaction systems directly communicate with each other. The concept was introduced in [6], and is related to the notion of a network of R systems [4]. A cdcR(p) system consists of a finite number of components, each component consists of a finite number of extended reactions which are of the same type. The components are defined over the same background set and in addition to performing standard reactions, communicate products to certain predefined target components. The components of the cdcR(p) system work in a synchronized manner, governed by the same clock. The products obtained as results of the reactions are associated with targets, i.e., with the label of the component which the product is sent to. The target component need not to be different from the sender component. After performing the reactions and the communication, the system performs a new transition, i.e. the procedure is repeated.

Now we recall the notion of a cdcR(p) system from [6].

A cdcR system communicating by products (a cdcR(p) system, for short), of degree n , $n \geq 1$, is an $(n+1)$ -tuple $\Delta = (S, A_1, \dots, A_n)$, where

- S is a finite nonempty set, the background set of Δ ;
- A_i , $1 \leq i \leq n$, is the i -th component of Δ , where
 - A_i is a finite nonempty set of extended reactions of type pc (pc -reactions, for short).
 - Each pc -reaction ρ of A_i is of the form $\rho : (R_\rho, I_\rho, \Pi_\rho)$, where R_ρ and I_ρ are nonempty subsets of S and $R_\rho \cap I_\rho = \emptyset$, and $\Pi_\rho \subseteq P_\rho \times \{1, \dots, n\}$, P_ρ is a nonempty subset of S . R_ρ, I_ρ, Π_ρ are called the set of reactants, the set of inhibitors, and the set of products with targets. A pair (b, j) , $1 \leq j \leq n$ in Π_ρ means that product b is communicated to component A_j .

The name pc -reaction refers to reaction communicating products.

The notions and notations concerning reaction systems are extended to cdcR(p) systems, we recall them from [6]. If it is clear from the context, for singleton set $\{\rho\}$ we use notation ρ .

A pc -reaction $\rho : (R_\rho, I_\rho, \Pi_\rho)$ is enabled for a set $U \subseteq S$ if $R_\rho \subseteq U$ and $I_\rho \cap U = \emptyset$ as in case of standard reaction systems; this fact is denoted by $en_\rho(U)$.

Let $\Delta = (S, A_1, \dots, A_n)$ be a cdcR(p) system and let $U \subseteq S$. Then, we define $res_{A_i}(U) = \{b \mid (b, j) \in \Pi_\rho, \rho \in A_i, en_\rho(U), 1 \leq j \leq n\}$.

We consider result all of the products obtained by performing the pc -reactions, including those ones that will leave the component by communication.

cdcR(p) systems operate by transitions, i.e., by changing their states. A state of a cdcR(p) system $\Delta =$

(S, A_1, \dots, A_n) is an n -tuple (D_1, \dots, D_n) where $D_i \subseteq S$, $1 \leq i \leq n$; D_i is called the state of component A_i , $1 \leq i \leq n$. Notice that D_i can be empty set.

A transition in Δ means that every component of the $\text{cdcR}(p)$ system performs all of its enabled pc -reactions on the current set of reactants and then communicates the obtained products to their target components, indicated in the corresponding pc -reaction. Notice that the same product from several components can be communicated to a component and by several pc -reactions.

The sequence of transitions starting with the initial state forms the state sequence in Δ . Observe that for a given initial state there is only one state sequence in Δ , i.e. the sequence of transitions is deterministic.

Let $\Delta = (S, A_1, \dots, A_n)$, $n \geq 1$, be a $\text{cdcR}(p)$ system. The sequence $\bar{D}_0, \dots, \bar{D}_j, \dots$ is called the state sequence of Δ starting with initial state \bar{D}_0 if the following conditions are met: For every \bar{D}_j , $j \geq 0$ where $\bar{D}_j = (D_{1,j}, \dots, D_{i,j}, \dots, D_{n,j})$, $1 \leq i \leq n$ it holds that $\bar{D}_{j+1} = (D_{1,j+1}, \dots, D_{i,j+1}, \dots, D_{n,j+1})$ with $D_{i,j+1} = \cup_{1 \leq k \leq n} \text{Com}_{k \rightarrow i}(\text{res}_{A_k}(D_{k,j}))$ where $\text{Com}_{k \rightarrow i}(\text{res}_{A_k}(D_{k,j})) = \{b \mid (b, i) \in \Pi_\rho, \rho : (R_\rho, I_\rho, \Pi_\rho) \in A_k, \text{en}_\rho(D_{k,j})\}$. Sequence $D_{i,0}, D_{i,1}, \dots$ is said to be the state sequence of component A_i of Δ , $1 \leq i \leq n$.

The state sequence does not end if $\text{res}_{A_i}(D_{i,j})$ is the empty set, since products can be communicated to the component in the coming steps.

Let $\Delta = (S, A_1, \dots, A_n)$, $n \geq 1$, be a $\text{cdcR}(p)$ system and let $\bar{D}_0, \bar{D}_1, \dots, \bar{D}_i, \dots$ be the state sequence of Δ starting with \bar{D}_0 . Then every pair $(\bar{D}_i, \bar{D}_{i+1})$, $i \geq 0$ is said to be a transition in Δ and is denoted by $\bar{D}_i \Longrightarrow \bar{D}_{i+1}$.

In [6] it was shown that to every $\text{cdcR}(p)$ system Δ a simulating R system \mathcal{A} can be constructed. Namely,

Theorem 1. *Let $\Delta = (S, A_1, \dots, A_n)$, $n \geq 1$, be a $\text{cdcR}(p)$ system and let $\bar{D}_0 = (D_{1,0}, \dots, D_{n,0})$ be the initial state of Δ . We can construct an R system $\mathcal{A} = (S', A')$, give an initial state W_0 of \mathcal{A} and define mappings $h_i : 2^{S'} \rightarrow 2^S$, $1 \leq i \leq n$ such that for each i , $1 \leq i \leq n$, the state sequence $D_{i,0}, D_{i,1}, \dots, D_{i,k}, \dots$ of component A_i of Δ is equal to the sequence $h_i(W_0), h_i(W_1), \dots, h_i(W_k), \dots$, where $W_0, W_1, \dots, W_k, \dots$, $k \geq 0$ is the state sequence of \mathcal{A} starting from initial state W_0 .*

The statement was proved by a so-called flattening technique (frequently used in the theory of P systems) where the notation of the reactants at the nodes indicates the location of the object (entity) as well. The reader interested in the details is referred to [6].

The reaction system \mathcal{A} obtained in this way is called the flattened reaction system or a flattened version of Δ . We recall the definition from [6].

Definition 1. *Let $\Delta = (S, A_1, \dots, A_n)$, $n \geq 1$, be a $\text{cdcR}(p)$ system. Let reaction system $\mathcal{A} = (S', A')$ be defined as follows. Let $S' = \{[x, i] \mid x \in S, 1 \leq i \leq n\}$ be the background set of \mathcal{A} . For any pc -reaction $\rho : (R_\rho, I_\rho, \Pi_\rho)$ of component A_i , we define reaction $\rho' : (R_{\rho'}, I_{\rho'}, P_{\rho'})$ of*

\mathcal{A} where $R_{\rho'} = \{[x, i] \mid x \in R_\rho\}$, $I_{\rho'} = \{[y, i] \mid x \in I_\rho\}$, $P_{\rho'} = \{[x, k] \mid (x, k) \in \Pi_\rho, 1 \leq k \leq n\}$. No other reaction is in \mathcal{A} . Then \mathcal{A} is called the flattened reaction system of Δ .

4 Properties of $\text{cdcR}(p)$ Systems

In [1] reaction systems as a modeling framework was examined and several formalizations of concepts in the focus of interest in bio-modeling were introduced and then studied: mass conservation, invariants, steady states, stationary processes, elementary fluxes, and periodicity. In this paper we extend some of these notions to networks of reaction systems, more precisely, to $\text{cdcR}(p)$ systems.

We first start with steady states from [1].

Definition 2. *Let $\mathcal{A} = (S, A)$ be a reaction system. We say that a nonempty set $W \subset S$ is a steady state of \mathcal{A} if $\text{res}_{\mathcal{A}}(W) = W$.*

Notice that this property means that no change can be experienced in this state in a process of evolution, i.e. if \mathcal{A} enters state W , then all elements following W in the state sequence will be equal to W .

Before defining the steady state for $\text{cdcR}(p)$ systems, we make some remarks. As it was shown in [6], to each $\text{cdcR}(p)$ system Δ a reaction system \mathcal{A} can be given, namely, its flattened version, which represents the components of Δ and its operation corresponds to the operation of Δ . This implies that if the flattened reaction system \mathcal{A} has a steady state W and Δ has n components, $n \geq 1$, then W corresponds to a state $\bar{D}_W = (W_1, \dots, W_n)$ of Δ where $W = \cup_{i=1}^n \bar{W}_i$, where $\bar{W}_i = \{[a, i] \mid a \in W_i\}$. Notice that W_j can be the empty set for some j , $1 \leq j \leq n$. By Theorem 1, \mathcal{A} is constructed in such way that $\text{res}_{\mathcal{A}}(W)$ corresponds to $\bar{D}'_W = (W'_1, \dots, W'_n)$, a state of Δ , where $\bar{D}_W \Longrightarrow \bar{D}'_W$ holds. If $\bar{D}_W = \bar{D}'_W$, then we call \bar{D}_W a steady state of Δ . Notice that in case of $\text{cdcR}(p)$ systems the reaction is extended, thus elements of S obtained by the extended reactions can be communicated to a node from other nodes.

Now we define the notion of a steady state of a $\text{cdcR}(p)$ system.

Definition 3. *Let $\Delta = (S, A_1, \dots, A_n)$, $n \geq 1$, be a $\text{cdcR}(p)$ system and let $\bar{D}_W = (W_1, \dots, W_n)$ be a state of Δ . Then \bar{D}_W is said to be a steady state of Δ if for $\bar{D}'_W = (W'_1, \dots, W'_n)$ where $D_W \Longrightarrow D'_W$ it holds that $W_i = W'_i$ for i , $1 \leq i \leq n$.*

Notice that for any W_i , $1 \leq i \leq n$, $\text{res}_{A_i}(W_i)$ consists of all products obtained by the performed pc -reactions, including those ones which will leave the component by communication. Thus, $W_i \neq \text{res}_{A_i}(W_i)$ may hold.

Next we will present a statement concerning a connection between steady states of $\text{cdcR}(P)$ systems and steady states of their flattened reaction systems.

Theorem 2. *Let $\Delta = (S, A_1, \dots, A_n)$, $n \geq 1$, be a $\text{cdcR}(p)$ system and let $\mathcal{A} = (S', A')$ be its flattened reaction system.*

- Let W be a steady state of \mathcal{A} . Then there exist mappings $g_i : 2^{S'} \rightarrow 2^S$, $1 \leq i \leq n$ and a state $\bar{D}_W = (W_1, \dots, W_n)$ of Δ such that $\bar{D}_W = (W_1, \dots, W_n)$ is a steady state of Δ and $g_i(W) = W_i$.
- Let $\bar{D}_W = (W_1, \dots, W_n)$ be a steady state of Δ . Then there exist mappings $h_i : 2^S \rightarrow 2^{S'}$, $1 \leq i \leq n$ and $W \subseteq S'$ such that $W = \cup_{i=1}^n h_i(W_i)$ is a steady state of \mathcal{A} .

Proof sketch. To prove the statement, we consider the definition of the flattened reaction systems of Δ . It is given by $\mathcal{A} = (S', A')$, where $S' = \{[x, i] \mid x \in S, 1 \leq i \leq n\}$ is the background set and for any pc -reaction $\rho : (R_\rho, I_\rho, \Pi_\rho)$ of component A_i of Δ , $1 \leq i \leq n$, we define reaction $\rho' : (R_{\rho'}, I_{\rho'}, P_{\rho'})$ of \mathcal{A} where $R_{\rho'} = \{[x, i] \mid x \in R_\rho\}$, $I_{\rho'} = \{[y, i] \mid x \in I_\rho\}$, $P_{\rho'} = \{[x, k] \mid (x, k) \in \Pi_\rho, 1 \leq k \leq n\}$. No other reaction is in A' . It is easy to see that if we define g_i such way that it orders to each reactant $[x, i]$ in \mathcal{A} a reactant x at component A_i , and by h_i we order to each reactant x of component A_i a reactant $[x, i]$ of \mathcal{A} , then we obtain from state W of \mathcal{A} state $\bar{D}_W = (W_1, \dots, W_n)$ of Δ and reversely. Furthermore if W is a steady state, then \bar{D}_W will be a steady state as well, and reversely. We leave the details to the reader.

Next we provide an example.

Example 1. Let $\Delta = (S, A_1, A_2, A_3)$ be a $cdcR(p)$ system where $S = \{a, b, c\}$ and components A_1, A_2 and A_3 are defined as follows:

$$A_1 = \{\rho_1 : (\{a, b\}, \{c\}, \{(a, 1), (b, 1)\})\},$$

$$A_2 = \{\rho_2 : (\{b, c\}, \{a\}, \{(b, 3), (c, 2)\}), \\ \rho_3 : (\{a, c\}, \{b\}, \{(a, 3), (c, 2)\})\},$$

$$A_3 = \{\rho_4 : (\{a, c\}, \{b\}, \{(a, 2), (c, 3)\}), \\ \rho_5 : (\{b, c\}, \{a\}, \{(b, 2), (c, 3)\})\}.$$

Let $\bar{D}_0 = (\{a, b\}, \{b, c\}, \{a, c\})$ be the initial state of Δ . For component A_1 , it is clear from the product $\{(a, 1), (b, 1)\}$ that after each transition the state does not change, it always remains $\{a, b\}$. On the other hand, states of components A_2 and A_3 keep changing due to the product with in-built communication.

The above example inspires us to distinguish between so-called "strong steady states" of a $cdcR(p)$ system where the states of the components do not change or so-called "weak steady states" where the support of the entire state remain unchanged but the states of the particular components may change. The support of the state of a $cdcR(p)$ system is the set of those elements of the background set that appear in some of the states of the particular components either as reactant or elements of a product (or both).

The study of weak steady states is an interesting open problem. Interesting questions are decidability problems as well. For example, it is known that given a reaction

system $\mathcal{A} = (A, S)$, deciding if there exists a nonempty steady state $W \subset S$ is an NP-complete problem.

In the following we deal with one other important property, called mass-conservation. First, we recall some auxiliary notions.

For a reaction system $\mathcal{A} = (S, A)$, the support set of \mathcal{A} is defined as $supp(\mathcal{A}) = \mathcal{R} \cup \mathcal{P}$ where $\mathcal{R} = \bigcup_{\rho \in A} R_\rho$ and

$$\mathcal{P} = \bigcup_{\rho \in A} P_\rho.$$

Next we define the notion of the support set for a component of a $cdcR(p)$ system and then for the system itself.

Definition 4. The support set for a particular component A_i of a $cdcR(p)$ system $\Delta = (S, A_1, \dots, A_n)$, $1 \leq i \leq n$, is defined as $supp(A_i) = R_i \cup \bar{P}_i$, where $R_i = \{a \mid a \in R_\rho, \rho \in A_i, a \in S\}$ and $\bar{P}_i = \{a \mid (a, j) \in \Pi_\rho, \rho \in A_i, a \in S, 1 \leq j \leq n\}$.

For a $cdcR(p)$ system $\Delta = (S, A_1, \dots, A_n)$, $n \geq 1$ the support set of Δ is defined as $supp(\Delta) = \bigcup_{i=1}^n supp(A_i)$.

We recall the notion of a conserved set of a reaction system [1].

Definition 5. Let $\mathcal{A} = (S, A)$ be a reaction system, then a set $M \subseteq supp(\mathcal{A})$ is conserved if for any $W \subseteq supp(\mathcal{A})$, $M \cap W \neq \emptyset$ if and only if $M \cap res_{\mathcal{A}}(W) \neq \emptyset$.

In this notion it is crucial that $supp(\mathcal{A}) \subset S$.

M has a special property, namely if it has a joint subset with a state W , then it has a joint subset with the state obtained after applying all enabled reactions to W as well.

This definition cannot be directly implemented for $cdcR(p)$ systems. Instead, we define a notion to describe conservation of sets.

Definition 6. Let $\Delta = (S, A_1, \dots, A_n)$, $n \geq 1$ be a $cdcR(p)$ system and let $M_i \subseteq S$, $1 \leq i \leq n$. We say that $M_i \subset supp(A_i)$ is a conserved set for component A_i , $i, 1 \leq i \leq n$ if the following holds. For any two states $\bar{D} = (D_1, \dots, D_n)$ and $\bar{D}' = (D'_1, \dots, D'_n)$ where $\bar{D} \Longrightarrow \bar{D}'$, it holds that if there exists $W_i \subset M_i$ such that $W_i \subset D_i$, then there exists $W'_i \subset M_i$ such that $W'_i \subset D'_i$ holds.

The above way of conservation concerns a particular component. Obviously, such conserved sets can appear at several components.

As in the case of steady states, we can find a connection between conserved sets of $cdcR(p)$ systems and their flattened reaction systems. Let $\Delta = (S, A_1, \dots, A_n)$, $n \geq 1$ be a $cdcR(p)$ system and let $\mathcal{A} = (S', A')$ be its flattened reaction system. By the construction of \mathcal{A} it can easily be seen that if $W_i \subset D_i$ and $W'_i \subset D'_i$, then $\bar{W}_i = \{[a, i] \mid a \in W_i\}$ and $\bar{W}'_i = \{[b, i] \mid b \in W'_i\}$ are subsets of $\bar{D}_i = \{[c, i] \mid c \in D_i\}$ and $\bar{D}'_i = \{[d, i] \mid d \in D'_i\}$, respectively. It would be useful to develop such notion that describe a distributed manner of conservation in the entire system.

5 Conclusions and Further Research Directions

In this paper we proposed steady states and mass conservation of communicating reaction systems by product communication. Using the concepts of the corresponding flattened reaction systems, we attempted to describe the ideas beyond the definitions. It will be a promising and useful research to study the concepts of invariants, stationary processes, elementary fluxes and periodicity of cdcR(p) systems. Another interesting research could be studying on all these bio-inspired properties for cdcR(r) (cdcR systems communicating reactions) and comparing all respective properties with cdcR(p).

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