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# Applications of the Chinese remainder theorem to reaction systems with duration

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ABSTRACT

The *reaction systems* introduced by Ehrenfeucht and Rozenberg have given rise to numerous contributions, both because of their capabilities in describing biochemical reactions, and because of their mathematical elegance and the resulting simply stated and yet often challenging problems. The present contribution deals with the mathematical structure of reaction systems. Reaction systems with *duration* were introduced to model decay in nature. As will be seen in this paper, the model enhanced with duration opens rich possibilities for dealing with sequence length, termination and cycles.



## 1. Introduction

A formal model of *reaction systems* was introduced in [5]. The original purpose was to model interactions between biochemical reactions. The reference [5] contains some of the original motivation and initial setup. Each reaction is characterized by its set of *reactants*, each of which has to be present for the reaction to take place, by its set of *inhibitors*, none of which is allowed to be present, and by its set of *products*, each of which will be present after a successful reaction. Thus, a single reaction is based on facilitation and inhibition. Everything is defined within a fixed finite *background set* $S$. The sets of reactants, inhibitors and products, $R$, $I$ and $P$, are nonempty subsets of $S$, the sets $R$ and $I$ being disjoint. A *reaction system* $RS$ consists of finitely many such triples $(R, I, P)$, called *reactions*. Thus, the model is mathematically very clean and simple, and so are the definitions of the basic operations. Yet many simply formulated problems turn out to be very challenging and many decidable questions turn out to be of high complexity. Since we are dealing with subsets of a finite set, most of the problems are decidable. Complexity of specific problems has been discussed in [7,8]. The latter reference exhibits problems in different complexity classes, going up to P-SPACE complete problems.

The model of reaction systems turned out to be suitable in different setups. Then also many variants of the systems and additions to them were introduced. The reference [1] constitutes a survey. A related very general approach is presented in [6]. However, in this paper we are mostly concerned with a specific variant only, originally introduced in [2], to model decay.

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## 2. Reaction systems with duration: basics

We now define the central notions, as well as the related operational notions. We emphasize that everything happens within the framework of a fixed finite background set $S$.

**Definition 1.** A *reaction* over the *finite background set* $S$ is a triple

$$\rho = (R, I, P),$$

where $R, I$ and $P$ are nonempty subsets of $S$ such that $R$ and $I$ do not intersect. The three sets are referred to as *reactants*, *inhibitors* and *products*, respectively. A *reaction system* $\mathcal{A}_S$ over the background set $S$ is a finite nonempty set

$$\mathcal{A}_S = \{\rho_i |\ 1 \leq i \leq k\}, \quad k \geq 1,$$

of reactions over $S$.

No specific assumptions are made about the set $P$. In particular, it may or may not contain elements of $R \cup I$. In this paper $S$ will always denote the background set. We will follow in this paper the original definition, where each of the sets $R, I, P$ is assumed to be nonempty. Some constructions are simpler if the inhibitor set $I$ is allowed to be empty [8].

We will omit the index $S$ from $\mathcal{A}_S$ whenever the background set is understood. The *cardinality* of a finite set $X$ is denoted by $\sharp X$. The *empty set* is denoted by $\emptyset$.

The following definition tells how a reaction system operates.

**Definition 2.** Consider a reaction $\rho = (R, I, P)$ over $S$ and a subset $T$ of $S$. The reaction $\rho$ is *enabled* with respect to $T$, in symbols $en_\rho(T)$, if $R \subseteq T$ and $I \cap T = \emptyset$. If $\rho$ is (resp. is not) enabled with respect to $T$, then we define the *result* by

$$res_\rho(T) = P \quad \big(\text{resp. } res_\rho(T) = \emptyset\big).$$

For a reaction system $\mathcal{A} = \{\rho_j |\ 1 \leq j \leq k\}, k \geq 1$, we define the *result* by

$$res_{\mathcal{A}}(T) = \bigcup_{j=1}^{k} res_{\rho_j}(T).$$

Reaction systems are often classified according to the maximal cardinalities of the sets of reactants and inhibitors. A reaction system $\mathcal{A}$ is a $(k,l)$ *system* if the conditions $\sharp R \leq k$ and $\sharp I \leq l$ are satisfied for every reaction $(R, I, P)$ in $\mathcal{A}$. It is *minimal* if $k = l = 1$. Various results concerning minimal reaction systems are contained in [4,9,11,13]. The reference [12] deals with the connection to propositional logic, and [14] the definition of arbitrary subset functions using minimal reaction systems.

We now come to the basic notions concerning sequences.

*Sequences* generated by reaction systems can be viewed as iterations of the operation $res_{\mathcal{A}}$. If $res_{\mathcal{A}}(Y) = Y'$, we use the notation

$$Y \Rightarrow_{\mathcal{A}} Y',$$

or simply $Y \Rightarrow Y'$. If

$$res_{\mathcal{A}}(X_i) = X_{i+1}, \quad 0 \leq i \leq m-1,$$

we write briefly

$$X_0 \Rightarrow X_1 \Rightarrow \cdots \Rightarrow X_m$$

and call $X_0, X_1, \ldots, X_m$ *states* of a *sequence* of *length* $m$ generated (or defined) by the reaction system $\mathcal{A}$.

It is important to notice that, whenever in a sequence $X_i = X_j$, $i \neq j$, then also $X_{i+1} = X_{j+1}$. As we will see, reaction systems with duration do not satisfy this condition.

Since there are only $2^{\sharp S}$ subsets of $S$, one of the following two alternatives always occurs for a sequence

$$X_0 \Rightarrow X_1 \Rightarrow \cdots \Rightarrow X_{m-1},$$

for large enough $m$.

1. $res_{\mathcal{A}}(X_{m-1}) = X_{m_1}$, for some $m_1 \leq m-1$. If $m_1$ is the largest number satisfying this inequality, we say that the sequence has (or ends with) a *cycle* of length $m - m_1$.