



Introducing time in reaction systems

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ABSTRACT

Reaction systems are a formal model of interactions between biochemical reactions. The main observation underlying the formulation of this model is that such interactions are based on two basic mechanisms: facilitation and inhibition. This paper continues the investigation of reaction systems, and in particular, it proposes a formal framework for introducing time into reaction systems. Within this framework one can formally define and investigate notions such as reaction times, creation times of compounds, their life spans, etc.

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0. Introduction

This paper continues research on reaction systems (see [1–3]) which are a formal model of interactions between biochemical reactions. The main idea behind reaction systems is that two main mechanisms underlying the regulation of biochemical reactions are facilitation and inhibition. These two mechanisms underlie the functioning of individual biochemical reactions as well as the interactions between individual biochemical reactions.

This reasoning leads to the formalization of a *reaction* as a triplet $a = (R_a, I_a, P_a)$, where R_a is the set of reactants, I_a is the set of inhibitors, and P_a is the set of products. Such a reaction a can take place (is *enabled*) in a state (set) T if all the reactants are present in T (hence $R_a \subseteq T$), and none of the inhibitors are present in T (hence $I_a \cap T = \emptyset$). If a is enabled in T , then P_a is produced, and so P_a is the *result* of applying a to T ; otherwise the result of applying a to T is the empty set.

These notions (of enabling and of the result) for single reactions are extended to sets of reactions as follows. A set A of reactions is enabled in state T if each reaction of A is enabled in T . Thus, unlike in standard theories of concurrent systems (see, e.g., [4] for Petri nets) there is no notion of *conflict* (between reactions *in a state*) involved in the definition of enabling of a set of reactions. This reflects our assumption about the “threshold supply” of elements (molecules): either an element is present and then there is “enough” of it, or an element is not present. Therefore there is no counting in reaction systems – in this sense reaction systems present qualitative rather than quantitative analysis of interactions between reactions.

If a set of reactions A is (enabled in and) applied to a state T , then the result of applying A to T is the cumulative result of applying all reactions in A to T : $res_A(T) = \bigcup_{a \in A} P_a$. In particular this means that if an element $x \in T$ is not in $\bigcup_{a \in A} P_a$, then it “disappears” – it is not sustained even if it was not at all “involved” in the reactions from A (i.e., even if x is not a reactant for any of the reactions from A). This reflects another important assumption we make: there is no permanency of elements – if nothing happens to an element, then it ceases to exist (the only way to keep an element present is to sustain it by suitable reactions). This assumption, motivated by organic chemistry, is again very different from traditional theories of concurrent systems (such as, e.g., Petri nets). Altogether, assumptions behind our model are often orthogonal to

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the assumptions underlying traditional formal models in computer science – see [1,2] for a more detailed discussion of this issue.

A *reaction system* is then just an ordered pair $\mathcal{A} = (S, A)$, where A is a finite set of reactions, and S is a finite (background) set such that $R_a \cup I_a \cup P_a \subseteq S$ for each $a \in A$. The dynamics of a reaction system is given through the notion of an interactive process. This is a sequence of states where each state is a subset of S given as the union of two sets: the result of transforming the previous state by A and a context set (which, e.g., may represent an interaction with the “environment”).

Our reasoning in constructing a framework for an abstract study of biochemical reactions based on reaction systems is that the basic notion of a reaction system can be extended/modified whenever needed in studies of specific issues concerning biochemical reactions. Thus in the study of the formation of modules (compounds) in an environment determined by biochemical reactions (such as a “molecular soup”) presented in [3], a reaction system was equipped with a binary relation \mathcal{R} on the set of potential states. Then, in a state sequence one can move from a state T to a state Q if the underlying reaction system prescribes such a move *and* the pair (T, Q) is admissible in \mathcal{R} (belongs to \mathcal{R}).

Clearly, there are situations where one needs to assign quantitative parameters to the states of a reaction system – one of such situations, viz., assigning time values/moments to states, is the topic of this paper. Our assumption is that such a numerical value can be assigned to a state T if there is a measurement of T yielding this value. This leads us to define measurement functions which are functions assigning reals to potential states of \mathcal{A} (hence to subsets of the background set S). Naturally, as, e.g., in measure theory, such measurement functions are required to be additive, i.e., for a measurement function f and two disjoint subsets Z_1, Z_2 of S we have $f(Z_1 \cup Z_2) = f(Z_1) + f(Z_2)$.

Then, a *reaction system with measurements* is a triplet $\mathcal{A} = (S, A, F)$, where (S, A) is a reaction system, and F is a finite set of measurement functions on (the subsets of) S .

In this paper, we are concerned with introducing time in reaction systems. In particular, we propose to define a time function (assigning time to consecutive states of state sequences) as a measurement function which has nonnegative values and is such that $f(T) < f(Q)$ if T, Q are two consecutive states of a state sequence with Q following T – this is “time flows forward” condition. The goal of this paper is to establish a formal framework for considering time in reaction systems. In particular, this will allow us to talk about issues such as reaction times, the time moments of states in a state sequence, the elapsed time between the holdings of states, and all kinds of (time) ratios.

The paper is organized as follows.

After establishing in Section 1 some basic notation and terminology, in Section 2 we recall the basic notions concerning reaction systems, and we introduce the notion of a reaction system with measurements. In Section 3 we introduce time functions as measurement functions, and then we define clocks as subsets of the background set that can measure time. Here time functions are first defined for single state sequences, and then extended to universal time functions that can measure time on all state sequences of a reaction system (more precisely on all the so-called active state sequences). In Section 4, we discuss the more obvious way of providing universal time-functions, viz., through external counters. They can be compared to dropping a watch to a Petri dish – one can see time while taking a snapshot of a Petri dish, but this time has no relationship to what is going on in the dish. A more interesting way of providing universal time for reaction systems is to use the so-called timers. In this way one gets the counting of time which is dependent on reactions going on in a reaction system (Petri dish). The formal notion of a timer is introduced in Section 5, examples of timers are given in Section 6, and in Section 7 we discuss the use of timers to provide universal time for reaction systems. Then in Section 8 we demonstrate how to use our framework for introducing time in reaction systems to determine reaction times. Most importantly, we demonstrate that using timers we can indeed have times of reactions dependent on the state of a system (which is a basic feature of reactions in organic chemistry). Then, based on our methodology of establishing reaction times, in Section 9 we demonstrate how to follow the dynamics of creating products/compounds in reaction systems. In particular, we discuss how to establish the time moment (between two consecutive states) when a compound is created as well as how to establish the life span of a compound. The discussion in Section 10 concludes this paper.

1. Preliminaries

Throughout the paper we use standard set-theoretical notation and terminology. We use \emptyset to denote the empty set. For a set A we use $|A|$ to denote its cardinality, and 2^A to denote the family of all subsets of A . For sets A and B , we use $A \cup B$ and $A \cap B$ to denote their union and intersection, respectively. We write $A \subseteq B$ if A is included in B . For a family \mathcal{F} of sets, we use $\bigcup \mathcal{F}$ and $\bigcap \mathcal{F}$ to denote the union and the intersection of all sets in \mathcal{F} , respectively.

For a sequence $\varrho = V_0, V_1, \dots, V_n$, its length is denoted by $|\varrho|$; hence $|\varrho| = n + 1$.

We use \mathbb{R} to denote the set of reals, and \mathbb{R}^+ to denote the set of positive reals. For a finite set $Z \subseteq \mathbb{R}$, $\max Z$ is the biggest real in Z , and ΣZ is the sum of all the reals in Z . A function $f : \mathcal{F} \rightarrow \mathbb{R}$, where \mathcal{F} is a family of sets closed under union, is *additive* if, for all disjoint $Z_1, Z_2 \in \mathcal{F}$, $f(Z_1 \cup Z_2) = f(Z_1) + f(Z_2)$. Note that if $\emptyset \in \mathcal{F}$, then $f(\emptyset) = 0$. If f is nonnegative (i.e., $f(Z) \geq 0$ for each $Z \in \mathcal{F}$), then we consider f to be a function with the range $\mathbb{R}^+ \cup \{0\}$ (i.e., $f : \mathcal{F} \rightarrow \mathbb{R}^+ \cup \{0\}$).

2. Reaction systems

In this section we recall (from [2]) some basic notions concerning reaction systems, and then we introduce the notion of a reaction system with measurements.

Definition 1. A reaction is a 3-tuple $a = (R, I, P)$ of finite sets.

For a reaction a as above: the set R , also denoted by R_a , is the *reactant set of a* ; the set I , also denoted by I_a , is the *inhibitor set of a* , and the set P , also denoted by P_a , is the *product set of a* . For a set A of reactions, $R_A = \bigcup_{a \in A} R_a$, $I_A = \bigcup_{a \in A} I_a$, and $P_A = \bigcup_{a \in A} P_a$.

If S is a set such that $R, I, P \subseteq S$, then we say that a is a *reaction in S* .

In this paper we assume that R_a, I_a , and P_a are nonempty, and $R_a \cap I_a = \emptyset$ for each reaction a .

Definition 2. (1) For a reaction a and a finite set T , the *result of a on T* , denoted $res_a(T)$, is defined by: $res_a(T) = P_a$ if $R_a \subseteq T$ and $I_a \cap T = \emptyset$, and $res_a(T) = \emptyset$ otherwise.

(2) For a set of reactions A and a set T , the *result of A on T* , denoted $res_A(T)$, is defined by: $res_A(T) = \bigcup_{a \in A} res_a(T)$.

If $R_a \subseteq T$ and $I_a \cap T = \emptyset$, then we say that a is *enabled on T* ; otherwise we say that a is *not enabled on T* . For a set of reactions A we say that A is *enabled on T* if each $a \in A$ is enabled on T .

Thus a reaction a is enabled on a set T if T separates R_a from I_a , i.e., $R_a \subseteq T$ and $I_a \cap T = \emptyset$. Similarly, a set of reactions A is enabled on T if T separates R_A from I_A .

Note that unlike in traditional theories of concurrency (such as Petri nets, see, e.g., [4]) there is no notion of conflict here when applying a set of reactions in a given state. This reflects our assumption about the “threshold supply” of elements in the *basic setup* of reaction systems: either an element is present and then there is “enough” of it, or an element is not present. Hence in the basic theory of reaction systems we do not have counting: it is a qualitative rather than a quantitative theory. On the other hand, there exists a natural notion of inconsistency of a set of reactions that is independent of a state to which the set is applied. Such inconsistency arises if reactants of some reactions are inhibitors for some other reactions.

A set A of reactions is *consistent* if $R_A \cap I_A = \emptyset$; otherwise A is *inconsistent*.

Definition 3. A *reaction system*, abbreviated *rs*, is an ordered pair $\mathcal{A} = (S, A)$ such that S is a finite set, and A is a finite set of reactions in S .

The set S is called the *background (set) of \mathcal{A}* .

Definition 4. Let $\mathcal{A} = (S, A)$ be a *rs*, and let $T \subseteq S$.

(1) The *result of \mathcal{A} on T* , denoted $res_{\mathcal{A}}(T)$, is defined by $res_{\mathcal{A}}(T) = res_A(T)$.

(2) The *T-activity of \mathcal{A}* , denoted by $en_{\mathcal{A}}(T)$, is the set $\{a \in A : a \text{ is enabled on } T\}$. If $en_{\mathcal{A}}(T) \neq \emptyset$, then T is *active (in \mathcal{A})*.

Note that since we assume that $P_a \neq \emptyset$ for every nonempty reaction a , the condition $en_{\mathcal{A}}(T) \neq \emptyset$ above is equivalent to the condition $res_{\mathcal{A}}(T) \neq \emptyset$.

The dynamic behaviour of reaction systems is expressed (formalized) through interactive processes which are defined as follows.

Definition 5. Let $\mathcal{A} = (S, A)$ be a *rs*. An *interactive process* in \mathcal{A} is a pair $\pi = (\gamma, \delta)$ of finite sequences such that, for some $n \geq 1$, $\gamma = C_0, C_1, \dots, C_n$, $\delta = D_1, \dots, D_n$, where $C_0, \dots, C_n, D_1, \dots, D_n \subseteq S$, $D_1 = res_{\mathcal{A}}(C_0)$, and $D_i = res_{\mathcal{A}}(C_{i-1} \cup D_{i-1})$ for each $2 \leq i \leq n$.

The sequence C_0, \dots, C_n is the *context sequence of π* , and the sequence D_1, \dots, D_n is the *result sequence of π* . Let $W_0 = C_0$, and $W_i = D_i \cup C_i$ for each $1 \leq i \leq n$. Then the sequence W_0, W_1, \dots, W_n is the *state sequence of π* , denoted by $sts(\pi)$, and W_0 is the *initial state of π* . For each $0 \leq j \leq n$, C_j is the *context of W_j* . If for each $1 \leq j \leq n$, $C_j \subseteq D_j$, then we say that $sts(\pi)$ is a *state sequence with no intervention by contexts*. The sequence E_0, E_1, \dots, E_{n-1} of subsets of A such that $E_i = en_{\mathcal{A}}(W_i)$ for all $0 \leq i \leq n-1$ is called the *activity sequence of π* , denoted by $act(\pi)$. If $act(\pi)$ consists of nonempty sets only, then $sts(\pi)$ is *active*, i.e., with a possible exception of the last state, all states in an active state sequence are active. The set of all state sequences of \mathcal{A} (i.e., all state sequences of all interactive processes in \mathcal{A}) is denoted by $STS(\mathcal{A})$, and the set of all active state sequences of \mathcal{A} is denoted by $ASTS(\mathcal{A})$.

Note that in general, in a state sequence a state W_i which is not active can be followed by an active state W_{i+1} – this happens when C_{i+1} is active (since W_i is not active, $W_{i+1} = C_{i+1}$).

Although the core theory of reaction systems is qualitative, as, e.g., it does not include counting, it can be extended so that quantitative parameters/values can be assigned to the states of a reaction system. Our assumption here is that a numerical value can be assigned to a state T if there is a measurement of T yielding this value, where a measurement of T is a real number assigned to T . Since in reaction systems states are sets, we are led to assigning real numbers to sets, and hence we deal with functions from all subsets of a given set (the background set of a reaction system) into reals. As usual (e.g., as in measure theory) we assume that such measurement functions are additive. Then the basic notion of a reaction system is extended to the notion of a reaction system with measurements defined as follows.

Definition 6. (1) A *measurement function for a $rs(S, A)$* is an additive function $f : 2^S \rightarrow \mathbb{R}$.

(2) A *reaction system with measurements*, abbreviated *rsm*, is a triplet $\mathcal{A} = (S, A, F)$ such that (S, A) is a *rs*, and F is a finite set of measurements functions.

The ordered pair (S, A) is called the *underlying reaction system of \mathcal{A}* , denoted by $und(\mathcal{A})$. Also, for $f \in F$, and $T \subseteq S$, $[T]_f = \{t \in T : f(t) \neq 0\}$.

As usual, we may notationally identify a singleton set $\{x\}$ with its element x – therefore we have written above $f(t)$ rather than $f(\{t\})$. All the notions and notations concerning reaction systems carry over to reaction systems with measurement (through their underlying reaction systems).

3. Time functions and clocks

In this section we will introduce time (functions) for reaction systems. This will be useful in the analysis of behaviour of reaction systems. For example, we will be able to determine that “something” (a reaction) occurs earlier than something else (another reaction), or we will be able to determine how much time elapsed between two states in a state sequence.

We begin by defining a time function for a single state sequence.

Definition 7. Let \mathcal{A} be a *rs*, and let $\tau = W_0, \dots, W_n \in STS(\mathcal{A})$. A *time function* for τ (in \mathcal{A}) is a nonnegative measurement function f for \mathcal{A} such that $f(W_i) < f(W_{i+1})$ for each $i \in \{0, \dots, n-1\}$. We say that τ is *timed* (by f) if there exists a time function (f) for τ .

We require that a time function is a *nonnegative* measurement function ($f : 2^S \rightarrow \mathbb{R}^+ \cup \{0\}$) as we do not want to have elements of the background that can set time back. The condition of strict monotonicity: $f(W_i) < f(W_{i+1})$, expresses the natural requirement that “time flows forward”. This allows one to express time ratios of measured quantities: e.g., if g is a measurement function, then, since $f(W_{i+1}) - f(W_i) \neq 0$, $\frac{g(W_{i+1}) - g(W_i)}{f(W_{i+1}) - f(W_i)}$ expresses time-relativised change of g in the transition from W_i to W_{i+1} . Note that if $\tau = W_0, \dots, W_n \in STS(\mathcal{A})$ is timed (by f), then, for all $i, j \in \{0, \dots, n\}$, $W_i \neq W_j$ whenever $i \neq j$ (as otherwise the strict monotonicity condition would be violated).

A clock is a device to measure time. Accordingly, within the framework of reaction systems, a clock is a subset of the background set that measures time correctly. Formally, this is expressed as follows.

Definition 8. Let \mathcal{A} be a *rs*, let $\tau = W_0, \dots, W_n \in STS(\mathcal{A})$, and let f be a time function for τ . A (τ, f) -clock is a subset K of S such that $f(W_i) = f(W_i \cap K)$ for each $i \in \{0, \dots, n\}$. We say that K is a *tight* (τ, f) -clock if no strict subset of K is a (τ, f) -clock.

Note that if $\tau \in STS(\mathcal{A})$ is timed by f , then there is a (τ, f) -clock. For example, S is a (τ, f) -clock. Also, $[S]_f$ is a (τ, f) -clock, which in general may be smaller than S . However $[S]_f$ does not have to be tight. As a matter of fact a tight (τ, f) -clock is unique, and it is defined by $K_{\tau, f} = \bigcup \{[W_i]_f : 0 \leq i \leq n\}$. It is the *minimal* (τ, f) -clock in the sense that if K is a (τ, f) -clock, then $K_{\tau, f} \subseteq K$. This follows from the observation that since $f(T) \geq 0$ for each $T \subseteq S$, and $f(K \cap W_i) = f(W_i)$ for each $i \in \{0, \dots, n\}$, it must be that $[W_i]_f \subseteq K$. The strict monotonicity property of time functions implies that the length of a timed state sequence is bounded, with the bound dependent on the cardinality of its minimal clock.

Lemma 9. Let \mathcal{A} be a *rs*, let $\tau = W_0, \dots, W_n \in STS(\mathcal{A})$ be timed, let f be a time function for τ , and let K be a (τ, f) -clock with $q = |K|$. Then $n \leq 2^q - 1$.

Proof. Since K is a (τ, f) -clock, $f(W_i) = f(W_i \cap K)$ for each $i \in \{0, \dots, n\}$. Since f is a time function for τ , $f(W_i) \neq f(W_j)$ whenever $i \neq j$, for all $i, j \in \{0, \dots, n\}$. Therefore $|\tau|$ is bounded by the number of subsets of K , which implies that $n + 1 \leq 2^q$. \square

Example 10. Let $\mathcal{A} = (S, A, \{f\})$ be a *rsm* defined as follows.

- (1) $S = D \cup \{b, e\}$, where $D = \{d_0, d_1, \dots, d_k\}$ for some $k \geq 1$ and $e, b \notin D$.
- (2) f is a nonnegative function such that $f(d_i) = 2^i$ for each $i \in \{0, \dots, k\}$, $f(b) = 0$, and $f(e) = 2^{k+2}$.
- (3) A is the union of the sets of reactions B_0, B_1, B_2, B_3, B_4 defined as follows:
 - $B_0 = (\{b\}, D \cup \{e\}, \{d_0\})$,
 - $B_1 = (\{\{d_j\}, \{d_0, e\}, \{d_0\}\} : j \in \{1, \dots, k\})$,
 - $B_2 = (\{\{d_0, \dots, d_{j-1}\}, \{d_j, e\}, \{d_j\}\} : j \in \{1, \dots, k\})$,
 - $B_3 = (\{\{d_j\}, \{d_i, e\}, \{d_j\}\} : i, j \in \{0, \dots, k\} \text{ and } i < j)$, and
 - $B_4 = (D, \{e\}, \{e\})$.

\mathcal{A} defines a binary counter, where subsets of D represent binary numbers: if $d_i \in Z \subseteq D$ for $i \in \{0, \dots, k\}$, then the binary number represented by Z has 1 on position 2^i . For example, $\{d_3, d_0\}$ represents 1001 (hence 9 in binary notation).

The reaction from B_0 will begin counting when started from 0 (represented by $\{b\}$).

Reactions from B_1 perform adding 1 to an even number.

Reactions from B_2 perform adding 1 to an odd number.

Reactions from B_3 sustain bits d_j which are not affected by carryover resulting by adding 1.

The reaction from B_4 introduces e , when the range of the representation by D (viz., $2^{k+1} - 1$) is reached.

This example illustrates a functioning of an *rsm* as a counter. It will be used (somewhat modified) in the sequel of this paper. However now we can use it to demonstrate that the bound from Lemma 9 cannot be improved (i.e., we may have $n = 2^q - 1$) – one can indeed time very long state sequences with small clocks.

To this aim consider the state sequence τ of \mathcal{A} , where $\tau = W_0, W_1, \dots, W_n$, where $W_0 = \{b\}$, and $W_{i+1} = res_{\mathcal{A}}(W_i)$ for each $i \in \{0, \dots, n\}$, and $n = 2^{k+1} - 1$. From the definition of A it follows that W_0, W_1, \dots, W_n are representations of consecutive binary numbers (beginning with 0), i.e., the values of f on τ are 0, 1, 2, 3, \dots , $2^{k+1} - 1$. Thus $W_1 = \{d_0\}$, $W_2 = \{d_1\}$, $W_3 = \{d_0, d_1\}$, \dots , and $W_n = D$. Since $f(b) = 0$, D is a (τ, f) -clock for τ ; as a matter of fact $D = K_{\tau, f}$. Moreover, $|\tau| = n + 1 = 2^{k+1}$, while $|D| = k + 1$. Thus $|\tau| = 2^{|D|}$.

Until now the time function was state sequence dependent: it was defined just for a single state sequence. We move now to define time function for reaction systems, i.e., one universal time function for all (active) state sequences of a reaction system.

Definition 11. Let \mathcal{A} be a *rs*. A *universal time function* for \mathcal{A} is a measurement function f for \mathcal{A} such that, for each $\tau \in \text{ASTS}(\mathcal{A})$, f is a time function for τ . If there is a universal time function (f) for \mathcal{A} , then we say that \mathcal{A} is *timed* (by f).

In this paper the time will be measured from *within* a *rsm* in the sense that a part of a system will be just measuring time. Thus the time moments of consecutive states of the whole system will correspond to the values of the time function on the states of this subsystem. Consequently, the passage of time is determined by the transformation of the states of this subsystem. This implies that the passage of time would have to stop when the system arrives at a state which is not active. For this reason in the definition of a universal time function we restrict ourselves to *active* state sequences only.

Recall that, for each *rs* $\mathcal{A} = (S, A)$, $[S]_f$ is a (τ, f) -clock for each $\tau \in \text{STS}(\mathcal{A})$ and each time function f for τ . Hence, Lemma 9 implies that in a timed *rs* \mathcal{A} , there is a common bound on the length of all active state sequences. However this may be really not restrictive, since, as shown in Example 10, small clocks can time very long state sequences: e.g., for $[S]_f = 100$ we can time state sequences of length 2^{100} .

The following lemma expresses an important property of universal time functions.

Lemma 12. Let $\mathcal{A} = (S, A)$ be a *rs*. A nonnegative measurement function f for \mathcal{A} is a universal time function for \mathcal{A} if and only if $f(T) < f(\text{res}_{\mathcal{A}}(T))$ for each active $T \subseteq S$.

Proof. Let $\mathcal{A} = (S, A)$ be a *rs* and let f be a nonnegative measurement function for \mathcal{A} .

- (i) Assume that f is a universal time function for \mathcal{A} , and let $T \subseteq S$ be active. Since $T, \text{res}_{\mathcal{A}}(T)$ is an active state sequence of \mathcal{A} , it follows from the definition of a universal time function that $f(T) < f(\text{res}_{\mathcal{A}}(T))$.
- (ii) Assume that $f(T) < f(\text{res}_{\mathcal{A}}(T))$ for each active $T \subseteq S$. Since f is nonnegative, this implies that if T, Q is an active state sequence of \mathcal{A} , then $f(T) < f(Q)$. Consequently, f is a time function for each $\tau \in \text{ASTS}(\mathcal{A})$, and hence f is a universal time function for \mathcal{A} . \square

4. Providing universal time functions by external counters

Clearly not every *rs* (*rsm*) is timed. For example, if a *rs* (*rsm*) contains an active state sequence with two states W, W' such that W preceeds W' and $W' \subseteq W$, then it is not timed, as $f(W') \leq f(W)$ for each measurement function f . However, we will demonstrate in this section that each *rsm* can be extended by equipping it with a counter so that the resulting *rsm* is timed. Moreover, this counter does not really “interfere” with the functioning of the original system (except for making sure that the composed *rsm* does not run if the counter doesn’t). We begin by constructing a counter.

Let $k \in \mathbb{N}^+$, and let $\mathcal{A}(k) = (S_k, A_k, F_k)$ be the *rsm* defined as follows.

$$S_k = \{c_0, \dots, c_k, d_0, \dots, d_k, e\}.$$

$$F_k = \{f_k\}, \text{ where the measurement function } f_k \text{ is defined by:}$$

$$f_k(c_i) = 0 \text{ for all } i \in \{0, \dots, k\},$$

$$f_k(d_i) = 2^i \text{ for all } i \in \{0, \dots, k\}, \text{ and}$$

$$f_k(e) = 2^{k+1}.$$

The intuition behind $\mathcal{A}(k)$ is that it is a binary counter that, without an intervention by context, is counting orderly up to $2^{k+1} - 1$, but, if “something goes wrong” (e.g., something “wrong” is added by a context), then it jumps to the “time stopper” e . Elements c_0, \dots, c_k represent zeros, and elements d_0, \dots, d_k represent ones in the binary representation of a number; this is formally set by the values of f on c_0, \dots, c_k and d_0, \dots, d_k . Then the time stopper e represents a number that is bigger than any number that can be represented using $c_0, \dots, c_k, d_0, \dots, d_k$; we have chosen to set $f(e) = 2^{k+1}$.

The set of reactions A_k is defined as the union of the sets of reactions B_1, \dots, B_7 defined below.

(1) B_1 consists of all reactions $(\{c_i, d_i\}, \{e\}, \{e\})$, for all $i \in \{0, \dots, k\}$.

The intuition behind B_1 is that if both c_i and d_i for some $i \in \{0, \dots, k\}$ belong to a current state, then the current state does not represent a binary number – thus something went wrong, and so $\mathcal{A}(k)$ introduces time stopper e (which is an inhibitor for every reaction in A_k).

(2) B_2 consists of all reactions $(\{u\}, \{c_i, d_i, e\}, \{e\})$, for all $i \in \{0, \dots, k\}$ and all $u \notin \{c_i, d_i, e\}$.

The intuition behind B_2 is that, for each $i \in \{0, \dots, k\}$, each good state must contain either c_i or d_i (as otherwise it does not represent a binary number) – thus if this is not the case, then $\mathcal{A}(k)$ introduces e .

(3) B_3 consists of all reactions $(\{c_i, d_j\}, \{e\}, \{d_j\})$, for all $i, j \in \{0, \dots, k\}$ such that $i < j$.

The intuition behind B_3 is that if a binary number contains a zero on position i , then a possible carry over from incrementing the number by one will not get to position j if $j > i$; thus d_j is sustained.

(4) B_4 consists of one reaction: $(\{c_0\}, \{e\}, \{d_0\})$.

This reaction is producing the successor of an even number.

(5) B_5 consists of all reactions $(\{d_0, \dots, d_i, c_{i+1}\}, \{e\}, \{c_0, \dots, c_i, d_{i+1}\})$ for all $i \in \{0, \dots, k-1\}$.

The reactions from B_5 produce the successor of an odd number.

(6) B_7 consists of all reactions $(\{c_i\}, \{d_j, e\}, \{c_j\})$ for all $i \in \{1, \dots, k\}$ and $j \in \{0, \dots, k-1\}$ such that $j < i$.

The intuition behind B_6 is that all the zeros in a binary number that are not changed into ones as the result of the successor function should be sustained.

(7) B_7 consists of one reaction, viz. $(\{d_0, \dots, d_k\}, \{e\}, \{e\})$.

The intuition behind B_7 is that this reaction represents the “end of time”: the successor of $2^{k+1} - 1$ cannot be represented in S_k .

Note that it follows from the construction of $\mathcal{A}(k)$ that a nonempty subset T of S_k is an active state of $\mathcal{A}(k)$ if and only if it does not contain e . If an active state T of $\mathcal{A}(k)$ represents a number x , then $\text{res}_{\mathcal{A}(k)}(T)$ represents $x + 1$ providing that $x + 1 < 2^{k+1} - 1$, otherwise $\text{res}_{\mathcal{A}(k)}(T)$ contains e . Hence $f_k(T) < f_k(\text{res}_{\mathcal{A}(k)}(T))$.

We will use now $\mathcal{A}(k)$ to extend an arbitrary *rsm* to a timed *rsm*. The extension is done as follows.

Let $\mathcal{A} = (S, A, F)$ be a *rsm*, let $k \geq 1$, and let $\mathcal{A}(k) = (S_k, A_k, \{f_k\})$ be a k -counter such that $S_k \cap S = \emptyset$. We define then the *rsm* $\mathcal{A}' = (S', A', F')$ as follows.

- (i) $S' = S \cup S_k$.
- (ii) $A' = A_e \cup A_k \cup G$, where
 - $A_e = \{(R_a, I_a \cup \{e\}, P_a) : a \in A\}$, and
 - $G = \{(\{u\}, S_k, \{e\}) : u \in S\}$.
- (iii) For each $g \in F$, we define the measurement function $g' : 2^{S'} \rightarrow \mathbb{R}$ as follows: for each $x \in S_k$, $g'(\{x\}) = 0$, and for each $x \in S$, $g'(\{x\}) = g(\{x\})$. The measurement function f_k is extended to the measurement function $f' : 2^{S'} \rightarrow \mathbb{R}$ as follows: for each $x \in S$, $f'(\{x\}) = 0$, and for each $x \in S_k$, $f'(\{x\}) = f_k(\{x\})$. Then we set $F' = \{g' : g \in F\} \cup \{f'\}$. (In defining g' and f' above we use the obvious fact that to specify a measurement function it suffices to give its values on all singleton sets).

In fact, \mathcal{A}' is essentially a “modified union” of \mathcal{A} and $\mathcal{A}(k)$, where $\mathcal{A}(k)$ influences the functioning of \mathcal{A} within \mathcal{A}' as follows (note that \mathcal{A} does not influence the functioning of $\mathcal{A}(k)$ within \mathcal{A}').

- (1) The time stopper e of $\mathcal{A}(k)$ inhibits each reaction.
- (2) The runs of \mathcal{A} without counting are inhibited by G (thus if the initial state of a state sequence of \mathcal{A}' is disjoint with $S_k - \{e\}$, then e is introduced and so the run is blocked).

The fact that \mathcal{A}' functions as \mathcal{A} with the counting of time performed by $\mathcal{A}(k)$ is more formally expressed by the following two properties (the straightforward proof of these properties is left to the reader).

- (I) For every $n \geq 1$, if $W_0, W_1, \dots, W_n \in \text{STS}(\mathcal{A})$ and $Z_0, Z_1, \dots, Z_n \in \text{ASTS}(\mathcal{A}(k))$, then $W_0 \cup Z_0, W_1 \cup Z_1, \dots, W_n \cup Z_n \in \text{ASTS}(\mathcal{A}')$ and $f'(W_i \cup Z_i) = f_k(Z_i)$ for all $i \in \{0, \dots, n\}$.
- (II) For each $U_0, U_1, \dots, U_n \in \text{ASTS}(\mathcal{A}')$, it holds that $S \cap U_0, S \cap U_1, \dots, S \cap U_n \in \text{STS}(\mathcal{A})$, $S_k \cap U_0, S_k \cap U_1, \dots, S_k \cap U_n \in \text{ASTS}(\mathcal{A}(k))$, and $f'(U_i) = f_k(S_k \cap U_i)$ for all $i \in \{0, \dots, n\}$.

We will prove now that \mathcal{A}' is timed by f' .

Lemma 13. *If $\tau = T, Q$ is an active state sequence of \mathcal{A}' , then $f'(T) < f'(Q)$.*

Proof. Since τ is active, $T \neq \emptyset$ and $e \notin T$.

By definition, $f'(T) = f'([T]_{f'})$.

We consider separately two cases.

(i) $[T]_{f'} = \emptyset$.

Then, by the definition of G , $e \in \text{res}_{\mathcal{A}'}(T)$, and so, by the value of $f'(e)$, $f'(T) < f'(\text{res}_{\mathcal{A}'}(T))$.

(ii) $[T]_{f'} \neq \emptyset$.

Since $e \notin T$, $[T]_{f'}$ is an active state of $\mathcal{A}(k)$. Therefore (see the comment after the definition of $\mathcal{A}(k)$), $f'([T]_{f'}) < f'(\text{res}_{\mathcal{A}(k)}([T]_{f'}))$. Since $S \cap S_k = \emptyset$, we get $f'(\text{res}_{\mathcal{A}(k)}([T]_{f'})) = f'(\text{res}_{\mathcal{A}'}([T]_{f'})) = f'(\text{res}_{\mathcal{A}'}(T))$. Hence, again, $f'(T) < f'(\text{res}_{\mathcal{A}'}(T))$.

Since in both cases $f'(T) < f'(\text{res}_{\mathcal{A}'}(T))$ and f' is nonnegative, we get $f'(T) < f'(Q)$. \square

Theorem 14. *\mathcal{A}' is a timed *rsm*.*

Proof. By Lemma 13, f' is a time function for each $\tau \in \text{ASTS}(\mathcal{A}')$. Therefore f' is a time function for \mathcal{A}' , and so \mathcal{A}' is timed. \square

Note that in our construction the counter $\mathcal{A}(k)$ got incorporated into \mathcal{A}' as an “external counter”: its counting is not influenced by the rest of \mathcal{A}' . It may be seen as a “clock dropped into a Petri dish” (representing \mathcal{A}), so that the snapshots of \mathcal{A} representing states in a state sequence contain now also the state of $\mathcal{A}(k)$. In other words, each snapshot (state) contains now a time certificate. These time certificates show an “external time” which is in no way influenced by (related to) the reactions of \mathcal{A} .

5. Timers

We will extend now reaction systems with measurements to timed reaction systems with measurement by equipping them with “devices” which provide time functions which are interacting with the “rest of the system”. These devices will be timers which are introduced in this section.

Definition 15. A timer is a *rsm* $\mathcal{A} = (S, A, F)$, where $F = \{f\}$, and there exists an element $e \in S$ such that the following five conditions hold (we set $D = S - \{e\}$ and assume $D \neq \emptyset$):

- (C1) $f(u) > 0$ for all $u \in S$,
- (C2) $f(e) > f(D)$,
- (C3) $e \in I_a$ for each $a \in A$, and
- (C4) $f(T) < f(\text{res}_{\mathcal{A}}(T))$ for each nonempty $T \subseteq D$.

Condition C1 requires that a timer does not have redundant elements, i.e., each element of (the background set of) a timer contributes to time counting.

Note that if $\mathcal{A} = (S, A, \{f\})$ is a timer, then an element $e \in S$ as in the definition above is unique, viz., it is the element of S for which f has the biggest value. As a matter of fact, the value $f(e)$ exceeds the sum of the values of f on all elements of D (condition C2). Also, e is an inhibitor for all reactions in \mathcal{A} (condition C3), which means that once introduced it stops the functioning of \mathcal{A}_f . For this reason, e is called *the end of time for* \mathcal{A} , denoted by $e_{\mathcal{A}}$; also we set $D_{\mathcal{A}} = S - \{e_{\mathcal{A}}\}$.

Condition C4 is the main technical requirement. Note that it implies that a nonempty $T \subseteq S$ is active if and only if $T \subseteq D$. Most importantly, it implies that f is a universal time function for \mathcal{A} . This is stated in the following lemma.

Lemma 16. Let $\mathcal{A} = (S, A, \{f\})$ be a timer.

- (1) For each $T \subseteq S$, $f(T) = 0$ if and only if $T = \emptyset$.
- (2) $e_{\mathcal{A}} \in \text{res}_{\mathcal{A}}(D_{\mathcal{A}})$.
- (3) f is a universal time function for \mathcal{A} .

Proof. ad(1) Since f is a measurement function, $T = \emptyset$ implies $f(T) = 0$. The reverse implication follows from condition C1.

ad(2) Condition C4 implies that $f(D_{\mathcal{A}}) < f(\text{res}_{\mathcal{A}}(D_{\mathcal{A}}))$, and so $\text{res}_{\mathcal{A}}(D_{\mathcal{A}})$ contains an element outside $D_{\mathcal{A}}$. Thus $e_{\mathcal{A}} \in \text{res}_{\mathcal{A}}(D_{\mathcal{A}})$.

ad(3) This follows directly from C4 and Lemma 12. \square

6. Examples of timers

In this section we give three examples of timers.

Example 17. Let $\mathcal{A} = (S, A, \{f\})$ be the *rsm* obtained from the *rsm* from Example 10 by the following modifications:

- (i) b is removed from S , i.e., $S = D \cup \{e\}$,
- (ii) f is now restricted to $D \cup \{e\}$, and
- (iii) the singleton set B_0 is removed from A , i.e., A is the union of the sets of reactions B_1, B_2, B_3, B_4 .

It is easily seen that \mathcal{A} satisfies conditions C1, \dots , C4 from Definition 15 (with $m = 2^{k+1} - 1$), and so \mathcal{A} is a timer. As a matter of fact, any choice of the value of $f(e)$ such that $f(e) \geq 2^{k+1}$ is good for satisfying condition C2 – we have chosen 2^{k+2} .

To illustrate the functioning of this timer let's choose $k = 3$, and the initial state $W_0 = \{d_2, d_3\}$. Then $\tau = W_0, W_1, W_2, W_3, W_4$ is an active state sequence (with no intervention by contexts), where

$$W_1 = \{d_0, d_2, d_3\},$$

$$W_2 = \{d_1, d_2, d_3\},$$

$$W_3 = \{d_0, d_1, d_2, d_3\}, \text{ and}$$

$$W_4 = \{e\}; \text{ note that } W_4 \text{ is not an active state.}$$

The values of f on τ are: 12, 13, 14, 15, 32, and so τ represents the counting by successor from 12 to 15, then jumping to 32 (when e is introduced).

It is important to notice that in this timer, for any two consecutive states W_i, W_{i+1} in an active state sequence, if $e \notin \text{res}_{\mathcal{A}}(W_i)$, then $f(\text{res}_{\mathcal{A}}(W_i)) - f(W_i) = 1$. Therefore we say that this timer counts by successor.

Example 18. Let $\mathcal{A} = (S, A, f)$ be the *rsm* defined as follows.

- (1) $S = D \cup \{e\}$, where $D = \{d_0, \dots, d_k\}$ for some $k \geq 1$, and $e \notin D$.
- (2) f is defined by: $f(d_i) = 1$ for all $i \in \{0, \dots, k\}$, and $f(e) = k + 3$.
- (3) A is the union of three sets of reactions B_1, B_2, B_3 defined as follows:
 - $B_1 = \{\{\{d_i, \dots, d_k\}, \{e, d_0, \dots, d_{i-1}\}, \{e\}\} : i \in \{0, \dots, k\}\}$,
 - $B_2 = \{\{\{d_i\}, \{e\}, \{d_i\}\} : i \in \{0, \dots, k\}\}$, and

$$B_3 = \{(\{d_i, \dots, d_j\}, \{e, d_0, \dots, d_{i-1}, d_{j+1}\}, \{d_{j+1}\}) : i, j \in \{0, \dots, k-1\} \text{ and } i \leq j\}.$$

\mathcal{A} defines a unary counter, where each $Z \subseteq D$ defines the number in unary notation, viz., $|Z|$. Given a nonempty $T \subseteq D$, the reactions from A transform T as follows.

By productions from B_1 , if there is $i \in \{0, \dots, k\}$ such that $d_j \in T$ for all $j \geq i$, and $d_j \notin T$ for all $j < i$, then $e \in \text{res}_{\mathcal{A}}(T)$ is signaling that unary counting was completed.

By productions from B_2 , each d_i in T is sustained, i.e., if $d_i \in T$, then $d_i \in \text{res}_{\mathcal{A}}(T)$ for all $i \in \{0, \dots, k\}$.

By productions from B_3 , d_t is added (i.e., $d_t \in \text{res}_{\mathcal{A}}(T)$) for the smallest t such that $d_t \notin T$, and $d_u \in T$ for some $u < t$.

Thus with no intervention by contexts, given nonempty $T \subseteq D$ with $m = \min\{i \in \{0, \dots, k\} : d_i \in T\}$, \mathcal{A} will function (count) as follows:

- (1) If T is not the suffix of D (i.e., D is not of the form $\{d_i, \dots, d_k\}$ for some $i \leq k$), then \mathcal{A} will count from $|T|$ to $k - m + 1$ by adding one in each step, and then \mathcal{A} will add $f(e) = k + 3$ (as a consequence of introducing e) and stop.
- (2) If T is the suffix of D , then \mathcal{A} will jump from the value $|T|$ to the value $|T| + f(e)$, and then stop.

It is easily seen that \mathcal{A} satisfies conditions C1, \dots , C4 from Definition 15 (with $m = k + 1$), and so \mathcal{A} is a timer.

To illustrate the functioning of this timer let's choose $k = 11$, and the initial state $W_0 = \{d_3, d_4, d_8, d_9\}$. Then $\tau = W_0, W_1, \dots, W_6$ is an active state sequence (with no intervention by contexts), where

$$W_1 = \{d_3, d_4, d_5, d_8, d_9\},$$

$$W_2 = \{d_3, d_4, d_5, d_6, d_8, d_9\},$$

$$W_3 = \{d_3, d_4, d_5, d_6, d_7, d_8, d_9\},$$

$$W_4 = \{d_3, d_4, d_5, d_6, d_7, d_8, d_9, d_{10}\},$$

$$W_5 = \{d_3, d_4, d_5, d_6, d_7, d_8, d_9, d_{10}, d_{11}\}, \text{ and}$$

$$W_6 = \{e, d_3, d_4, d_5, d_6, d_7, d_8, d_9, d_{10}, d_{11}\}.$$

Clearly, W_6 is not an active state as it contains e which inhibits every reaction.

Thus, in this state sequence, first the gap $\{d_5, d_6, d_7\}$ is filled in sequentially in the order d_5, d_6, d_7 , then the gap $\{d_{10}, d_{11}\}$ is filled in sequentially in the order d_{10}, d_{11} , and then, since the counting was completed, e is introduced, and the system becomes inactive.

Note that the system could be activated again if context adds a nonempty subset of D : for example if this context $C_7 = \{d_1, d_3\}$, then $W_7 = C_7$ and so W_7 is active with $\text{res}_{\mathcal{A}}(W_7) = \{d_1, d_2, d_3\}$.

The values of f on τ are: 4, 5, 6, 7, 8, 9, 23, and so τ represents counting by successor from 4 to 9, then jumping to 23 (when e is introduced), and stopping afterwards. It is important to note that also this timer counts by successor.

Example 19. Let $\mathcal{A} = (S, A, \{f\})$ be the *rsm* which is identical to the *rsm* from Example 18 except that A contains an additional group of reactions $B_4 = \{(\{d_i, d_j\}, \{d_\ell, e\}, \{d_\ell\}) : i, j, \ell \in \{0, \dots, k\} \text{ and } i < \ell < j\}$.

Thus this *rsm* also counts in unary, except that if nonempty $T \subseteq D$ has a “gap” (i.e., there are $i, j \in \{0, \dots, k\}$ such that $j > i, d_j, d_i \in T$ and $d_\ell \notin T$ for all $\ell \in \{i+1, \dots, j-1\}$), then each such gap is filled in by 1's (i.e., corresponding d_ℓ 's) in one step. Hence in one counting step increments bigger than one may be added.

It is easily seen that adding B_5 to the set of reactions from the *rsm* from Example 18 does not influence the satisfiability of conditions C1, \dots , C4 from Definition 15, and so also \mathcal{A} is a timer.

To illustrate the functioning of this timer let's again (as in the previous example) choose $k = 11$ and the initial state $W_0 = \{d_3, d_4, d_7, d_9\}$. Then $\tau = W_0, W_1, W_2, W_3, W_4$ is an active state sequence (with no intervention by contexts), where

$$W_1 = \{d_i : 3 \leq i \leq 9\},$$

$$W_2 = \{d_i : 3 \leq i \leq 10\},$$

$$W_3 = \{d_i : 3 \leq i \leq 11\}, \text{ and}$$

$$W_4 = \{e\} \cup \{d_i : 3 \leq i \leq 11\}.$$

Clearly, W_4 is not an active state as it contains e which inhibits every reaction.

Note that here, already in the first transition from W_0 to W_1 , all the gaps, viz. $\{d_5, d_6\}$ and $\{d_8\}$ were filled in at once. From then on, as in the previous example, d_{10} and then d_{11} were produced, followed by the production of e . The values of f on τ are: 4, 7, 8, 9, 23. Note that filling in all gaps at once gave the jump of the value of f from 4 to 7. Then, as in the previous example, the values increased by one until e was introduced. Thus the essential difference with the two previous examples is that this timer *does not* count by successor.

7. Using timers to provide universal time

In this section we will demonstrate how to equip *rsms* with universal time functions using timers. The difference with Section 4, where we used external counters, is that now the timer part of the resulting *rsm* interacts *both* ways with the rest of the system. As we will see in the sequel of the paper, this is a fundamental difference as it allows for defining reaction times (rates) in such a way that they depend on the state of the system.

We will need the following useful notion.

For a *rsm* $\mathcal{A} = (S, A, F)$ and $f \in F$, the *f-restriction* of \mathcal{A} , is the *rsm* system $\mathcal{A}_f = ([S]_f, [A]_f, \{f'\})$, where $[A]_f = \{a \in A : R_a \cup I_a \cup P_a \subseteq [S]_f\}$, and f' is f restricted to the subsets of $[S]_f$.

Definition 20. Let $\mathcal{A} = (S, A, F)$ be a rsm, and let $f \in F$ be nonnegative.

(1) We say that f defines a timer for \mathcal{A} if

- (i) \mathcal{A}_f is a timer,
- (ii) for each $u \in S - [S]_f$ there exists $Z \subseteq S$ such that $Z \cap [S]_f \neq \emptyset$ and $(\{u\}, [S]_f, Z) \in A$,
- (iii) for each $a \in A$, $e_{\mathcal{A}_f} \in I_a$.

(2) We say that \mathcal{A} contains a timer (based on f) if there exists $f \in F$ which defines a timer for \mathcal{A} .

Thus f defines a timer for \mathcal{A} if the f -restriction of \mathcal{A} is a timer, each set of elements U from outside the background set of \mathcal{A}_f (i.e., $U \subseteq S - [S]_f$) will introduce some elements from the timer \mathcal{A}_f if no element of $[S]_f$ is present in a current state, and moreover the end of time element of \mathcal{A}_f inhibits all reactions from \mathcal{A} .

In the notation from the above definition, we say that \mathcal{A}_f is a timer for \mathcal{A} , and for $T \subseteq S$, $[T]_f$ is the state of \mathcal{A}_f in T .

We will demonstrate now that if f defines a timer for \mathcal{A} , then f is a universal time function for \mathcal{A} .

Lemma 21. Let $\mathcal{A} = (S, A, F)$ be a rsm, and let $f \in F$ be such that it defines a timer for \mathcal{A} . If $T \subseteq S$ is active in \mathcal{A} , then $f(T) < f(\text{res}_{\mathcal{A}}(T))$.

Proof. Note that since T is active, it must be that $T \neq \emptyset$ and $e \notin T$.

There are two possible cases which we will consider separately.

(1) $[S]_f \cap T = \emptyset$.

Then $f(T) = 0$, and by (ii) of Definition 20, $f(\text{res}_{\mathcal{A}}(T)) > 0$. Thus $f(T) < f(\text{res}_{\mathcal{A}}(T))$.

(2) $[S]_f \cap T \neq \emptyset$.

Since $f(T) = f(T \cap [S]_f)$ and \mathcal{A}_f is a timer and $[S]_f \cap T \neq \emptyset$, by C4 from Definition 15 we get $f(T) = f(T \cap [S]_f) < f(\text{res}_{\mathcal{A}_f}(T \cap [S]_f))$.

Since no production in \mathcal{A}_f can be inhibited by an element from $S - [S]_f$, $f(\text{res}_{\mathcal{A}_f}(T \cap [S]_f)) \leq f(\text{res}_{\mathcal{A}_f}(T))$.

Therefore $f(T) = f(T \cap [S]_f) < f(\text{res}_{\mathcal{A}}(T))$.

Since cases (1) and (2) are exhaustive, the lemma holds. \square

Theorem 22. Let $\mathcal{A} = (S, A, F)$ be a rsm, and let $f \in F$. If f defines a timer for \mathcal{A} , then f is a universal time function for \mathcal{A} .

Proof. The theorem follows from Lemmas 21 and 12. \square

Thus if $f \in F$ defines a timer for \mathcal{A} , then $[S]_f$ is a universal clock for \mathcal{A} , and \mathcal{A}_f specifies the functioning of this clock. However the time counting by f may be influenced by productions from $A - [A]_f$ (the “rest of the system”). Intuitively, it is the rest of the system that specifies the set of reactions that one is really interested in, while \mathcal{A}_f specifies the timing mechanism for counting time. Note that F may contain several measurement functions that define timers for \mathcal{A} with some of them better than others for specific considerations (applications).

When we write down an active state sequence W_0, W_1, \dots, W_n for a reaction system, then the sequence of indices $0, 1, 2, \dots, n$ is external to the system itself – the same holds for most models of computation. This often leads to conclusion that one unit of time elapses between each W_i and W_{i+1} which often is neither justified nor intended.

When we deal with reaction systems with measurements and f defines a timer for the system considered, then for a given state sequence W_0, W_1, \dots, W_n its consecutive time indices are really $f(W_0), f(W_1), \dots, f(W_n)$. These time indices are internal to the system – they are determined (computed) by the system itself (viz., by \mathcal{A}_f). Moreover, in general quite a lot can be said about what happens between the state with the time index $f(W_i)$ and the state with the time index $f(W_{i+1})$ in a given state sequence. This is the subject of the remaining part of this paper.

8. Counting time: Reaction times

We move now to the important issue of determining the time duration of sets of reactions. The basic underlying unit of time measurement is the tick of the timer \mathcal{A}_f determined by f . The value of this tick is state dependent, and it is formally defined as follows.

Let $\mathcal{A} = (S, A, F)$ be a rsm, and let $f \in F$ define a timer (\mathcal{A}_f) for \mathcal{A} .

For $U \subseteq D_{\mathcal{A}_f}$, $\text{tic}_U(\mathcal{A}_f) = f(\text{res}_{\mathcal{A}_f}(U)) - f(U)$ is the tick of \mathcal{A}_f in U . Then, for an active state T of \mathcal{A} , we define $\text{tic}_T(\mathcal{A}_f) = \text{tic}_{[T]_f}(\mathcal{A}_f)$ (note that since T is an active state of \mathcal{A} , $e_{\mathcal{A}_f} \notin [T]_f$ and so $\text{tic}_{[T]_f}(\mathcal{A}_f)$ is well defined). Hence $\text{tic}_T(\mathcal{A}_f)$ is the increase of the value of f contributed by \mathcal{A}_f in T ; thus $\text{tic}_T(\mathcal{A}_f) = f(\text{res}_{\mathcal{A}_f}([T]_f)) - f(T)$.

We will establish now a couple of basic properties of the tick of \mathcal{A}_f .

The first property says that the only case when timer \mathcal{A}_f produces a tick equal zero is when its state is the empty set.

Lemma 23. For each $U \subseteq D_{\mathcal{A}_f}$, $\text{tic}_U(\mathcal{A}_f) = 0$ if and only if $U = \emptyset$.

Proof. If $U = \emptyset$, then $\text{res}_{\mathcal{A}_f}(U) = \emptyset$ and so $\text{tic}_U(\mathcal{A}_f) = f(\emptyset) - f(\emptyset) = 0$.

If $U \neq \emptyset$, then, by C4 from Definition 15, $f(\text{res}_{\mathcal{A}_f}(U)) > f(U)$ which implies that $\text{tic}_U(\mathcal{A}_f) \neq 0$. \square

The second property says that the ticks of \mathcal{A}_f establish the minimal discernability for measuring time in reaction systems. The time interval between two consecutive states T, Q in an active state sequence cannot be smaller than the tick of \mathcal{A}_f in T .

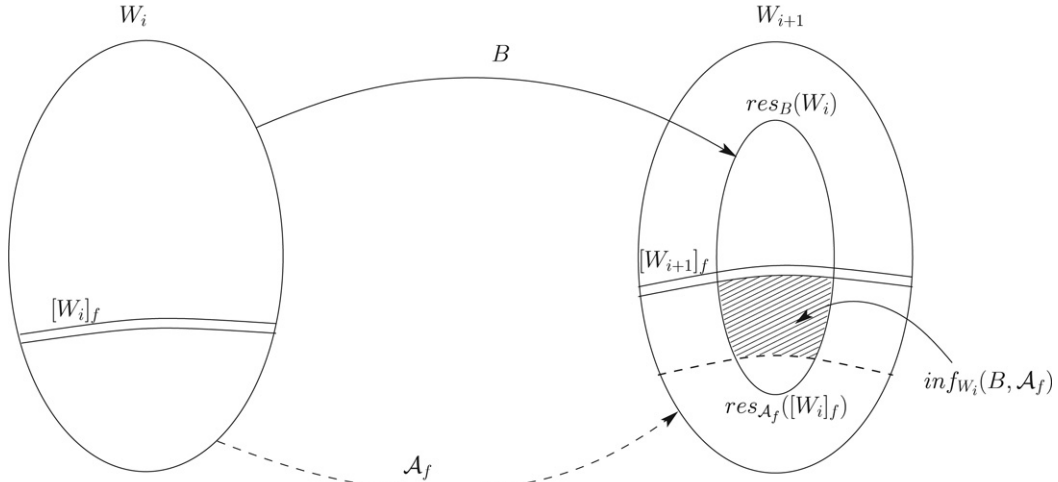


Fig. 1.

Lemma 24. For each active $T \subseteq S$, $f(\text{res}_{\mathcal{A}}(T)) - f(T) \geq \text{tic}_{[T]_f}(\mathcal{A}_f)$.

Proof. Since no reaction in \mathcal{A}_f is inhibited by an element from $S - [S]_f$, $\text{res}_{\mathcal{A}_f}([T]_f) \subseteq \text{res}_{\mathcal{A}}(T)$. Since $f(T) = f([T]_f)$ and f is nonnegative, this implies that $f(\text{res}_{\mathcal{A}}(T)) - f(T) \geq f(\text{res}_{\mathcal{A}_f}([T]_f)) - f([T]_f) = \text{tic}_{[T]_f}(\mathcal{A}_f)$ (again note that since T is active, $\text{tic}_{[T]_f}(\mathcal{A}_f)$ is defined). \square

In order to determine the time (duration) of a set of reactions in a given state, we need a number of auxiliary notions.

For a consistent $B \subseteq A$, $[P_B]_f$ is the total contribution of B to \mathcal{A}_f . Then, for $T \subseteq S$ such that $B \subseteq \text{en}_{\mathcal{A}}(T)$, $[P_B]_f - \text{res}_{\mathcal{A}_f}([T]_f)$ is the influence of B on \mathcal{A}_f in T , denoted by $\text{inf}_T(B, \mathcal{A}_f)$. Thus if $\text{inf}_T(B, \mathcal{A}_f) \neq \emptyset$, then B changes the state of \mathcal{A}_f (after T is transformed by \mathcal{A}) by adding (by union) $\text{inf}_T(B, \mathcal{A}_f)$ to $\text{res}_{\mathcal{A}_f}([T]_f)$; otherwise B does not change the time keeping function of \mathcal{A}_f in $[T]_f$. Clearly, the change of the value of time function f caused by B in T amounts to adding $f(\text{inf}_T(B, \mathcal{A}_f))$ to $f(\text{res}_{\mathcal{A}_f}([T]_f))$. Accordingly, $f(\text{inf}_T(B, \mathcal{A}_f))$ is called the delay by B on T , and denoted by $\text{del}_T(B)$.

Thus, when f is a time function which defines a timer for \mathcal{A} , the ticks of \mathcal{A}_f determine the basic time passage for state transitions in state sequences of \mathcal{A} . In an active state sequence $\tau = W_0, \dots, W_i, W_{i+1}, \dots, W_n$ if we assume that in the state transition from W_i to W_{i+1}

- (1) the influence of the set of reactions from outside \mathcal{A}_f on \mathcal{A}_f in W_i is empty, and that
- (2) the context C_{i+1} does not influence \mathcal{A}_f (i.e., $[C_{i+1}]_f \subseteq \text{res}_{\mathcal{A}_f}(W_i)$),

then $\text{tic}_T(W_i)$ is the transition time from W_i to W_{i+1} . This basic transition rhythm is in general state dependent. Hence the value of the tick of \mathcal{A}_f in the transition from W_i to W_{i+1} may be different than the value of the tick of \mathcal{A}_f in the transition from W_j to W_{j+1} when $j \neq i$. Whether or not it is actually different depends on the properties of \mathcal{A}_f , and on the properties of states W_i and W_j .

Our basic assumption is that for a (consistent) set of reactions B the reaction time for B is dependent on the current state W_i (in which B is enabled). What B actually does (as far as the time properties of τ are concerned) is adding to the set $\text{res}_{\mathcal{A}_f}([W_i]_f)$ its own influence on \mathcal{A}_f in W_i . The situation is illustrated in Fig. 1.

The counting of time by \mathcal{A}_f together with the influence by B , determines then the reaction time of B in W_i . This is formalized as follows (recall that, by definition, $\text{inf}_T(B, \mathcal{A}_f)$ is disjoint with $\text{res}_{\mathcal{A}_f}([T]_f)$).

Definition 25. Let $\mathcal{A} = (S, A, F)$ be a rsm, and let $f \in F$ be such that it defines a timer for \mathcal{A} . For $T \subseteq S$ and $B \subseteq A$ such that $B \subseteq \text{en}_{\mathcal{A}}(T)$, the reaction f -time for B in T , denoted by $f\text{-time}_T(B)$, is defined by $f\text{-time}_T(B) = f(\text{inf}_T(B, \mathcal{A}_f) \cup \text{res}_{\mathcal{A}_f}([T]_f)) - f(T)$.

Whenever f is understood from the context of considerations, we may use the term reaction time for B in T , and the notation $\text{time}_T(B)$.

Thus, intuitively, if $\text{del}_T(B) = 0$, then the reaction time for B would be just a tick of \mathcal{A}_f in T . This is formally proved as follows.

Lemma 26. For \mathcal{A} , f , T and B as in Definition 25, $f\text{-time}_T(B) = \text{del}_T(B) + \text{tic}_{[T]_f}(\mathcal{A}_f)$.

Proof. By definition, $f\text{-time}_T(B) = f(\text{inf}_T(B, \mathcal{A}_f) \cup \text{res}_{\mathcal{A}_f}([T]_f)) - f(T)$. Since $(\text{inf}_T(B, \mathcal{A}_f) \cap \text{res}_{\mathcal{A}_f}([T]_f)) = \emptyset$, $f\text{-time}_T(B) = f(\text{inf}_T(B, \mathcal{A}_f)) + f(\text{res}_{\mathcal{A}_f}([T]_f)) - f(T) = \text{del}_T(B) + (f(\text{res}_{\mathcal{A}_f}([T]_f)) - f([T]_f)) = \text{del}_T(B) + \text{tic}_{[T]_f}(\mathcal{A}_f)$. \square

Since the smallest time unit we have for counting time in the transformation of W_i to W_{i+1} (in an active state sequence $\tau = W_0, \dots, W_i, W_{i+1}, \dots, W_n$) is the tick of \mathcal{A}_f in W_i , the reaction time of a set of reactions B in W_i is at least one tick. On the other hand this reaction time cannot exceed the time interval between W_{i+1} and W_i . This is formally stated in the following lemma.

Lemma 27. Let \mathcal{A}, f, T and B be as in Definition 25, and let $Q \subseteq S$ be such that $T, Q \in \text{ASTS}(\mathcal{A})$. Then $\text{tic}_{[T]_f}(\mathcal{A}_f) \leq f\text{-time}_T(B) \leq f(Q) - f(T)$.

Proof. By Lemma 26, $\text{tic}_{[T]_f}(\mathcal{A}_f) \leq f\text{-time}_T(B)$. On the other hand, since $(\text{inf}_T(B, \mathcal{A}_f) \cup \text{res}_{\mathcal{A}_f}([T]_f)) \subseteq Q$, $f(\text{inf}_T(B, \mathcal{A}_f) \cup \text{res}_{\mathcal{A}_f}([T]_f)) \leq f(Q)$. Therefore $f\text{-time}_T(B) \leq f(Q) - f(T)$. \square

We point out that our basic setup is to consider reaction times for sets of reactions rather than for single reactions. The reason for this choice is that in general one cannot infer the delay by a set of reactions B (on a given state T) by knowing the delays by all single reactions in B . The dependence of the delay by B on the delay by individual reactions from B may vary a lot. It satisfies the following formula:

$$\max\{\text{del}_T(\{b\}) : b \in B\} \leq \text{del}_T(B) \leq \Sigma\{\text{del}_T(\{b\}) : b \in B\}.$$

The exact dependence relies on the intersection properties of the family of sets $\{\text{inf}_T(\{b\}, \mathcal{A}_f) : b \in B\}$.

Knowing the influence of a set of reactions B on \mathcal{A}_f in an active state T we can determine the completion moment of B in T , denoted by $t_T(B, f)$, as follows: $t_T(B, f) = f(\text{inf}_T(B, \mathcal{A}_f)) + f(\text{res}_{\mathcal{A}_f}([T]_f))$.

9. Sets in time: Life span of sets

Now that we have determined how to measure reaction times we move to the related issue of determining the time moments of creating sets of objects (subsets of S) and their life span.

For an active state sequence T, Q , when we consider a formation in time of subsets of Q , we will restrict our considerations to the subsets of $\text{res}_{\mathcal{A}}(T)$. The reason is that if a subset of Q contains elements which are not in $\text{res}_{\mathcal{A}}(T)$, then it contains elements of true context (i.e., elements of context that are not in $\text{res}_{\mathcal{A}}(T)$). But, in general, we really have no indication when (in the time interval between $f(T)$ and $f(Q)$) such elements are added to Q .

For a nonempty $Z \subseteq \text{res}_{\mathcal{A}}(T)$, the creation moment of Z in T , denoted $cm_T(Z, f)$, is defined by $cm_T(Z, f) = \min\{t_T(B, f) : B \subseteq \text{en}_{\mathcal{A}}(T) \text{ and } Z \subseteq P_B\}$. In general, Z may be included in the product of many different sets of reactions B enabled in T . The creation moment of Z is chosen as the minimal completion moment among all these sets B .

It is important in this context to note that among all the subsets of Q we distinguish those that are “physical”, i.e., are the results of transforming a subset of T by a set of reactions enabled in T (this distinction is essential for considerations in [3]). Thus the definition of $cm_T(Z, f)$ implies that we are interested in the earliest moment when Z was created as a part of forming of a physical subset.

Note that it follows directly from the definition of the creation moment that if $Z = Z_1 \cup Z_2$, then $cm_T(Z_1, f) \leq cm_T(Z, f)$ and $cm_T(Z_2, f) \leq cm_T(Z, f)$. On the other hand it may be the case that both $cm_T(Z_1, f) < cm_T(Z, f)$ and $cm_T(Z_2, f) < cm_T(Z, f)$. This may happen when, e.g., a set of reactions B_1 that introduces Z_1 and takes minimal time, and a set of reactions B_2 that introduces Z_2 and takes minimal time are such that both $\text{inf}_T(B_1, f)$ and $\text{inf}_T(B_2, f)$ are strict subsets of $\text{inf}_T(B_1, f) \cup \text{inf}_T(B_2, f)$, and $B_1 \cup B_2$ is a subset of $\text{en}_{\mathcal{A}}(T)$ with a minimal completion time among all the subsets of $\text{en}_{\mathcal{A}}(T)$ that produce Z .

Since the shortest reaction time for any set of reactions in an active state Q is $\text{tic}_Q(\mathcal{A}_f)$, it is reasonable to assume that if $\tau = T, Q$ is an active state sequence with active Q , then for any set Z created by \mathcal{A} in T (i.e., $Z \subseteq \text{res}_{\mathcal{A}}(T)$) its life span (between T and Q) is the time period from the moment of creation of Z in T until (and including) the time moment $f(Q) + \text{tic}_Q(\mathcal{A}_f)$. Until this time moment no set of reactions enabled on Q will be completed, and so no change w.r.t. Q will take place. If however Q is not active, then \mathcal{A}_f will not tic in Q , and so the life span of Z is counted until (and including) $f(Q)$. This is more formally expressed as follows.

Given an active state sequence $\tau = W_0, \dots, W_n$ and $i \in \{0, \dots, n-1\}$, for each $U \subseteq \text{res}_{\mathcal{A}}(W_i)$ we define the life span of U between W_i and W_{i+1} , denoted by $\ell_{S_{W_i, W_{i+1}}}(U)$ as follows: $\ell_{S_{W_i, W_{i+1}}}(U) = (f(W_{i+1}) + \text{tic}_{W_{i+1}}(\mathcal{A}_f)) - cm_{W_i}(U)$ if $\text{res}_{\mathcal{A}}(W_{i+1}) \neq \emptyset$, and $\ell_{S_{W_i, W_{i+1}}}(U) = f(W_{i+1}) - cm_{W_i}(U)$ if $\text{res}_{\mathcal{A}}(W_{i+1}) = \emptyset$ (which may happen only if $i+1 = n$).

The completion moment of B is well-determined (and signaled by the creation of its product P_B). On the other hand it is not so clear how to determine the beginning/initiation moment of B . Suppose that we consider an active state sequence W, T, Q and a set of reactions B such that $B \subseteq \text{en}_{\mathcal{A}}(T)$. The completion moment of B in T is $t_T(B)$, but if $R_B \subseteq \text{res}_{\mathcal{A}}(W)$ and $cm_W(R_B) < f(T)$, then B could be initiated at $cm_W(R_B)$ and hence before $f(T)$. This is illustrated in Fig. 2, where $\Delta_{B,T}$ is a possible activity interval of B . Clearly, if the activity interval for B would be defined in this way, then we would have to modify our definition of reaction time for B by adding to it the time interval $f(T) - cm_W(R_B)$.

Thus, in general, for sets of reactions B_1, B_2, \dots, B_m enabled in T we could have then the situation depicted in Fig. 3. Hence B_1, B_2, \dots, B_m may be acting asynchronously in T , and this asynchronicity can be detected through our detailed time analysis. If we would deal with “external time counting” where the reaction time for sets of reactions is not state dependent then the activity intervals for sets of reactions enabled in B would stretch from $f(T)$ to $f(Q)$ implying that the sets of reactions enabled in T act synchronously.

10. Discussion

The goal of this paper is to propose a formal framework for introducing time in reaction systems. To achieve this goal we considered reaction systems with measurements, where a time function is a nonnegative measurement function satisfying

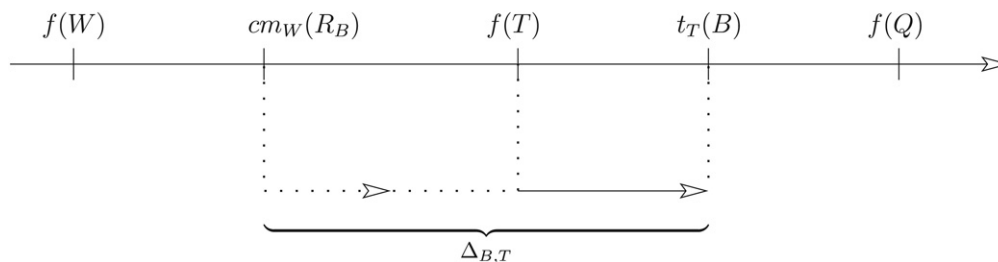


Fig. 2.

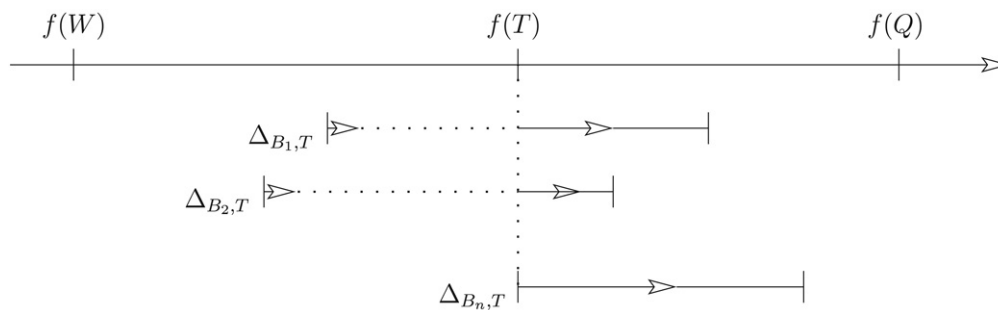


Fig. 3.

the “time flows forward” condition: $f(W_i) < f(W_{i+1})$ for any two consecutive states W_i, W_{i+1} in an active state sequence. Then we demonstrated how to provide universal time functions by external counters and by timers. The former method yields time measurement in a way “totally detached” from the functioning of the reaction system for which we want to measure time. The latter method provides a way of time measurement that is “intrinsic” to the measured reaction system: the time counting is influenced by reactions of the system. This method is the preferred method as it naturally allows reaction times to be dependent on the state of a system. Indeed, we have formally defined reaction times, and then we have also defined time-related parameters of elements and their sets (compounds) such as the creation time and the life span (in the time interval between two consecutive states of an active state sequence).

Note that “time flows forward” condition that we required to be satisfied by time functions allows one to define all kinds of rates useful in the analysis of reaction systems. This is perhaps best explained through examples.

Let $\mathcal{A} = (S, A, F)$ be a *rsm*, and let T, Q be two consecutive states from an active state sequence of \mathcal{A} (hence $res_{\mathcal{A}}(T) \neq \emptyset$, and $res_{\mathcal{A}}(T) \subseteq Q$). Let $f \in F$ be a global time function for \mathcal{A} , and let $\Delta = f(Q) - f(T)$; thus $\Delta \neq 0$. Let $B \subseteq en_{\mathcal{A}}(T)$. We can define the the following characteristics of this “situation” (T, Q, B) :

- (1) *surviving elements*: $sur(T, Q, B) = R_B \cap P_B$,
- (2) *used elements*: $usd(T, Q, B) = R_B - sur(T, Q, B)$,
- (3) *produced elements*: $prd(T, Q, B) = P_B - sur(T, Q, B)$.

Now let $g \in F$ be a (different) measuring function that measures some quantity α .

Since the transition from T to Q happens within Δ time units, we get the following ratios:

- (i) $\frac{g(prd(T, Q, B)) - g(T)}{\Delta}$, the rate of total change of g (in the interval between T and Q),
- (ii) $\frac{g(prd(T, Q, B)) - g(usd(T, Q, B))}{\Delta}$, the rate of efficiency of g (in the interval between T and Q),
- (iii) $\frac{g(usd(T, Q, B))}{\Delta}$, the rate of consumption of α (in the interval between T and Q), and
- (iv) $\frac{g(prd(T, Q, B))}{\Delta}$, the rate of production of α (in the interval between T and Q).

Since $\Delta \neq 0$, all of these rates are well-defined.

Finally we want to comment on extending time functions to *all* state sequences (currently they are defined for *active* state sequences). To this aim we need the notion of a *block* of a state sequence defined as follows.

Let $\tau = W_0, \dots, W_n \in STS(\mathcal{A})$.

If $\tau \in ASTS(\mathcal{A})$, then τ is the *block* of τ .

If $\tau \notin ASTS(\mathcal{A})$, then let $W_{i_1}, W_{i_2}, \dots, W_{i_r}$, with $r \geq 1$ and $i_1 < i_2 < \dots < i_r$, be all not active states of τ . These states split τ into *segments* $\sigma_1 = W_0, \dots, W_{i_1}, \sigma_2 = W_{i_1+1}, \dots, W_{i_2}, \dots, \sigma_r = W_{i_{r-1}+1}, \dots, W_{i_r}$, and if $i_r \neq n$ then also $\sigma_{r+1} = W_{i_r+1}, \dots, W_n$. A segment σ_j is a *block* of τ if $\sigma_j \in ASTS(\mathcal{A})$.

We can extend now the notion of a time function to an arbitrary $\tau \in STS(\mathcal{A})$ as follows. A nonnegative measurement function f for \mathcal{A} is a time function for τ if f satisfies the “time flows forward” condition for each block of τ .

Thus, if τ is not active, then the value of f is set by each $W_{i_j}, 1 \leq j \leq r$, to $f(res_{\mathcal{A}}(W_{i_j})) = 0$, and then (if $i_j \neq n$) reset by the context of $W_{i_{j+1}}$ to $f(W_{i_{j+1}})$. If σ_{j+1} is a block, then $f(W_{i_{j+1}})$ will be the initial value of clocks for σ_{j+1} .

Now that the notion of a time function is defined for all state sequences, the notion of a universal time function extends to all state sequences as well.

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