Available online at www.sciencedirect.com
ScienceDirect
Theoretical Computer Science 376 (2007) 3–16
Theoretical Computer Science
www.elsevier.com/locate/tcs

Events and modules in reaction systems

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Abstract

Reaction systems are a formal model of interactions between biochemical reactions. They are based on the observation that two basic mechanisms behind the functioning of biochemical reactions are facilitation and inhibition. In this paper we continue the investigation of reaction systems, and in particular we introduce the notion of a module, and then we investigate the formation and evolution of modules. Among others we prove that reaction systems can be viewed as self-organizing systems, where the organizing goal is to ensure a specific property of the set of all modules (of a state of a process).
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Keywords: Natural computing; Biochemical reactions; Partial orders

0. Introduction

Two main mechanisms behind the functioning of biochemical reactions are facilitation and inhibition; these mechanisms are also central for the interaction between biochemical reactions. This observation underlies the theory of reaction systems introduced in [2] (see also [1]) which is a formal framework for the investigation of biochemical reactions, and especially interactions between them.

More specifically, a biochemical reaction is formalized as follows. A (formal) *reaction* is 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*. The intuition behind this formal notion of a reaction corresponds in a straightforward way to the functioning of a biochemical reaction: reaction a converts/transforms the set of reactants R_a into the product set P_a providing that it is not inhibited by (one or more) inhibitors from I_a. Therefore, more formally, the result of applying reaction a to a set T, denoted by $res_a(T)$, is conditional: if T separates R_a from I_a (i.e., if R_a is included in T and I_a is disjoint with T), then a is enabled on (applicable to) T, otherwise a is not enabled on (not applicable to) T. If a is enabled on T, then a transforms the set of reactants into the product set, and so $res_a(T) = P_a$; otherwise $res_a(T)$ is the empty set.

Then the notion of transformation by a single reaction is extended to sets of reactions, and the dynamics of *reaction systems* (which are essentially sets of reactions) is investigated through the notion of an interactive process. Such a

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doi:10.1016/j.tcs.2007.01.008

process is essentially a sequence of states, where each state is a set (a subset of the background set fixed for a given reaction system) which is a union of two sets: the result of transforming the previous state in the sequence and a context set (which may, e.g., represent an interaction with "the rest of the system" or "the environment").

In [2] we have introduced the basic definitions (and motivations behind them) concerning reaction systems, illustrated them by examples, related them to some traditional models of computation (such as elementary net systems and boolean functions), and proved some basic properties.

In this paper we investigate the formation and evolution of modules in a reaction system $\mathcal{E}$. A subset Q_i of a state W_i in a state sequence τ is just that: a (mathematical) subset of W_i. However, when W_i is transformed into W_{i+1} by $\mathcal{E}$, Q_i gets transformed into Q_{i+1} which then gets a physical/material interpretation: it is a subset of W_{i+1} which is the product of reactions of $\mathcal{E}$ acting on Q_i. Such "physical" subsets are called *modules*. Now if we follow the transformation of the state W_{i+1} we get the transformation of Q_{i+1} into the successor module Q_{i+2}. In this way following the fate/evolution of a subset Q_i of W_i we obtain the sequence of modules $Q_{i+1}, Q_{i+2}, \ldots$; such a sequence is called an *event* (tracing the evolution of Q_i). This paper presents a formal study of modules and events tracing their evolution. We refer the reader to [3] for the background concerning the importance of modules in biology, and the need for a precise definition of a module in various biological contexts.

The paper is organized as follows.

In Preliminaries we recall basic mathematical notions, terminology and notation to be used in this paper. We also prove a technical result concerning lattices that is used later in the paper. In Section 2 we recall from [2] basic notions concerning reaction systems, and in Section 3 we introduce a generalization of reaction systems, called extended reaction systems that are investigated in this paper. In Section 4 we introduce events and modules, and in Section 5 we introduce snapshots — the snapshot of a state is the set of all its modules. In Section 6 we investigate the structure of snapshots. In particular we prove that an extended reaction system is a self-organizing system whose organizing goal is to achieve a specific property of snapshots (called separability). As a corollary we prove that when a state sequence stabilizes, then the set of modules of a snapshot forms a lattice. In Section 7 we present a more abstract study of snapshots where the partial order of sets is replaced by an abstract partial order (the set identity of nodes of a partial order is lost).

1. Preliminaries

Throughout the paper we use standard set-theoretical notation and terminology.

We use $\emptyset$ to denote the empty set, and, for a set A, 2^A denotes the set of all subsets of A. For sets A and B, we use $A \cup B$, $A \cap B$, and $A - B$ to denote their union, intersection and difference, 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. The top of $\mathcal{F}$ is the set $X \in \mathcal{F}$ such that $Z \subseteq X$ for each $Z \in \mathcal{F}$, and the bottom of $\mathcal{F}$ is the set $Y \in \mathcal{F}$ such that $Y \subseteq Z$ for each $Z \in \mathcal{F}$. Clearly, if the top/bottom exists, then it is unique. We use $\mathbb{N}$ to denote the set of nonnegative integers, and $\mathbb{N}^+$ to denote the set of positive integers. For a bijection f we use f^{-1} to denote the inverse of f.

A *partial order* is an ordered pair $\varphi = (P, \leq)$, where P is a set and $\leq$ is a binary relation on P which is reflexive, antisymmetric and transitive. For $X \subseteq P$, $z \in P$ is an upper bound of X if $x \leq z$ for all $x \in X$; if also $z \leq t$ for each upper bound t of X, then z is the supremum of X, denoted $sup(X)$. For $X \subseteq P$, $z \in P$ is a lower bound of X if $z \leq x$ for all $x \in X$; if also $t \leq z$ for each lower bound t of X, then z is the infimum of X, denoted $inf(X)$. When $sup(P)$ exists then it is called the top of φ, denoted by $\top$. When $inf(P)$ exists then it is called the bottom of φ, denoted by $\bot$. If $sup(\{x, y\})$ and $inf(\{x, y\})$ exist for all $x, y \in P$, then φ is a *lattice*, and if $sup(X)$ and $inf(X)$ exist for all $X \subseteq P$, then φ is a *complete lattice*. Thus φ is a lattice if *every* finite subset $X \subseteq P$ has both supremum and infimum, and φ is a complete lattice if *every* subset $X \subseteq P$, finite or infinite, has both supremum and infimum. Clearly, a finite lattice (i.e., P is finite) is always complete, and a complete lattice has always the top and the bottom. Of particular interest for this paper will be lattices of the form $(\mathcal{L} \subseteq)$, where $\mathcal{L} \subseteq 2^Z$, for some set Z.

Note that a partial order $\varphi = (P, \leq)$ is a graph, where P is the set of nodes and $\leq$ is the set of edges. To provide a more compact representation of φ, one defines the *Hasse graph* of φ which is the graph $(P, \varrho_{\leq})$, where

$$\varrho_{\leq} = \{(x, y) : x \leq y \text{ and for no } z \in P - \{x, y\}, (x, z) \in \leq \text{ and } (z, y) \in \leq\}.$$

Thus the Hasse graph of φ results from φ by removing the "transitive" edges.

We will introduce now a couple of set-theoretic notions and prove a technical result concerning complete lattices that will be needed in this paper.

Let $\mathcal{F}_1, \mathcal{F}_2$ be nonempty families of sets. We say that $\mathcal{F}_1$ is *embedded in* $\mathcal{F}_2$ if for each $U \in \mathcal{F}_1$ and each $V \in \mathcal{F}_2$, $U \subseteq V$.

Let $\mathcal{L}$ be a family of sets and let $\mathcal{F}_1, \mathcal{F}_2 \subseteq \mathcal{L}$. We say that $\mathcal{F}_1$ is *separated from* $\mathcal{F}_2$ *in* $\mathcal{L}$ if there exists $U \in \mathcal{L}$ such that $\bigcup \mathcal{F}_1 \subseteq U \subseteq \bigcap \mathcal{F}_2$.

The following characterization of complete lattices will be used in Section 6 (although in this paper we will consider finite partial orders only, the following result is proved for arbitrary, i.e., also infinite, lattices).

Lemma 1.1. *Let $\mathcal{L}$ be a family of sets. Then $(\mathcal{L}, \subseteq)$ is a complete lattice if and only if*

(i) *$\mathcal{L}$ has both the top and the bottom,*
(ii) *if $\mathcal{F}_1, \mathcal{F}_2 \subseteq \mathcal{L}$ are such that $\mathcal{F}_1$ is embedded in $\mathcal{F}_2$, then $\mathcal{F}_1$ is separated from $\mathcal{F}_2$ in $\mathcal{L}$.*

Proof. (1) Assume that $(\mathcal{L}, \subseteq)$ is a complete lattice.
- (1i) Since $(\mathcal{L}, \subseteq)$ is complete, $\mathcal{L}$ has both the top and the bottom.
- (1ii) Assume that $\mathcal{F}_1, \mathcal{F}_2 \subseteq \mathcal{L}$ are such that $\mathcal{F}_1$ is embedded in $\mathcal{F}_2$. Since $(\mathcal{L}, \subseteq)$ is a complete lattice, $sup(\mathcal{F}_1) \in \mathcal{L}$. Clearly $\bigcup \mathcal{F}_1 \subseteq sup(\mathcal{F}_1)$ and, because $\mathcal{F}_1$ is embedded in $\mathcal{F}_2$, $sup(\mathcal{F}_1) \subseteq Z$ for each $Z \in \mathcal{F}_2$; hence $sup(\mathcal{F}_1) \subseteq \bigcap \mathcal{F}_2$. Therefore $\mathcal{F}_1$ is separated from $\mathcal{F}_2$ in $\mathcal{L}$.

(2) Assume that $\mathcal{L}$ satisfies conditions (i) and (ii) from the statement of the lemma.
- (2.1) Let $\mathcal{F}_1$ be an arbitrary nonempty subfamily of $\mathcal{L}$. Let $\mathcal{F}_2 = \{Z \in \mathcal{L} : T \subseteq Z \text{ for each } T \in \mathcal{F}_1\}$; thus $\mathcal{F}_2$ is the set of upper bounds of $\mathcal{F}_1$ in $(\mathcal{L}, \subseteq)$. Since, by condition (i), $\mathcal{L}$ contains the top element, $\mathcal{F}_2 \neq \emptyset$. By definition of $\mathcal{F}_2$, $\mathcal{F}_1$ is embedded in $\mathcal{F}_2$, and so, by condition (ii), there exists $U \in \mathcal{L}$ such that $\bigcup \mathcal{F}_1 \subseteq U$ and $U \subseteq \bigcap \mathcal{F}_2$. Since $U \in \mathcal{L}$ and $\bigcup \mathcal{F}_1 \subseteq U$, $U \in \mathcal{F}_2$. Since $U \subseteq \bigcap \mathcal{F}_2$, $U \subseteq Q$ for each $Q \in \mathcal{F}_2$. Thus $U = sup(\mathcal{F}_1)$. Consequently, any $\mathcal{F}_1 \subseteq \mathcal{L}$ has a supremum.
- (2.2) Analogously one proves that any subfamily of $\mathcal{L}$ has an infimum. It follows from (2.1) and (2.2) that every $\mathcal{F} \subseteq \mathcal{L}$ has both the supremum and infimum, and so $(\mathcal{L}, \subseteq)$ is a complete lattice.

The lemma follows now from (1) and (2). □

2. Reaction systems

In this section we recall from [2] the basic notions of reaction systems.

Two basic mechanisms underlying the functioning of biochemical reactions are facilitating and inhibiting. A biochemical reaction can take place if all of its reactants are present and all inhibitors are absent. Then, when a reaction takes place it produces the product. This reasoning is reflected in the formal definition of a reaction.

Definition 2.1. A *reaction* is a 3-tuple $a = (R, I, P)$ of finite sets.

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

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 $P_A = \bigcup_{a \in A} P_a$.

The reaction $(\emptyset, \emptyset, \emptyset)$ is called the *empty reaction* and denoted by Φ.

Definition 2.2. (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: $res_A(T) = \bigcup\{res_a(T) \mid a \in A\}$.

If $R_a \subseteq T$ and $I_a \cap T = \emptyset$, then we say that a is *enabled by* T; otherwise we say that a is *not enabled by* T. Then for a set of reactions A we say that A is *enabled by* T if each $a \in A$ is enabled by T. Thus a reaction a is enabled on a set T if T separates R_a from I_a : $R_a \subseteq T$ while $I_a \cap T = \emptyset$. Similarly a set of reactions A is enabled on T if T separates R_A from I_A.

We are ready now to recall a central notion of this paper.

Definition 2.3. A *reaction system*, abbreviated rs, is an ordered pair $\mathcal{A} = (S, A)$ such that S is a finite set, and A is a set of reactions in S.

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

The main notion concerning the functioning of a reaction system is defined as follows.

Definition 2.4. For a reaction system $\mathcal{A} = (S, A)$ and a set $T \subseteq S$, the *result of* $\mathcal{A}$ *on* T, denoted $res_{\mathcal{A}}(T)$, is defined by $res_{\mathcal{A}}(T) = res_A(T)$. The set $\{a \in A \mid a \text{ is enabled by } T\}$ is called the T*-activity of* $\mathcal{A}$ (or *activity of* $\mathcal{A}$ *on* T), denoted by $en_{\mathcal{A}}(T)$.

We may drop the subscript $\mathcal{A}$ in our notations whenever $\mathcal{A}$ is understood from the context of considerations.

We assume that, for each nonempty reaction a, $R_a \cap I_a = \emptyset$, $I_a \neq \emptyset$, and $P_a \neq \emptyset$.

Example 2.5. Let $\mathcal{A} = (S, A)$ be the rs such that $S = \{1, 2, 3, 4, 5\}$, and $A = \{a_1, a_2, a_3, a_4\}$, where $a_1 = (\{1\}, \{2\}, \{2\})$, $a_2 = (\{2\}, \{1\}, \{1\})$, $a_3 = (\{3\}, \{4\}, \{3\})$, $a_4 = (\{4\}, \{3\}, \{4\})$.
Intuitively, a_1 with a_2 form a flip-flop (for 1 and 2), a_3 and a_4 exclude each other, and $\{a_1, a_2\}$, $\{a_3, a_4\}$ are "mutually independent".

(i) For $T_1 = \{1, 2, 3\}$, $res_{a_1}(T_1) = res_{a_2}(T_1) = res_{a_4}(T_1) = \emptyset$, and $res_{a_3}(T_1) = \{3\}$. For $A_1 = \{a_1, a_2\}$, $res_{A_1}(T_1) = \emptyset$, and for $A_2 = \{a_1, a_3\}$, $res_{A_2}(T_1) = \{3\}$. Also, $res_{\mathcal{A}}(T_1) = \{3\}$.
(ii) For $T_2 = \{1, 3\}$, $res_{a_1}(T_2) = \{2\}$, $res_{a_2}(T_2) = \emptyset$, $res_{a_3}(T_2) = \{3\}$, and $res_{a_4}(T_2) = \emptyset$. For A_1, A_2 as above, $res_{A_1}(T_2) = \{2\}$, and $res_{A_2}(T_2) = \{2, 3\}$. Also, $res_A(T_2) = \{2, 3\}$.

Definition 2.6. Let $\mathcal{A} = (S, A)$ be a rs. An *interactive process* π in $\mathcal{A}$ is a pair of finite sequences $\pi = (\gamma, \delta)$ such that, for some $n \geq 1$, $\gamma = C_0, C_1, \ldots, C_n$, $\delta = D_1, \ldots, D_n$ where $C_0, \ldots, C_n, D_1, \ldots, D_n \subseteq S$, $D_1 = res_{\mathcal{A}}(C_0)$ and, for each $2 \leq i \leq n$, $D_i = res_{\mathcal{A}}(C_{i-1} \cup D_{i-1})$.

We will use the "arrow notation" $\pi : C_0 \to (D_1, C_1) \to \cdots \to (D_n, C_n)$ to represent an interactive process π as above.

The sequence $C_0, \ldots, C_n$ is the *interaction sequence of* π, and the sequence $D_1, \ldots, D_n$ is the *result sequence of* π. For each $1 \leq i \leq n$, we define $W_i = C_i \cup D_i$, and $W_0 = C_0$. The sequence $W_0, W_1, W_2, \ldots, W_n$ is called the *state sequence of* π, denoted by $sts(\pi)$, while W_0 is called the *initial state of* π. For each $0 \leq j \leq n$, the set C_j is called the *context of* W_j. Thus, for all $1 \leq i \leq n$, the ith result of π (i.e., D_i) is obtained from the state $(i-1)$ of π by applying $res_{\mathcal{A}}$. The sequence $E_0, E_1, \ldots, E_{n-1}$ of subsets of A such that $E_i = en_{\mathcal{A}}(W_i)$, for all $1 \leq i \leq n-1$, is called the *activity sequence of* π, denoted by $act(\pi)$. Also, STS($\mathcal{A}$) denotes the set of all *state sequences of* $\mathcal{A}$ (i.e., all state sequences of all interactive processes in $\mathcal{A}$).

Example 2.7. We continue Example 2.5.

(i) Since $res_{\mathcal{A}}(\{1, 3\}) = \{2, 3\}$ and $res_{\mathcal{A}}(\{2, 3\}) = \{1, 3\}$, $\pi_1 : \{1, 3\} \to (\{2, 3\}, \emptyset) \to (\{1, 3\}, \emptyset) \to (\{2, 3\}, \emptyset)$ is an interactive process in $\mathcal{A}$. Moreover, $sts(\pi_1) = \{1, 3\}, \{2, 3\}, \{1, 3\}, \{2, 3\}$, and $act(\pi_1) = \{a_1, a_3\}, \{a_3\}$.
(ii) $\pi_2 : \{1, 3\} \to (\{2, 3\}, \{1\}) \to (\{3\}, \emptyset) \to (\{3\}, \emptyset)$ is an interactive process in $\mathcal{A}$ with $sts(\pi_2) = \{1, 3\}, \{1, 2, 3\}, \{3\}, \{3\}$, and $act(\pi_2) = \{a_1, a_3\}, \{a_1, a_2, a_3\}, \{a_3\}$.
(iii) $\pi_3 : \{1, 3\} \to (\{2, 3\}, \{4\}) \to (\{1\}, \emptyset) \to (\{2\}, \{4\}) \to (\{1, 4\}, \emptyset)$ is an interactive process in $\mathcal{A}$ with

$$sts(\pi_3) = \{1, 3\}, \{2, 3, 4\}, \{1\}, \{2, 4\}, \{1, 4\}, \quad \text{and}$$
$$act(\pi_3) = \{a_1, a_3\}, \{a_2\}, \{a_1\}, \{a_2, a_4\}.$$

(iv) $\pi_4 : \{1, 3\} \to (\{2, 3\}, \{1, 4\}) \to (\emptyset, \{1, 3\}) \to (\{2, 3\}, \{1, 4\}) \to (\emptyset, \emptyset)$ is an interactive process in $\mathcal{A}$ with

$$sts(\pi_4) = \{1, 3\}, \{1, 2, 3, 4\}, \{1, 3\}, \{1, 2, 3, 4\}, \emptyset, \quad \text{and}$$
$$act(\pi_4) = \{a_1, a_3\}, \emptyset, \{a_1, a_3\}, \emptyset.$$

(v) $\pi_5 : \{1, 3\} \to (\{2, 3\}, \{1, 4\}) \to (\emptyset, \emptyset) \to (\emptyset, \{1, 2, 3, 4\}) \to (\emptyset, \emptyset)$ is an interactive process in $\mathcal{A}$ with

$$sts(\pi_5) = \{1, 3\}, \{1, 2, 3, 4\}, \emptyset, \{1, 2, 3, 4\}, \emptyset, \quad \text{and}$$
$$act(\pi_5) = \{a_1, a_3\}, \emptyset, \emptyset, \emptyset.$$

(vi) $\pi_6 : \{3\} \to (\{3\}, \emptyset) \to (\{3\}, \{4\}) \to (\emptyset, \{4\}) \to (\{4\}, \emptyset)$ is an interactive process in $\mathcal{A}$ with

$$sts(\pi_6) = \{3\}, \{3\}, \{3, 4\}, \{4\}, \{4\} \quad \text{and}$$
$$act(\pi_5) = \{a_3\}, \{a_3\}, \emptyset, \{a_4\}.$$

3. Extended reaction systems

In this paper we consider a generalization of a reaction system which results by equipping it with a restriction relation which determines which pairs of sets can form consecutive states in state sequences. A possible interpretation for a restriction relation is observability: only some successions of states are observable.

Definition 3.1. An *extended reaction system, ers* for short, is an ordered pair $\mathcal{E} = (\mathcal{A}, R)$, where $\mathcal{A} = (S, A)$ is a rs, and $R \subseteq 2^S \times 2^S$.

We refer to $\mathcal{A}$ as the *underlying reaction system of* $\mathcal{E}$, denoted by $und(\mathcal{E})$, and to R as the *restriction relation of* $\mathcal{E}$. We will also write $\mathcal{E}$ as a 3-tuple (S, A, R).

All the relevant notions, terminology and notation concerning reaction systems carry over to extended reaction systems (through their underlying reaction systems). However, the notion of an interactive process gets modified as follows.

Definition 3.2. Let $\mathcal{E} = (S, A, R)$ be an ers. An *interactive process in* $\mathcal{E}$ is an interactive process $\pi = (\gamma, \delta)$ in $und(\mathcal{E})$ such that $sts(\pi) = W_0, \ldots, W_n$ satisfies the *restriction condition*: for all $0 \leq i \leq n-1$, $(W_i, W_{i+1}) \in R$.

We assume in this paper that extended reaction systems satisfy also the *prolongation condition*: if $W_0, \ldots, W_n \in STS(\mathcal{E})$, $n \geq 1$, for an ers $\mathcal{E} = (S, A, R)$, then there exists a $W \subseteq S$ such that also $W_0, \ldots, W_n, W \in STS(\mathcal{E})$.

Definition 3.3. Let $\mathcal{E} = (S, A, R)$ be an ers, and let $t \in S$. We say that t is *periodic* (*in* $\mathcal{E}$) if there exists $n \in \mathbb{N}^+$ such that, for each $W_0, \ldots, W_n \in STS(\mathcal{E})$, $t \in W_0$ if and only if $t \in W_n$. The smallest n satisfying this condition is the *period of* t, denoted by $per_{\mathcal{E}}(t)$.

We use $per(\mathcal{E})$ to denote the set of periodic elements of $\mathcal{E}$.

Example 3.4. Let $\mathcal{E} = (\mathcal{A}, R)$ be the ers such that $\mathcal{A} = (S, A)$ is the rs from Example 2.5, and $R \subseteq 2^S \times 2^S$ is defined by: $(X, Y) \in R$ if and only if ($1 \in X$ if and only if $2 \in Y$ and $1 \notin Y$) and ($2 \in X$ if and only if $1 \in Y$ and $2 \notin Y$).

(i) Both 1 and 2 are periodic elements in $\mathcal{E}$, and $per_{\mathcal{E}}(1) = per_{\mathcal{E}}(2) = 2$.
(ii) Inspecting the interactive processes $\pi_1, \ldots, \pi_6$ from Example 2.7, we notice (by considering their state sequences) that only π_1, π_3 and π_6 satisfy the prolongation condition. Thus π_1, π_3, and π_6 are also interactive processes in $\mathcal{E}$, while neither π_2 nor π_4 nor π_5 is an interactive process in $\mathcal{E}$.

Note that the notion of a periodic element is intrinsic for *extended* reaction systems. Elements of reaction systems cannot be periodic, which (somewhat informally) can be shown as follows.
Let $\mathcal{A} = (S, A)$ be a rs, and assume that $t \in S$ is a periodic element of $\mathcal{A}$. Assume, e.g., that $per_{\mathcal{A}}(t) = 3$.
Let $\tau = W_0, W_1, W_2, W_3 \in STS(\mathcal{A})$ be such that $t \in W_0$.
We modify τ to $\tau' = W_0, W_1, W_2', W_3'$ as follows.
Let $\pi = C_0 \to (D_1, C_1) \to (D_2, C_2) \to (D_3, C_3)$ be an interactive process in $\mathcal{A}$ such that $sts(\pi) = \tau$. Let $Z_t = \{a \in en_{\mathcal{A}}(W_2) : t \in P_a\}$, and, for each $a \in Z_t$, let y_a be an arbitrary element of I_a. Then let $U_t = \{y_a : a \in Z_t\}$ — hence U_t contains at least one inhibiting element for each reaction in Z_t. Now, we modify context C_2 by adding U_t to it, obtaining $C_2' = C_2 \cup U_t$ and $W_2' = D_2 \cup C_2'$, and we modify context C_3 by removing t from it (if it was there), obtaining $C_3' = C_3 - \{t\}$ and $W_3' = W_3 \cup C_3'$. Since $t \notin C_3'$ and t cannot be produced by $en_{\mathcal{E}}(W_2')$, $t \notin W_3'$, contradicting the fact that $per_{\mathcal{A}}(t) = 3$; hence contradicting the fact that t is periodic. Thus $\mathcal{A}$ cannot contain periodic elements.

The existence of periodic elements in extended reaction systems leads to a more refined view of states.

Definition 3.5. Let $\mathcal{E} = (S, A, R)$ be an ers.

(1) For $T \subseteq S$, the *periodic part of* T, denoted $per_{\mathcal{E}}(T)$, is defined by $per_{\mathcal{E}}(T) = T \cap per(\mathcal{E})$.

(2) Let $\tau = W_0, \ldots, W_n \in STS(\mathcal{E})$, and let $1 \leq i \leq n$.
  (2.1) The *truly produced i-part of* τ, denoted by $trp_\tau(i)$, is defined by $trp_\tau(i) = res_{\mathcal{E}}(W_{i-1}) - per_{\mathcal{E}}(W_i) = res_{\mathcal{E}}(W_{i-1}) - per(\mathcal{E})$.
  (2.2) The *true i-context* of τ, denoted by $trc_\tau(i)$, is defined by $trc_\tau(i) = W_i - (per_{\mathcal{E}}(W_i) \cup trp_\tau(i)) = W_i - (per_{\mathcal{E}}(W_i) \cup res_{\mathcal{E}}(W_{i-1}))$.

Example 3.6. We continue Example 3.4.

(i) Consider the interactive process π_1.
Let $\tau_1 = sts(\pi_1) = W_0, W_1, W_2, W_3$, hence $W_0 = W_2 = \{1, 3\}$, and $W_1 = W_3 = \{2, 3\}$. We have then $per_{\mathcal{E}}(W_0) = per_{\mathcal{E}}(W_2) = \{1\}, per_{\mathcal{E}}(W_1) = per_{\mathcal{E}}(W_3) = \{2\}$, $trp_{\tau_1}(1) = trp_{\tau_1}(2) = trp_{\tau_1}(3) = \{3\}$, and $trc_{\tau_1}(1) = trc_{\tau_1}(2) = trc_{\tau_1}(3) = \emptyset$.
(ii) Consider the interactive process π_3.
Let $\tau_3 = sts(\pi_3) = W_0, W_1, W_2, W_3, W_4$, hence $W_0 = \{1, 3\}, W_1 = \{2, 3, 4\}, W_2 = \{1\}, W_3 = \{2, 4\}$, and $W_4 = \{1, 4\}$. Then $per_{\mathcal{E}}(W_0) = per_{\mathcal{E}}(W_2) = per_{\mathcal{E}}(W_4) = \{1\}, per_{\mathcal{E}}(W_1) = per_{\mathcal{E}}(W_3) = \{2\}$, $trp_{\tau_3}(1) = \{3\}, trp_{\tau_3}(2) = trp_{\tau_3}(3) = \emptyset, trp_{\tau_3}(4) = \{4\}, trc_{\tau_3}(1) = trc_{\tau_3}(3) = \{4\}$, and $trc_{\tau_3}(2) = trc_{\tau_3}(4) = \emptyset$.
(iii) Consider the interactive process π_6.
Let $\tau_6 = sts(\pi_6) = W_0, W_1, W_2, W_3, W_4$, hence now $W_0 = W_1 = \{3\}, W_2 = \{3, 4\}, W_3 = W_4 = \{4\}$. Then $per_{\mathcal{E}}(W_i) = \emptyset$, for $0 \leq i \leq 4$, $trp_{\tau_6}(1) = trp_{\tau_6}(2) = \{3\}, trp_{\tau_6}(3) = \emptyset, trp_{\tau_6}(4) = \{4\}, trc_{\tau_6}(1) = trc_{\tau_6}(4) = \emptyset$, and $trc_{\tau_6}(2) = trc_{\tau_6}(3) = \{4\}$.

4. Events

Given a state $W_i, i \geq 1$, in a state sequence τ, a subset U of W_i is just that: a mathematical (notion of a) subset. However, if we consider the subset $res_{E_i}(U)$ of W_{i+1}, then it is not only a mathematical subset of W_{i+1}, but also the result/product of the set E_i of reactions acting on U. Since reactions in an ers are in our framework formal models of biochemical reactions, we may interpret $res_{E_i}(U)$ as a material/physical object. If we now follow the fate/evolution of U as it gets transformed by the consecutive sequence of sets of reactions $E_i, E_{i+1}, \ldots$ then we get an event (or a generalized event) which is formally defined as follows.

Definition 4.1. Let $\mathcal{E} = (S, A, R)$ be an ers, let $\tau = W_0, \ldots, W_n \in STS(\mathcal{E})$, let $i, j \in \{1, \ldots, n\}$ be such that $i \leq j$, and let $\omega = Q_i, \ldots, Q_j$ be such that $Q_i \subseteq W_i, \ldots, Q_j \subseteq W_j$.

(i) ω is a *generalized event in* τ if
  (i.1) there is $U \subseteq W_{i-1}$ such that $Q_i = (res_{E_{i-1}}(U \cup per_{\mathcal{E}}(W_{i-1}))) \cap trp_\tau(i)$, and
  (i.2) for each $k \in \{i+1, \ldots, j\}$, $Q_k = (res_{E_{k-1}}(Q_{k-1} \cup per_{\mathcal{E}}(W_{k-1}))) \cap trp_\tau(k)$, where, for each $0 \leq j \leq n-1$, $E_j = en_{\mathcal{E}}(W_j)$.
(ii) ω is an *event* (*in* τ) if ω is a generalized event such that all $Q_i, \ldots, Q_{j-1}$ are nonempty.

One should note that in the definition of Q_i (see (i.1) above) one transforms $U \cup per_{\mathcal{E}}(W_{i-1})$ by E_{i-1}, rather than U alone. The reason is that periodic elements of W_{i-1} are present in W_{i-1} independently of how W_{i-1} was obtained, and therefore they will always participate in the transformation by E_{i-1}. Similarly, Q_i is not defined as $res_{E_{i-1}}(U \cup per_{\mathcal{E}}(W_{i-1}))$, but rather as $(res_{E_{i-1}}(U \cup per_{\mathcal{E}}(W_{i-1}))) \cap trp_\tau(i) = res_{E_{i-1}}(U \cup per_{\mathcal{E}}(W_{i-1})) - per(\mathcal{E})$, because the periodic elements of W_i are there independently of the transformation of $U \cup per_{\mathcal{E}}(W_{i-1})$ by E_{i-1}, and so we do not count them as produced by transforming $U \cup per_{\mathcal{E}}(W_{i-1})$. Analogous remarks hold for the definition of Q_k in (i.2) above.

For U and ω as above, we say that ω *is tracing the fate of* U. The sets $Q_i, \ldots, Q_j$ are called the *modules* of ω, and, for $i \leq k \leq j$, Q_k is the *k-module of* ω. We also say that ω is a *generalized (i, j)-event in* τ, and that ω is *running from i to j* (and it is *passing through each* $k \in \{i, \ldots, j\}$); when $i = j$ then we say that ω is an *i-event*. Then, for each pair (r, s) such that $i \leq r \leq s \leq j$, the generalized event $Q_r, \ldots, Q_s$ is a *restriction of* ω; if $(r, s) \neq (i, j)$, then $Q_r, \ldots, Q_s$ is a *strict restriction of* ω.

It will be convenient to have a notation for the transformation used in Definition 4.1. Thus, for each $i \in \{1, \ldots, n-1\}$ and each $Q \subseteq W_i$, we use $tran_{\tau,i}(Q)$ to denote the set $(res_{E_i}(Q \cup per_{\mathcal{E}}(W_i))) \cap trp_\tau(i+1) = res_{E_{i-1}}(U \cup per_{\mathcal{E}}(W_{i-1})) - per(\mathcal{E})$.

We give now a classification of events which is helpful in the understanding of the nature of evolution of modules in reaction systems.
An event ω is called (using the notation from Definition 4.1):

- *trivial* if $i = j$ and $Q_i = \emptyset$,
- *maverick* if $Q_i \neq \emptyset$, but $Q_{i+1} = \emptyset$,
- *reduced* if all modules of ω are nonempty,
- *complete* if it is not a strict restriction of any event, and
- *maximal* if it is not a strict restriction of any reduced event.

Example 4.2. We continue Example 3.6.
(i) Consider the interactive process π_1.

- $\{3\}$ is a 1-event, it is tracing the fate of $\{1, 3\}$ and of $\{3\}$; it is also a 2-event tracing the fate of $\{2, 3\}$ and of $\{3\}$, and a 3-event tracing the fate of $\{1, 3\}$ and of $\{3\}$.
- $\{3\}, \{3\}$ is a $(1, 2)$-event tracing the fate of $\{1, 3\}$ and of $\{3\}$; it is also a $(2, 3)$-event tracing the fate of $\{2, 3\}$ and $\{3\}$.
- $\{3\}, \{3\}, \{3\}$ is a complete $(1, 3)$-event tracing the fate of $\{1, 3\}$ and $\{3\}$.
- $\emptyset$ is a (trivial) 1-event tracing the fate of $\emptyset$ and of $\{1\}$; it is also a 2-event tracing the fate of $\emptyset$ and of $\{2\}$, and a 3-event tracing the fate of $\emptyset$ and of $\{1\}$. It is a trivial event.

(ii) For the interactive process π_3

- $\{3\}$ is a 1-event, it is tracing the fate of $\{1, 3\}$ and $\{3\}$.
- $\{4\}$ is a 4-event, it is tracing the fate of $\{2, 4\}$ and $\{4\}$.
- $\emptyset$ is a 1-event tracing the fate of $\{2\}$ and $\emptyset$; it is also a 2-event tracing the fate of *every* subset of W_1, it is also a 3-event tracing the fate of $\{1\}$ and $\emptyset$, and a 4-event tracing the fate of $\{2\}$ and $\emptyset$.

(iii) For the interactive process π_6

- $\{3\}$ is a 1-event, it is tracing the fate of $\{3\}$; it is also a 2-event tracing the fate of $\{3\}$.
- $\{4\}$ is a 4-event, it is tracing the fate of $\{4\}$.
- $\{3\}, \{3\}$ is a $(1, 2)$-event tracing the fate of $\{3\}$.
- $\{3\}, \{3\}, \emptyset$ is a $(1, 3)$-event tracing the fate of $\{3\}$.
- $\{3\}, \{3\}, \emptyset, \emptyset$ is a generalized $(1, 4)$-event (but not an event) tracing the fate of $\{3\}$.
- $\emptyset$ is a 1-event tracing the fate of $\emptyset$; it is also a 2-event tracing the fate of $\emptyset$, and a 3-event tracing the fate of *every* subset of W_2, and a 4-event tracing the fate of $\emptyset$.
- $\emptyset, \emptyset$ is a generalized $(1, 3)$-event tracing the fate of $\emptyset$; it is also a generalized $(2, 3)$-event tracing the fate of $\emptyset$, and a generalized $(3, 4)$-event tracing the fate of every subset of W_2.
- $\emptyset, \emptyset, \emptyset$ is a generalized $(1, 3)$-event tracing the fate of $\emptyset$; it is also a generalized $(2, 4)$-event tracing the fate of $\emptyset$.
- $\emptyset, \emptyset, \emptyset, \emptyset$ is a generalized $(1, 4)$-event tracing the fate of $\emptyset$.

Although empty sets are mathematically convenient they have very limited physical interpretation. Therefore *in this paper we consider only events*. In an event the empty set may occur only as the last module signaling the "death" of an event. In a generalized event empty modules may occur in many ways, allowing also "rising from the grave", where the nonempty module follows the empty module.

5. Modules and snapshots

We move now to investigate formal properties of events. We begin by the merging property of events: when an event ω merges with an event ω' in state W_i (i.e., the module of ω in W_i is a subset of the module of ω' in W_i) then they remain merged as they evolve through the consecutive states $W_{i+1}, W_{i+2}, \ldots$.

Lemma 5.1. *Let $\mathcal{E}$ be an ers, and let $\tau = W_0, \ldots, W_n \in STS(\mathcal{E})$. Let $1 \leq i < j \leq n$, and let $\omega = Q_i, \ldots, Q_j$ and $\omega' = Q'_i, \ldots, Q'_j$ be (i, j)-events in τ. If $Q_i \subseteq Q'_i$, then $Q_k \subseteq Q'_k$ for all $k \in \{i, \ldots, j\}$.*

Proof. This follows directly from Definition 4.1(i.2). □

Events trace the fate (the evolution) of subsets of states in a given state sequence. In our framework one can view events as the prime mechanism for the formation of modules. When an event ω is passing through a state W_k it leaves a "trace" there, viz., its k-module. The set of all such traces left by all events passing through W_k form the snapshot of W_k. This is formally defined as follows.

Definition 5.2. Let $\mathcal{E} = (S, A, R)$ be an ers, let $\tau = W_0, \ldots, W_n \in STS(\mathcal{E})$ and let $1 \leq k \leq n$.

(i) A *k-module of τ* is a subset $Q \subseteq W_k$ for which there exists an event ω in τ passing through k such that Q is the k-module of ω.
(ii) The *k-snapshot of τ*, denoted by $snp_\tau(k)$, is the set of all k-modules of τ.

Given a state sequence $\tau = W_0, W_1, \ldots, W_n$ we get the corresponding sequence of snapshots $snp_\tau(1), \ldots, snp_\tau(n)$, called the *snapshot sequence of τ* (denoted by $snp(\tau)$) and a *snapshot sequence of $\mathcal{E}$*. We will also use $\mathcal{S}_i$ to denote $snp_\tau(i)$; thus $\mathcal{S}$ with a possible subscript is reserved to denote a snapshot (in the same way as we use W to denote a state). Thus, $snp(\tau) = \mathcal{S}_1, \ldots, \mathcal{S}_n$.

Now for each $1 \leq k \leq n-1$, we define the partial function $next_{\tau,k} : snp_\tau(k) \to snp_\tau(k+1)$ as follows. For $Q \in snp_\tau(k)$, $next_{\tau,k}(Q) = Q'$ if and only if there exists an event ω in τ such that Q is the nonempty k-module of ω, and Q' is the nonempty $(k+1)$-module of ω. If we extend the $next_{\tau,k}$ function also to pairs (Q, Q'), where Q is nonempty but Q' may be empty, then we obtain $suc_{\tau,k}$ function.
We will use the notations $next_k$ and suc_k whenever τ is clear from the context of considerations.

Example 5.3. We continue Example 4.2.

(i) For the interactive process π_1, the snapshot sequence is $\mathcal{S}_1, \mathcal{S}_2, \mathcal{S}_3$, where $\mathcal{S}_1 = \mathcal{S}_2 = \mathcal{S}_3 = \{\{3\}, \emptyset\}$.
(ii) For the interactive process π_3, the snapshot sequence is $\mathcal{S}_1, \mathcal{S}_2, \mathcal{S}_3, \mathcal{S}_4$, where $\mathcal{S}_1 = \{\{3\}, \emptyset\}$, $\mathcal{S}_2 = \mathcal{S}_3 = \{\emptyset\}$, $\mathcal{S}_5 = \{\{4\}, \emptyset\}$.
(iii) For the interactive process π_6, the snapshot sequence is $\mathcal{S}_1, \mathcal{S}_2, \mathcal{S}_3, \mathcal{S}_4$, where $\mathcal{S}_1 = \mathcal{S}_2 = \{\{3\}, \emptyset\}$, $\mathcal{S}_3 = \{\emptyset\}$, and $\mathcal{S}_4 = \{\{4\}, \emptyset\}$.

Example 5.4. Let $\mathcal{E} = (S, A, R)$ be the ers such that $S = \{1, 2, 3, 4, 5, 6\}$, $A = \{b_1, b_2, b_3, b_4\}$ with $b_1 = (\{1\}, \{2\}, \{1, 6\})$, $b_2 = (\{2\}, \{2\}, \{1, 6\})$, $b_3 = (\{3\}, \{5\}, \{1, 3\})$, $b_4 = (\{1, 4\}, \{5\}, \{4\})$, and $R \subseteq 2^S \times 2^S$ is defined by: $(X, Y) \in R$ if and only if ($1 \in X$ if and only if $1 \in Y$). Hence $per(\mathcal{E}) = \{1\}$ and $per_{\mathcal{E}}(1) = 1$.

Consider the interactive process π in $\mathcal{E}$ such that $\pi : \{1, 3, 4\} \to (\{1, 3, 4, 6\}, \{2\}) \to (\{1, 3, 4\}, \{2\}) \to (\{1, 3, 4\}, \{5\}) \to (\{6\}, \{1, 2, 3, 4\})$. Hence $\tau = sts(\pi) = W_0, W_1, W_2, W_3, W_4$, where $W_0 = \{1, 3, 4\}$, $W_1 = \{1, 2, 3, 4, 6\}$, $W_2 = \{1, 2, 3, 4\}$, $W_3 = \{1, 3, 4, 5\}$, $W_4 = \{1, 2, 3, 4, 6\}$, and $act(\tau) = \{b_1, b_3, b_4\}$, $\{b_3, b_4\}$, $\{b_3, b_4\}$, $\{b_1\}$.

Here are some events in τ.

– $\{3, 4, 6\}, \{3, 4\}, \{3, 4\}, \{6\}$ is a maximal $(1, 4)$-event (tracing the fate of $\{1, 3, 4\}$ and $\{3, 4\}$).
– $\{3, 6\}, \{3\}, \{3\}, \{6\}$ is a maximal $(1, 4)$-event.
– $\{4, 6\}, \{4\}, \{4\}, \{6\}$ is a maximal $(1, 4)$-event.
– $\{6\}, \emptyset$ is a maverick $(1, 2)$-event.

The snapshot sequence of τ is $\mathcal{S}_1, \mathcal{S}_2, \mathcal{S}_3, \mathcal{S}_4$, where $\mathcal{S}_1 = \{\{3, 4, 6\}, \{3, 6\}, \{4, 6\}, \{6\}\}$, $\mathcal{S}_2 = \mathcal{S}_3 = \{\{3, 4\}, \{3\}, \{4\}, \emptyset\}$, and $\mathcal{S}_4 = \{\{6\}\}$.

We will relate now the transformation of a module Q common to two states W_k and W'_ℓ from possibly different state sequences τ and τ', providing that the two states are in the same "phase", i.e., they have the same set of periodic elements. Assume that Q is the k-module of an event ω of τ and it is also the ℓ-module of an event ω' of τ'. It turns out that if $W_k \subseteq W'_\ell$, then the successor of Q in ω' is a subset of the successor of Q in ω. The intuition behind this result is that, because of the inhibiting mechanism, for an i-module Q, everything outside Q in W_i (i.e., $W_i - Q$) is an "adversary" of Q in the production of its successor module.

Lemma 5.5. *Let $\mathcal{E}$ be an ers, and let $\tau, \tau' \in STS(\mathcal{E})$, where $\tau = W_0, \ldots, W_n$ and $\tau' = W'_0, \ldots, W'_m$, with $n, m \geq 2$. Let $k \in \{1, \ldots, n-1\}$, and $\ell \in \{1, \ldots, m-1\}$ be such that $per_{\mathcal{E}}(W_k) = per_{\mathcal{E}}(W'_\ell)$. Let $Q \in snp_\tau(k) \cap snp_{\tau'}(\ell)$ be nonempty. If $W_k \subseteq W'_\ell$, then $suc_{\tau',\ell}(Q) \subseteq suc_{\tau,k}(Q)$.*

Proof. Let $und(\mathcal{E}) = (S, A)$.
Note that $suc_{\tau',\ell}(Q) = (res_{B'}(Q \cup per_{\mathcal{E}}(W'_\ell))) \cap trp_{\tau'}(\ell+1)$, where $B' = \{a \in en_{\mathcal{E}}(W'_\ell) : a \in en_{\mathcal{E}}(Q \cup per_{\mathcal{E}}(W'_\ell))\}$. Clearly,

$$B' = \{a \in A : R_a \subseteq Q \cup per_{\mathcal{E}}(W'_\ell) \text{ and } I_a \cap W'_\ell = \emptyset\}. \tag{1}$$

On the other hand, $suc_{\tau,k}(Q) = (res_B(Q \cup per_{\mathcal{E}}(W_k))) \cap trp_\tau(k+1)$, where $B = \{a \in en_{\mathcal{E}}(W_k) : a \in en_{\mathcal{E}}(Q \cup per_{\mathcal{E}}(W_k))\}$. Clearly,

$$B = \{a \in A : R_a \subseteq Q \cup per_{\mathcal{E}}(W_k) \text{ and } I_a \cap W_k = \emptyset\}. \tag{2}$$

Since $W_k \subseteq W'_\ell$, $\{a \in A : I_a \cap W'_\ell = \emptyset\} \subseteq \{a \in A : I_a \cap W_k = \emptyset\}$. Thus, since $per_{\mathcal{E}}(W_k) = per_{\mathcal{E}}(W'_\ell)$, (1) and (2) implies that $B' \subseteq B$. Since $per_{\mathcal{E}}(W_k) = per_{\mathcal{E}}(W'_\ell)$, this implies that $(res_{B'}(Q \cup per_{\mathcal{E}}(W'_\ell))) \cap trp_{\tau'}(\ell+1) = res_{B'}(Q \cup per_{\mathcal{E}}(W'_\ell)) - per(\mathcal{E}) \subseteq res_B(Q \cup per_{\mathcal{E}}(W_k)) - per(\mathcal{E}) = (res_B\ (Q \cup per_{\mathcal{E}}(W_k))) \cap trp_\tau(k+1)$.
Consequently, $suc_{\tau',\ell}(Q) \subseteq suc_{\tau,k}(Q)$. □

6. The structure of snapshots

Since each snapshot $\mathcal{S}_k$ is a family of sets (subsets of W_k), $(\mathcal{S}_k, \subseteq)$ is a partial order. In this section we analyze in detail the structure of these partial orders.

Lemma 6.1. *Let $\mathcal{E}$ be an ers, let $\tau = W_0, \ldots, W_n \in STS(\mathcal{E})$, and let $1 \leq k \leq n$. Then the partial order $(\mathcal{S}_k, \subseteq)$ contains both the bottom and the top.*

Proof. (1) Consider W_{k-1} and choose $U = \emptyset$.
By Definition 4.1, $Q_k = tran_{\tau,k-1}(U)$ is the first module of an event beginning in k, and so $Q_k \in \mathcal{S}_k$. It is also clear from Definition 4.1 that $Q_k \subseteq Q$ for each $Q \in \mathcal{S}_k$. Therefore Q_k is the bottom element of $(\mathcal{S}_k, \subseteq)$.
(2) Consider W_{k-1} and choose $U = W_{k-1}$.
By Definition 4.1, $Q_k = tran_{\tau,k-1}(U)$ is the first module of an event beginning in k, and so $Q_k \in \mathcal{S}_k$. It is also clear from Definition 4.1 that $Q \subseteq Q_k$ for each $Q \in \mathcal{S}_k$. Therefore Q_k is the top element of $\mathcal{S}_k$.
Lemma 6.1 follows now from (1) and (2). □

We will use $\bot_k$ and $\top_k$ to denote the bottom and the top elements of $\mathcal{S}_k$ respectively. Note that by Lemma 5.1, $next_k(\top_k) = \top_{k+1}$, for $k \in \{1, \ldots, n-1\}$. Also, if $next_k(\bot_k)$ is defined, then $next_k(\bot_k) = \bot_{k+1}$.

Because the empty module $\emptyset$ has really no "physical interpretation", but rather it is a signaling of the termination (the death) of an event, it is convenient to consider snapshots with $\emptyset$ removed. Accordingly, given a snapshot sequence $\mathcal{S}_1, \ldots, \mathcal{S}_n$ we set $\bar{\mathcal{S}}_k = \mathcal{S}_k - \{\emptyset\}$, for each $1 \leq k \leq n$. Then we also modify the $next_k$ functions to $rnext_k$ functions, where, for each $1 \leq k \leq n-1$, $rnext_k$ is $next_k$ restricted to $\bar{\mathcal{S}}_k$.

We state and prove now an important property of snapshots.

Theorem 6.2. *Let $\mathcal{E}$ be an ers, let $\tau = W_0, W_1, \ldots, W_n$, with $n \geq 2$, be a state sequence of $\mathcal{E}$, and let $\mathcal{S}_k, \mathcal{S}_{k+1}$ be two consecutive snapshots of τ for some $1 \leq k \leq n-1$. If $\mathcal{F}_1, \mathcal{F}_2 \subseteq \bar{\mathcal{S}}_k$ are nonempty families of sets such that $\mathcal{F}_1$ is embedded in $\mathcal{F}_2$ and $next_k$ is defined on all modules in $\mathcal{F}_1 \cup \mathcal{F}_2$, then $next_k(\mathcal{F}_1)$ is separated from $next_k(\mathcal{F}_2)$ in $\mathcal{S}_{k+1}$.*

Proof. Let $\mathcal{S}_k, \mathcal{S}_{k+1}$ and $\mathcal{F}_1, \mathcal{F}_2$ be as in the statement of the theorem. Let $U = tran_{\tau,k}(\bigcup \mathcal{F}_1)$. From the definition of U it follows that $U \in \mathcal{S}_{k+1}$.
Note that, for each $V \in \mathcal{F}_1$, $V \cup per_{\mathcal{E}}(W_k) \subseteq \bigcup \mathcal{F}_1 \cup per_{\mathcal{E}}(W_k)$. Since $next_k$ is defined on all modules in $\mathcal{F}_1$, this implies that,

$$\text{for each } V \in \mathcal{F}_1, \quad next_k(V) \subseteq U. \tag{1}$$

Also, since $\mathcal{F}_1$ is embedded in $\mathcal{F}_2$, for each $Z \in \mathcal{F}_2$, $\bigcup \mathcal{F}_1 \cup per_{\mathcal{E}}(W_k) \subseteq Z \cup per_{\mathcal{E}}(W_k)$. Since $next_k$ is defined on all modules in $\mathcal{F}_2$, this implies that,

$$\text{for each } Z \in \mathcal{F}_2, \quad U \subseteq next_k(Z). \tag{2}$$

Since $U \in \mathcal{S}_{k+1}$, it follows then from (1) and (2) that $next_k(\mathcal{F}_1)$ is separated in $\mathcal{S}_{k+1}$ from $next_k(\mathcal{F}_2)$. Thus the theorem holds. □

Thus one can view (extended) reaction systems as self-organizing systems, where a possible goal of its interactive processes is to ensure (improve on) separability!

A run of an ers $\mathcal{E}$ (i.e., an interactive process of $\mathcal{E}$) produces a sequence of snapshots $\mathcal{S}_1, \ldots, \mathcal{S}_k, \ldots, \mathcal{S}_n$ where in general there may be no (mathematical) similarity between two consecutive snapshots $\mathcal{S}_k$ and $\mathcal{S}_{k+1}$. But when a "strong similarity" between $\mathcal{S}_k$ and $\mathcal{S}_{k+1}$ occurs one gets stability. A natural way to define a strong similarity is to require that $rnext_k$ is an isomorphism between $(\bar{\mathcal{S}}_k, \subseteq)$ and $(\bar{\mathcal{S}}_{k+1}, \subseteq)$. When this happens, we get a *local* stability — it is local because it may happen that then again there is no similarity between $\mathcal{S}_{k+1}$ and $\mathcal{S}_{k+2}$. This is formalised as follows.

Definition 6.3. Let $\mathcal{E}$ be an ers, let $\tau = W_0, W_1, \ldots, W_n \in STS(\mathcal{E})$, with $n \geq 2$, and let $\mathcal{S}_k, \mathcal{S}_{k+1}$ be two consecutive snapshots of τ for some $1 \leq k \leq n-1$. We say that $(\mathcal{S}_k, \mathcal{S}_{k+1})$ is a *locally stable situation* if $rnext_k$ is an isomorphism between $(\bar{\mathcal{S}}_k, \subseteq)$ and $(\bar{\mathcal{S}}_{k+1}, \subseteq)$.

It turns out that local stability is reflected in the structure of the corresponding snapshots: if $(\mathcal{S}_k, \mathcal{S}_{k+1})$ is a locally stable situation, then both $\mathcal{S}_k$ and $\mathcal{S}_{k+1}$ are complete lattices.

Corollary 6.4. *Let $\mathcal{E}$ be an ers, let τ be a state sequence, and let $\mathcal{S}, \mathcal{S}'$ be two consecutive snapshots of τ. If $(\mathcal{S}, \mathcal{S}')$ is a locally stable situation, then both $(\mathcal{S}, \subseteq)$ and $(\mathcal{S}', \subseteq)$ are complete lattices.*

Proof. Let $\tau, \mathcal{S}$, and $\mathcal{S}'$ be as in the statement of the corollary, say $\tau = W_0, W_1, \ldots, W_n$, with $n \geq 2$, and $\mathcal{S} = \mathcal{S}_k$, $\mathcal{S}' = \mathcal{S}_{k+1}$, for some $1 \leq k \leq n-1$. We define the function $mnext_k : \mathcal{S}_k \to \mathcal{S}_{k+1}$ as follows:

(i) if $next_k(\perp_k)$ is defined, then $mnext_k(Q) = next_k$, and
(ii) if $next_k(\perp_k)$ is not defined, then $mnext_k(Q) = next_k(Q)$ for all $Q \in \mathcal{S}_k$ such that $Q \neq \perp_k$, and $mnext_k(\perp_k) = \perp_{k+1}$. Thus $mnext_k$ is $next_k$ possibly modified on $\perp_k$.

Let $\mathcal{F}_1, \mathcal{F}_2$ be arbitrary two nonempty subfamilies of $\mathcal{S}_{k+1}$ such that $\mathcal{F}_1$ is embedded in $\mathcal{F}_2$.

Since $(\mathcal{S}_k, \mathcal{S}_{k+1})$ is a locally stable situation, $rnext_k$ is an isomorphism between $(\bar{\mathcal{S}}_k, \subseteq)$ and $(\bar{\mathcal{S}}_{k+1}, \subseteq)$. It follows then from the definition of $mnext_k$ that $mnext_k$ is an isomorphism between $(\mathcal{S}_k, \subseteq)$ and $(\mathcal{S}_{k+1}, \subseteq)$. Therefore, $\mathcal{F}'_1 = mnext_k^{-1}(\mathcal{F}_1)$ and $\mathcal{F}'_2 = mnext_k^{-1}(\mathcal{F}_2)$ are subfamilies of $\mathcal{S}_k$ such that $\mathcal{F}'_1$ is embedded in $\mathcal{F}'_2$. Hence, by Theorem 6.2, $mnext_k(\mathcal{F}'_1) = \mathcal{F}_1$ is separated from $mnext_k(\mathcal{F}'_2) = \mathcal{F}_2$ in $\mathcal{S}_{k+1}$. Since $\mathcal{F}_1, \mathcal{F}_2$ are two arbitrary nonempty subfamilies of $\mathcal{S}_{k+1}$ such that $\mathcal{F}_1$ is embedded in $\mathcal{F}_2$, it follows from Lemmas 6.1 and 1.1 that $(\mathcal{S}_{k+1}, \subseteq)$ is a complete lattice. Because $(\mathcal{S}_k, \subseteq)$ is isomorphic with $(\mathcal{S}_{k+1}, \subseteq)$, also $(\mathcal{S}_k, \subseteq)$ is a complete lattice. Hence the corollary holds. □

We end this section by pointing out that having $\bar{\mathcal{S}}_k = \bar{\mathcal{S}}_{k+1}$ does not necessarily imply that $rnext_k$ is an isomorphism of $\bar{\mathcal{S}}_k$ onto $\bar{\mathcal{S}}_{k+1}$.

Example 6.5. Let $\mathcal{E} = (S, A, R)$ be the ers such that $S = \{f, h, p, q, z\}$, $A = \{a_1, a_2, a_3, a_4\}$ with $a_1 = (\{q\}, \{f\}, \{u, v\})$, $a_2 = (\{p\}, \{f\}, \{u\})$, $a_3 = (\{z\}, \{f\}, \{u\})$, $a_4 = (\{u, v\}, \{f\}, \{u, v\})$, and $R = 2^S \times 2^S$. Hence R is not restrictive; thus in fact we consider the rs $\mathcal{A} = (S, A)$.

Consider the interactive process π in $\mathcal{E}$ such that $\pi : \{h, p, q\} \to (\{u, v\}, \{z\}) \to (\{u, v\}, \emptyset)$.

Hence $\tau = sts(\pi) = W_0, W_1, W_2$, where $W_0 = \{h, p, q\}$, $W_1 = \{u, v, z\}$, $W_2 = \{u, v\}$, and $act(\tau) = \{a_1, a_2\}, \{a_3, a_4\}$.

There is only one reduced event, viz., $(1, 2)$-event $\{u, v\}, \{u, v\}$, and only one maverick event, viz., $(1, 2)$-event $\{u\}, \emptyset$. Also, event $\{u, v\}$, event $\{u\}$, and event $\emptyset$ are both 1-events and 2-events. As a matter of fact, $\mathcal{S}_1 = \mathcal{S}_2 = \{\{u, v\}, \{u\}, \emptyset\}$. On the other hand, $rnext_1$ is not an isomorphism between $\bar{\mathcal{S}}_1$ and $\bar{\mathcal{S}}_2$, as it is not defined on $\{u\}$.

7. Abstract view of snapshots

In this section we view snapshots in a more abstract way. Given a snapshot $\mathcal{S}_k$ (of a state W_k in a state sequence τ) we replace $(\mathcal{S}_k, \subseteq)$ by a partial order (a graph) $G_k = (M_k, \subseteq)$ isomorphic with $(\mathcal{S}_k, \subseteq)$, where M_k is an arbitrary subset of a given a priori universal set $\mathcal{N}$ of nodes. Then, as is standard in the theory of partial orders, we consider the Hasse graph H_k of G_k. Similarly we replace $\bar{\mathcal{S}}_k$ by $\overline{G}_k$ and then by $\overline{H}_k$, which we will call the *abstract k-snapshot of τ*. Thus in this section the snapshot sequence $snp(\tau) = \mathcal{S}_1, \ldots, \mathcal{S}_k$ of a state sequence τ will be replaced by the *abstract snapshot sequence of* $\tau : \overline{H}_1, \ldots, \overline{H}_k$.

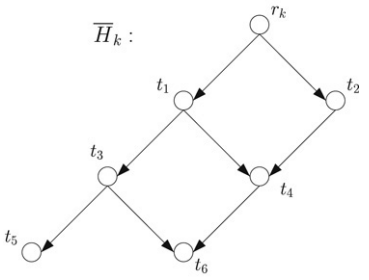

Fig. 7.1.

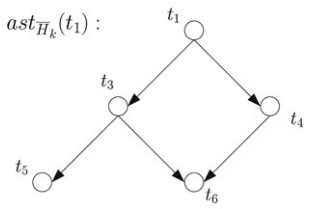

Fig. 7.2.

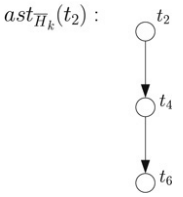

Fig. 7.3.

In considering G_k rather than $\mathcal{S}_k$ we lose all the "absolute" information about the sets in $\mathcal{S}_k$, i.e., in general, given a node z in M_k we do not know what set in 2^S it represents, we even do not know the cardinality of a represented set. We have here only "relative" information, viz., the relationship to some other sets in $\mathcal{S}_k$ (represented by the edges of G_k).

Given the abstract snapshot sequence $\overline{H}_1, \ldots, \overline{H}_n$, for each $1 \leq k \leq n-1$, the restricted function, $rnext_k : \bar{\mathcal{S}}_k \to \bar{\mathcal{S}}_{k+1}$ translates naturally into its abstract version $arnext_k : \overline{H}_k \to \overline{H}_{k+1}$.

Although the sequence $\overline{H}_1, \ldots, \overline{H}_n$ is an abstract view of $snp(\tau)$, together with the functions $arnext_k$, for $1 \leq k \leq n-1$, it allows one to deduce various facts about events and modules in τ which are independent of "implementation", i.e., independent of the composition of sets (subsets of S) represented by nodes in Hasse graphs $\overline{H}_1, \ldots, \overline{H}_n$.

Thus, e.g., for a node z in $\overline{H}_k$ one can define the *abstract structure of* z (*in* $\overline{H}_k$) as the subgraph of $\overline{H}_k$ rooted at z, denoted by $ast_{\overline{H}_k}(z)$. For example, for $\overline{H}_k$ given in Fig. 7.1, the abstract structures of t_1 and t_2 are given in Figs. 7.2 and 7.3, respectively.

As another example of reasoning in this abstract setting, assume that the abstract snapshot sequence together with the functions $arnext_1$ and $arnext_2$ is as given in Fig. 7.4 (where *arnext* functions are represented by boldface directed segments between $\overline{H}_1$ and $\overline{H}_2$, and between $\overline{H}_2$ and $\overline{H}_3$). Then, we conclude that there is only one reduced (1, 3)-event (corresponding to the *abstract* reduced event r_1, q_1, p_1), there are five reduced (1, 2)-events, and five reduced (2, 3)-events. Also, there are three reduced events merging in a 2-module (corresponding to q_7), and three reduced events merging in a 3-module (corresponding to p_2). Moreover, there are two maverick (1, 2)-events (corresponding to t_5 and t_6), and two maverick (2, 3)-events (corresponding to q_7 and q_8). Note that, given $asnp(\tau)$ and the corresponding functions $arnext_k$, one can also detect locally stable situations in τ.

Let us consider now the abstract snapshot sequence $\mu = \overline{H}_1, \overline{H}_2, \overline{H}_3, \overline{H}_4, \overline{H}_5, \overline{H}_6, \overline{H}_7$ together with the corresponding functions $arnext_k : \overline{H}_k \to \overline{H}_{k+1}$ as given in Fig. 7.5. This is a very simple example: all Hasse graphs

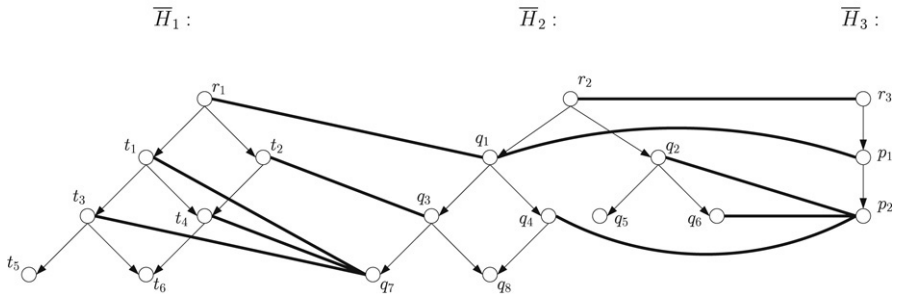

Fig. 7.4.

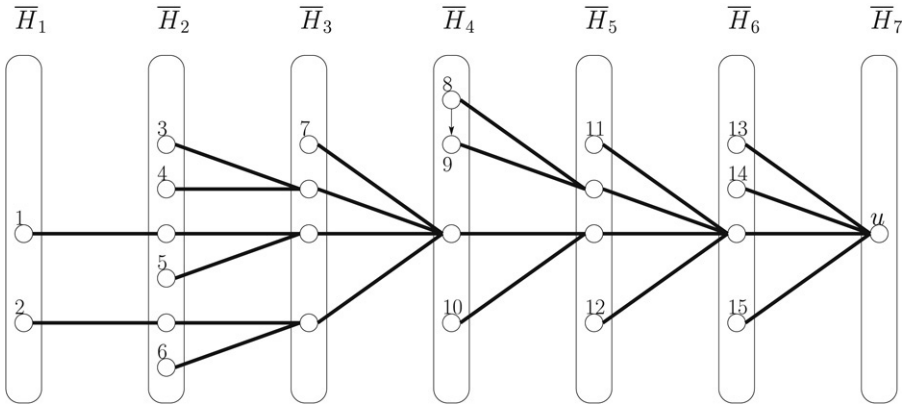

Fig. 7.5.

Fig. 7.6.

with the exception of $\overline{H}_4$ are discrete (i.e., they have the empty sets of edges), and there is only one edge in $\overline{H}_4$. There are 15 events merging in the (abstract) module u — we have numbered the modules originating these 15 events by 1 through 15.

It is easily seen that, in general, for a given ers $\mathcal{E}$ the number of events that can merge in an arbitrary module (of some state of some state sequence of $\mathcal{E}$) can be unbounded — i.e., there does not exist a positive integer s such that for each (nonempty) module Q in each state sequence τ of $\mathcal{E}$ the number of events of τ merging in Q is bounded by s. The generic situation preventing a common bound is shown in Fig. 7.6: a long path with many edges (or paths) flowing into it. Such a situation may be troublesome when analyzing the origins (causes) of modules.

Note that when events merge into the empty module they all terminate/die. It would be convenient to have a somewhat analogous situation for nonempty modules: sometimes when events merge in a nonempty module some of them terminate. Towards this aim we will use the following *antecedent reduction rule*. Let $\tau = W_0, W_1, \ldots, W_n$ be a state sequence, let $1 \leq k \leq n-1$, and let u be a node in $\overline{H}_k$. If abstract events ω_1, ω_2 merge in u, where ω_1 originates in $\overline{H}_i$ and ω_2 originates in $\overline{H}_j$ with $i < j$, then ω_1 "wins", i.e., ω_2 discontinues (it ends in $\overline{H}_{k-1}$).
A possible interpretation of the ancienity reduction rule is: when we already have a cause (an explanation) for the formation of module u, a younger cause (an explanation coming later) can be neglected.

Applying the ancienity reduction rule to the situation in Fig. 7.5 we get the situation in Fig. 7.7. We note that now we have only two events merging in u (viz., the events originating in modules 1 and 2). As a matter of fact, the ancienity rule guarantees an a priori bound on the number of events that can merge in a single nonempty module.

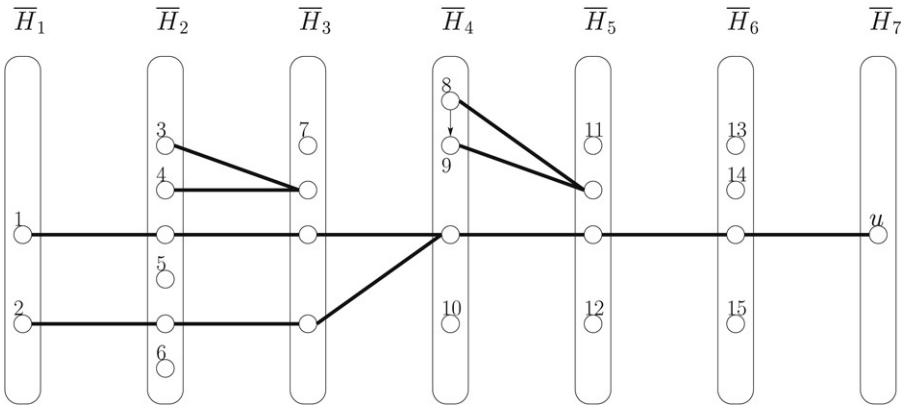

Fig. 7.7.

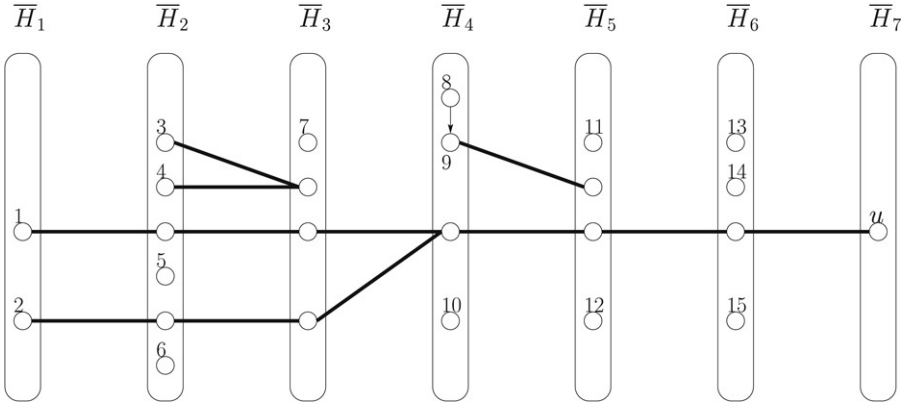

Fig. 7.8.

Theorem 7.1. *Let $\mathcal{E}$ be an ers. There exists a positive integer s such that, for each state sequence $W_0, W_1, \ldots, W_n$ of $\mathcal{E}$, each $k \in \{1, \ldots, n-1\}$, and each $u \in \overline{H}_k$, the number of events merging in u under the ancienity reduction rule does not exceed s.*

Proof. Let $\mathcal{E} = (S, A, R)$ be an ers, let $W_0, \ldots, W_n \in STS(\mathcal{E})$, let $k \in \{1, \ldots, n-1\}$ and let $u \in \overline{H}_k$. Let $\omega_1, \ldots, \omega_r$ be all abstract events in $asnp(\tau)$ that merge in u under the ancienity reduction rule. Let, for each $j \in \{1, \ldots, r\}$, i_j be the positive integer such that ω_j originates in $\overline{H}_{i_j}$. Since we consider the ancienity reduction rule, all integers i_j must be equal — say they are all equal to i. Therefore the number of events merging in u under the ancienity successor rule cannot exceed the number of nodes in $\overline{H}_i$, which is certainly bounded by $s = |2^S| - 1$. Thus the theorem holds. □

There is another reduction rule that seems to be natural from the biological point of view — it is the following *subset reduction rule*.

Let $\tau = W_0, W_1, \ldots, W_n$ be a state sequence, let $1 \leq k \leq n-1$, and let u be a node in $\overline{H}_k$. If abstract events ω_1, ω_2 merge in u, z is the abstract module of ω_1 in $\overline{H}_{k-1}$, and v is the abstract module of ω_2 in $\overline{H}_{k-1}$, with $z \leq v$ in $\overline{H}_{k-1}$, then ω_1 "wins", i.e., ω_2 discontinues (it ends in $\overline{H}_{k-1}$).

A possible interpretation of the subset reduction rule is the parsimony principle: a simpler/smaller explanation is retained. The subset reduction rule is illustrated in Fig. 7.8, where it is applied to the situation in Fig. 7.7.

Acknowledgements

The authors are indebted to Marloes van der Nat for the expert typing of the manuscript, to R. Brijder and H.J. Hoogeboom for useful comments on the first version of the manuscript, and to R. Brijder for his help with producing the figures for this paper.

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