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Standard and ordered zoom structures

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ABSTRACT

Reaction systems are a formal framework for investigating *dynamic* bioprocesses which was inspired by the functioning of the living cell. Zoom structures formalize a *static* depository of knowledge of a discipline of knowledge/science and in particular they allow one to deal with the hierarchical nature of biology. Exploration systems combine reaction systems with zoom structures allowing one to explore a discipline of science such as biology taking into account both its static and dynamic aspects. In order to facilitate applications of exploration systems, in this paper we consider (i) a subclass of zoom structures called standard zoom structures as well as (ii) augmenting both zoom structures and reaction systems by total ordering of their domains (background sets).

1. Introduction

The original motivation behind *reaction systems* (see, e.g., [1–4]) was to model the functioning of the living cell (at a high level of abstraction). The main idea is that the underlying "skeleton" of this functioning is formed by interactions of biochemical reactions that take place in the living cell. Moreover, these interactions are driven by two mechanisms, facilitation and inhibition: the reactions may facilitate or inhibit each other. Thus, the living cell can be considered to be a reactor with a finite number of reactions that can take place within it, and the dynamic behavior is formed by (discrete) processes resulting from the interactions of reactions that are enabled in consecutive states.

Formally, a reaction system is defined as an ordered pair $\mathcal{A} = (S, A)$, where S is a finite set of *entities* called the *background set* and A is a finite set of (formal) *reactions*. The background set provides all the entities needed to define reactions in A as well as other entities needed to define dynamical processes running in $\mathcal{A}$ (e.g., entities that form the *contexts* of these processes which formalize the influence of the environment on the functioning of the living cell).

Reaction systems capture two essential aspects of the functioning of the living cell: *non-permanency* of its entities (reflecting the bioenergetics of the living cell) and the fact that the living cell is an *open system* (the functioning of the living cell depends on its interactions with the environment). However, an important aspect of biological systems, viz., *hierarchical structures* occurring on both physical and methodological levels, is not addressed by reaction systems.

This aspect is addressed by *zoom structures* (introduced in [5]) which formalize the integrating structure of a depository of knowledge of a discipline of science, e.g., biology. The core of this integrating structure is a well-founded partial order which provides a "vertical" structuring of the deposited knowledge. More formally, a zoom structure $\mathcal{Z}$ consists of its *domain* D and a binary *relation* E on D such that the transitive closure E^+ of E is a well-founded partial order. Moreover:

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- D is partitioned into a finite number of *component domains* with each of them indexed/labeled by one of the *domain indices*, and
- E is partitioned into a finite number of *component relations* with each of them indexed/labeled by one of the *relation indices*.

The vertical structuring of $\mathcal{Z}$ by E^+ allows one to introduce *inzooms* which integrate knowledge from different levels (of this vertical structuring). More specifically, an inzoom is a finite sequence $(x_1, x_2, \ldots, x_n)$ of elements from the domain of a given zoom structure such that following this sequence (inzooming) beginning with x_1 one investigates the structure of x_1 with an increasing level of detail. Thus, e.g., an inzoom may relate the knowledge from species level, to organism level, to cellular level, to molecular level, to atomic level, ...

As a matter of fact, it is advocated in [5] that one considers inzooms rather than single elements of the domain as basic units for representing and analyzing biological systems. For example, it is proposed that an inzoom is a basic unit of observation and a state of a biosystem is a finite set of inzooms.

Although reaction systems were introduced because of a specific biological motivation, from the formal point of view the notion of a reaction system is an abstract set-theoretical notion. The background set can be *any set* and the formal reactions from the set of reactions specify the dynamical processes in the "universe" defined by the background set (the states of these dynamical processes are subsets of the background set).

In particular a reaction system $\mathcal{A} = (S, A)$ can specify dynamic processes running within a zoom structure $\mathcal{Z}$ by setting the background set S to be a set of inzooms from $\mathcal{Z}$ (we say that $\mathcal{A}$ is *rooted in* $\mathcal{Z}$). Then the dynamic processes specified by $\mathcal{A}$ will be running within the part of $\mathcal{Z}$ determined by the inzooms from S.

We get in this way an attractive combination: a zoom structure $\mathcal{Z}$ which is a *static* depository of knowledge and reaction systems rooted in $\mathcal{Z}$ which specify *dynamic* processes based on the knowledge deposited in $\mathcal{Z}$. This combination allows one to explore a discipline of science for which $\mathcal{Z}$ forms a depository of knowledge. Accordingly, an *exploration system* is defined as an ordered pair $\mathcal{E} = (\mathcal{Z}, \mathcal{F})$, where $\mathcal{Z}$ is an extended zoom structure and $\mathcal{F}$ is a family of reaction systems rooted in $\mathcal{Z}$. Roughly speaking an *extended* zoom structure is a zoom structure with a family of relations added to it in order to express some "additional" (to component relations) relationships holding between some elements of the domain of $\mathcal{Z}$.

The current paper is a companion paper for [5]. We introduce here standard zoom structures as well as ordered zoom structures and ordered reaction systems. The goal of introducing these special classes is to facilitate applications of zoom structures.

In the general notion of a zoom structure its domain is partitioned into a finite number of indexed/labeled component domains and its relation is partitioned into a finite number of indexed/labeled component relations. In *standard zoom structures* we propose four specific types of component domains and four specific types of component relations that can be used in forming domains and relations of zoom structures. The specific types of component domains and component relations that we propose are based on our long experience in modeling biological processes.

In *ordered zoom structures* (*ordered reaction systems*) we augment that the domain (the background set, respectively) by an ordering so that it becomes an ordered set.

The paper is organized as follows.

In Section 2 we establish some basic terminology and notation concerning binary relations, while in Section 3 we briefly recall some basic notions, notation, and terminology from [5].

In Section 4 standard zoom structures are introduced and, as an illustration of their use, in Section 5 we demonstrate how to specify families of reaction systems by standard zoom structures.

In Section 6 we introduce ordered reaction systems and ordered zoom structures, and then in Section 7 we extend the example from Section 5 to ordered zoom structures demonstrating their usefulness in specifying inzooms (of standard zoom structures). A short discussion in Section 8 concludes this paper.

2. Preliminaries

Throughout the paper we use standard mathematical terminology and notation. Perhaps the following points require a terminological and notational clarification.

A *binary relation* is an ordered pair $R = (D, G)$, where D is a set and $G \subseteq D \times D$. For $(x, y) \in G$, we also write xGy. Also, G^+ denotes the *transitive closure* of G and the transitive closure of R is $R^+ = (D, G^+)$.

In this paper, G is a *partial order* of D if it is irreflexive and transitive – the so defined partial order is often referred in the literature as a *strict* partial order. Then G is a *total order* or simply an *order* if for all $x, y \in D$ with $x \neq y$, either $(x, y) \in G$ or $(y, x) \in G$. We also say that R is a partial order or *partially ordered set* (an order or *ordered set*, if G is a total order).

We say that relation $R = (D, G)$ is *well-founded* if there is no infinite sequence $x_0, x_1, x_2, \ldots$ of elements of D such that $x_i G x_{i-1}$ for each $i \geq 1$.

A *partition* $\mathcal{P}$ of a set D is a family of nonempty disjoint subsets of D (*blocks* of $\mathcal{P}$) the union of which equals D. In an *indexed partition* each block is labeled by an index from a given set of indices.

For a positive integer n we use $[n]$ to denote the interval $\{1, \ldots, n\}$.