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Behavioural observations of cell movements with timing aspects

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ABSTRACT

We use membrane systems to define a formalism inspired by cell biology in which mobility and timing are explicitly specified. In order to reason about the behaviours of complex biological systems, we introduce several observational equivalences over mobile membranes with lifetimes. These equivalences based on observations correspond to several combinations of mobility operations that can be performed, timing aspects of the objects involved in mobility and their explicit positions inside membranes. Various relationships between these observational equivalences are proved. Moreover, we use the ambient logic to provide a logical characterization for located observational equivalence.

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1. Introduction

Biologists increasingly recognize that formal methods can help to avoid resources consumption in lab experiments [1]. The field of computational methods in systems biology provides formal frameworks for modelling and simulating complex biological systems. During the last years, formalisms as membrane systems [2] and Petri nets [3] have been applied to biology. Process calculi like π-calculus [4], mobile ambients [5] and kappa calculus [6] have been designed and used to describe cellular/molecular mechanisms. These formalisms may have an important impact in understanding how the biological systems work, giving also several ways to describe, manipulate, analyse and verify them.

In order to understand better how the biological systems behave, an appropriate formalism can be used to highlight the important properties of a system (by ignoring unimportant aspects). A suitable model should be relevant and understandable, providing a conceptual framework for expressing desirable features of the system in order to prove some of its useful properties. The formalisms should be able to describe faithfully the behaviour of the complex systems, to provide both qualitative and quantitative reasoning, as well as to allow comparisons between behaviours of some related systems.

Observational equivalence could represent an important notion in biology needed for analysing and comparing the systems behaviours based on their observations. For example, an artificial organ should be functionally equivalent to the natural organ, meaning that both are observed to behave in a similar manner. Recently, it was shown that the vas deferens of humans, canines, and bulls are equivalent in many ways [7].

The paper is organized as follows. In Section 2 we introduce a formalism inspired by cell biology in which timing, mobility and explicit locations can be specified. In Section 3 we define several observational equivalences that could be used to compare the observed behaviours of (biological) systems sensitive to time and mobility. We consider systems of mobile membranes with lifetimes having three observational coordinates: one involving the mobility operations that can be performed, another given by the position (explicit location) inside a membrane, and a third one involving the timing aspects. In Section 4 we use the ambient logic of Cardelli and Gordon [5] to provide a logical

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characterization of one of the coarsest observational equivalences defined in Section 3. Conclusion and references end the paper.

This article is the extended version of [8]. In comparison with [8], here we have a much ampler Introduction and a logical characterization of a new observational equivalence defined in Section 4. Moreover, we add several examples and explanations for a better description of our model.

2. Timing aspects in cell movements

Inspired by the compartments of biological cells and their movement, we have defined a rule-based model of mobile membranes [9]. The structure of the cell is represented by a set of hierarchically embedded regions, each one delimited by a surrounding boundary (called membrane), and all of them contained inside an external special membrane called *skin*. A membrane without other membranes inside is called elementary. The molecular species (ions, proteins, agents, etc.) floating inside cellular compartments are represented by multisets of objects described by means of symbols or strings over a given alphabet. Chemical reactions (e.g., $H_2 + O \rightarrow H_2O$) are represented by evolution rules that operate on multisets of objects written as $H^2 + O \rightarrow H_2O$, meaning that we have two objects H and an object O producing an object H_2O. The biologically inspired rules we use in this paper are endocytosis (moving an elementary membrane inside a neighbouring membrane), exocytosis (moving an elementary membrane outside the membrane where it is placed), and elementary division (dividing an elementary membrane).

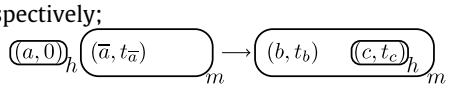
Timing is an important aspect in biological systems: evolution of real systems frequently involves various temporal interdependence among components; e.g., "the life span of intracellular proteins varies from as short as a few minutes for mitotic cyclins, which help regulate passage through mitosis, to as long as the age of an organism for proteins in the lens of the eye" [10].

We consider lifetimes associated to objects (as done in [11]), and use a global clock to simulate the passage of time. The endocytosis and exocytosis rules work whenever the involved membranes "agree" on the movement by using dual objects a and $\overline{a}$ in the involved membranes. An object a marks the active part of the movement (is ready to interact when its lifetime reaches 0), while an object $\overline{a}$ marks the passive part (is ready to interact during its entire lifetime).

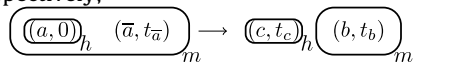
Definition 1. A system of mobile membranes with lifetimes is a construct

$\Pi_t = (O_t, H, \mu, w_{t,1}, \ldots, w_{t,n}, R_t)$, where:

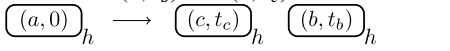
1. $n \geq 1$ (the degree of the system);
2. $O_t = O \times \mathbb{N}$ is a set of objects with lifetimes, where O is an alphabet (its elements are called objects), and (a, t_a) represents an object a and its lifetime $t_a \geq 0$;
3. H is a finite set of labels for membranes;
4. $\mu \subset H \times H$ is the membrane structure (a tree-like structure); $(i, j) \in \mu$ denotes that a membrane labelled by j is inside a membrane labelled by i;
5. $w_{t,1}, w_{t,2}, \ldots, w_{t,n}$ are multisets over O_t describing the initial multisets of objects with their lifetimes placed in the n regions of μ;
6. The finite set R_t contains the rules for mobile membranes [9], where lifetimes for objects are added, and rules are used to manipulate the lifetimes of objects. The rules of R_t have the following forms, where $(a, 0)$, (a, t_a), $(a, t_a - 1)$, $(\overline{a}, t_{\overline{a}})$, (c, t_c), $(b, t_b) \in O_t$ and $h, m \in H$:
   (a) $[\,(a, 0)\,]_h[\,(\overline{a}, t_{\overline{a}})\,]_m \rightarrow [\,[\,(c, t_c)\,]_h(b, t_b)\,]_m$; (endo)
   an elementary membrane h containing $(a, 0)$ enters the adjacent membrane m containing $(\overline{a}, t_{\overline{a}})$; $(a, 0)$ and $(\overline{a}, t_{\overline{a}})$ are rewritten to (c, t_c) and (b, t_b), respectively;



   (b) $[\,[\,(a, 0)\,]_h(\overline{a}, t_{\overline{a}})\,]_m \rightarrow [\,(c, t_c)\,]_h[\,(b, t_b)\,]_m$; (exo)
   an elementary membrane h containing $(a, 0)$ exits the parent membrane m containing $(\overline{a}, t_{\overline{a}})$; $(a, 0)$ and $(\overline{a}, t_{\overline{a}})$ are rewritten to (c, t_c) and (b, t_b), respectively;



   (c) $[\,(a, 0)\,]_h \rightarrow [\,(c, t_c)\,]_h[\,(b, t_b)\,]_h$; (elementary division)
   if containing $(a, 0)$, a membrane h is divided into two membranes with the same label h, and $(a, 0)$ is rewritten to (b, t_b) and (c, t_c).



   (d) $(a, t_a) \rightsquigarrow (a, t_a - 1)$; (lifetime decrementing)
   (e) $(a, 0) \rightsquigarrow \varepsilon$, for $(a, 0) \in O_t$. (object degradation).

In terms of computation, we are working with membrane configurations. A computation is performed in the following way: starting from an initial configuration of the system, the evolution takes place by applying sequentially rules from the set R_t. A rule is applicable to a membrane configuration when all the involved objects and membranes appearing in its left hand side are available. In rules (a)–(c), the lifetime of the involved active objects a is 0, namely the involved objects elapsed their lifetime. It can be noticed that the lifetime of the involved passive objects can be different from 0, since they just offer information to the moving membrane. When a membrane is divided, then all its inner objects are replicated in the two new membranes. When there is no rule from R_t applicable, then a lifetime decreasing step is performed using the rules (d) and (e): all the objects from a current configuration have either their lifetimes decreased by one or are eliminated from the system (depending on the value of their lifetime).

Definition 2. The set $\mathcal{M}(\Pi_t)$ of membrane configurations M in a system Π_t is inductively defined as follows:

- if $i \in H$ denotes the label of an elementary membrane and u_t is a multiset over O_t, then $\langle i; u_t \rangle \in \mathcal{M}(\Pi_t)$ is an elementary membrane configuration;
- if $M_1, \ldots, M_n \in \mathcal{M}(\Pi_t)$, $n \geq 1$, $i \in H$ and u_t is a multiset over O_t, then $\langle i; u_t, M_1 \| \ldots \| M_n \rangle \in \mathcal{M}(\Pi_t)$ is a composite membrane configuration. $M_1 \parallel M_2$ denotes two membrane configurations M_1 and M_2 placed in parallel using the parallel composition operator $\|$.

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