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Complex Functional Rates in the Modeling of Nano Devices (Extended Abstract)

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Abstract

We give an overview of recent work on the rule-based modeling of nano devices. In particular, our experience in the modeling of a nanoscale elevator suggested us to enhance rule-based modeling with *complex functional rates* that can be used to express rates that depend on the current state of the entire complexes in which the reacting molecules reside.

Keywords: Rule-based modeling, nano devices, functional rates

1 The CompReNDe project

In this overview we briefly describe *CompReNDe* (Compositional and executable Representations of Nano Devices), an interdisciplinary project of the Chemistry and Computer Science departments of the University of Bologna aimed at combining the expertises of two groups, one specialized in the design and construction of devices and machines of molecular size [3,2] and the other one qualified in formal models, based on the theory of process calculi, for describing and analyzing molecular systems [14]. Such expertises have been joined together in order to deliver a programming model for describing molecular machines that is also amenable to automated simulations and verifications by means of existing algorithms.

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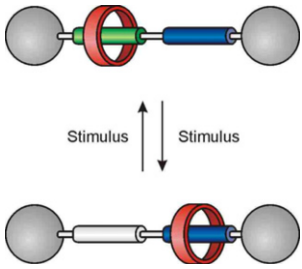

Fig. 1. Schematic representation of a two-station rotaxane and its operation as a controllable molecular shuttle.

The CompReNDe research activity started with the initial goal of formalizing a *[2]rotaxane* [29] with the Kappa-calculus [14] in order to simulate its behavior. [2]rotaxanes [29] (simply rotaxanes in the following) are systems composed of a molecular axle surrounded by a ring-type (macrocyclic) molecule. Bulky chemical moieties ("stoppers") are placed at the extremities of the axle to prevent the disassembly of the system. In rotaxanes containing two different recognition sites on the axle ("stations"), it is possible to switch the position of the macrocyclic ring between the two stations by an external energy input as illustrated in Figure 1. Several rotaxanes of this kind, known as *molecular shuttles*, have been developed (see [7] and the references therein) and used for building more complex systems [21,2].

The Kappa-calculus is a formal language idealizing molecular interactions as a particular kind of graph-rewriting. Molecules are nodes with fixed numbers of sites and molecular bonds are arcs connecting sites. Complexes are connected graphs built over such nodes and bonds. Reactions are modeled by rewriting rules that can modify the internal state of nodes, create bonds to represent *complexations*, and destroy bonds to represent *decomplexations*.

One of the distinct features of Kappa is the *"don't care, don't write"* approach: in a reaction, the reactants are not mandatorily fully described, but they can be identified by a pattern, i.e. an abstract description that can be matched by several different concrete molecules. In this way, a rule contains the description of only those parts of the complexes that are actually involved in a reaction.

The Kappa-calculus was selected as the best candidate for the modeling of the rotaxane for two main reasons: the graph-based modeling approach allowed for a natural representation of the rotaxane components and their bindings, and the rewriting rules could be used to easily represent both the chemical reaction representing the stimulus and the subsequent mechanical movement. In particular, reactions could be expressed according to the *"don't care, don't write"* approach thus focusing only on those sub-elements of the rotaxane that are actually involved.

In [9,10] we have reported about our experience in the modeling of the rotaxane by using the Kappa-calculus. One of the most interesting observations was that Kappa was not expressive enough to model complexes in which the modification of the internal state of one molecule influenced the behavior of other molecules in the same complex. To overcome this limitation, we introduced nano-K, an extension of Kappa with *instantaneous reactions* used to implement instantaneous protocols