

# Computational Nature of Biochemical Reactions

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The functioning of a living cell consists of a (huge) number of individual biochemical reactions. These reactions are regulated, where the two main regulation mechanisms are: facilitation/acceleration and inhibition/retardation. The interaction between individual biochemical reactions takes place through their influence on each other, and this influence is through facilitation or inhibition (or both).

We present a formal model of reaction systems – its goal is to analyze/understand, on an abstract level, some aspects of the functioning of a living cell, and in particular to analyze the interaction between biomolecular reactions. Therefore in the theory of reaction systems the formalization of an individual reaction relies on the above mentioned two regulation mechanisms, while the interaction between individual reactions does not have to be formalized: it is there “for free”.

In this approach reactions are primary while structures are secondary: reactions *create* states (rather than *transform* states as is the case in traditional approaches in computer science). We also assume the “threshold” supply of elements (molecules) – if an element is present, then there is “enough” of it; thus we perform a qualitative rather than quantitative analysis of functioning of reaction systems. Moreover we do not assume permanency of elements but rather their sustainability: if nothing happens to an element (it is not a reactant for any active reaction), then it ceases to exist (“life must be sustained”).

Altogether we argue that the axioms/assumptions underlying models of biochemical reactions and their interactions are *very* different from the axioms underlying models of computation in computer science. Thus, although reaction systems formalize (massively) concurrent systems, such as living cells, the basic set up here is very different than, e.g., for Petri Nets.

We present the basic theory of reaction systems, and illustrate it through examples coming both from biology and computer science. We demonstrate how the investigation of (suitably defined) computations in reaction systems allows one to understand their functioning. In particular one can define and investigate in this framework topics such as malfunctioning, or the formation of functional units (modules).