



Automaton model of protein: Dynamics of conformational and functional states



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ABSTRACT

In this conceptual paper we propose to explore the analogy between ontic/epistemic description of quantum phenomena and interrelation between dynamics of conformational and functional states of proteins. Another new idea is to apply theory of automata to model the latter dynamics. In our model protein's behavior is modeled with the aid of two dynamical systems, ontic and epistemic, which describe evolution of conformational and functional states of proteins, respectively. The epistemic automaton is constructed from the ontic automaton on the basis of functional (observational) equivalence relation on the space of ontic states. This reminds a few approaches to emergent quantum mechanics in which a quantum (epistemic) state is treated as representing a class of prequantum (ontic) states. This approach does not match to the standard *protein structure-function paradigm*. However, it is perfect for modeling of behavior of intrinsically disordered proteins. Mathematically space of protein's ontic states (conformational states) is modeled with the aid of p -adic numbers or more general ultrametric spaces encoding the internal hierarchical structure of proteins. Connection with theory of p -adic dynamical systems is briefly discussed.

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1. Introduction

In this note we apply automata theory (Sakarovitch, 2009; Anashin, 2012a, Anashin, 2012b), to modeling dynamics of proteins' states. The protein automaton model is presented by exploring the scientific methodology which plays the important role in foundations of quantum physics. This methodology is based on joint exploring of the two descriptive levels: *ontic and epistemic*. The ontic description is about reality "as it is" and the epistemic description is about observations, see (Atmanspacher et al., 2001; 2002; 2005), see also (Khrennikov, 2003a, 2003b, 2004a). Now we want to apply this methodology to molecular biology. Conformational states of proteins are treated as ontic states and functional states or states approachable for observations as epistemic states. Such a separation of two descriptive levels is very fruitful in creation of an adequate model of dynamics of proteins' states. Moreover, it matches well with automata theory (Sakarovitch, 2009): automata without output represent dynamics of ontic states, in our case conformational states, and automata with outputs represent dynamics of epistemic states, in our case functional/observational states.

We do not pretend that proteins are genuine quantum systems; we just want to use the methodology of ontic-epistemic states designed for quantum mechanics, see appendix 1 for discussion. The starting point linking dynamics of proteins with factorization models of quantum phenomena is the observation that the space of conformational states of a protein is huge and the concrete conformational states can be unobservables. Thus, as in quantum physics, one has to proceed with two types of states: ontic states (conformational states of a protein) and epistemic states (observable states representing various functions of a protein). We remark that, for a protein, the number of epistemic states is small, since each protein is a highly specialized biological machine with a few functions. At the same time the number of conformational states is huge.

In short we plan to model protein's state dynamics as functioning of an automaton without output having a huge configuration space (of conformational states); by adding output to this automaton we construct the model of observations of protein's functional states (epistemic states). Such an observational output produces factorization of the space of conformational states and can be mathematically represented as new "factorized automaton". In the framework of this automaton-model we discuss a number of conceptual problems related to production of functional states of proteins from conformational states. *We emphasize that this is a concept-type paper.* Our main aim is to present the concept of the *automaton-protein*. We also rise a series of questions which have to be clarified to make this model closer to the real biological situation, section 7. We plan to work on these questions in coming publications.

This model of protein's behavior does not match the standard *protein structure-function paradigm* formulated more than one hundred years ago (Fischer, 1894), (Redfern et al., 2008). (In the operational terms by this paradigm the ontic and epistemic descriptions can be unified in the straightforward manner.) At the same time the ontic/epistemic operational approach is perfect for modeling of behavior of intrinsically disordered proteins (Dunker

et al., 2001), see section 2 for the discussion on recent studies of the molecular biological features of proteins' functioning.

We want that the paper will be readable for biologists. Therefore we try to minimize the mathematical apparatus in the use. The basic mathematical formalism under consideration is theory of *automata*, see (Sakarovitch, 2009) and section 3 for definition. We illustrate our model by a few illustrative examples, see Figs. 1–3.

The presented model can be formulated in more advanced mathematical terms; in particular, by formalizing the mathematical structure of the ontic state space. We discuss shortly this problem appendix 2. The most natural model of proteins' state space is based on so called *p*-adic numbers, where $p > 1$ is a natural number. For *p* prime, these numbers are widely used in theory of dynamical systems, physics, biology and psychology (Anashin, 1994; De Smedt and Khrennikov, 1997; Khrennikov, 1997; Anashin, 2002, 2006; Khrennikov and Nilson, 2004; Fan et al., 2007; Vuillemin, 2000; Smyshlyayeva, 2013; Kozyrev, 2006a, 2006b, 2010; Dragovich and Dragovich, 2009, 2010; Khrennikov, 2009; Khrennikov, 1998, 2010a, 2014; Albeverio et al., 1999; Khrennikov, 2014; Murtagh, 2012a; Murtagh, 2012b; Murtagh, 2013; Iurato, 2013, 2015). We remark a kind of similarity between the *p*-adic state representation of protein's state dynamics and application of *p*-adic dynamical systems to encryption of data, see Anashin (1994; 2002; 2006). Thus one may speculate that nature encrypted functioning of proteins by using methods of *p*-adic cryptography. This is an interesting idea, but in this paper we cannot elaborate it in more detail (in particular, such elaboration would lead to exploration of advanced mathematics of theory of *p*-adic dynamical systems).

Finally, we remark that statistics of quantum observations has some peculiarities (Khrennikov, 2016), see also appendix 1 with discussion on the Bell inequality. In physics it is known that automata-dynamics can generate some features of quantum statistics (Atmanspacher et al., 2001). In this note we show that biological systems such as proteins (and others having huge configuration space of internal states and just a few functional/observational states) can demonstrate special statistical features (even generation of *p*-adic probabilities corresponding to the absence of statistical stabilization of frequencies of outputs, see (Khrennikov, 1994a) (Khrennikov, 1997), for such probabilities and their role in non-Archimedean physics and biology).

2. Dynamics of proteins conformational and functional states from the perspective of molecular biology

In this section we apply the ontic-epistemic approach to state dynamics (which we borrow from quantum foundations) to the protein dynamics.

By the *protein structure-function paradigm*, any protein function is determined by a fixed three-dimensional structure (Redfern et al., 2008). This paradigm has been dominating in molecular biology during more than one hundred years, see Fischer (1894) for one of the pioneer studies. At the same time it was challenged during many years including experimental evidences of its violation. Nevertheless, it stayed firmly as the cornerstone of molecular biology; only the discovery of *intrinsically disordered proteins* (IDPs), Dunker et al. (2001), Dyson and Wright (2005), Dunker et al.

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