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**BNO: An ontology for describing the behaviour of complex biomolecular networks**

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**Abstract**

The use of semantic technologies, such as ontologies, to describe and analyse biological systems is at the heart of systems biology. Indeed, understanding the behaviour of cells requires a large amount of context information. In this paper, we propose an ontology entitled “Biomolecular Network ontology” using the OWL language. The BNO ontology standardises the terminology used by biologists experts to address issues including semantic behaviour representation, reasoning and knowledge sharing. The main benefit of this proposed ontology is the ability to reason about dynamical behaviour of complex biomolecular networks over time. We demonstrate our proposed ontology with a detailed example, the bacteriophage T4 gene 32 use case.

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1. Introduction

To understand how our body works it is extremely crucial to focus on the behaviour of the cells and how cells correctly respond to their environments. Indeed, cells are exposed to several environmental stimuli. These detectable change in the cell’s environment can be internal such as the increased concentration of intracellular components, or external effects such as the ones of taking medication. In general, cell adaptation to these stimuli refers to changes in the state of the cell molecular components. These molecular components interact together creating a complex biomolecular network that consists of a set of nodes, denoting the molecular components and a set of edges, denoting the interactions among these cellular components. These networks are considered as systems that dynamically evolve from a state to another so that the cell can adapt itself to changes in its environment. This issue has already been addressed in Wu et al. ’s research\textsuperscript{1}, where they introduce and define the transittability of biomolecular networks as their steering from an undesired state to a desired state\textsuperscript{1}.

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Our research team has already proposed a platform to simulate the state changes in complex biomolecular networks. Our approach is based on semantic technologies. Moreover, intense research in molecular biology has led to major discoveries in cellular components, producing accumulation of a large volume of knowledge about these components. It would therefore be helpful to exploit this knowledge to increase the understanding the behaviour of complex biomolecular networks. In fact, ontologies with their clearly-defined and well-structured descriptions are vital tools for the effective application of ‘omic’ information through computational approaches.

Our previous works propose a semantic architecture for modelling the behaviour of complex biomolecular networks over time. This semantic architecture is based on four ontologies: the Gene Ontology (GO), the Simple Event Model Ontology (SEMO), the Time Ontology (TO) and our development, the Biomolecular Network Ontology (BNO). This semantic approach aims at enriching the structural description of biomolecular networks by contextual knowledge concerning their state transitions, the events that can steer these transitions and the complete temporal context linked to this information.

In this article, we detail and describe the Biomolecular Network Ontology, that aims at giving a formal and semantic representation that models all the necessary biological knowledge to study and reason on complex biomolecular networks. This semantic representation wishes to meet the following goals: (1) Determine the structure of a biomolecular network by identifying its heterogeneous components and the relations among them; (2) Define the specific functions of all molecules and the different nature of interactions they provide; (3) Understand how a cell works through the semantic interpretation of knowledge involved in the network’s behaviour; (4) Perturb the network with stimuli by changing the concentration of an element and observe its behaviour; (5) Reasoning and inferring new knowledge; (6) Simulate and identify the different states of the biomolecular network over time.

The presentation of this work is structured as follows. Section 2 reviews the necessary preliminaries from complex biomolecular networks and ontologies, and presents a brief state of the art on the existing ontologies in systems biology. Section 3 describes our proposed biomolecular network ontology in more detail. Section 4 provides a case study to demonstrate how the proposed ontology can be used for reasoning on the bacteriophage T4 gene 32 whereas concluding remarks are in Section 5.

2. Background and related work

In this section, we describe approaches close to our works. Especially, we discuss those that use ontologies and semantic information to enable and improve understanding of cells.

2.1. Complex Biomolecular Networks

The cell is a complex system consisting of thousands of diverse molecular entities (genes, proteins and metabolites) which interact with each other physically, functionally and logically creating a biomolecular network. The complexity of the biomolecular network appears by its decomposition into three levels: the genome level models the genetic material of an organism, the proteome level describes the entire set of proteins and the metabolism level contains the complete set of small-molecule chemicals. Depending on the type of their cellular components and their interactions, we can distinguish the three basic types of networks: the Gene Regulatory networks (GRNs), the Protein-Protein-Interaction networks (PPINs) and the Metabolic networks (MNs), that were logically and semantically formalized in our previous works.

2.2. Ontologies in systems biology

The use of ontological reasoning for interoperable data management is an increasingly accepted method in the field of systems biology research. Indeed, over the past decades has emerged an incredible amount of ontologies in the

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1 http://www.geneontology.org
3 https://www.w3.org/TR/owl-time/
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