A Bioinspired Computing Approach to Model Complex Systems

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Abstract. The use of models is intrinsic to any scientific activity. In particular, formal/mathematical models provide a relevant tool for scientific investigation. This paper presents a new Membrane Computing based computational paradigm as a framework for modelling processes and real-life phenomena. P systems, devices in Membrane Computing, are not used as a computing paradigm, but rather as a formalism for describing the behaviour of the system to be modelled. They offer an approach to the development of models for biological systems that meets the requirements of a good modelling framework: relevance, understandability, extensibility and computability.

Keywords: Membrane Computing · Multienvironment P systems · Multicompartmental P systems · Population Dynamics P systems

1 Introduction

Scientists regularly use abstractions with the aim to describe and understand the reality they are examining. Computational modelling is the process of representing real world problems in mathematical terms in an attempt to find solutions to their associated complex systems. A formal model is an abstraction of the real-world onto a mathematical/computational domain that highlights some key features while ignoring others that are assumed to be secondary. A formal model should not be considered as representation of the truth, but instead as a statement of our current knowledge of the phenomenon under research.

It is desirable for a model to fulfill four properties: relevance, understandability, extensibility and computability [19]. A formal model must be relevant capturing the key features while ignoring others assumed to be secondary. The abstract formalism used should adequately match the informal concepts and ideas from the investigated phenomenon. Mathematical models should also be extensible to higher level of organizations, like tissues, organs, organisms, etc, in the case of cellular systems. Finally, a formal model should be able to be implemented in a computer so that we can run simulations to study the dynamics of the system in different scenarios, as well as the qualitative and quantitative reasoning about its properties.

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One of the main objectives of any model is to provide a predictive capability, that is, the possibility to make guesses in terms of plausible hypotheses related to the dynamics of the observed phenomenon in different scenarios that are of interest to experts.

Cellular systems and population biology often depend on many parameters related to the observed behaviours. Since they define the dynamics of the system, parameters must satisfy some conditions, which can be referred to as the invariants of the associated behaviour. Some of these invariants can be expressed by rules and can be obtained by carrying out experiments, while others cannot be measured or they are very expensive to estimate. Therefore, before simulations can be performed in order to make predictions, we need to calibrate our model. Several parameters values are tested by calibration and the results corresponding to the state parameters are compared with the observed/expected behaviour of the system for the same state parameters. In some cases, the design of the model has to be reconsidered [15].

Nowadays ordinary/partial differential equations (ODEs/PDEs) constitute the most widely used approach in modelling complex systems. Nevertheless, in some cases such as molecular interaction networks in cellular systems, any model described by means of a system of ODEs/PDEs is based on two assumptions: (a) cells are assumed to be well stirred and homogeneous volumes so that concentrations do not change with respect to space; and (b) chemical concentrations vary continuously over time in a deterministic way. This assumption is valid if the number of molecules specified in the reaction volume are sufficiently large and reactions are fast.

Membrane Computing is an emergent branch of Natural Computing introduced by G. Paun at the end of 1998. This new computing paradigm starts from the assumption that processes taking place in the compartmental structure of a living cell can be interpreted as computations. In contrast to differential equations, P systems explicitly correspond to the discrete character of the components of a complex system and use rewriting/evolution rules on multisets of objects which represent the variables of the system. The inherent stochasticity, external noise and uncertainty in cellular systems is captured by using stochastic or probabilistic strategies. A general bioinspired computing modelling framework, called multienvironment P systems is introduced.

The paper is structured as follows. First, the framework of multienvironment P systems is defined in a formal way. Section 3 is devoted to multicompartmen- tal P systems, the stochastic approach. Besides, four case studies at cellular level are presented in this Section. Population dynamics P systems, the probabilistic approach, are studied in Section 4 and three case studies related to real ecosystems are described. Finally, some conclusions are drawn.

2 Multienvironment P System

A multienvironment P system of degree \((m, n, q)\) taking \(T\) time units is a tuple

\[(G, \Gamma, \Sigma, \mu, T, \Pi_1, \ldots, \Pi_n, \mathcal{R}, E_1, \ldots, E_m, \mathcal{R}_E)\]