George Eleftherakis Petros Kefalas
Gheorghe Păun Grzegorz Rozenberg
Arto Salomaa (Eds.)

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Membrane Computing

8th International Workshop, WMC 2007
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Revised Selected and Invited Papers

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In Memory of Nadia Busi

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Preface

This volume contains a selection of papers presented at the Eighth Workshop on Membrane Computing, WMC8, which took place in Thessaloniki, Greece, during June 25–28, 2008. The first three workshops on membrane computing were organized in Curtea de Argeş, Romania – they took place in August 2000 (with the proceedings published in *Lecture Notes in Computer Science*, volume 2235), in August 2001 (with a selection of papers published as a special issue of *Fundamenta Informaticae*, volume 49, numbers 1–3, 2002), and in August 2002 (with the proceedings published in *Lecture Notes in Computer Science*, volume 2597). The next four workshops were organized in Tarragona, Spain, in July 2003, in Milan, Italy, in June 2004, in Vienna, Austria, in July 2005, and in Leiden, The Netherlands, in July 2006, with the proceedings published as volumes 2933, 3365, 3850, and 4361, respectively, of *Lecture Notes in Computer Science.*

The 2007 edition of WMC was organized by the South-East European Research Centre in Thessaloniki, under the auspices of the European Molecular Computing Consortium (EMCC). Special attention was paid to the interaction of membrane computing with biology and computer science, focusing on the biological roots of membrane computing, on applications of membrane computing in biology and medicine, and on possible electronically based implementations.

The pre-proceedings of WMC8 were published by the South-East European Research Centre, Thessaloniki, and they were available during the workshop. Each paper was refereed by two members of the Program Committee. Most of the papers selected for the present volume were significantly modified according to the discussions that took place during the workshop.

The volume includes all five invited talks as well as 22 regular papers, and so it presents a representative snapshot of current research in membrane computing (a comprehensive source of information about this fast-emerging area of natural computing is `http://psystems.disco.unimib.it`).

The Program Committee consisted of Gabriel Ciobanu (Iaşi, Romania), Erzsébeth Csuhaj-Varjú (Budapest, Hungary), Rudolf Freund (Vienna, Austria), Pierluigi Frisco (Edinburgh, UK), Marian Gheorghe (Sheffield, UK), Oscar H. Ibarra (Santa Barbara, USA), Petros Kefalas (Thessaloniki, Greece) – Co-chair, Vincenzo Manca (Verona, Italy), Giancarlo Mauri (Milan, Italy), Linqiang Pan (Wuhan, China), Gheorghe Păun (Bucharest, Romania) – Co-chair, Mario J. Pérez-Jiménez (Seville, Spain), and Athina Vakali (Thessaloniki, Greece).

The workshop was sponsored by City College, Thessaloniki, and the South-East European Research Centre (SEERC).

The editors are indebted to the members of the Program Committee, to all participants of WMC8, and in particular to the contributors to this volume.

Special thanks go to the organizers for their efficiency, and to Springer for the pleasant cooperation in the timely production of this volume.

At the beginning of September 2007, Nadia Busi passed away, after a short and severe illness. She was one of the most active researchers in membrane computing and the present volume includes the paper she presented at WMC8, one of the last conferences Nadia attended. Nadia will be remembered as a passionate researcher as well as a very nice person. As a token of respect and friendship that she enjoyed in our community, we devote this volume to her memory.

Rest in peace, Nadia. We all miss you.

October 2007

George Eleftherakis
Petros Kefalas
Gheorghe Păun
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Psim: A Computational Platform for Metabolic P Systems

Luca Bianco[1] and Alberto Castellini[2]

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Abstract. Although born as unconventional models of computation, P systems can be conveniently adopted as modeling frameworks for biological systems simulations. This choice brings with it the advantage of producing easier to be devised and understood models than with other formalisms. Nevertheless, the employment of P systems for modeling purposes demands biologically meaningful evolution strategies as well as complete computational tools to run simulations on. In previous papers a strategy of evolution known as the *metabolic algorithm* has been presented; here a simulation tool called *Psim* (current version 2.4) is discussed and a case study of its application is also given.

1 Introduction

Membranes play a prominent role in living cells [1,20]. In fact, membranes not only act as a separation barrier indispensable to create different environments within cells boundaries, but they can also physically constitute a kind of "working board" whereby enzymes can activate and perform their duties on substrates. Other examples of the crucial role of membranes within cells are their ability to perform selective uptakes and expulsion of chemicals as well as being the interface of the cell with the surrounding environment allowing communication with neighboring cells.

P systems originate from the recognition of this important role of membranes and, by abstracting from the functioning and structure of living cells, they provide a novel computation model rooted in the context of formal language theory [34,36].

P systems investigations are nowadays focused on several research lines that make the field "a fast Emerging Research Front" in computer science (as stated by the Institute for Scientific Information). In particular, theoretical investigations on the power of the computational model have been carried on and important results have been achieved so far in order to characterize the computational power of many elements of P systems (such as objects and membranes) and,

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from a complexity viewpoint, P systems have been employed as well in the solution of NP hard problems. For a constant up to date bibliography of P systems we refer the reader to [39].

Parallel to these lines some more practical investigations are under way too. These studies exploit the resemblance of P systems to biological membranes in order to develop computational models of interesting biological systems. P systems seem to be particularly suitable to model biological systems, due to their direct correspondence of many elements (namely membranes, objects-chemicals and rules-reactions), even in their basic formulation, with real biological entities building the system to be modeled. Moreover, many extensions have been proposed to the standard formulation of P systems, such as some biologically relevant communication mechanisms [28,33,11], energy account [37] and active membranes [35] among others, which show the flexibility of the model. In this way, discrete mathematical tools can be used to represent interesting biological realities to be investigated. A further step is that of simulating all systems described in this way to get more information about their internal regulatory mechanisms and deeper insights into their underlying elements.

Although born as a non-conventional model of computation inspired by nature, P systems can therefore be employed as a simulation framework in which to embed the in silico simulation of interesting biological systems. The strength of this choice is, as said, the advantage that P systems share with biological systems many of their features and this leads to easy-to-devise and easy-to-understand descriptions of the studied realities. In fact, the membrane construct in P systems has a direct counterpart into biological membranes: objects correspond to all chemicals, proteins and macromolecules swimming in the aqueous solution within the cell and, eventually, rewriting rules represent biochemical reactions taking place in the controlled cellular environment. Other formalisms have been employed as modeling and simulation frameworks too, such as Π calculus [29], Petri nets [38] and Ambient calculus [10], but in their case the very same notions of membranes, chemicals and reactions need to be reinterpreted and immersed in the particular representation formalism in a less immediate way.

Nevertheless, the employment of P systems as a modeling framework for biological systems posed, from a purely computational viewpoint, some new challenges to cope with, such as the identification of suitable, biologically meaningful, strategies for system evolution and the development of new automatic tools to describe, simulate and analyze the investigated system.

In previous works a novel strategy for systems evolution, called *metabolic algorithm* has been introduced [6,27,8], an hybrid (deterministic-stochastic) variant of which has been proposed as well [5]. Other strategies of evolution are known, such as *Dynamical Probabilistic P systems* [32,31] and *Multi-compartmental Gillespie's algorithm* [30,2].

Here we will focus on the metabolic algorithm in its deterministic version which has been confronted with the dynamics of several systems (a collection of case studies can also be found in [4]). Some examples of investigated systems by means of the metabolic algorithm are the Belousov-Zhabotinsky reaction

(in the Brusselator formulation) [6,8], the Lotka-Volterra dynamics [6,27,7,14], the SIR (Susceptible-Infected-Recovered) epidemic [6], the leukocyte selective recruitment in the immune response [16,6], the Protein Kinase C activation [8], circadian rhythms [12] and mitotic cycles in early amphibian embryos [26]. In order to cope with the demand of computational tools to simulate the dynamics of P systems, we developed a first simulator called *Psim* [6], which has now been extended with several new features as will be explained later on. The new version of the simulator is freely available for download at [15].

The remaining of the discussion will firstly introduce (section 2) some theoretical aspects of the simulation framework we developed and some recent advances will be mentioned too. Section 3 will then be devoted to the newer version of the simulator itself and a practical case study will be given as well in such a way to show to the reader how to set up a simulation with the interface of Psim.

2 MP Systems

MP systems (Metabolic P systems) [21,26,24,23] are a special class of P systems [34,36], introduced for expressing the dynamics of metabolic (or, more generally speaking, biological) systems. Their dynamics is computed by means of a deterministic algorithm called *metabolic algorithm* which transforms populations of objects according to a *mass partition* principle, based on suitable generalizations of chemical laws.

A definition of MP systems follows, as given in [4].

Definition 1 (MP system). *An MP system of level $n-1$ (i.e., with $n \in \mathbb{N}$ membranes) is a construct*

$$\Pi = (T, \mu, Q, R, F, q_0)$$

in which:

- *T is a finite set of symbols (or objects) called the* alphabet*;*
- *μ is the hierarchical membrane structure, constituted by n membranes, labeled uniquely from 0 to $n-1$, or equivalently, associated in a one-to-one manner to labels from a set L of $n-1$ distinct labels;*
- *Q is the set of the possible* states *reachable by the MP system. Each element $q \in Q$ is a function $q : T \times L \longrightarrow \mathbb{R}$, from couples objects-membranes to real values. A value $q(X, l)$, with $X \in T$ and $l \in L$ gives the amount of objects X inside a membrane labeled l, with respect to a conventional unit measure (grams, moles, individuals, ...);*
- *R is the finite set of* rewriting rules*. Each $r \in R$ is specified according to the boundary notation [3]. In other words, each rule r has the form $\alpha_r \longrightarrow \beta_r$, where α_r, β_r are strings defined over the alphabet T enhanced with indexed parenthesis representing membranes. As an example, an hypothetical rule can have the form: $\alpha[_1\beta \longrightarrow \gamma[_1\delta$, with $\alpha, \beta, \gamma, \delta \in T^*$, meaning that α and β are respectively changed in γ and δ, where all objects within α and γ are outside membrane labeled 1, whereas elements of β and δ are placed inside membrane 1;*

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