Analysis and Simulation of Dynamics in Probabilistic P Systems*

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Abstract. We introduce dynamical probabilistic P systems, a variant where probabilities associated to the rules change during the evolution of the system, as a new approach to the analysis and simulation of the behavior of complex systems. We define the notions for the analysis of the dynamics of these systems and we show an application for the investigation of the properties of the Brusselator (a simple scheme for the Belousov-Zhabothinskii reaction).

1 Introduction

P systems [8] are a class of distributed and parallel computing devices, inspired by the structure and the functioning of cells. The basic model consists of a cell-like membrane structure, composed by several compartments where multisets of objects evolve according to given rules, in a nondeterministic and maximally parallel manner. A computation device is obtained starting from an initial configuration and letting the system evolve. In the following, we assume that the reader is familiar with the basic notions and the terminology underlying P systems. We refer, for details, to [9]. Updated information about P systems can be found at http://psystems.disco.unimib.it/.

Many research studies around P systems concentrates on computational power aspects. In this paper, we propose a new approach for the investigation and the application of P systems, which consists in interpreting them as tools for the description and the analysis of the *dynamical* behavior of complex systems. A similar approach is considered also in [3,10,12], where different methods are used to investigate several biological and chemical processes, among which one can find the Belousov-Zhabothinskii reaction. As said, membrane systems are inspired from the functioning of the cell, hence it is natural to consider them for

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modelling different cellular processes and natural living systems, with the final goal of producing new tools and acquiring useful information for the scientists (mainly, biologists) working on the modelled system. Some first steps in this direction have already been made, see [4] for various applications.

Since we are interested in describing the evolution of a complex system, and since changes of many different conditions can have direct influence on the reaction parameters and behavior, the basic non-deterministic model of P systems is not suitable to describe these kind of processes. Indeed, many efforts have been recently done to introduce the notion of probability in P systems. The first definition of a probabilistic P system appeared in [7], where probabilities are assigned to evolution rules, an initial probability distribution is defined in each region, and vectors related to each rule specify which rules can be applied at the next step. Though, two assumptions are made which seem quite unnatural from a biological point of view: priority relations among rules are used and, above all, probability values are initially assigned and never change during a computation, which corresponds to a *static* nature of the system. In [6] some more proposals for approaching probabilistic P systems are suggested: priority relations are no more formally considered, though they are implicitly included in computations, since one does not consider a stochastic application of rules. Lately, P systems with probabilistic rules have been also applied for the investigation of cellular phenomena and structures, such as respiration and photosynthesis processes in [2], mechanosensitive channels in [1].

In order to overcome the limitations outlined above, we propose a new version of probabilistic P systems, where probability values are *dynamically* assigned to evolution rules, according to the form of the current multiset. Moreover, the application of rules is stochastic (we will talk about *evolution* instead of *computation*).

The paper is structured as follows. In Section 2 we give the formal definition of dynamical probabilistic P systems, in Section 3 we introduce some notions which will then be used to analyze, via software tools, the behavior of such systems. In Section 4 we show an application to the Brusselator, a well known and simplified theoretical scheme which describes the Belousov-Zhabotinskii reaction (BZ, in short). Finally, in Section 5 we present the conclusion and give some perspective for future work.

2 Dynamical Probabilistic P Systems

In this section we give the definition of a probabilistic P system, where the probabilities associated to the rules vary during the evolution of the system. The method for evaluating probabilities and the way the system works are explained in details. Then, we extend the definition to consider families of P systems of this type, whose members differ among each other for the choice of some parameters, but not for the main structure.

We assume the reader to be familiar with the basic notions and notations of P systems [9]. Some prerequisites about multisets are here recalled.

Let V be an alphabet, we denote by V^* the set of all strings over V, by λ the empty string, and by $V^+ = V^* \setminus \{\lambda\}$ the set of non-empty strings. A multiset over V is a map $M : V \to \mathbb{N}$, where $M(a)$ is the multiplicity of any symbol $a \in V$, $\mathbb{N}$ is the set of natural numbers. A multiset M over $V = \{a_1, \ldots, a_l\}$ can be explicitly represented by the string $x = a_1^{M(a_1)} a_2^{M(a_2)} \ldots a_l^{M(a_l)}$, for all $a_i \in V$ such that $M(a_i) \neq 0$, and by all its possible permutations. By interpreting a multiset in the corresponding form of a string x, we can denote by $|x|$ its *length* and by $|x|_a$ the number of occurrences of a symbol a in x. The set of symbols from V occurring in x is denoted by $alph(x)$. Moreover, to every string $x \in V^*$ we can associate the *Parikh vector* $\Psi_V(x) = (|x|_{a_1}, |x|_{a_2}, \ldots, |x|_{a_l})$.

Definition 1. A *dynamical probabilistic P system* (DPP, in short) of degree n is a construct $\Pi = (V, O, \mu, M_0, \ldots, M_{n-1}, R_0, \ldots, R_{n-1}, E, I)$ where:

- V is the alphabet of the system, $O \subseteq V$ is the set of *analyzed symbols*;
- μ is a membrane structure consisting of n membranes labelled with the numbers $0, \ldots, n-1$. The skin membrane is labelled with 0;
- M_i, $i = 0, \ldots, n-1$, is the multiset over V initially present inside membrane i;
- R_i, $i = 0, \ldots, n-1$, is a finite set of evolution rules associated with membrane i. An evolution rule is of the form $r : u \xrightarrow{k} v$, where u is a multiset over V, v is a string over $V \times (\{here, out\} \cup \{in_j \mid 1 \leq j \leq n-1\})$ and $k \in \mathbb{R}^+$ is a constant associated to the rule;
- $E = \{V_E, M_E, R_E\}$ is called the *environment*, it consists of an alphabet $V_E \subseteq V$, a *feeding multiset* M_E over V_E and a finite set of *feeding rules* R_E of the type $r : u \to (v, in_0)$, for u, v multisets over V_E;
- $I \subseteq \{0, \ldots, n-1\} \cup \{\infty\}$ is the set of labels of the *analyzed regions* (the label ∞ corresponds to the environment).

The alphabet O and the set I specify which symbols and regions (environment included) are of peculiar importance in Π, namely those elements whose evolution will be actually analyzed and simulated.

Definition 2. Let Π be a DPP. We call the *parameters* of Π the set $\mathcal{P}$ consisting of: (1) the multisets $M_0, \ldots, M_{n-1}, M_E$ initially present in μ and in E, (2) the constants associated to all rules in $R_0, \ldots, R_{n-1}$.

Note that the alphabets V, O, V_E, the membrane structure μ, the form of the rules in $R_0, \ldots, R_{n-1}, R_E$ and the set I of analyzed regions do not belong to the set of parameters of Π. We call these components the *main structure* of Π. We can now extend Definition 1 and consider a *family* of DPPs, where the main structure is equal for all members of the family, while the parameters can change from member to member.

Definition 3. A *family* of DPPs is defined as $\mathcal{F} = \{(\Pi, \mathcal{P}_i) \mid \Pi$ is a DPP and $\mathcal{P}_i$ is the set of parameters of $\Pi, i \geq 1\}$.

Hence, given any two elements $(\Pi, \mathcal{P}_1), (\Pi, \mathcal{P}_2) \in \mathcal{F}$, it holds $\mathcal{P}_1 \neq \mathcal{P}_2$ for the choice of (all or some) values in $\mathcal{P}_1$ and $\mathcal{P}_2$. For instance, one can choose to

analyze the same DPP with some different settings of initial conditions, such as different initial multisets and/or different rule constants (this can be useful when not all of them are previously known) and/or different feeding multisets.

In the following, we will talk about the *evolution*, not computation, of a DPP, since we are not interested in generating languages but in simulating biological or chemical systems. The family $\mathcal{F}$ describes a general model of the biological or chemical system of interest and, for any choice of the parameters, we can investigate the evolution of the corresponding fixed DPP.

A fixed initial configuration of Π depends on the choice of $\mathcal{P}$, hence it consists of the multisets initially present inside the membrane structure, the chosen rule constants and the feeding multiset, which is given as an input to the skin membrane from the environment at each step of the evolution by applying the feeding rules. Different strategies in the feeding process can be used: for instance, one can use the feeding rules to keep at a constant value the concentrations of chemicals involved in a certain reaction (see Section 4 for an application of this strategy to the BZ), or to increase the concentrations of substances mimicking the biological transport from the extracellular space. We assume that, as long as the system evolves, the environment contains as many symbols as they are needed to continuously feed the system.

At each step of the evolution, all applicable rules are simultaneously applied and all occurrences of the left-hand sides of the rules are consumed, hence the parallelism is maximal at both levels of objects and of rules. For simplicity, in this paper we assume that the system evolves according to a universal clock, that is, all membranes and the application of all rules are synchronized. The applied rules are chosen according to the probability values dynamically assigned to them; the rules with the highest normalized probability value will be more frequently tossed. In simulations, the tossing process is obtained by means of a random number generator, as described below. If some rules compete for objects and have the same probability values, then objects are nondeterministically assigned to those rules.

The probability associated to each rule in any set R_i, $i = 0, \ldots, n-1$, is a function of its constant and of the current multiset occurring in membrane i, and it is evaluated as follows. Let $V = \{a_1, \ldots, a_l\}$, M_i be the multiset inside membrane i, $r : u \xrightarrow{k} v$ a rule in R_i; let $u = a_1^{\alpha_1} \ldots a_s^{\alpha_s}$, $alph(u) = \{a_1, \ldots, a_s\}$ and $H = \{1, \ldots, s\}$. To obtain the actual normalized probability p_i of applying r with respect to all other rules that are applicable in membrane i at the same step, we need to evaluate the non-normalized probability $\widetilde{p_i}(r)$ of r, which depends on the constant associated to r and on the left-hand side of r, namely:

$$\widetilde{p_i}(r) = \begin{cases} 0 & \text{if } M_i(a_h) < \alpha_h \text{ for some } h \in H \\ k \cdot \prod_{h \in H} \dfrac{M_i(a_h)!}{\alpha_h!(M_i(a_h) - \alpha_h)!} & \text{if } M_i(a_h) \geq \alpha_h \text{ for all } h \in H \end{cases} \quad (1)$$

that is, whenever the current multiset inside membrane i contains *all* occurrences of *all* symbols appearing in the left-hand side of rule r (second case in Equation (1)), then $\widetilde{p}_i(r)$ is dynamically defined according to the current multiset inside membrane i: we choose α_h copies of each symbol a_h among all its $M_i(a_h)$ copies currently available in the membrane itself. In other words, we consider all possible distinct combinations of the symbols appearing in $alph(u)$. Thus, $\widetilde{p}_i(r)$ corresponds to the probability of having a collision among reactant objects, which are considered undistinguishable.

If $R_i = \{r_1, \ldots, r_m\}$, the normalized probability of any rule r_j is

$$p_i(r_j) = \frac{\widetilde{p}_i(r_j)}{\sum_{j=1}^{m} \widetilde{p}_i(r_j)}. \tag{2}$$

In the simulations, the parallel application of the rules is done by splitting one parallel step into several sequential sub-steps. It is possible to separate each single parallel step into two stages, exploiting the fact that the probability distribution and the applicability of the rules are functions only of the left-hand side of the rules and their constants. In the first stage objects are assigned to rules by means of a random number generator, while in the second one the multiset is updated using a stored trace of the rules previously tossed. It should be pointed out that, during the first stage, the probability distribution of the rules has to be kept constant, otherwise the application of the rules would become sequential. A detailed description of he simulation algorithm will appear elsewhere.

Remark 1. A different probability distribution over rules could be obtained by using the classical *rate law* of Chemistry, though the approach used in Equation (1) is more accurate from the combinatorial point of view (see also [5], where a similar approach is considered). Indeed, at high concentrations (multiplicities) the two approaches are undistinguishable, but at lower ones our choice is preferable since it accounts for the exact number of all possible tuples of evolving objects.

3 Analysis of the Dynamics in DPP

In this section we introduce some notions that will be used for the analysis of the behavior of a DPP via software tools, whose complete description and functioning will appear in a forthcoming paper. The final goal is to introduce an appropriate definition of the phase space, thus creating a bridge between P systems and well known tools from the Physics of dynamical systems. Usually, the evolution of a physical system is completely determined by means of the motion equations, a set of differential equations inferred by the system properties. In the case of P systems this role should be accomplished by the evolution rules, which create a one-to-one mapping between the application of each rule and the relative displacement of the system in the phase space.

First of all, to keep trace of the system evolution we extend the definition of the alphabet $V = \{a_1, \ldots, a_l\}$ of Π by introducing the parameter *time*, that is, we define the space $\widetilde{V} := V \times \mathbb{N} = V \times \{\text{time}\}$.

Definition 4. Let $M = \{a_1^{\alpha_1} \dots a_l^{\alpha_l}\}$ be a multiset over V, where $\alpha_i \geq 0$ for all $h = 1, \dots, l$. We call a *t-multiset* the structure $M = \{a_1^{\alpha_1}, \dots, a_l^{\alpha_l}, t\} \in \widetilde{V}$.

By abuse of notation, we will denote both the multiset over V and the t-multiset in $\widetilde{V}$ with the same symbol M, being it clear when one considers also the time component or not. To represent a t-multiset in the space $\widetilde{V}$ we define its position relatively to the t-multiset $O = \{0, \dots, 0\}$ of $\widetilde{V}$ (the first l components of O are the null multiplicities of the symbols from V). We need also to extend the notion of Parikh vector to the space $\widetilde{V}$ as $\Psi_{\widetilde{V}}(M) = (\alpha_1, \dots, \alpha_l, t)$. This is necessary if we want to distinguish among two multisets having the same total numbers of symbols but different multiplicities for (at least) one symbol from V.

Definition 5. The *position* of a t-multiset $M \in \widetilde{V}$ is the vector $\overrightarrow{M} = \Psi_{\widetilde{V}}(M)$. The vector $\overrightarrow{O} = \Psi_{\widetilde{V}}(O)$ is called the *origin* of $\widetilde{V}$.

From Definition 5 it follows that the positions of t-multisets $\overrightarrow{O}$ and $\overrightarrow{M}$ are vectors in the space $\mathbb{N}^{l+1}$. The next step is to introduce a scalar product in $\mathbb{N}^l$, to naturally define the notion of distance between t-multisets, thus giving the structure of an euclidean space to $\mathbb{N}^l$. By convention, in the following we will always denote the components of a generic position $\overrightarrow{M}_i$ as the $l+1$-tuple $(\alpha_{i,1}, \alpha_{i,2}, \dots, \alpha_{i,l}, t_i)$.

Definition 6. Let $\overrightarrow{M}_i, \overrightarrow{M}_j$ be two positions in $\mathbb{N}^l \times \mathbb{N}$. The *distance* between $\overrightarrow{M}_i, \overrightarrow{M}_j$ is a function $d : \mathbb{N}^{l+1} \times \mathbb{N}^{l+1} \longrightarrow \mathbb{R}^+$ defined as

$$d^2(\overrightarrow{M_i}, \overrightarrow{M_j}) = \sum_{k=1}^{m} (\alpha_{i,k} - \alpha_{j,k})^2 \ . \tag{3}$$

Note that the two positions $\overrightarrow{M}_i, \overrightarrow{M}_j$ in Definition 6 need not to be necessarily one the evolution of the other (that is, the multiset inside the same membrane taken into different time steps). In fact, given a family $\mathcal{F}$ of DPP and two positions $\overrightarrow{M}_i, \overrightarrow{M}_j$, the following cases may hold: (*i*) $\overrightarrow{M}_i, \overrightarrow{M}_j$ occur in distinct time steps, in the same membrane of the same DPP with equal setting $\mathcal{P}$; (*ii*) $\overrightarrow{M}_i, \overrightarrow{M}_j$ occur in distinct or equal time steps, in different membranes of the same DPP with equal setting $\mathcal{P}$; (*iii*) $\overrightarrow{M}_i, \overrightarrow{M}_j$ occur in distinct or equal time steps, in the same membrane of the same DPP with different settings $\mathcal{P}_1$, $\mathcal{P}_2$; (*iv*) $\overrightarrow{M}_i, \overrightarrow{M}_j$ occur in distinct or equal time steps, in different membranes of the same DPP with different settings $\mathcal{P}_1$, $\mathcal{P}_2$. That is, we might be interested in looking at the multiset occurring inside a membrane during its evolution, or comparing two multisets of different membranes of the same DPP (in equal or different time steps), or else two multisets inside the same (or even a different) membrane but analyzed in two different evolutions of the *family* of the DPP. In each of the four cases, the distance gives information about "how far" the states in the two trajectories are (that is, the t-multisets in the two evolutions).

In particular, given any couple of positions $\overrightarrow{M}_i, \overrightarrow{M}_j$ of the same DPP (for the same or different set of fixed parameters $\mathcal{P}$), we can say that they are *simultaneous* if they exist at the same time step. This concept can be useful mainly when one considers a membrane structure with degree $n > 1$, where many multisets are co-evolving.

Definition 7. Let $\overrightarrow{M}_i, \overrightarrow{M}_j$ be two positions in $\mathbb{N}^{l+1}$. The *displacement* between $\overrightarrow{M}_i, \overrightarrow{M}_j$ is a function $\overrightarrow{u} : \mathbb{N}^{l+1} \times \mathbb{N}^{l+1} \longrightarrow \mathbb{Z}^l$ defined as

$$\overrightarrow{u}(\overrightarrow{M_i}, \overrightarrow{M_j}) = (\alpha_{i,1} - \alpha_{j,1}, \ldots, \alpha_{i,l} - \alpha_{j,l}) \ . \tag{4}$$

Note that the displacement can be either a positive or negative value, and it tells how the system "moves"; in details, it tells how the multiplicities in the positions $\overrightarrow{M}_j$ differ from those in $\overrightarrow{M}_i$. Hence, it gives more information than the distance, since it also considers the direction of the variation. Indeed, it is also possible to construct the *versor* $\widehat{u} : \mathbb{N}^{l+1} \times \mathbb{N}^{l+1} \longrightarrow \mathbb{R}^l$ of the displacement which only gives the information about the direction of $\overrightarrow{u}$:

$$\widehat{u}(\overrightarrow{M_i}, \overrightarrow{M_j}) = \left(\frac{\alpha_{i,1} - \alpha_{j,1}}{d(\overrightarrow{M_i}, \overrightarrow{M_j})}, \ldots, \frac{\alpha_{i,l} - \alpha_{j,l}}{d(\overrightarrow{M_i}, \overrightarrow{M_j})} \right) \ . \tag{5}$$

Note that $\overrightarrow{u} = \widehat{u} \cdot d$, by definition.

The last step before arriving to the definition of the phase space consists in defining the velocity, which carries on the information about the time the displacement between two t-multisets (in the same DPP, with equal initial settings) needs to take place. That is, it tells how fast the evolution from one state of the DPP to the other is.

Definition 8. Let $\overrightarrow{M_i}, \overrightarrow{M_j}$ be two positions with $t_i \neq t_j$ occurring inside the same membrane of a DPP (for a fixed choice of the parameters). The *average velocity* between $\overrightarrow{M_i}, \overrightarrow{M_j}$ is a function $\overrightarrow{v} : \mathbb{N}^{l+1} \times \mathbb{N}^{l+1} \longrightarrow \mathbb{R}^l$ defined as

$$\overrightarrow{v}(\overrightarrow{M_i}, \overrightarrow{M_j}) = \left(\frac{\alpha_{i,1} - \alpha_{j,1}}{t_i - t_j}, \ldots, \frac{\alpha_{i,l} - \alpha_{j,l}}{t_i - t_j} \right) \ . \tag{6}$$

When $t_i - t_j = 1$, which is the minimal time increment allowed in P systems, then the average velocity $\overrightarrow{v}(\overrightarrow{M_i}, \overrightarrow{M_j})$ becomes the "instantaneous" velocity between time steps t_j and $t_i = t_j + 1$, that we denote by $\overrightarrow{v}(\overrightarrow{M_j})$. Note that if $\overrightarrow{M_i}$ is the position evolved from $\overrightarrow{M_j}$ in the same membrane, then the instantaneous velocity gives the variation of that multiset in a single time step.

We are now ready to define the phase space for a DPP, which is constructed as the cartesian product of the phase spaces of all membranes in the DPP. Let $\overrightarrow{M}^i = (\alpha_1, \ldots, \alpha_l, t)$ be the position of the t-multiset inside membrane i at time t, and let $\overrightarrow{v}(\overrightarrow{M}^i) = (v_1, \ldots, v_l)$ be its instantaneous velocity.

Definition 9. We call a *phase point* of $\overrightarrow{M}^i$ the vector $\overrightarrow{\varphi_t}^i = (\alpha_1, \ldots, \alpha_l, v_1, \ldots, v_l) \in \mathbb{N}^l \times \mathbb{R}^l$, for any fixed $t \in \mathbb{N}$.

The phase point represents the state of membrane i at any given time t. The evolution of the multiset in membrane i can be described by the *phase curve*, which is a function $\overrightarrow{\varphi}^i : \mathbb{N} \longrightarrow \mathbb{N}^l \times \mathbb{R}^l$ such that $\overrightarrow{\varphi}^i(t) = \overrightarrow{\varphi_t}^i$.

The space $\Phi^i \subseteq \mathbb{N}^l \times \mathbb{R}^l$ is the set of all the points $\overrightarrow{\varphi_t}^i$ corresponding to an evolution of the multiset inside any membrane.

Definition 10. Let Π be a DPP of degree n, for some $n \geq 1$. The space $\Phi^i \subseteq \mathbb{N}^l \times \mathbb{R}^l$ is called the phase space of the membrane i, $\Phi^E \subseteq \mathbb{N}^l \times \mathbb{R}^l$ is the phase space of the environment. The space $\Phi_\Pi = \Phi^0 \times \cdots \times \Phi^{n-1} \times \Phi^E \subseteq (\mathbb{N}^l \times \mathbb{R}^l)^{n+1}$ is called the *phase space* of the DPP.

Hence, the phase space of a DPP describes the evolution of the whole system, with respect to both the change of all multisets and the passing of time. Actually, in analyzing the behavior of a given DPP, we will be interested in considering only the phase space restricted to the regions specified in the set I (see Definition 1). Similarly, only the evolution of symbols from O will be analyzed for the multisets present in the regions appearing in I.

4 Case Study: The Belousov-Zhabotinskii Reaction

The BZ chemical reaction is considered the prototype oscillator and exhibits an extraordinary variety of temporal and spatial phenomena. Its oscillating behavior is one of the most widely studied, both theoretically and experimentally, thus making this reaction a suitable workbench for the capabilities of DPP. Its basic mechanism consists in the oxidation of malonic acid, in acid medium, by bromate ions and catalyzed by cerium, which has two states. The sustained periodic oscillations are observed in the cerium ions. The Brusselator is a simplified theoretical scheme introduced in [11] to explain the nonlinear oscillating behavior, and after that was carefully studied in, e.g., [13]. Despite the fact that it is physically unrealistic, as it involves a trimolecular state, it is recognized to be the skeleton for the explanation of the oscillating behavior in chemical reactions. Moreover, it has a very simple description: $A \xrightarrow{k_1} X, B+X \xrightarrow{k_2} Y+D, 2X+Y \xrightarrow{k_3} 3X, X \xrightarrow{k_4} E$.

In this section we describe the Brusselator in terms of DPP and we show the analysis and some results obtained from the simulations. Indeed, in order to describe a chemical or a biological system evolving over time, a kind of rule able to react to the variation of occurrences of symbols (that is, concentrations of substances) is needed. For this purpose, we believe that the dynamical probabilistic rules are really suitable, so we consider the DPP defined as $\Pi_{BZ} = (V, O, \mu, M_0, R_0, E_{BZ}, 0)$ where

- $V = \{A, B, X, Y\}$, $O = \{X, Y\}$;
- $\mu = [_0\,]_0$;
- $M_0 = \{A^{m_1} B^{m_2} X^{m_3} Y^{m_4}\}$;
- R_0 consists of the rules

$$r_1 : A \xrightarrow{k_1} X$$
$$r_2 : BX \xrightarrow{k_2} Y$$
$$r_3 : XXY \xrightarrow{k_3} XXX$$
$$r_4 : X \xrightarrow{k_4} \lambda$$

for some $k_1, \ldots, k_4 \in \mathbb{R}^+$;

– the environment E_{BZ} is given by the alphabet {A,B}, the multiset $M_{E_{BZ}} = \{A^{n_1}, B^{n_2}\}$, for some $n_1, n_2 \in \mathbb{N}$, and the feeding rules $R_{E_{BZ}} = \{r_5 : A \longrightarrow (A, in_0), r_6 : B \longrightarrow (B, in_0)\}$.

Note that, with respect to the original equations in the Brusselator, we choose not to consider the chemicals D and E since they are not relevant for the system evolution. According to Definition 2, the set of parameters of Π_{BZ} is $\mathcal{P}_{BZ} = \{m_1, \ldots, m_4, k_1, \ldots, k_4, n_1, n_2\}$. A family $\mathcal{F}_{BZ}$ can be given by considering different values for the elements in $\mathcal{P}_{BZ}$.

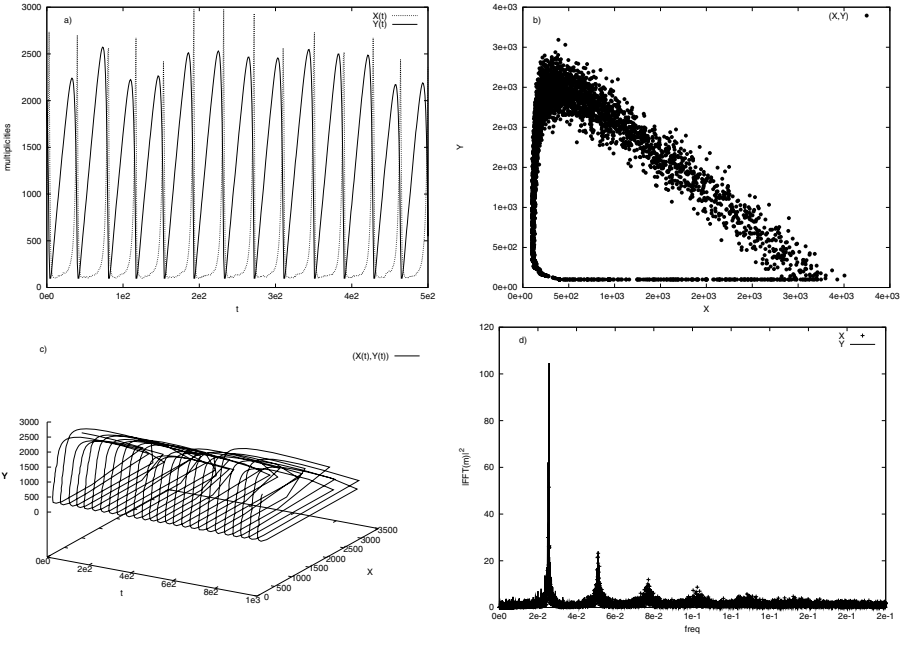

Fig. 1. Quasi-periodic cycle

The simulations based on the DPP approach have shown all the dynamical behaviors which characterize the continuously stirred BZ (see for example [3,5,13]); here we present the quasi periodic oscillations (in Figure 1, for $\mathcal{P}^{qp}_{BZ}$=$\{100, 100, 1000, 2000, 50, 0.5, 5 \cdot 10^{-5}, 5, 100, 100\}$) and the attractor (in Figure 2, for $\mathcal{P}^{att}_{BZ} = \{100, 100, 1000, 2000, 1, 1, 1, 1, 100, 100\}$). A fading transition from one to the other is possible by tuning the parameters in $\mathcal{P}_{\mathcal{BZ}}$. Since

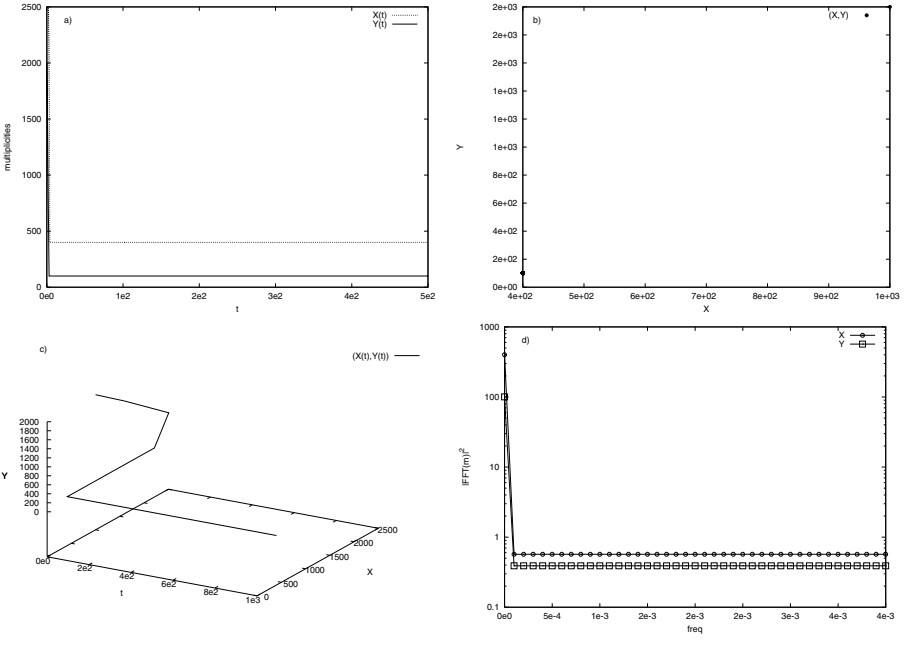

Fig. 2. Attractor

in the literature about the Brusselator the phase plane has been widely identified with the X-Y plane, our attention is focused on the dynamic of these symbols. A first characterization of the system dynamic can be obtained by looking directly to the temporal evolution of the two variables: Fig.1.(a) and Fig.2.(a) allow to discriminate the quasi periodic oscillation of the first case from the attracted dynamic of the second one. Fig.1.(b) and Fig.2.(b) show the phase space of membrane 0: in the first case we obtain a limit cycle, in the second case only the initial multiset (point at right-up corner) and the attractor (point at left-bottom corner) can be displayed. Fig.1.(c) and Fig.2.(c) show the evolution of multiplicities of X and Y; the projection on $X - Y$ plane of these pictures obviously correspond to Fig.1.(b), Fig.2.(b), respectively. Finally, Fig.1.(d) and Fig.2.(d) show the spectra: in the first case, the spectrum shows the highest peak, corresponding to the principal oscillation frequency, and some other harmonics, plus the stochastic contribute which is spread all over the other frequencies; in the second case (where the Y axis is in logarithmic scale), the spectrum corresponds to a δ of Dirac centered in the 0 frequency (the height of δ is equal to the mean value of the multiplicities of X and Y), since this is the Fourier transform of a constant (in time) signal.

Remark 2. To make clear the definitions of Section 3, we give some examples by extracting three t-multisets from the simulated evolution of $(\Pi_{BZ}, \mathcal{P}^{qp}_{BZ})$. Chosen the t-multisets $M_{39} = \{100, 100, 1921, 1029, 39\}$, $M_{40} = \{100, 100, 2701, 262, 40\}$, $M_{53} = \{100, 100, 109, 1055, 53\}$, their positions are $\overrightarrow{M}_{39} = (100, 100, 1921, 1029,$

39), $\overrightarrow{M}_{40} = (100, 100, 2701, 262, 40)$, $\overrightarrow{M}_{53} = (100, 100, 109, 1055, 53)$. The distance between M_{53} and M_{39} is $d(\overrightarrow{M}_{53}, \overrightarrow{M}_{39}) = (0 + 0 + (-1812)^2 + 26^2)^{1/2} \approx 1812.19$, while the displacement is $\overrightarrow{u}(\overrightarrow{M}_{53}, \overrightarrow{M}_{39}) = (0, 0, -1812, 26)$. The versor associated to this displacement is $\hat{u}(\overrightarrow{M}_{53}, \overrightarrow{M}_{39}) = (0, 0, -\frac{1812}{1812.19}, \frac{26}{1812.19}) \approx (0, 0, -0.99, 0.0014)$, which says that the predominant direction of the motion is along the X axes (that is, the highest variation occurs for the multiplicities of the symbol X). The average velocity $\overrightarrow{v}(\overrightarrow{M}_{53}, \overrightarrow{M}_{39}) = (0, 0, -\frac{1812}{14}, \frac{26}{14}) \approx (0, 0, -129.43, 1.86)$ is quite different from the instantaneous one, which is $\overrightarrow{v}(\overrightarrow{M}_{39}) = (0, 0, 780, -767)$ (evaluated between time steps 39 and 40).

5 Conclusions and Future Work

In this paper we introduced dynamical probabilistic P systems as a new approach for describing and analyzing complex biological or chemical processes. We also sketched some novel definitions, such as timed-multisets, the position and displacement of a multiset, the phase space of a P system, which are needed for the investigations of dynamical properties of the system of interest.

In particular, we applied such system to the analysis of well-known Belousov-Zhabotinskii reaction, showing that we can simulate the behavior of chemical oscillator reactions. Indeed, the interaction of two or more oscillating systems is of interest for many biological processes and systems, as it constitutes an important factor to keep alive an organism or a complex system constituted by several sub-components of different types.

The future work will consist in a further deep investigation of our model, both from a theoretical and an experimental point of view, e.g., by considering also non-synchronized evolutions, as well as in its use for the analysis of complex cellular processes. For instance, we are currently applying dynamical probabilistic P systems and the tools here introduced to the analysis of the role of protein p53 in cell growth arrest and apoptosis.

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