On the Dynamics of PB Systems: a Petri Net View

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Abstract. We study dynamical properties of PB systems, a new computational model of biological processes, and propose a compositional encoding of PB systems into Petri nets. Building on this relation, we show that three properties: *boundedness*, *reachability* and *cyclicity*, which we claim are useful in practice, are all decidable.

1 Introduction

We study the complexity of dynamical properties of PB systems, a new computation model introduced by Bernardini and Manca [1] for modeling biological processes. PB systems extend a previous model by Păun [9,10,11] using a notion of nested structure of *membranes*, which recalls the hierarchical structures of the living cell. Each region, delimited by a membrane, contains some *objects*, or *molecules* to stick to the biological metaphor. The configuration of membranes may evolve according to two kinds of rules: *transformation rules*, defined locally to each membrane, which model basic chemical reactions with rewriting rules over multisets; and *communication rules*, which model the ability of some molecules to transit through membranes. (Gated-pore reactions are a typical instance of such rules.)

In [1], the authors start investigating the dynamics of PB systems. The main focus is on periodicity, a central notion of biological processes. Indeed, many important biological processes have a periodic or quasi-periodic behavior, such as the ATP cycle, for instance. In this paper, we study a new notion of periodic systems, called *cyclicity*, and also study two other dynamical properties, which are familiar to the area of verification of concurrent systems, namely boundedness and reachability.

Boundedness is a property of systems whose production and consumption of resources (during a finite lapse of time) may be bounded. From a biological point of view, boundedness can be interpreted as a property of *sustainable development*, in the sense that long-lived processes in a cell are not allowed to store more and more chemical components. (Clearly, a cell can accumulate only a finite amount of material.) Reachability is the problem of deciding whether a system may reach a given state during its execution. This is one of the most critical property in the verification of systems as most of the *safety properties* of mechanical and computing systems can be reduced to the problem of checking whether a system may reach a "bad state". (Another quality of reachability is that many other properties may be recursively reduced to it.) In the context of PB systems, reachability may take a biological interpretation. Assume we are modeling the drug absorption activity of some cell. The system starts with some initial drug density in the outermost region of the cell and, during evolution, the drug start circulating and concentrating in membranes. From a biochemical viewpoint, one can be interested if, upon evolutions, the density of drug in the cell reaches some critical value, that is, if it reaches some special configuration of our PB system.

We prove that cyclicity (another form of periodicity), boundedness and reachability are all decidable problems for PB systems. These results are essentially obtained by encoding PB systems as Petri nets [14], a distinguished model of concurrent computation, and by transferring known difficult complexity results on Petri nets. Using our encoding result, it is also possible to easily transfer the decision procedures for these problems and therefore to obtain efficient algorithms in specific cases.

Relating two apparently different formal models of computations is always fruitful. Indeed, the transfer of results from one model to the other often leads to a deeper understanding of the concepts involved or to the discovery of new results. In the present case for example, the notion of *periodicity*, that is central to the study of PB systems, appears almost overlooked in Petri nets, and we can conjecture that the search for a good definition of *periodic behavior*, that will fit the biological sense associated to this adjective, will be challenging. (There exists a notion of cyclic Petri net, quite distant from the notion of periodic system found in [1].) We can draw a parallel here with the search for a comprehensive notion of *fairness* in concurrent computation, which initiated the definition of a whole family of formal characterizations, or with the formal definitions of the concepts of *secrecy* and *authentication* in the study of cryptographic protocols, which are still elusive.

The paper is structured as follows. Next section gives basic definitions on multisets and periodic sequences of multisets. Section 3 and 4 define PB systems and PBE systems, respectively. Petri nets and related notions are introduced in Section 5. Section 6 contains our full abstraction result and illustrates the construction of the Petri net associated with a PB/PBE system. Before concluding, we prove several decidability results which can be deduced from the relation between Petri net and PB systems.

2 Basic Definitions

In this section, we recall some preliminary definitions about multisets and periodic sequences. The interested reader may find complete informations in [1,10,11]. Consider a finite alphabet Σ of abstract symbols called *objects*. A *multiset* over

Σ is a mapping $u : \Sigma \to \mathbb{N}$. For any $a \in \Sigma$, the value $u(a)$ is the number of objects of type a in the multiset u, also called the multiplicity of a in u. Given two multisets u, v over Σ, we write $u \doteq v$ the equality of the two multisets u and v, and $u \prec v$ if the multiset u is included in v, that is, $u(a) \leq v(a)$ for all $a \in \Sigma$.

A multiset u over Σ can be conveniently encoded by a string over the alphabet Σ, say $w = a_1^{u(a_1)} \dots a_n^{u(a_n)}$. This representation is not unique and any permutation of w gives an admissible encoding. In this paper, we will interchangeably use the expressions "the multiset represented by the string w", "the multiset w" or "the string w", we shall also use the notation $w(a)$ for the multiplicity of a in the multiset w.

An infinite sequence $(w_i)_{i\in\mathbb{N}}$ of multisets is *ultimately periodic* if there exists $t_0, p \in \mathbb{N}$ such that for all $t \in \mathbb{N}$ and $1 \leq j \leq p$:

$$w_{t_0+j} \doteq w_{t_0+pt+j} \quad . \tag{1}$$

An infinite sequence $(w_i)_{i\in\mathbb{N}}$ of multisets is *ultimately almost periodic* if there exists $t_0, p \in \mathbb{N}$ such that for all $t \in \mathbb{N}$ and $1 \leq j \leq p$:

$$w_{t_0+j} \prec w_{t_0+pt+j} \quad . \tag{2}$$

The least integers p and t_0 satisfying (1) or (2) are called the *period* and the *transient* of $(w_i)_{i\in\mathbb{N}}$, respectively. An ultimately periodic sequence with a null transient (i.e. $t_0 = 0$) is called *periodic*. Similarly, an ultimately almost periodic sequences with a null transient is called *almost periodic*.

3 PB systems

In this section we briefly recall basic definitions about PB systems (see [1] for more on this subject).

Definition 1 (PB system). *A PB system is a structure $\Pi = \langle \Gamma, M, R, \mu_0 \rangle$, where Γ is a finite alphabet of symbols, M is a finite tree representing the* membrane *structure, R is a finite set of rules and μ_0 is the* initial configuration*, that is a mapping from membranes of Π (nodes in M) to multisets of objects from Γ. Rules can be of the following two forms:*

1. $u.u' \,[_i\, v'.v \;\to\; u.v' \,[_i\, u'.v$ (communication rules)
2. $[_i\, u \;\to\; [_i\, v$ (transformation rules)

where $u, u', v, v' \in \Gamma^\star$ and i is a node in M.

A *configuration* (for Π), μ, is a distribution of objects from Γ in membranes of Π. We say that there is a transition $\mu \to \mu'$ if μ' can be obtained from μ by applying a rule in R. A *computation* with initial configuration μ_0 is a sequence of transitions $\mu_0 \to \mu_1 \to \mu_2 \dots$

Our definition of PB systems slightly differs from the original version found in [1]. First, we explicitly consider the spatial distribution of membranes instead of relying on structural conditions about initial configurations (for example the property of being well-parenthesized). Second, we do not distinguish an output membrane. Indeed, this distinguished membrane is only used to define the "final result" of an evolution whereas, in this paper, we are exclusively interested in dynamical aspects of the system.

Another, more significant difference, appears in the definition of the operational semantics. In our model, following typical algebraic models of concurrent computation like CCS and Petri nets, reduction rules are applied in an "asynchronous" and non-deterministic manner, whereas the operational semantics of P-systems is usually based on a *maximum-parallel* reduction relation (in which configurations evolve by applying the maximal number of non-interfering transition rules). While the two kinds of semantics may not always be simply related, it is easy to see that a configuration reachable using the maximum-parallel reduction strategy is also reachable in our setting.

A PB system with initial configuration μ_0 is *ultimately periodic* (resp. *ultimately almost periodic*) if there exists a computation with initial configuration μ_0 which is ultimately periodic (resp. ultimately almost periodic).

It is important to remark that, due to non-determinism, there are possibly infinitely many computations originating from the same initial configuration. Anyway, we call ultimately periodic (resp. ultimately almost periodic) a system with initial configuration μ_0 which admits at least one ultimately periodic (resp. ultimately almost periodic) computation. Taking inspiration from Petri nets terminology, we say that a PB has *structurally* the property P if P holds for all possible initial configurations. In Section 7, we give results on periodic and structurally periodic systems and propose an adequate condition for a system to enjoy these properties. We also prove (Proposition 5) that almost every periodic PB-system also exhibits an infinite number of aperiodic computations. More precisely, we prove that "uniformly periodic" systems, such that all computations are periodic (with or without the same period), are restricted to systems with a unique, deterministic, computation.

4 PBE systems

In [1], the authors provide an interesting extension of PB systems: PB systems with environment (or PBE for short). In this model, there is an *environment* regularly providing molecules at the boundaries of the outermost membrane of the PB system. These molecules evolve according to special rules of the environment and can interact with the PB system. The intuition behind this model is that the environment provides resources for the PB system and, eventually, collects garbages. To simplify our presentation, we consider an abridged model of environment, but much of our results can be extended to the full definition found in [1].

Definition 2 (PBE system). *A PBE system is a structure* $\Pi = \langle \Gamma, M, R, E, R_E, \mu_0 \rangle$*, where* $\langle \Gamma, M, R, \mu_0 \rangle$ *is a PB system, and* $E = w_1 \cdot \cdots \cdot w_k$ *is a se-*

quence of multisets over Γ, and R_E is a finite set of environment rules*, that is, transformation rules acting on the multisets contained in the environment E.*

A configuration ν of a PBE system is a triple (t, e, μ) where $t \in \mathbb{N}$ is the cycle step for the environment, $e \in \Gamma^*$ is the current environment content and μ is the configuration of the PB system. We use the notation $E(t)$ for the t^{th} element of the sequence E and, since an environment correspond to a cyclic behavior, we extend this definition to all indices $t \in \mathbb{N}$ assuming that $E(t + k) = E(t)$.

A transition from the configuration $\nu = (t, e, \mu)$ is obtained in two steps:

1. apply to e a rule in $R_E \cup R$ and add $E(t)$ to e;
2. apply to μ a rule in R and increment t by 1.

Similarly to previous sections, we denote this fact by $\nu \rightarrow \nu'$. Remark that, at this point, all definitions of dynamical properties about PB systems extend in a natural manner to PBE systems.

5 Petri Nets

Petri nets are a very popular model for the analysis and representation of concurrent systems that has draw much attention from the community of verification of concurrent systems. Interestingly enough, the Petri net model was proved equivalent to the vector addition systems [6] of Karp and Miller, a simple mathematical structure defined to analyze the computations of vector-parallel architectures. Correspondingly, in this paper, we show an equivalent result relating Petri nets with a model for "biological computation", the PB systems of Bernardini and Manca.

The interest of relating PB systems with the (seemingly different) Petri net model of computation is that collected works on Petri nets span over more than twenty five years and have lead to several important results on decidability issues, new notions of equivalences and modal logics for expressing temporal and behavioral properties (with the associated model-checking algorithms). We may therefore hope to transfer these results to the setting of PB systems.

Definition 3 (Petri net). *A Petri net N is a tuple $\langle P, T, F, \mu_0 \rangle$ where P and T are two disjoint finite sets, and $F : (P \times T) \cup (T \times P) \rightarrow \mathbb{N}$ is a flow function and μ_0 is the* initial marking*. A* marking*, μ, is a mapping $P \rightarrow \mathbb{N}$ from places to integers. The elements of S and T are called* places *and* transitions*, respectively, and the elements of F are called* arcs*.*

Given a Petri net $N = \langle P, T, F, \mu_0 \rangle$, a *marking*, μ, associates an integer, $\mu(p)$, to every places $p \in P$. The intuition is that every place contains a bag of *tokens* and that transitions may take tokens from some places to others following the arcs which are connected to it. An arc $F(p, t) = n$ represents a flow from the place p to the transition t carrying (and necessitating at least) n tokens; an arc $F(t, p) = n$ represents a flow from the place t to the place p; and $F(p, t) = F(t, p) = 0$ represents no connection at all.

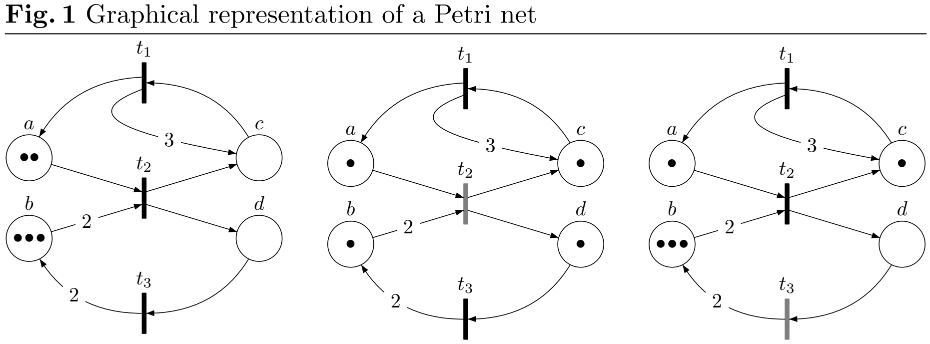
A transition t is *firable* from a marking μ, written $\mu \xrightarrow{t}$, if for all places $p \in P$, it holds $F(p,t) \leq \mu(p)$. If t is firable from μ, firing t from μ leads to a new marking μ', a relation denoted $\mu \xrightarrow{t} \mu'$, such that for all $p \in P$ we have $\mu'(p) = \mu(p) - F(p,t) + F(t,p)$. A marking μ' is *reachable* from μ, denoted $\mu \xrightarrow{*} \mu'$, if there exists a sequence of transitions $t_0, t_1, \ldots, t_n$ such that

$$\mu \xrightarrow{t_0} \mu_{t_0} \xrightarrow{t_1} \mu_{t_1} \cdots \xrightarrow{t_n} \mu_{t_n} = \mu' \ .$$

The set of all Petri nets is a semi-group and nets may be composed using a simple operation, called *parallel composition*, defined as follows. The parallel composition of the nets $N_1 = (S_1, T_1, F_1, \mu_1)$ and $N_2 = (S_2, T_2, F_2, \mu_2)$, denoted $N_1 \| N_2$, is the net obtained by simply merging the set of places, transitions and arcs, that is, $N_1 \| N_2 = (S_1 \cup S_2, T_1 \cup T_2, F_1 + F_2, \mu_1 + \mu_2)$, where addition of functions is defined place-wise. (Note that this operator strongly relies on the names chosen for places and transitions.)

There is a standard graphical representation of Petri net, exemplified in Figure 1. Circles represent places, black bars represent transitions and directed weighted edges represent arcs. (A missing label is equivalent to a weight of 1.) A marking, μ, is represented by groups of $\mu(p)$ tokens located at each place p in the net. For example, a marking that assigns the integer 2 to the place p is represented by two tokens (depicted $\bullet$) located in p. The first net depicted in Figure 1 corresponds to a Petri net with 4 places (labeled a, b, c and d) and 3 transitions, in the configuration $a \to 2, b \to 3$ (or equivalently to the multiset $aabbb$). The second figure shows the system after the firing of transition t_2. In this state, only the transitions t_1 and t_3 are enabled and they may fire concurrently (one transition may not hamper the firing of the other). Last figure shows the state of the system after the firing of t_3.

Fig. 1 Graphical representation of a Petri net



6 Encoding PB and PBE systems

In this section we define an encoding of PB systems into Petri nets that preserves reduction. This encoding allows one to deduce fundamental results on the dynamics of PB systems from known results about Petri nets.

Consider the PB system $\Pi = \langle \Gamma, M, R, \mu_0 \rangle$. The encoding of Π is decomposed into two separate steps. First, we associate to each membrane i of Π a Petri net N_i that corresponds to transformation rules — that is rules that are purely local to one membrane. Second, the nets N_i are merged into a larger Petri net and special transitions between the sub-nets N_i are added in order to code communication rules. The resulting Petri net, denoted $[\![\Pi]\!]$, is obtained compositionally from the rules in Π. Moreover, the size of $[\![\Pi]\!]$ is proportional to the size of Π.

Remark that Petri nets do not explicitly model locality, like in PB systems, but the hierarchical structure of membranes is reflected by the communication links between sub-nets.

For every membrane $i \in T$, define the Petri net $N_i = \left\langle S_i, T_i, F_i, \mu_0^i \right\rangle$ as follows. There is one place $a_i \in N_i$ for every symbol $a \in \Gamma$, and one transition t_ρ for every transformation rule $\rho \in R$ that acts on the membrane i. The flow function F_i is the function such that for any rule $\rho : [_i\, u \to [_i\, v$ (with $u, v \in \Gamma^\star$) we have $F(a_i, t_\rho) = u(a)$ and $F(t_\rho, a_i) = v(a)$ for all $a \in \Gamma$. The initial marking μ_0^i is the mapping associating to each place a_i (i.e. a is a molecule in Γ) the number of molecules a in the membrane i.

Now, consider the Petri net $N = \langle S, T, F, \omega \rangle$ obtained by merging the nets N_i for $i \in M$, that is $\|_{i \in M} N_i$, extended with one transition for every communication rules in Π. (By construction, the places and transitions used in the N_i are all distinct.) The set of places of N is $S = \bigcup_{i \in M} S_i$, and the set of transitions, T, is equal to R, the set of rule (names) of Π, that is, the union of $(\bigcup_{i \in M} T_i)$ (the names of the transformations rules of Π) with the names of the communications rules of Π. The initial marking ω is the union of the markings μ_0^i, for all $i \in M$. In the sequel, this marking is denoted $[\![\mu_0]\!]$.

The flow function F of N is the union of the functions F_i, for $i \in M$, and such that for any communication rule $\rho : u.u'[_i\, v'.v \to u.v'[_i\, u'.v$ and all $a \in \Gamma$, given j is the (unique) name of the membrane containing membrane i, we have $F(a_j, t_\rho) = u.u'(a)$, and $F(a_i, t_\rho) = v'.v(a)$, and $F(t_\rho, a_i) = u'.v(a)$, and $F(t_\rho, a_j) = u.v'(a)$.

It is easy to see that the Petri net $[\![\Pi]\!]$ has $|\Sigma||M|$ places, the product of the number of symbols by the number of membranes, and $|R|$ transitions.

Theorem 1. *Given a PB system $\Pi = \langle \Gamma, M, R, \mu_0 \rangle$, if $\mu \to \mu'$ in Π then there exists a firable transition $[\![\mu]\!] \to [\![\mu']\!]$ in $[\![\Pi]\!]$. Conversely, if $[\![\mu]\!] \to [\![\mu']\!]$ in $[\![\Pi]\!]$ then $\mu \to \mu'$ in Π.*

Proof. By case analysis on the transition rules of Π.

Example 1. The Petri net given in Figure 1 corresponds to a simple PB system, Π, made of a single membrane, 4 different types of atoms i.e. $\Gamma = \{a, b, c, d\}$, and the following 3 transformations rules:

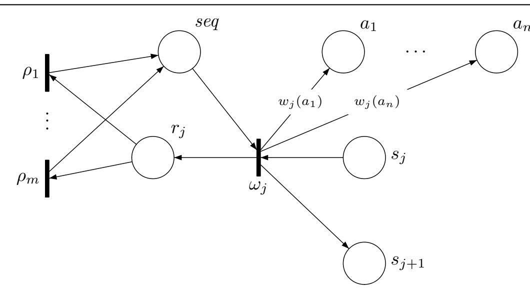
$$\begin{array}{l} t_1 : [\, c \quad\;\; \to [\, accc \\ t_2 : [\, abb \to [\, cd \\ t_3 : [\, d \quad\;\; \to [\, bb \end{array}$$

The distribution of tokens in $[\![\Pi]\!]$ corresponds to the initial configuration $aabbb$. □

We show that an environment, E (with the implicit associated set of rules R_E), may also be interpreted as a Petri net, and we provide a compositional encoding, $[\![\langle E, R_E\rangle]\!]$, of E. What is more surprising is that the action of controlling a PB system, Π, by an environment, E, corresponds to the parallel composition of the nets encoding Π and E. Therefore all the results given in this paper for PB systems can also be lifted to PBE systems.

Assume E is the environment $E(j) = w_j \in \Gamma^\star$ for all $j \in 1..k$, with $\Gamma = \{a_1, \ldots, a_n\}$. We suppose a fixed set of rules for the PB systems, say $\{\rho_1, \ldots, \rho_m\}$. The Petri net $[\![\langle E, R_E\rangle]\!]$ is the parallel composition of the nets E_i (depicted in Figure 2) for all $i \in 1..k$, together with the Petri net encoding R_E (build exactly like the net N_i in the encoding of PB systems). We give more intuitions on the encoding of E in the following example.

Fig. 2 The Petri net E_j: encoding one step of the environment E



The encoding of the PBE system $\langle \Gamma, M, R, E, R_E, \mu_0\rangle$ is the parallel composition $[\![\langle \Gamma, M, R, \mu_0\rangle]\!] \| [\![\langle E, R_E\rangle]\!]$.

Theorem 2. *Given a PBE system $\Pi = \langle \Gamma, M, R, E, R_E, \mu_0\rangle$, if $\mu \to \mu'$ in Π then there exists a firable transition $[\![\mu]\!] \to [\![\mu']\!]$ in Π. Conversely, if $[\![\mu]\!] \to [\![\mu']\!]$ in $[\![\Pi]\!]$ then $\mu \to \mu'$ in Π.*

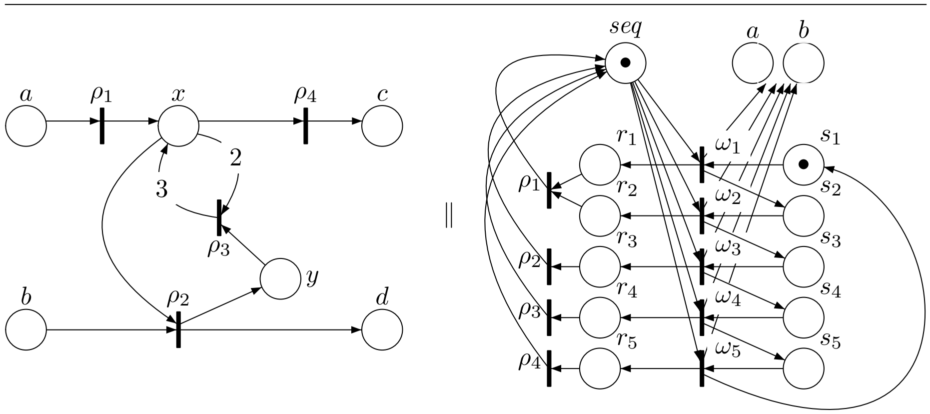
The example given in Figure 3 displays the Petri net corresponding to the Brusselator (with an empty initial configuration): a model of chemical oscillations based on the famous Belousov-Zhabotinsky used as an example in [1]. The

Brusselator is a system over the alphabet $\{a, b, c, d, x, y\}$, with only one membrane and the following set of rules:

$$\begin{aligned} \rho_1 &: [\, a &&\rightarrow [\, x \\ \rho_2 &: [\, bx &&\rightarrow [\, yd \\ \rho_3 &: [\, xxy &&\rightarrow [\, xxx \\ \rho_4 &: [\, x &&\rightarrow [\, c \end{aligned}$$

We also give an encoding of the environment $E = (ab, \{\rho_1\}) \cdot (ab, \{\rho_1\}) \cdot (ab, \{\rho_2\}) \cdot (ab, \{\rho_3\}) \cdot (ab, \{\rho_4\})$, with $R_E = \emptyset$. We encode a simple example of *PBE with resources*, an extension of PBE systems such that each element in the environment sequence E specifies also the set of reactions that may take place in the controlled PB systems. The intuition behind this extension is that an environment, beyond bringing repeatedly new molecules to the system, may also promote or hinder some chemical reactions. To build the encoding of an environment with resources, it is enough to erase from the nets E_j (for all $j \in 1..k$) the arcs between r_j and the rule names not mentioned in $E(j)$.

Fig. 3 Encoding of the Brusselator and its environment



The net $[\![\langle E, \emptyset\rangle]\!]$ given in Figure 3 is essentially a linked chain of transitions and places $(s_1; \omega_1; \ldots; s_5; \omega_5; s_1)$ which sequentially enables the transitions ω_i for $i \in 1..5$ and then loops. In this example, the transition ω_i corresponds to the i^{th} component of the environment, of the form $(ab, \{\rho_j\})$ in our example. When fired, a transition ω_i generates a token in the places a and b (modeling the fact that the environment brings a molecule a and a molecule b in the Brusselator) and a token in the place r_j. To ensure the synchronization between firings in the (encoding of the) Brusselator and firings in the environment, we also rely on an extra-place, *seq*, which ensure that a transition ρ_j in $[\![\Pi]\!]$ may only fire after a firing of some transition ω_j in $[\![\langle E, \emptyset\rangle]\!]$ and conversely.

7 Decidability results

In this section, we go back over some significant complexity results on Petri nets. Theorems 1 and 2 allow to transfer these results to PB/PBE systems. We begin with the study of two dynamical properties typical of the verification of concurrent systems, boundedness and reachability, and conclude with the study of different notions of periodicity.

Reachability and boundedness are two general properties of interest when working on Petri nets. Given a net, N, with initial marking, μ_0, we say that the marking μ is *reachable* from N if there exists a sequence of firings $\mu_0 \to \mu_1 \to \ldots \to \mu_n = \mu$ of the net. We say that a net is *bounded* if its set of reachable markings is finite. A bounded net implies that there exists some integer k bounding the number of tokens that may be present at each place (the net is said to be k-safe).

The boundedness and reachability problems are decidable, even if they tend to have a very large complexity in theory. (Petri nets are an important source of natural non-primitive problems!) A good survey of the known decidability issues for Petri nets, from which the results in this section are taken, is given in [4].

The best known-algorithm to test whether a Petri net is bounded may require an exponential space in the size of the net. More precisely, it may require at most space $2^{cn \log n}$ for some constant c. (This complexity is almost optimal because Lipton proved [7] that deciding boundedness requires at least space $2^{c\sqrt{n}}$.) The same property is much simpler if we require the boundedness of the net N for all possible initial markings. In this case, the net N is said to be *structurally bounded*. Indeed, using a clever reduction involving linear programming, Memmi and Roucairol proved [8] that the structural boundedness problem has only a polynomial time complexity.

As a corollary, we prove that boundedness is a decidable property for PB systems. We say that a PB system Π, with initial configuration μ_0, is *bounded* if there are only finitely many configurations which are reachable starting from μ_0 (that is, if $[\![\Pi]\!]$ is a bounded net).

Theorem 3 (Boundedness). *Given a PB system Π and an initial configuration μ_0, it is decidable to know whether Π is bounded.*

For the complexity of the reachability problem, there exists only an exponential space lower bound [7], while the known algorithms require non-primitive recursive space. However, tighter complexity bounds are known for many restricted classes of nets: it is EXPSPACE-complete for symmetric Petri nets, such that every transition t has a symmetric transition whose occurrence "undoes" the effect of t; it is NP-complete for Petri nets without cycles; ...

Many complexity problems can be reduced to the boundedness or the reachability problem. Thus, most of the usual properties of interest for verification purposes are decidable. Intuitively, these decidability results follow from the monotonic nature of Petri net reductions: if a transition may fire for some marking M, it may also fire for a marking with more tokens (say $M+L$ where addition of markings is defined place-wise). Disregarding the simplicity of this intuition, formal proofs of these results have proved very complicated. In the case of the reachability problem, for example, and in spite of important research efforts, the decidability results remained elusive for nearly 30 years. Therefore, it is interesting to transfer these difficult results to the setting of PB systems. For example, we may directly obtain the following properties using our main theorem.

Theorem 4 (Reachability). *Given a PB system Π, with initial configuration μ_0, and a configuration μ, it is decidable to prove that there exists an integer $n \geq 0$ and a sequence of transitions $\mu_0 \to \mu_1 \to \cdots \to \mu_n = \mu$ in Π.*

As a corollary, we prove that periodicity is a decidable property.

Proposition 1 (Periodicity). *Given a PB system Π with initial configuration μ_0, it is decidable to know if it is periodic.*

Proof. From Theorem 4, considering μ_0 both as an initial and as a target configuration.

Many variants of the reachability property are recursively equivalent to it. We mention these problems here since they can be related to properties of biological processes, the subject that motivated the definitions of PB systems.

- The home states problem. A marking of a Petri net is a *home state* if it is reachable from every reachable state. That is, it is always possible to cycle through a home state. The home state problem consists in deciding, given a net N and a marking μ, if μ is a home state. A Petri net is called *cyclic* if its initial marking is a home state.
- The sub-marking reachability problem. The equivalent of reachability for sub-markings, that is partially specified markings, such that only the number of tokens on some places is given. On PB system, this problem is equivalent to checking whether there is some reachable configuration which contains some given numbers of molecules in some given membranes.
- Deadlock problem. It consists in proving that every reachable marking enables at least one transition. That is, the system may infinitely evolve without stopping. The deadlock problem is reducible in polynomial time to the reachability problem [2].

The decidability of the deadlock problem can be directly restated in terms of evolutions in a PB system.

Proposition 2 (Non-termination). *Given a PB system Π and an initial configuration μ_0, it is decidable to know whether all computations starting with μ_0 are infinite.*

We have already proved that periodicity is a decidable property, that is, it is decidable to know whether a PB system admit at least one periodic computation. The remainder of this section further develops the study of periodic behaviors. We start by a result relating boundedness and the existence of an ultimately periodic computation.

Proposition 3 (Ultimate periodicity). *Consider a PB system Π and an initial configuration μ_0. If Π is bounded then Π is ultimately periodic.*

Proof. Assume $[\![\Pi]\!]$ with initial configuration $[\![\mu_0]\!]$ is bounded. If Π halts then we are done. Otherwise, let U be the set of configurations which are reachable starting from μ_0. Consider a computation $(\mu_i)_{i\in\mathbb{N}}$ of Π. (Since the system may not halt, the computation is necessarily infinite.) We have $\mu_i \in U$ for all $i \in \mathbb{N}$ and U has finite cardinality, therefore there exists $j_0, p \in \mathbb{N}$ such that $\mu_{j_0} = \mu_{j_0+p}$ (we may assume that j_0 is minimal with this property). Therefore, we may build a periodic sequence of computations of Π, say $(\omega_i)_{i\in\mathbb{N}}$, such that $\omega_i = \mu_i$ for all $i \leq j_0$ and $\omega_i = \mu_{(i-j_0) \mod p}$ otherwise. Hence Π is ultimately periodic.

Since structural boundedness (the property that a net is bounded for all possible initial markings) is decidable, the previous proposition gives an adequate condition for structural ultimate periodicity. This condition can be efficiently checked since structural boundedness is in PTIME [8].

Propositions 1 and 2 only refer to the existence of one periodic computation. In the study of biological systems, we may be interested in a stronger property, akin to the notion of regularity in discrete dynamical systems, namely that every computation of a PB system, Π, may be "approximated" by a sequence of periodic computations of Π. Taking our inspiration from the decidability of the home states problem (and therefore of the problem of testing whether a net is cyclic), we give a sufficient condition for regularity.

Proposition 4 (Cyclicity). *Consider a PB system Π, if $[\![\Pi]\!]$ is cyclic then every finite computation of Π may be extended into an infinite periodic computation of Π.*

Periodicity and regularity are not precise enough to wholly characterize the global dynamic of the systems. In particular, the following proposition shows that a system with at least two different periodic computations has an extremely complex dynamics. This result suggests that, when looking after systems that exhibit simple, repetitive behavior, one should concentrate on "almost degenerated systems", with practically no internal concurrency and only one cyclic computation.

Proposition 5. *If a PB system, Π, has at least two distinct periodic computations then the following three statements hold:*

- *the system Π has (at least) a countable set of periodic computations;*
- *the system Π has a countable set of ultimately periodic computations;*
- *the system Π has an uncountable set of aperiodic computations.*

Proof. Assume there are at least two periodic computations in Π, that is, at least two cycles, C of length p and D of length q, in the "transitions graph" associated to Π. From any infinite boolean sequence, w, we may built a valid computation of Π, say C_w, as follows.

We build the computation sequence C_w gradually, as the limit of a sequence of computations $(C_i)_{i\in\mathbb{N}}$. Intuitively, C_w is obtained as the concatenation of the sequence of transitions in C and the sequence of transitions in D, following the value of the bits in w. For example, the sequence $0110\ldots$ will correspond to the computation $C \cdot D \cdot D \cdot C \cdot \ldots$.

Let $\#_b(w, j)$ be the number of occurrences of the boolean b in the prefix of size j of w and let r equals $p.\#_0(w, j) + q.\#_1(w, j)$. At step 0, define $C_0(i) = C(i \bmod p)$ for all indices $i \in \mathbb{N}$. At step j, if $w(j) = 0$ then define $C_j(i) = C(i - r)$ for all indices $i \in \mathbb{N}$ such that $r \leq i \leq r + p$ and $C_j(i) = C_{j-1}(i)$ otherwise. Conversely, if $w(j) = 1$ then define $C_j(i) = D(i - r)$ for all indices $i \in \mathbb{N}$ such that $r \leq i \leq r + q$ and $C_{j-1}(i)$ otherwise. Let $C_w = \lim_{j\to\infty} C_j$.

For every infinite sequence of boolean w, the sequence of transitions C_w is a valid computation of Π. Therefore, for every different periodic sequence w (there is a countable number of such sequences), we obtain a different periodic computation C_w of Π. Moreover, choose a real number x in $[0, 1]$ and let w be its binary expansion. If x is rational then C_w is ultimately periodic and if x is not rational then C_w is aperiodic. Therefore there is a countable set of ultimately periodic computations of the form C_w in Π and an uncountable set of aperiodic computations of the form C_w in Π.

Before concluding, we remark that most of the results presented here may not be preserved if we slightly extend the semantics of PB systems. Indeed, we have seen that most of interesting dynamical properties on "standard" Petri nets are decidable. The situation is much different when Petri nets are extended with inhibitor arcs, that is with transitions that get enabled when a given place is empty. The reachability problem is still decidable for nets with only one inhibitor arc [13], but it is a folklore result that reachability is undecidable for nets with (at least two) inhibitors arcs (see for example [12]).

By our main theorem, it follows that many problems on PB systems will become undecidable if we extend this model with rules that may react to the absence of a molecule (intuitively, the opposite of a catalysing rule).

Theorem 5. *The reachability problem is undecidable for PB systems extended with communication or transformation rules that may react to the absence of a molecule.*

Likewise, boundedness and reachability are undecidable problems for Transfer and Reset Petri nets [3], two extensions of Petri nets with special arcs that may transfer or reset the full content of some place. (On the other hand, the coverability problem is decidable.) This last result shed light on the potential complexity of extensions of PB-systems with mobile or volatile membranes.

8 Conclusions and further discussions

This paper offers a compositional encoding of PB and PBE systems into Petri nets. We may relate this encoding to a compilation process, where PB systems take the part of the high-level programs (in which to model biological reactions) and Petri nets amount to the target assembly language (in which to apply optimizations and decision procedures). Most particularly, this encoding allows us to transfer several decidability results from Petri nets to PB/PBE systems and may be used as a safeguard when looking for (decidable) extensions to this model.

We foresee several domains in which this newly established connection between Petri nets and PB systems may be fruitful. For example, in the creation of tools for reasoning on PB systems, since many logics and associated model-checking tools have been developed for Petri nets, or in the study of stochastic or timed versions of PB systems [5,15]. Another example is the study of the *controller synthesis* problem, an important current issue in Petri nets theory: given a system N, the problem is to build a *controlling system*, E, such that the composition of N with E satisfies some specific property — for instance it has a cyclic behavior. In the context of PBE system, an extension of PB systems [1] defined in Section 4, the synthesis problem can be directly connected to the problem of finding a suitable environment which "drives" some specific behavior.

More profoundly, our work on the relation between PB systems and Petri net calls for a deeper study of the appropriate notion(s) of periodicity. It is clear that, from a biological point of view, periodicity plays a fundamental role in the dynamical behavior of systems. Our point is that it may be more subtle than it seems to precisely express the kind of periodicity needed in order to express real biological properties. Definitions based on a single computation sequence (see Section 3) seems too weak when applied to a non-deterministic process. Cyclicity (see Proposition 4) may be another possible alternative.

Acknowledgment

This article has been typeset using the GasTEX macro package. The authors warmly thanks Roberto Amadio and Rémi Morin for useful discussions.

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