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Concurrency in Boolean networks

Thomas Chatain · Stefan Haar · Juraj
Kolčák · Loïc Paulevé · Aalok Thakkar

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Abstract Boolean networks (BNs) are widely used to model the qualitative dynamics of biological systems. Besides the logical rules determining the evolution of each component with respect to the state of its regulators, the scheduling of components updates can have a dramatic impact on the predicted behaviours. In this paper, we explore the use of Contextual Petri Nets (CPNs) to study dynamics of BNs with a concurrency theory perspective. After showing bi-directional translations between CPNs and BNs and analogies between results on synchronism sensitivities, we illustrate that usual updating modes for BNs can miss plausible behaviours, i.e., incorrectly conclude on the absence/impossibility of reaching specific configurations. Taking advantage of CPN semantics enabling more behaviour than the generalized asynchronous updating mode, we propose an encoding of BNs ensuring a correct abstraction of any multivalued refinement, as one may expect to achieve when modelling biological systems with no assumption on its time features.

T. Chatain, S. Haar, J. Kolčák, A. Thakkar
Inria Saclay-Île-de-France
LSV, CNRS, & ENS Paris-Saclay
Université Paris-Saclay, France
E-mail: thomas.chatain@lsv.fr
E-mail: stefan.haar@lsv.fr
E-mail: juraj.kolcak@lsv.fr
Present address: of A. Thakkar
Department of Computer and Information Science
University of Pennsylvania
Philadelphia, PA 19104, USA
E-mail: athakkar@seas.upenn.edu

L. Paulevé
CNRS, LRI UMR 8623, Univ. Paris-Sud – CNRS
Université Paris-Saclay, France
E-mail: loic.pauleve@lri.fr

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1 Introduction

Boolean networks (BNs) model dynamics of systems where several components (nodes) interact. They specify for each node an update function to determine its next value according to the configuration (global state) of the network. In addition, an *update mode* for scheduling the node updates has to be specified to determine the set of reachable configurations.

BNs are increasingly used to model dynamics of biological networks, such as gene networks and cellular signalling pathways. In these practical applications, it is usual to assess the accordance of a BN with the concrete modeled system by checking if the observed behaviours are reproducible by the abstract BN [37, 42, 18]. For instance, if one observe that the system can reach a configuration y from configuration x , one may expect it is indeed the case in the BN model. Whenever it is not the case, it typically means that the designed Boolean functions do not model the system correctly, and thus should be fixed prior to further analysis. With this perspective, the choice of the update mode is crucial, as it is known to have a strong influence on the reachable configurations of the network.

More fundamentally, the relationships between different updating modes has been extensively studied for function-centered models such as cellular automata [38, 5] and Boolean networks [26, 41, 21, 3, 30, 31], on which this article is focused.

Interestingly, the study of updating mechanisms in networks and their effect on the emerging global dynamics has also been widely addressed in the field of discrete and hybrid concurrent systems, especially with Petri nets [24, 8, 9, 44, 45]. Petri nets are a classical formal framework for studying concurrency, offering a fine-grained specification of the *conditions* (partial configurations) for *events* (partial configuration changes). This decomposed view of causality and effect of updates enables capturing events which can indifferently occur sequentially or in parallel, and events having conflicts (triggering one would pre-empt the application of the second).

In the literature, many variants of Petri nets have been employed to model and simulate various biological processes [22, 33, 10], but little work considered the link between the theoretical work on concurrency in Petri nets and the theoretical work in Boolean networks. In [39, 11, 13], encodings of BNs and their multi-valued extension in certain classes of Petri nets have been proposed, often as a mean to take advantage of existing dynamical analysis already implemented for Petri nets, e.g., model-checking.

This paper aims at building a bridge between the theoretical work in BNs on the one hand and Contextual Petri Nets (CPNs) on the other. Based on bidirectional connections between the two formalisms, we use a classical result from Petri nets to show the PSPACE-completeness of reachability in asyn-

chronous BNs. Then, we exhibit analogies of results on update mode comparisons. Importantly, we show how the concurrent view of updates brings new updating modes for BNs, enabling new behaviours and meeting with a correct abstraction of multi-level systems. This result is illustrated on a small BN which occurs in different models of actual biological networks, and for which the usual updating modes fail to capture behaviours existing in refined models.

Outline. Sect. 2 gives basic definitions of BNs, their asynchronous, synchronous, and generalized asynchronous update mode, and their influence graph. Sect. 3 defines safe CPNs and their atomic, step, and interval semantics. Sect. 4 brings encodings of BNs into safe CPNs and vice-versa, the latter allowing to derive that reachability in BNs is PSPACE-complete. Sect. 5 establishes an analogy between the results on synchronism sensitivity in BNs and Petri nets. Sect. 6 provides an encoding of the interval semantics of CPNs into asynchronous BNs, initially published in the conference paper [15]. Sect. 7 first illustrates the benefits of the interval semantics on a simple BN showing that usual BN semantics can miss plausible behaviours. Then, an extension of the interval semantics is proposed in order to meet with a correct abstraction of behaviours achievable in a multivalued refinement. Finally, Sect. 8 summarizes the contributions and discusses further work.

Notations. If S is a finite set, $|S|$ denotes its cardinality. $\mathbb{B} = \{0, 1\}$, and we write \wedge, \vee, \neg for logic operators *and, or, not*; given a set of literals $L = \{l_1, \dots, l_k\}$, $\bigwedge_L \equiv l_1 \wedge \dots \wedge l_n$ with $\bigwedge_\emptyset = 1$, and $\bigvee_L \equiv l_1 \vee \dots \vee l_n$ with $\bigvee_\emptyset = 0$.

2 Boolean networks with function-centered specification

Given a *configuration* $x \in \mathbb{B}^n$ and $i \in \{1, \dots, n\}$, we denote x_i the i^{th} component of x , so that $x = x_1 \dots x_n$. Given two configurations $x, y \in \mathbb{B}^n$, the components that differ are noted $\Delta(x, y) \triangleq \{i \in \{1, \dots, n\} \mid x_i \neq y_i\}$.

Definition 1 (Boolean network) A Boolean network (BN) of dimension n is a collection of functions $f = \langle f_1, \dots, f_n \rangle$ where $\forall i \in \{1, \dots, n\}, f_i : \mathbb{B}^n \rightarrow \mathbb{B}$.

Given $x \in \mathbb{B}^n$, we write $f(x)$ for $f_1(x) \dots f_n(x)$.

Fig. 1 (a) shows an example of BN of dimension 3.

When modelling biological systems, each node $i \in \{1, \dots, n\}$ usually represents a biochemical species, being either active (or present, value 1) or inactive (or absent, value 0). Each function f_i indicates how the evolution of the value of i is influenced by the current value of other components $j \in \{1, \dots, n\}$. However, this description can be interpreted in several ways, therefore several updating modes coexist for BNs, depending on the assumptions about the order in which the evolutions predicted by the f_i apply.

The (fully) *asynchronous updating* assumes that only one component is updated at each time step. The choice of the component to update is non deterministic.

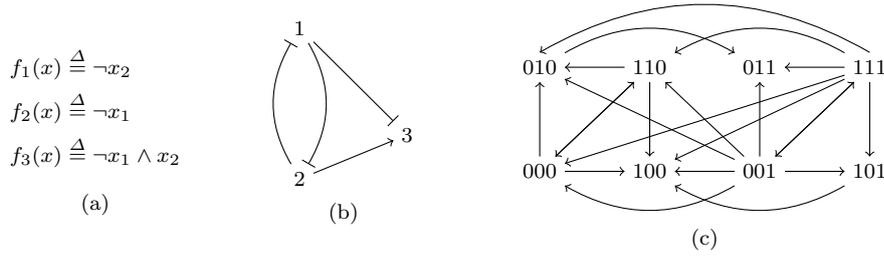


Fig. 1 (a) Example BN f of dimension 3; (b) Influence graph $G(f)$; positive edges are with normal tip; negative edges are with bar tip; (c) Transition relations between states in \mathbb{B}^n according to the generalized asynchronous semantics of f .

Definition 2 (Asynchronous updating) Given a BN f , the binary irreflexive relation $\xrightarrow[\text{async}]{} \subseteq \mathbb{B}^n \times \mathbb{B}^n$ is defined as:

$$x \xrightarrow[\text{async}]{} y \iff \exists i \in \{1, \dots, n\}, \Delta(x, y) = \{i\} \wedge y_i = f_i(x) .$$

We write $\xrightarrow[\text{async}]{}^*$ for the transitive closure of $\xrightarrow[\text{async}]{}.$

The *synchronous updating* can be seen as the opposite: *all* components are updated at each time step. This leads to a purely deterministic dynamics.

Definition 3 (Synchronous updating) Given a BN f , the binary irreflexive relation $\xrightarrow[\text{sync}]{} \subseteq \mathbb{B}^n \times \mathbb{B}^n$ is defined as:

$$x \xrightarrow[\text{sync}]{} y \iff x \neq y \wedge \forall i \in \{1, \dots, n\}, y_i = f_i(x) .$$

By forcing all the components to evolve synchronously, the synchronous updating makes a strong assumption on the dynamics of the system. In many concrete cases, for instance in systems biology, this assumption is clearly unrealistic, at least because the components model the quantity of some biochemical species which evolve at different speeds.

As a result, the synchronous updating fails to describe some behaviours, like the transition $010 \rightarrow 011$ represented in Fig. 1 (c) which represents the activation of species 3 when species 1 is inactive and species 2 is active ($f_3(010) = 1$). There are also transitions which are possible in the synchronous

but not in the asynchronous updating, for instance $000 \rightarrow 110$. Remark that 110 is not even reachable from 000 in the asynchronous updating.

The *generalized asynchronous updating* generalizes both the asynchronous and the synchronous ones: it allows updating synchronously any nonempty subset of components.

Definition 4 (Generalized asynchronous updating) Given a BN f , the binary irreflexive relation $\xrightarrow[\text{gen}]{f} \subseteq \mathbb{B}^n \times \mathbb{B}^n$ is defined as:

$$x \xrightarrow[\text{gen}]{f} y \stackrel{\Delta}{\iff} x \neq y \wedge \forall i \in \Delta(x, y) : y_i = f_i(x) .$$

Clearly, $x \xrightarrow[\text{async}]{f} y \Rightarrow x \xrightarrow[\text{gen}]{f} y$ and $x \xrightarrow[\text{sync}]{f} y \Rightarrow x \xrightarrow[\text{gen}]{f} y$. The converse propositions are false in general. It is even false that $x \xrightarrow[\text{gen}]{f} y$ implies $x \xrightarrow[\text{async}]{f} y \vee x \xrightarrow[\text{sync}]{f} y$.

Note that we forbid “idle” transitions ($x \rightarrow x$) whatsoever the updating mode.

Other updating modes like sequential or block sequential have also been considered in the literature on cellular automata and Boolean networks [5, 3], and usually lead to transitions allowed by the generalized asynchronous updating.

For each node $i \in \{1, \dots, n\}$ of the BN, f_i typically depends only on a subset of nodes of the network. The *influence graph* of a BN (also called interaction or causal graph) summarizes these dependencies by having an edge from node j to i if f_i depends on the value of j . Formally, f_i depends on x_j if there exists a configuration $x \in \mathbb{B}^n$ such that $f_i(x)$ is different from $f_i(x')$ where x' is x having solely the component j different ($x'_j = \neg x_j$). Moreover, assuming $x_j = 0$ (therefore $x'_j = 1$), we say that j has a positive influence on i (in configuration x) if $f_i(x) < f_i(x')$, and a negative influence if $f_i(x) > f_i(x')$. It is possible that a node has different signs of influence on i in different configurations (leading to non-monotonic f_i). It is worth noticing that different BNs can have the same influence graph.

Definition 5 (Influence graph) Given a BN f , its *influence graph* $G(f)$ is a directed graph $(\{1, \dots, n\}, E_+, E_-)$ with *positives* and *negatives* edges such that

$$(j, i) \in E_+ \stackrel{\Delta}{\iff} \exists x, y \in \mathbb{B}^n : \Delta(x, y) = \{j\}, x_j < y_j, f_i(x) < f_i(y)$$

$$(j, i) \in E_- \stackrel{\Delta}{\iff} \exists x, y \in \mathbb{B}^n : \Delta(x, y) = \{j\}, x_j < y_j, f_i(x) > f_i(y)$$

A (directed) cycle composed of edges in $E_+ \cup E_-$ is said *positive* when it is composed by an even number of edges in E_- (and any number of edges in E_+), otherwise it is *negative*.

The influence graph is an important object in the literature of BNs [40, 2]. For instance, many studies have shown that one can derive dynamical features of a BN f by the sole analysis of its influence graph $G(f)$. Importantly, the presence of negative and positive cycles in the influence graph, and the way they are intertwined can help to determine the nature of attractors (that are the smallest sets of configurations closed by the transition relationship) [35], and derive bounds on the number of fixpoints and attractors a BN having the same influence graph can have [34, 1, 4].

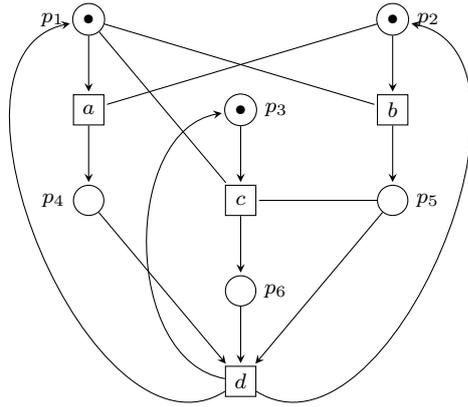


Fig. 2 A contextual Petri net (CPN). Neither atomic semantics or step semantics allow d to fire, while the more permissive non-atomic semantics allows it.

3 Contextual Petri Nets with transition-centered specifications

In the semantics of BNs, each node computes its next value according to the value of the other nodes. We have seen in previous section that this general rule does not suffice to define the precise behaviour and several updating modes can be considered.

This situation is very similar to what happens in contextual Petri nets (CPNs), where, more for a matter of concurrency, read arcs have been introduced to model read-only access to resources. Interestingly, the introduction of read arcs in Petri nets has also led to several variants of the semantics. In this section, we present some of them, mainly taken from [14]. Next, relying on a natural encoding of BNs in CPNs (Sect. 4), we will establish a correspondence between updating modes for BNs and semantics of CPNs. In particular, we transpose the *interval semantics* of CPNs to a new semantics for BNs (Sect. 6) which retrieves some plausible scenarios that were missed by other updating modes.

3.1 Contextual Petri Nets

We consider only *safe* contextual Petri nets (CPNs), i.e. CPNs where there is never more than one token in a place.

Definition 6 (Contextual Petri Net (CPN)) A *contextual Petri net* is a tuple $(P, T, pre, cont, post, M_0)$ where P and T are finite sets of *places* and *transitions* respectively, pre and $post$ map each transition $t \in T$ to its (nonempty) *preset* denoted $\bullet t \triangleq pre(t) \subseteq P$, its (possibly empty) *con-*

text denoted $\underline{t} \triangleq \text{cont}(t) \subseteq P \setminus \bullet t$ and its (possibly empty) postset denoted $t^\bullet \triangleq \text{post}(t) \subseteq P$; $M_0 \subseteq P$ is the *initial marking*. We usually denote $\bullet \underline{t} \triangleq \bullet t \cup \underline{t}$.

For simplicity, we assume that for every transition t , its context is disjoint from its preset and postset.

A CPN is represented as a graph with two types of nodes: places (circles) and transitions (rectangles). Presets are represented by arrows from places to transitions, postsets by arrows from transitions to places, and contexts by undirected edges, called read arcs, between places and transitions. The initial marking is represented by tokens in places. Fig. 2 shows an example of CPN. The transition a , for instance, has p_1 in its preset, p_2 in its context and p_4 in its postset.

3.2 Atomic Semantics

A *marking* of a safe contextual Petri net is a set $M \subseteq P$ of marked places. A Petri net starts in its *initial marking* M_0 . A transition $t \in T$ is *enabled* in a marking M if all the places of its preset and context are marked, i.e. $\bullet t \cup \underline{t} \subseteq M$. Then t can *fire* from M , leading to the marking $M' \triangleq (M \setminus \bullet t) \cup t^\bullet$. In this case, we write $M \xrightarrow[\text{atom}]{N,t} M'$ or simply $M \xrightarrow[\text{atom}]{N} M'$.

Again, we consider only *safe* contextual Petri nets, that is we assume that if a transition $t \in T$ is enabled in a marking M , then $(M \setminus \bullet t) \cap t^\bullet = \emptyset$.

Definition 7 (Atomic semantics, a-run) We call *firing sequence* of N under the atomic semantics, or *a-run*, any sequence $\sigma \triangleq (t_1 \dots t_n)$ of transitions for which there exist markings M_1, \dots, M_n such that for all $i \in \{1, \dots, n\}$, firing t_i from M_{i-1} is possible and leads to M_i .

For instance, the net in Figure 2 has two possible firing sequences: (a) and (bc) . However, it is never possible to fire d because that would require to fire both a and b first, and firing one of a, b disables the other.

3.3 Non-atomic Semantics

In this section, we discuss two semantics for concurrent firing of multiple transitions. One is the well-known *step semantics* [23], in which multiple transitions can fire simultaneously. This is typically the case of a and b in the net of Figure 2, which are enabled simultaneously and have disjoint presets, but cannot fire together according to the atomic semantics. The step semantics can be interpreted as first checking whether all members of a set of transitions can fire, and then firing them either simultaneously or one by one, in any order. We then recall the *interval semantics* introduced in [14], which allows a more liberal choice of checking and firing transitions in a set.

We present the semantics under the assumption that the underlying net is safe even under these two semantics, which allow more possibilities than the atomic one.

3.3.1 Step Semantics

We first recall the step semantics [23].

Definition 8 (Step semantics, s-run) Let N be a CPN. A *step* is a set S of transitions of N . It can fire from configuration M and lead to configuration M' , written $M \xrightarrow[\text{step}]{N,S} M'$ or simply $M \xrightarrow[\text{step}]{N} M'$, if

- every $t \in S$ is enabled in M ,
- the presets of the transitions in S are disjoint, and
- $M' = (M \setminus \bigcup_{t \in S} \bullet t) \cup \bigcup_{t \in S} t \bullet$.

We call *s-run* of N any sequence $\sigma \triangleq (S_1 \dots S_n)$ of *steps* for which there exist markings M_1, \dots, M_n such that for all $i \in \{1, \dots, n\}$, step S_i can fire from M_{i-1} and leads to M_i .

A variant of step semantics, called maximal step semantics has received interest in the literature [25, 19].

Definition 9 (Maximal step semantics) The firing rule for the maximal step semantics is defined as $M \xrightarrow[\text{mstep}]{N,S} M'$ (or simply $M \xrightarrow[\text{mstep}]{N} M'$) iff $M \xrightarrow[\text{step}]{N,S} M'$ and no larger step $S' \supsetneq S$ can fire from M .

In the example of Figure 2, the step semantics allows one to fire a and b in one step since they are both enabled in the initial state and $\bullet a \cap \bullet b = \emptyset$. This gives the s-run $(\{a, b\})$ in addition to the others which were already possible under the atomic semantics; for instance the a-run involving b followed by c , (denoted (bc) for the atomic semantics), is simply rewritten as the s-run $(\{b\}\{c\})$ under the step semantics. However, transition d remains dead since none of these s-runs contains all of a , b , and c .

The intuitive model underlying the step semantics is that all the transitions in the step can first check, in any order, whether they are enabled and not in conflict with one another. Once the checks have been performed, they can all fire, again in any order. Put differently, if we denote the checking phase of a transition t by t^- and its firing phase by t^+ , then every step consists of any permutation of the actions of type t^- (for all transitions t in the step), followed by any permutation of the actions t^+ . The notion introduced in Definition 10 formalizes this intuition.

Definition 10 (s^\pm -run) For every s-run $(T_1 \dots T_n)$ of a contextual Petri net N , every concatenation $u_1^- . u_1^+ . \dots . u_n^- . u_n^+$ of sequences u_i^- and u_i^+ , is a s^\pm -run of N , where every u_i^- is a permutation of the set $\{t^- \mid t \in T_i\}$ and every u_i^+ is a permutation of the set $\{t^+ \mid t \in T_i\}$ (remember that T_i is a set of transitions of N).

For example, the s-run $(\{b\}\{c\})$ yields the s^\pm -run $(b^-b^+c^-c^+)$ and the s-run $(\{a, b\})$ yields four s^\pm -runs: $(a^-b^-a^+b^+)$, $(a^-b^-b^+a^+)$, $(b^-a^-a^+b^+)$ and $(b^-a^-b^+a^+)$.

3.3.2 Splitting Transitions for Understanding Steps

Definition 10 formalizes a semantics of CPNs, in which the firing of a transition does not happen atomically, but in two steps, the checking of the pre-conditions and the actual execution. In this section, we generalize this idea.

The left-hand side of Figure 3 shows a part of the net in Figure 2, which consists of transition a with its preset $\{p_1\}$, context $\{p_2\}$, and postset $\{p_4\}$. The construction on the right-hand side of 3 illustrates the idea of splitting firing transitions into two phases:

- Every transition t is split into t^- and t^+ .
- Every place p is duplicated to p^c (meaning token in p available for consumption) and p^r (meaning token in p available for reading).

Similar ideas about splitting transitions can be found in several works, for instance in [43].

Intuitively, if we apply this construction to all transitions from Figure 2, then the s^\pm -runs of that net correspond to a-runs of the newly constructed net. The following Definition 11 provides the precise details of the construction.

Definition 11 (*split*(N)) For every contextual Petri net $N = (P, T, pre, cont, post, M_0)$, we define the contextual Petri net $split(N) \triangleq (P', T', pre', cont', post', M'_0)$ where

- T' contains two copies, denoted t^- and t^+ of every transition $t \in T$.
- P' contains two copies, denoted p^c and p^r of every place $p \in P$, plus one place p_t per transition $t \in T$.
- $\bullet t^- \triangleq \{p^c \mid p \in \bullet t\}$
- $\underline{t}^- \triangleq \{p^r \mid p \in \underline{t}\}$
- $t^- \bullet \triangleq \{p_t\}$
- $\bullet t^+ \triangleq \{p^r \mid p \in \bullet t\} \cup \{p_t\}$
- $\underline{t}^+ \triangleq \emptyset$
- $t^+ \bullet \triangleq \{p^c \mid p \in t^\bullet\} \cup \{p^r \mid p \in t^\bullet\}$
- $M'_0 \triangleq \{p^c \mid p \in M_0\} \cup \{p^r \mid p \in M_0\}$

We now formally prove the intuition mentioned above:

Lemma 1 *Every s^\pm -run σ^\pm of N is a a-run of $split(N)$. Moreover σ^\pm reaches the marking $\{p^c \mid p \in M\} \cup \{p^r \mid p \in M\}$, where M is the marking of N reached after the s-run σ from which σ^\pm is obtained.*

Proof We proceed by induction on the length of σ . The case $\sigma = ()$ is trivial. Now, let $\sigma^\pm = u_1^- . u_1^+ . \dots . u_n^- . u_n^+$ be a s^\pm -run obtained from a s-run

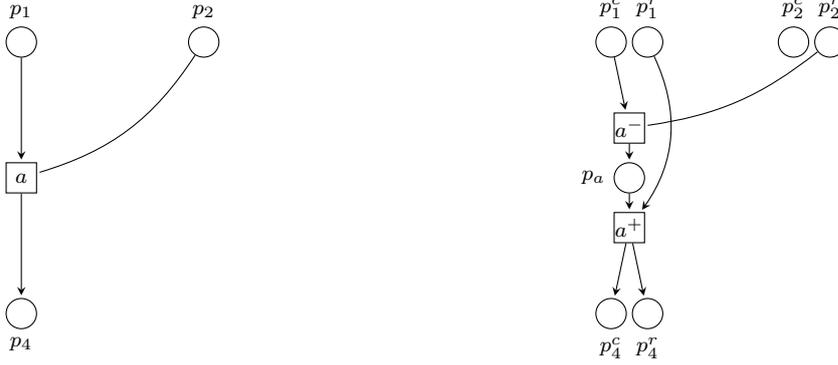


Fig. 3 The splitting of transition a (left) into a^- and a^+ (right).

$\sigma = (T_1 \dots T_n)$, assume the property true for $u_1^-.u_1^+ \dots u_{n-1}^-.u_{n-1}^+$ and denote M_{n-1} the marking reached after $(T_1 \dots T_{n-1})$. By induction hypothesis, $u_1^-.u_1^+ \dots u_{n-1}^-.u_{n-1}^+$ reaches the marking $\{p^c \mid p \in M_{n-1}\} \cup \{p^r \mid p \in M_{n-1}\}$ of $\text{split}(N)$. The fact that T_n is a valid step from M_{n-1} implies that $\bigcup_{t \in T_n} \bullet t \subseteq M_{n-1}$ and that the presets of the transitions in T_n are disjoint. This allows one to fire all the $t^-, t \in T_n$ in any order and reach the marking $\{p^c \mid p \in M_{n-1} \setminus \bigcup_{t \in T_n} \bullet t\} \cup \{p^r \mid p \in M_{n-1}\} \cup \{p_t \mid t \in T_n\}$ of $\text{split}(N)$. Now the $t^+, t \in T_n$, are all enabled and their presets are disjoint. They can in turn be fired in any order, reaching the desired marking of $\text{split}(N)$. \square

Note that the converse of Lemma 1 does not hold. For instance, for the net N from Figure 2, the net $\text{split}(N)$ admits the a-run $a^-b^+c^-c^+a^+$, which is not an s^\pm -run of N .

3.3.3 Interval Semantics

We have seen that the construction $\text{split}(N)$ admits firing sequences that cannot be mapped back to executions under either the atomic or the step semantics. In this section, we shall introduce the *interval semantics*, which is more general than the step semantics, and whose interpretation on a net N does correspond to the feasible executions in $\text{split}(N)$.

Definition 12 (Interval semantics, i-run) Every a-run of $\text{split}(N)$ is called *i-run* of N , or run of N under the interval semantics.

Coming back to the example of Figure 2, transition d can fire under the interval semantics, for instance after the i-run $a^-b^+c^-c^+a^+d^-d^+$ where transitions b and c complete the firing during the period in which a fires. Under the atomic semantics, a and b are in conflict, which prevents d from firing. Under the step semantics, a and b can fire in the same step, but then c cannot fire. Under the interval semantics, d can also fire.

Recall that we introduced t^- and t^+ to represent different phases during the execution of transition t . An obvious question is whether the new semantics can lead to runs in which a transition ‘gets stuck’ during its execution. The following Lemma 2 affirms that this is not the case: once t^- is fired, nothing can hinder t^+ from firing, too.

Definition 13 (complete marking) A marking of $split(N)$ is *complete* if no p_t is marked.

In particular, the initial marking is complete.

Definition 14 (complete i-run) An i-run is *complete* if every t^- is matched by a t^+ .

Lemma 2 *Every i-run can be completed: for every i-run σ , there exists a suffix μ which matches all the unmatched t^- , and such that $\sigma\mu$ is an i-run. Moreover, complete i-runs (and only them) lead to complete markings.*

Proof As long as a t^- is unmatched, $\bullet t^+$ remains included in the marking: no other transition consumes these tokens. Hence it suffices to fire all the t^+ corresponding to the unmatched t^- , in any order. \square

Now, relating $split(N)$ with the original net N , we map naturally every marking M of N to the complete marking M' of $split(N)$ defined as $M' \triangleq \{p^c \mid p \in M\} \cup \{p^r \mid p \in M\}$. We get of course that

$$M_1 \xrightarrow[\text{atom}]{N,t} M_2 \implies M'_1 \xrightarrow[\text{atom}]{N,t^-} \xrightarrow[\text{atom}]{N,t^+} M'_2,$$

but in general the interval semantics induces more runs: for every markings M_1 and M_2 of N , we write $M_1 \xrightarrow[\text{istep}]{N}^* M_2$ when $M'_1 \xrightarrow[\text{atom}]{N}^* M'_2$.

4 Encodings

4.1 Coding Boolean Networks in safe Contextual Petri nets

The translation of BNs into safe Petri nets has been already addressed in the literature (e.g. [10,11,13,12]). We provide here a similar encoding of BNs into safe CPNs, with the explicit specification of the context of transitions, and with notations that will be used in Sect. 5. The encoding can be easily generalized to multi-valued networks to safe CPNs, following [13,32].

BNs translate into a special type of CPNs:

- *complemented*: for every place p there is exactly one distinct place \bar{p} such that

$$\bullet p = \bar{p}^\bullet \wedge p^\bullet = \bullet \bar{p} \wedge \forall t \in T : p \in \underline{t} \Rightarrow \bar{p} \notin \underline{t};$$

The initial marking M_0 and any reachable marking M satisfy

- *Boolean*: there is a surjection $var : P \rightarrow \{1, \dots, n\}$ such that

$$\forall p, p' \in P : var(p) = var(p') \Leftrightarrow p' \in \{p, \bar{p}\},$$

and, subsequently, a mapping $val : P \rightarrow \mathbb{B}$ which satisfies

$$\forall p \in P : val(p) + val(\bar{p}) = 1.$$

Moreover, any reachable marking M satisfies

$$\forall p \in P : p \in M \Leftrightarrow \bar{p} \notin M.$$

- *transition dichotomy*: every transition $t \in T$ has exactly one input place p and as unique output place \bar{p} . If $val(p) = 0$ then call t the *up-transition* $\mathbf{up}(var(p))$ of $var(p)$, otherwise the *down-transition* $\mathbf{dw}(var(p))$ of $var(p)$.

Let us consider a BN f of dimension n . Every component $v \in \{1, \dots, n\}$ gives rise to two places v_0 and v_1 representing the two values possible for v . Then there is a transition v^+ for each conjunctive clause of the disjunctive normal form of $(\neg x_v \wedge f_v(x))$, and a transition v^- for each conjunctive clause of the disjunctive normal form of $(x_v \wedge \neg f_v(x))$, such that

$$\bullet(v^+) = (v^-)^\bullet = \{v_0\} \text{ and } \bullet(v^-) = (v^+)^\bullet = \{v_1\},$$

and where the contexts of the transitions are given by the conjunctive clauses minus literals related to v .

Fig.4 show the translation of the BN of Fig. 1 into CPN.

Hereafter, Definition 15 gives a formalization of this encoding, and Theorem 1 states its correctness with respect to the asynchronous, synchronous, generalized asynchronous updating modes, and CPN atomic, maximal step, and step semantics, respectively. Given a Boolean formula F , we write $\text{DNF}[F]$ for the set of conjunctive clauses in F 's disjunctive normal form. A clause $C \in \text{DNF}[F]$ is then a set of literals, positives or negatives. It is worth noticing that the resulting CPN can have a number of transitions exponential in the number of literals in the Boolean functions.

Definition 15 Given a BN f of dimension n and a configuration y , (f) is the CPN $(P, T, pre, cont, post, M_0)$ such that

- $P = \{1, \dots, 2n\}$ are the places;
- $T, pre, cont, post$ are the smallest sets such that for each $i \in \{1, \dots, n\}$, for each clause $C \in \text{DNF}[\neg x_i \wedge f_i(x)]$ (resp. $C \in \text{DNF}[x_i \wedge \neg f_i(x)]$), there is a transition $t \in T$ such that $\bullet t = \{i\}$ (resp. $\bullet t = \{i + n\}$), $t^\bullet = \{i + n\}$ (resp. $t^\bullet = \{i\}$), and $\underline{t} = \{j \mid [\neg x_j] \in C, j \neq i\} \cup \{j + n \mid [x_j] \in C, j \neq i\}$;
- $M_0 = (y)$

where, for any configuration $x \in \mathbb{B}^n$, $(x) \triangleq \{i + nx_i \mid i \in \{1, \dots, n\}\}$.

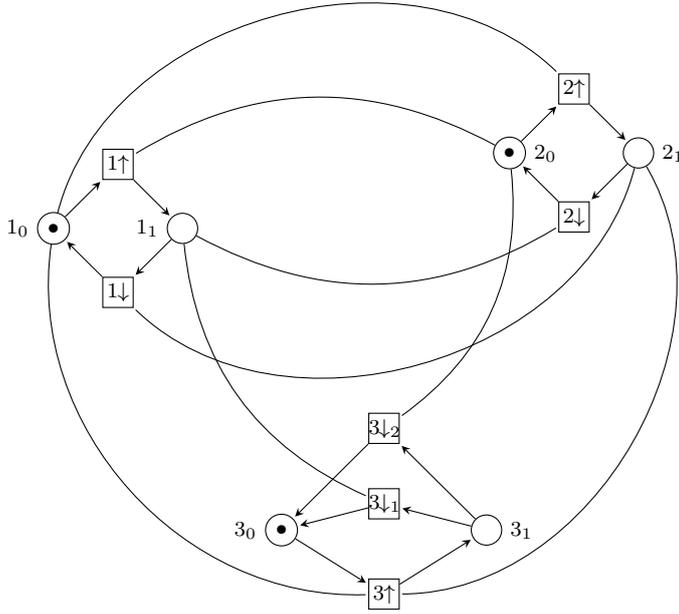


Fig. 4 CPN encoding of the BN of Fig. 1 $\langle f_1(x) = \neg x_2, f_2(x) = \neg x_1, f_3(x) = \neg x_1 \wedge x_2 \rangle$ and configuration 000

Theorem 1 Given a BN f of dimension n , for any configurations $x, y \in \mathbb{B}^n$,

$$\begin{aligned} x \xrightarrow[\text{async}]{f} y &\iff \langle x \rangle \xrightarrow[\text{atom}]{\langle f \rangle} \langle y \rangle, \\ x \xrightarrow[\text{sync}]{f} y &\iff \langle x \rangle \xrightarrow[\text{mstep}]{\langle f \rangle} \langle y \rangle, \\ x \xrightarrow[\text{gen}]{f} y &\iff \langle x \rangle \xrightarrow[\text{step}]{\langle f \rangle} \langle y \rangle. \end{aligned}$$

Proof For any $i \in \{1, \dots, n\}$, $f_i(x) \neq x_i$ if and only if there exists a transition t of $\langle f \rangle$ where $\bullet t \cup \underline{t} \subseteq \langle x \rangle$.

4.2 Coding Contextual Petri Nets in Boolean Networks

We have given above a translation of BNs into (a special class of) CPNs. The comparison of both models also leads us into the opposite direction.

In the following, fix a safe CPN $N = (P, T, pre, cont, post, M_0)$. The BN associated to N has $|P| + |T|$ components, where the first $|P|$ components encode the marking of the corresponding place, and the $|T|$ other components encode the occurring transitions. Without loss of generality, we assume that

places and transitions range over indexes from 1 to $|P| + |T|$, i.e., $P \cup T \equiv \{1, \dots, |P| + |T|\}$. In order to simplify the encodings, we assume moreover the contextual Petri nets to be *loop-free*, i.e. for every transition $t \in T$, $\bullet t \cap t^\bullet = \emptyset$. It is well known that loops can be replaced by read arcs without any effect on the (atomic) semantics.

Transporting the *dynamics*, i.e. the actual *firing* of transitions, into the framework of BNs constitutes the non-trivial part of the translation. A CPN transition typically has more than one output place, while the functions in BNs write on one single variable. Our encoding decomposes the firing of a CPN transition into several updates of the BN. Essentially, when components corresponding to the pre-condition and context of a transition t , and if no other transition t' is already occurring, the t^{th} component of the BN can be updated to 1. Then, the components related to the input and output places can be updated (in any order) to apply their respective un-marking and marking. Once all these components have been updated, the t^{th} component can be updated to 0.

It results that a transition t is occurring, encoded by the value 1 of the t^{th} component, if and only if either (i) no transition is occurring, and all components corresponding to places in the pre-condition and context of t have value 1, or (ii) t is already occurring and at least one input (resp. output) place has not been unmarked (resp. marked) yet. A component corresponding to a place p has value 1 if and only if either one of transition producing p is occurring, or if it has already value 1 and none transition consuming it is occurring.

Hereafter, Definition 16 provides a formalization of the encoding of a safe CPN into a BN, and Theorem 2 states its correctness in the scope of the asynchronous updating (atomic); note that the correctness also holds for the generalized asynchronous (step semantics) and synchronous (maximal step semantics) updating. For the sake of simplicity, we assume the CPN is loop-free, i.e., for every transition t , $\bullet t \cap t^\bullet = \emptyset$; it is well known that loops can be replaced by read arcs without any effect on the (atomic) semantics.

Definition 16 Given a safe CPN $N = (P, T, pre, cont, post, M_0)$, $\llbracket N \rrbracket$ is the BN of dimension $|P| + |T|$ such that

$$\begin{aligned} \forall p \in P, \llbracket N \rrbracket_p(x) &= \left(\bigvee_{t \in \bullet p} x_t \right) \vee \left(x_p \wedge \bigwedge_{t \in p^\bullet} \neg x_t \right) \\ \forall t \in T, \llbracket N \rrbracket_t(x) &= \left(\bigwedge_{p \in \bullet t} x_p \wedge \bigwedge_{t' \in T} \neg x_{t'} \right) \\ &\quad \vee \left(x_t \wedge \left(\bigvee_{p \in t^\bullet} \neg x_p \vee \bigvee_{p \in \bullet t} x_p \right) \right) \end{aligned}$$

Given a marking $M \subseteq P$ of \mathcal{N} , the corresponding configuration of $\llbracket N \rrbracket$ is $\llbracket M \rrbracket \in \mathbb{B}^n$ where $\forall p \in M, \llbracket M \rrbracket_p = 1$, $\forall p \in P \setminus M, \llbracket M \rrbracket_p = 0$, and $\forall t \in T, \llbracket M \rrbracket_t = 0$.

Theorem 2 For a safe CPN $N = (P, T, pre, cont, post, M_0)$, and any pair of markings $M, M' \subseteq P$, one has

$$M \xrightarrow[\text{atom}]{N}^* M' \iff \llbracket M \rrbracket \xrightarrow[\text{async}]{\llbracket N \rrbracket}^* \llbracket M' \rrbracket$$

Proof If $M = M'$, the proof is trivial; in the following we consider $M \neq M'$.

(\Rightarrow) Let us assume that $M \xrightarrow[\text{atom}]{N} M'$. Then there exists $t \in T$ such that $\bullet \underline{t} \subseteq M$ and $M' = (M \setminus \bullet t) \cup t^\bullet$. Thus, $\llbracket N \rrbracket_t(\llbracket M \rrbracket) = 1$, and therefore, there exists $y \in \mathbb{B}^n$ such that $x \xrightarrow[\text{async}]{\llbracket N \rrbracket} y$ with $\delta(x, y) = \{t\}$. Then, assuming $\bullet t \cap t^\bullet = \emptyset$, for each place $p \in \bullet t$, because $t \in p^\bullet$ and $y_p = 1$, $\llbracket N \rrbracket_t(y) = 0$, and for each place $p \in t^\bullet$, because $t \in \bullet p$, $\llbracket N \rrbracket_p = 1$. Therefore, by updating the components p for $p \in \bullet t \cup t^\bullet$ in any ordering, we obtain a configuration z where all components are 0 except the components $p, \forall p \in M'$, and the component t . Then, because $\llbracket N \rrbracket_t(z) = 0$, this latter component can be set to 0, resulting in the configuration $\llbracket M' \rrbracket$.

(\Leftarrow) Let us assume that there exists $y \in \mathbb{B}^{|P|+|T|}$ such that $\llbracket M \rrbracket \xrightarrow[\text{async}]{\llbracket N \rrbracket} y$. Necessarily, there is a unique $t \in T$ such that $y_t = 1$; moreover, $\bullet t \cup \underline{t} \subseteq M$. Remark that as long as the t^{th} component of a configuration x is 1, none of the other components t' for $t' \in T, t' \neq t$ can be set to 1 (because $\llbracket N \rrbracket_{t'}(x) = 0$). Moreover, remark that in the configuration y , $\{p \in P \mid y_p \neq \llbracket N \rrbracket_p\} = \bullet t \cup t^\bullet$, and that the component t can be set to 0 only when all these latter components have been updated. Therefore, with $M'' = (M \setminus \bullet t) \cup t^\bullet$, we obtain that $\llbracket M \rrbracket \xrightarrow[\text{async}]{\llbracket N \rrbracket}^* \llbracket M'' \rrbracket$ and $M \xrightarrow[\text{atom}]{N} M'' \square$

The reachability problem consists in deciding if there exists a sequence of transitions from a given configuration (marking) x to a given configuration y . The reachability problem is PSPACE-complete in safe CPNs with asynchronous update mode [17]. By linear reduction to BNs, we therefore obtain that reachability in BNs is PSPACE-hard:

Corollary 1 *Reachability in asynchronous BNs is PSPACE-hard.*

Finally, one can remark that deciding the reachability in BNs is in PSPACE: given a BN of dimension n and the initial configuration x , let us define a counter using n bits, initially with value 0. Then, while the counter has value strictly less than 2^n and the current configuration is not equal to y , non-deterministically apply an update, and increase the counter by one.

Theorem 3 *Reachability in asynchronous BNs is PSPACE-complete.*

5 Synchronism sensitivity

For a given BN or CPN, changing the update/firing policy (from synchronous to asynchronous) may have little impact on the reachable states in some cases.

In others, it may render global states accessible, or exclude previously feasible paths. We say that a network of the latter category is *synchronism sensitive*. The authors of [30] have analyzed this sensitivity in BNs; in this section, we perform an analogous analysis for CPNs. As we will show, the characterization of synchronism sensitivity in safe CPNs boils down to the existence of *preemption cycles*, defined below, among the transitions that are enabled in a given marking. Moreover, we show that when instantiated on a CPN encoding a BN (according to Sect. 4.1), the general characterization of synchronism sensitivity in CPNs allows to recover the results of synchronism sensitivity in BNs with respect to their influence graph [30], with a slight generalization relaxing the locally monotonicity constraints of BNs.

5.1 Synchronism sensitivity in BNs

Following [30], given a BN f of dimension n where, $\forall i \in \{1, \dots, n\}$, f_i is monotonic, a positive (resp. negative) edge (j, i) of its influence graph $G(f)$ is *frustrated* in a configuration $x \in \mathbb{B}^n$ iff $x_i \neq x_j$ (resp. $x_i = x_j$). A (directed) cycle in $G(f)$ is *critical* in x iff all its edges are frustrated.

Then, the synchronism sensitivity in BNs can be characterized with respect to their influence graphs as follows.

Lemma 3 ([30], **Prop. 1**) *A critical cycle must be NOPE: **n**egative with **o**dd length or **p**ositive with **e**ven length.*

Theorem 4 ([30]) *Synchronism-sensitivity, i.e. the presence of some synchronous transition that cannot be sequentialized, in a locally monotonic BN f requires the existence of a critical cycle, and thus of a NOPE-cycle in its influence graph $G(f)$.*

5.2 Synchronism Sensitivity in CPNs

Given any safe CPN $N = (P, T, pre, cont, post, M_0)$, call a pair $(\tau, M) \in 2^T \times 2^P$ such that τ is s-enabled but not a-enabled in M a *witness of synchronism sensitivity* or, extending [30], *normal*.

As in [8], we say for any two transitions $t_1, t_2 \in T$ that t_1 *preempts*¹ t_2 , written $t_1 \rightsquigarrow t_2$ iff the context of t_2 intersects the preset of t_1 :

$$t_1 \rightsquigarrow t_2 \iff \Delta \bullet t_1 \cap t_2.$$

Theorem 5 *Let $(\tau, M) \in 2^T \times 2^P$ such that M s-enables τ .*

1. *If $\tau = \{t_1, \dots, t_n\}$ is a preemption cycle, i.e.*

$$t_1 \rightsquigarrow t_2 \rightsquigarrow \dots \rightsquigarrow t_{n-1} \rightsquigarrow t_n,$$

then (τ, M) is normal.

¹ for readers familiar with [8]: we will only need this *immediate* preemption relation \rightsquigarrow here, not the full asymmetric conflict obtained by adding causal precedence

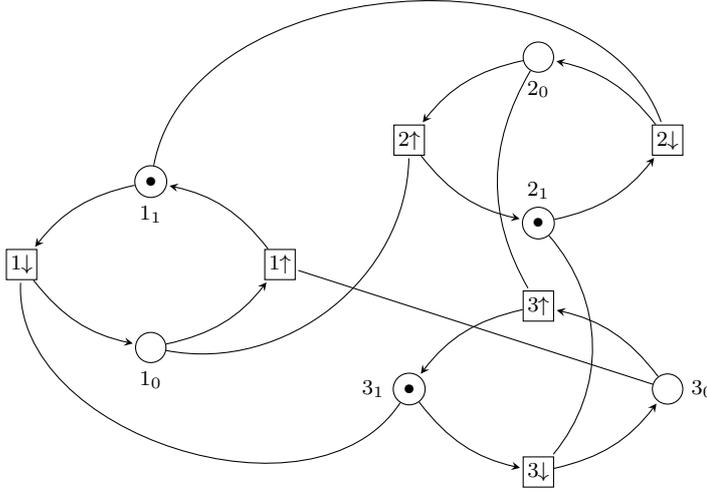


Fig. 5 A translation of the BN $\langle f_1(x) = \neg x_3, f_2(x) = \neg x_1, \neg f_3(x) \rangle = x_3$ and the configuration 111 into CPN. The step $\tau = \{1\downarrow, 2\downarrow, 3\downarrow\}$ is normal and reflects the negative-odd cycle of the BN.

2. Conversely, if (τ, M) is normal, then τ contains a preemption cycle.

Proof: Part 1 follows immediately from the assumptions. For Part 2, take any transition $t_1 \in \tau$. If there is no place $p \in t$ such that $p \in \bullet t_2$ for some $t_2 \in \tau$, remove t_1 from τ and start over. Otherwise, we have $t_2 \rightsquigarrow t_1$, and inspect $(\bullet t_2)$ as above. Since $|\tau| = n$, this process terminates after at most n steps, yielding either a decomposition of τ , or a preemption chain of length at most n , or a preemption cycle of length at most n . Only the last case corresponds to τ being normal. \square

As an immediate consequence, we note the following minimality result:

Corollary 2 Let τ be such that (τ, M) is normal, but every $\emptyset \subset \tau' \subseteq \tau$ (with proper inclusions) is a -enabled, i.e. (τ', M) is not normal. Then τ is a minimal preemption cycle.

In Fig. 5, $\tau = \{1\downarrow, 2\downarrow, 3\downarrow\}$ illustrates a preemption cycle, which is also normal in the marking shown; $\tau' = \{1\uparrow, 2\uparrow, 3\uparrow\}$ is another preemption cycle which is not enabled, but would become enabled after firing τ . In Fig. 6, $\tau'' = \{1\uparrow, 2\downarrow\}$ is a preemption cycle, which is normal in the marking shown.

5.3 Application to CPNs encoding BNs

We will now study how the characterization of synchronism sensitivity carries over to CPNs which encode BNs following the transformation described in

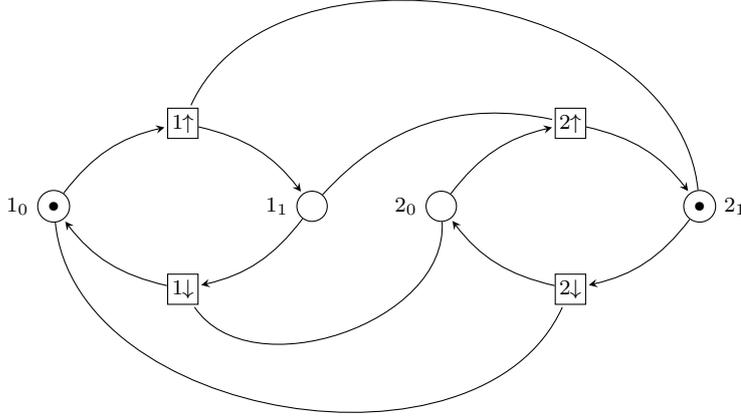


Fig. 6 A translation of the BN $(f_1(x) = x_2, f_2(x) = x_1)$ and configuration 01 into CPN.

Sect. 4.1. Remember that in this setting, each transition t of the CPN satisfy $\bullet t = \{p\}$ and $t\bullet = \{\bar{p}\}$ with $\text{var}(p) = \text{var}(\bar{p})$ and $\text{val}(p) + \text{val}(\bar{p}) = 1$. Thus, t corresponds either to an up-transition $\mathbf{up}(\text{var}(p))$ iff $\text{val}(p) = 0$ (i.e., $\text{val}(\bar{p}) = 1$), or to a down-transition $\mathbf{dw}(\text{var}(p))$ iff $\text{val}(p) = 1$ (i.e., $\text{val}(\bar{p}) = 0$).

Let us assume that the contexts of transitions are minimal, i.e., the DNF being the disjunction of all the context of all the up- (resp. down-) transitions of a node is minimal. Given a transition $t = \mathbf{up}(v_i)$ (resp. $t = \mathbf{dw}(v_i)$), for each $p \in \underline{t}$ with $\text{var}(p) = v_j$, the sign of the influence from v_j to v_i is positive iff $\text{val}(p) = 1$ (resp. $\text{val}(p) = 0$) and negative otherwise.

Consider a preemption cycle $t_1 \rightsquigarrow \dots \rightsquigarrow t_n \rightsquigarrow t_1$, and any arc (t_i, t_{i+1}) - identifying $i = 1$ and $i = n + 1$ - in this cycle. By definition, there exists a place $p \in P$ with $\text{var}(p) = v_j = \text{var}(t_i)$ such that $\{p\} = \bullet t_i \cap \underline{t_{i+1}}$, and a place $q \in P$ with $\text{var}(q) = v_k = \text{var}(t_{i+1})$ and $\{q\} = \bullet t_{i+1}$. If $t_i = \mathbf{up}(v_j)$ (i.e., $\text{val}(p) = 0$), and $t_{i+1} = \mathbf{dw}(v_k)$ (i.e., $\text{val}(q) = 1$), we say that the type of (t_i, t_{i+1}) is $0 - 1$, written $[\nearrow]$, and witnesses a positive influence of $\text{var}(t_i)$ on $\text{var}(t_{i+1})$. Similarly, if $t_i = \mathbf{dw}(v_j)$ and $t_{i+1} = \mathbf{up}(v_k)$, the type of (t_i, t_{i+1}) is $1 - 0$, written $[\searrow]$, witnessing a positive influence of $\text{var}(t_i)$ on $\text{var}(t_{i+1})$; if $t_i = \mathbf{up}(v_j)$ and $t_{i+1} = \mathbf{up}(v_k)$, the type of (t_i, t_{i+1}) is $0 - 0$, written $[\rightarrow]$, witnessing a negative influence of $\text{var}(t_i)$ on $\text{var}(t_{i+1})$; and if $t_i = \mathbf{dw}(v_j)$ and $t_{i+1} = \mathbf{dw}(v_k)$, the type of (t_i, t_{i+1}) is $1 - 1$, written $[\dashrightarrow]$, witnessing a negative influence of $\text{var}(t_i)$ on $\text{var}(t_{i+1})$.

As a consequence, in any preemption cycle, the numbers of type $[\nearrow]$ arcs and of type $[\searrow]$ must be equal, while nothing can be said in general about the number of $[\rightarrow]$ and $[\dashrightarrow]$ arcs. Since $[\rightarrow]$ and $[\dashrightarrow]$ correspond to arcs with

negative signs in the BN's influence graph, adding them in a cycle does not change the cycle's NOPE status (it only changes from negative-odd to positive-even, or vice versa).

Lemma 4 *Let $\{t_1, \dots, t_n\}$ be a preemption cycle in τ . Then the product of the signs of associated arcs (t_i, t_{i+1}) for $i \in \{1, \dots, n-1\}$ and (t_n, t_1) is positive iff n is even.*

Proof: By construction, the types of adjacent arcs have to match: type \nearrow and type \rightarrow arcs can only be followed by \searrow or \rightarrow , and analogously, types \rightarrow and \searrow need a successor arc of type \nearrow or \rightarrow . Hence the word $w \in \{\rightarrow, \nearrow, \searrow, \rightarrow\}^*$ associated to the preemption cycle must not contain the infixes $\rightarrow\searrow$, $\nearrow\nearrow$, $\nearrow\rightarrow$, $\searrow\searrow$, $\searrow\rightarrow$ or $\rightarrow\nearrow$, and not even $\rightarrow\rightarrow$ or $\rightarrow\searrow$. Since w also has to be cyclic, this implies that

1. between any occurrences of \rightarrow and \rightarrow (\rightarrow and \rightarrow), at least one occurrence of \nearrow (\searrow) is required;
2. between any two occurrences of \nearrow (\searrow), at least one occurrence of \searrow (\nearrow) is required;

therefore $|w|_{\nearrow} = |w|_{\searrow}$, which in turn implies the result. \square

Example 1 The preemption cycle $\tau = \{1\downarrow, 2\downarrow, 3\downarrow\}$ in Fig. 5 is of type $\rightarrow\rightarrow\rightarrow$, that of $\tau' = \{1\uparrow, 2\uparrow, 3\uparrow\}$ of type $\rightarrow\rightarrow\rightarrow$; the preemption cycle $\tau'' = \{1\uparrow, 2\downarrow\}$ in Fig. 6 is of type $\nearrow\searrow$.

6 Encoding the Interval Semantics with Boolean Networks

In this section, we show how the interval semantics for CPNs (Sect. 3.3.3) can be modelled using BNs with *asynchronous* updating. The resulting BNs subsume the generalized asynchronous updating mode, and enable new reachable configurations, while preserving important dynamical and structural (influence graph) properties.

Interval semantics adds the possibility to trigger, within a single step, transitions that become enabled by the firing transitions. Essentially, we model its application to BNs as follows. Each node $i \in \{1, \dots, n\}$ is decoupled in two nodes: a “write” node storing the next value ($2i-1$) and a “read” node for the current value ($2i$). The decoupling is used to store an ongoing value change, while other nodes of the system still read the current (to be changed) value of the node. A value change is then performed according to the automaton given in Fig. 7: assuming we start in both write and read node with value 0, if $f_i(x)$ is true, then the write node is updated to value 1. The read node is updated in a second step, leading to the value where both write and read nodes are 1. Then, if $f_i(x)$ is false, the write node is updated first, followed, in a second stage by the update of the read node.

Once the write node ($2i-1$) has changed its value, it can no longer revert back until the read node has been updated. Hence, if $f_i(x)$ become false in

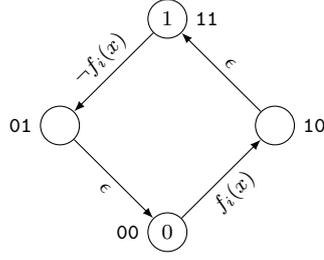


Fig. 7 Automaton of the value change of a node i in the interval semantics. The states marked 0 and 1 represents the value 0 and 1 of the node. The labels $f_i(x)$ and $\neg f_i(x)$ on edges are the conditions for firing the transitions; ϵ indicates that the transitions can be done without condition. The states are labeled by the corresponding values of nodes $(2i-1)(2i)$ in our encoding.

the intermediate value 10, the read node will still go through value 1 (possibly enabling transitions) before the write node can be updated to 0, if still applicable.

6.1 Encoding

From the automaton given in Fig. 7, one can derive Boolean functions for the write $(2i-1)$ and read $(2i)$ nodes. It results in the following BN \tilde{f} , encoding the interval semantics for the BN f :

Definition 17 (Interval semantics for Boolean networks) Given a BN f of dimension n , \tilde{f} is a BN of dimension $2n$ where $\forall i \in \{1, \dots, n\}$,

$$\begin{aligned} \tilde{f}_{2i-1}(z) &\triangleq (f_i(\gamma(z)) \wedge (\neg z_{2i} \vee z_{2i-1})) \vee (\neg z_{2i} \wedge z_{2i-1}) \\ \tilde{f}_{2i}(z) &\triangleq z_{2i-1} \end{aligned}$$

where $\gamma(z) \in \mathbb{B}^n$ is defined as $\gamma(z)_i \triangleq z_{2i}$ for every $i \in \{1, \dots, n\}$.

Given $x \in \mathbb{B}^n$, $\alpha(x) \in \mathbb{B}^{2n}$ is defined as $\alpha(x)_{2i-1} = \alpha(x)_{2i} \triangleq x_i$ for every $i \in \{1, \dots, n\}$.

A configuration $z \in \mathbb{B}^{2n}$ is called *consistent* when $\alpha(\gamma(z)) = z$.

The function $\gamma : \mathbb{B}^{2n} \rightarrow \mathbb{B}^n$ maps a configuration of the interval semantics to a configuration of the BN f by projecting on the read nodes. The function $\alpha : \mathbb{B}^n \rightarrow \mathbb{B}^{2n}$ gives the interval semantics configuration of a configuration of the Boolean network f , where the read and write nodes have a consistent value.

The correctness of our encoding is given with respect to the interval semantics applied to the CPN translation of the BN. It follows from the correspondence between split transitions of the CPN and update of read and write nodes of the encoded BN: for any Petri net transition t of the CPN (f), the

triggering of t^- matches with the update of the “write node” for $var(t^\bullet)$ of the BN, and the triggering of t^+ matches with the update of the “read node” for $var(t^\bullet)$ of the BN.

Theorem 6 *Given a BN f of dimension n , for all $x, y \in \mathbb{B}^n$,*

$$\langle x \rangle \xrightarrow[\text{istep}]{(f)}^* \langle y \rangle \iff \alpha(x) \xrightarrow[\text{async}]{\tilde{f}}^* \alpha(y) .$$

6.2 Consistency

The above theorem shows that the asynchronous semantics of the Boolean network encoding our interval semantics can reproduce any behaviour of the generalized asynchronous semantics. The aim of this section is to show that the interval semantics still preserves important constraints of the BN on its dynamics. In particular, we show the one-to-one relationship between the fixpoints of the BN and its encoding for interval semantics; and that the influences are preserved with their sign.

Lemma 5 states that from any configuration of encoded BN, one can always reach a configuration which corresponds to a configuration of the original BN (i.e., a configuration $z \in \mathbb{B}^{2n}$ such that $\alpha(\gamma(z)) = z$):

Lemma 5 (Reachability of consistent configurations) *For any $z \in \mathbb{B}^{2n}$ such that $\alpha(\gamma(z)) \neq z$, $\exists y \in \mathbb{B}^n : z \xrightarrow[\text{async}]{\tilde{f}}^* \alpha(y)$.*

Proof For each $i \in \{1, \dots, n\}$ such that $z_{2i-1} \neq z_{2i}$, we update the $2i$ node, in whatever order. This leads to the configuration $z' \in \mathbb{B}^{2n}$ where $\forall i \in \{1, \dots, n\}$, $z'_{2i} = z'_{2i-1} = z_{2i-1}$. Hence, by picking $y = \gamma(z)$, we obtain $z \xrightarrow[\text{async}]{\tilde{f}}^* \alpha(y)$. \square

The one-to-one relationship between fixpoints of f and fixpoints of \tilde{f} is given by the following lemma:

Lemma 6 (Fixpoint equivalence) $\forall x \in \mathbb{B}^n, f(x) = x \Rightarrow f(\alpha(x)) = \alpha(x)$; and $\forall z \in \mathbb{B}^{2n}, \tilde{f}(z) = z \Rightarrow \alpha(\gamma(z)) = z \wedge f(\gamma(z)) = \gamma(z)$.

Proof Let $x \in \mathbb{B}^n$ be such that $f(x) = x$. We have that $\alpha(x)_{2i-1} = \alpha(x)_{2i} = x_i = f_i(x)$. Hence, $\tilde{f}_{2i-1}(\alpha(x)) = f_i(\gamma(\alpha(x))) = f_i(x) = \alpha(x)_{2i-1}$; and $\tilde{f}_{2i}(\alpha(x)) = \alpha(x)_{2i-1} = \alpha(x)_{2i}$. Thus, $\tilde{f}(\alpha(x)) = \alpha(x)$.

Let $z \in \mathbb{B}^{2n}$ be such that $\tilde{f}(z) = z$. For each $i \in \{1, \dots, n\}$, because $\tilde{f}_{2i}(z) = z_{2i}$, by the definition of \tilde{f}_{2i} , we obtain that $z_{2i} = z_{2i-1}$. Thus, $\alpha(\gamma(z)) = z$. Moreover, as $(\neg z_{2i} \vee z_{2i-1})$ reduces to true and $(\neg z_{2i} \wedge z_{2i-1})$ reduces to false, $\tilde{f}_{2i-1}(z) = f_i(\gamma(z)) = z_{2i-1} = \gamma(z)_i$. Therefore, $f(\gamma(z)) = \gamma(z)$. \square

6.3 Influence graph

As defined in Sect. 2, the influence graph provides a summary of the causal dependencies between the value changes of nodes of the BN. We show that our encoding of interval semantics preserves the causal dependencies of the original network, and in particular, preserves the cycles and their signs.

From the definition of \tilde{f} , one can derive that all the influences in f are preserved in \tilde{f} , and no additional influences between different variables i, j are created by the encoding. This latter fact is addressed by the following lemma:

Lemma 7 *For any $i, j \in \{1, \dots, n\}$, $i \neq j$, there is a positive (resp. negative) edge from j to i in $G(f)$ if and only if there is a positive (resp. negative) edge from $2j$ to $2i - 1$ in $G(\tilde{f})$.*

Proof Let us define $x, y \in \mathbb{B}^n$ such that $\Delta(x, y) = \{j\}$, and $z, z' \in \mathbb{B}^{2n}$ such that $z = \alpha(x)$ and $\Delta(z, z') = \{2j\}$, i.e., $z'_j = y_j$. Because $z_{2i} = z_{2i-1}$ and, as $i \neq j$, $z'_{2i} = z'_{2i-1}$, we obtain that $\tilde{f}_{2i-1}(z) = f_i(x)$ and $\tilde{f}_{2i-1}(z') = f_i(y)$. \square

Lemma 8 *For any $i \in \{1, \dots, n\}$,*

- a. *there is a positive self-loop on $2i - 1$ in $G(\tilde{f})$ if and only if there exists $x \in \mathbb{B}^n$ such that $f_i(x) = x_i$;*
- b. *there is never a negative self-loop on $2i - 1$ in $G(\tilde{f})$;*
- c. *there is never a positive edge from $2i$ to $2i - 1$ in $G(\tilde{f})$;*
- d. *there is a negative edge from $2i$ to $2i - 1$ in $G(\tilde{f})$ if and only if there exists $x \in \mathbb{B}^n$ such that $f_i(x) \neq x_i$;*
- e. *there is always exactly one edge from $2i - 1$ to $2i$ in $G(\tilde{f})$ and it is positive.*

Proof (a) Let us consider $z, z' \in \mathbb{B}^{2n}$ such that $\Delta(z, z') = \{2i - 1\}$ with $z_{2i-1} = 0$: $\tilde{f}_{2i-1}(z) = 0 = \neg \tilde{f}_{2i-1}(z') \Leftrightarrow [(z_{2i} = 0 \wedge f_i(\gamma(z)) = 0) \vee (z_{2i} = 1 \wedge f_i(\gamma(z)) = 1)] \Leftrightarrow f_i(\gamma(z)) = z_{2i}$. (b) Let us consider $z, z' \in \mathbb{B}^{2n}$ such that $\Delta(z, z') = \{2i - 1\}$ with $z_{2i-1} = 0$ and $\tilde{f}_{2i-1}(z) = 1 = \neg \tilde{f}_{2i-1}(z')$. Thus, $z_{2i} = 0$, therefore, $\tilde{f}_{2i-1}(z') = z'_{2i-1} = 1$, which is a contradiction. (c) Let us consider $z, z' \in \mathbb{B}^{2n}$ such that $\Delta(z, z') = \{2i\}$ with $z_{2i} = 0$: if $z_{2i-1} = z'_{2i-1} = 0$, then $\tilde{f}_{2i-1}(z) \geq \tilde{f}_{2i-1}(z')$; if $z_{2i-1} = z'_{2i-1} = 1$, then $\tilde{f}_{2i-1}(z) \geq \tilde{f}_{2i-1}(z')$; therefore there cannot be a negative edge from $2i$ to $2i - 1$ in $G(\tilde{f})$. (d) $\exists z, z' \in \mathbb{B}^{2n}$: $\Delta(z, z') = \{2i\}$, $z_{2i} = 0$, $\tilde{f}_{2i-1}(z) = 1 = \neg \tilde{f}_{2i-1}(z') \Leftrightarrow [(z_{2i-1} = z'_{2i-1} = 0 \wedge f_i(\gamma(z)) = 1) \vee (z_{2i-1} = z'_{2i-1} = 1 \wedge f_i(\gamma(z')) = 0)] \Leftrightarrow \exists x \in \mathbb{B}^n : f_i(x) = \neg x_i$. (e) By \tilde{f}_{2i} definition.

From Lemma 8, one can deduce that if there is a positive self-loop on i in $G(f)$, then there is a positive self-loop on $2i - 1$ in $G(\tilde{f})$; and if there is a negative self-loop on i in $G(f)$, then there is a negative edge from $2i$ to $2i - 1$ in $G(\tilde{f})$.

We can then deduce that the positive and negative cycles of $G(f)$ are preserved in $G(\tilde{f})$. It is worth noting that the encoding may also introduce negative cycles between $2i - 1$ and $2i$ and positive self-loops on $2i - 1$, for some $i \in \{1, \dots, n\}$.

Lemma 9 *To each positive (resp. negative) cycle in $G(f)$ of length $k > 1$, there exists a corresponding positive (resp. negative) cycle in $G(\tilde{f})$ of length $2k$. To each positive self-loop in $G(f)$ corresponds one positive self-loop in $G(\tilde{f})$; to each negative self-loop in $G(f)$ corresponds a negative cycle in $G(\tilde{f})$ of length 2.*

Proof For cycle of length $k > 1$, by Lemma 7 and by the fact that there is a positive edge from $2i - 1$ to $2i$ in $G(\tilde{f})$: each edge (i, j) in the cycle in $G(f)$ is mapped to the string $(2i, 2j - 1)(2j - 1, 2j)$, giving a cycle in $G(\tilde{f})$ of the same sign. Correspondence of self-loops is given by Lemma 8 \square

7 Beyond Generalized Asynchronicity and Interval Semantics

BNs are widely used to model the qualitative dynamics of biological networks, notably of signalling and gene regulation networks.

A major concern is the impact of the chosen updating mode on the validation of the model. Indeed, it is usual to assess the accordance of a BN with measurement data, including time series: it is expected that the observed behaviours can be reproduced in the abstract model. With this perspective, the computation of reachable configurations in BNs is key. For example, let assume we observe (in the concrete system) that a given component (e.g., gene) gets eventually activated: if the reachability analysis of the BN concludes that no reachable state has this component active, the model would likely be rejected by the modeller.

In biological applications, the analysis of BNs merely splits into two scientific sub-communities: the one preferring the synchronous updating mode, and the one preferring the asynchronous updating mode. The generalized asynchronous updating, which subsumes synchronous and asynchronous, seems a good compromise but it received very little attention in practice. It should be noted that most of computational tools rely only on synchronous or asynchronous modes, which can provide a partial explanation.

Is the generalized asynchronous mode the ultimate updating mode when analysing reachable configurations in BNs for biological systems? If little is known on time and speed features of the system and the reachability analysis with generalized asynchronicity concludes on the absence of the observed state, can we safely invalidate the model?

In the following motivating example (Sect. 7.1), we show that the generalized asynchronous updating can miss transitions, hence reachable configurations, which correspond to particular, but plausible, behaviours. Thus, the resulting analysis can be misleading on the absence of some behaviours, notably regarding the reachability of attractors (configurations reachable on the long-run), and may lead to reject valid models. It is worth noting that the network considered in the example is embedded in many actual models of biological networks, e.g., [28, 29, 42].

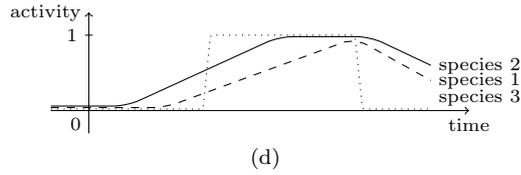


Fig. 8 A possible evolution of the activity of species modelled by the BN of Fig. 1 (species 1 in dashed line, species 2 plain, species 3 dotted).

As introduced in Sect. 3, the interval semantics of CPNs takes advantage of the fine-grained specification of causality of transitions to enable new behaviours, i.e., new reachable states, which can be caused by specific ordering and duration of updates. We show in Sect. 7.2 that using the encoding of BNs into CPNs provided in Sect. 4.1 and applying the interval semantics correctly recover the missing reachable configurations in our motivating example.

Finally, in Sect. 7.3 we explore further extensions of the interval semantics resulting in correct over-approximation of the configurations reachable by any multi-valued refinement of the BN.

7.1 Motivating example

Let us consider the BN defined in Fig. 1. The BN and its influence graph suggest that the activity of species 3 increases when 1 is inactive and 2 is active. In any scenario starting from 000 where 3 eventually increases, 2 has to increase to trigger the increase of 3. Hence, according to the generalized asynchronous updating represented in Fig. 1 (c), the only transition which represents an increase of 3 is $010 \rightarrow 011$. After this, no transition is possible.

But, assuming the BN abstracts continuous evolution of activities, the following scenario, pictured in Fig. 1(d), becomes possible: initially, the inactivity of species 1 causes an increase of the activity of species 2, represented in plain line on the figure. Symmetrically, the absence of species 2 causes an increase of the activities of species 1 (dashed line). This corresponds to the evolution described by the arrow $000 \rightarrow 110$ in Fig. 1(b) and leads to a (transient) configuration where species 1 and 2 are present.

Assume that 1 and 2 activity increase slowly. After some time, however, the activity of 2 becomes sufficient for influencing positively the activity of 3, while there is still too little of species 1 for influencing negatively the activity of 3. Species 3 can then increase. In the scenario represented in the figure, 3 (dotted line) increases quickly, and then 1 and 2 continue to increase. In summary, the activity of species 3 increased from 0 to 1 *during* the increase of 1 and 2, which was not predicted by the generalized asynchronous updating (Fig. 1(b)).

One could argue that in this case, one should better consider more fine-grained models, for instance by allowing more than binary values on nodes in order to reflect the different activation thresholds. However, the definition of

the refined models would require additional parameters (the different activation thresholds) which are unknown in general. Our goal is to allow capturing these behaviours already in the Boolean abstraction, so that any refinement would remove possible transitions, and not create new ones.

7.2 Application of the Interval Semantics of CPNs

Let us consider the BN f in Fig. 1 and its CPN encoding (f) in Fig. 4. Starting from the marking (000) , $1\uparrow^- 2\uparrow^- 2\uparrow^+ 3\uparrow^- 3\uparrow^+ 1\uparrow^+$ is a *complete i-run* (Def. 14) of the interval semantics, and leads to the marking (111) .

Similarly, let us consider the encoding of the interval semantics in the BN \tilde{f} , as defined in Sect. 6. We obtain the following possible sequence of asynchronous iterations of \tilde{f} :

$$\begin{array}{ccccccc} 00\ 00\ 00 & \xrightarrow[\text{async}]{\tilde{f}} & 10\ 00\ 00 & \xrightarrow[\text{async}]{\tilde{f}} & 10\ 10\ 00 & \xrightarrow[\text{async}]{\tilde{f}} & 10\ 11\ 00 \\ & & \xrightarrow[\text{async}]{\tilde{f}} & & \xrightarrow[\text{async}]{\tilde{f}} & & \xrightarrow[\text{async}]{\tilde{f}} \\ & & 10\ 11\ 10 & \xrightarrow[\text{async}]{\tilde{f}} & 10\ 11\ 11 & \xrightarrow[\text{async}]{\tilde{f}} & 11\ 11\ 11 \end{array}$$

Therefore, with the interval semantics, the configuration 111 of f is reachable from 000, contrary to the generalized asynchronous semantics. This is due to the decoupling of the update of node 1: the activation of 1 is delayed which allows activating node 3 beforehand.

7.3 Beyond the Interval Semantics

Our interval semantics (Definition 17) decouples the update of a node in order to allow the interleaving of transitions during the interval when the next value has been computed (write node) but not applied yet (read node still with the before-update value). This also implies that, during this interval, the other nodes have access only to the before-update value. A third feature of the interval semantics is the enforcement of the update application: once an update is triggered (write node gets a different value than the read node), no further update on the same node is possible until the update has been applied. Thus, if for instance the update triggers a change of value from 0 to 1, the interval semantics guarantees that the read node will eventually have the value 1.

These two aspects, restricted access to the before-update value of nodes and enforcement of update application, were essentially motivated by our choice that our interval semantics should simulate the synchronous update of nodes used in the classical synchronous and generalized asynchronous semantics, as stated in Theorem 6. However, one could go further and consider extended interval semantics which relax either the restricted access to the before-update value of nodes, or the enforcement of update application, or both.

In terms of modeling, the restriction to before-update values in our interval semantics can be seen as an asymmetry in the consideration of transitions:

the resource modified by the transition is still available during the interval of update, whereas the result is only available once the transition finished. When modelling biological systems, it translates into considering only species which are slow to reach their activity threshold.

Actually, the choice of whether the before-update, after-update or both values are available during the update may be done according to the knowledge of the modeled system. Our construction can easily be adapted for giving access, depending on the node, to the after-update value instead of the before-update value. For instance, if the node i should follow closely value changes of node i , then node j should access the after-update value (write node) of i , whereas, as in our motivating example, if i is slow to update compared to j , node j should access the before-update value (read node) of i .

7.3.1 Most Permissive Semantics for Boolean Networks

Finally, one could also consider a more permissive symmetric version which would allow the access of both before-update and after-update values. This choice may be very reasonable when not much is known about the system, for instance about the relative speed of the nodes.

This leads us to define a *most permissive semantics* for Boolean networks which is defined as a 3-valued semantics in order to represent non instantaneous updates: a configuration can now assign value $\frac{1}{2}$ to a node, in addition to the usual 0 and 1, and the updates are done in two stages: if the network is in a configuration x where for some i , we have $x_i = 0$ and $f_i(x) = 1$, the update of x_i will be in two stages, going through an intermediate configuration y with $y_i = \frac{1}{2}$. In this intermediate configuration y , other updates can occur before the completion of the update of node i , and they will be allowed to use either the value 0 or 1 for node i . In the end, for a 3-valued configuration $x \in \{0, \frac{1}{2}, 1\}^n$, we allow all the intermediate values to be approximated either as 0 or as 1. The possible approximations are defined as the set $Approx(x)$ of Boolean configurations $x' \in \mathbb{B}^n$ such that, for every $i \in \{1, \dots, n\}$,

- $x'_i = 0$ if $x_i = 0$,
- $x'_i = 1$ if $x_i = 1$,
- otherwise x'_i can be either 0 or 1.

Definition 18 (Most permissive semantics for Boolean networks)

Given a BN f , the binary irreflexive relation $\frac{f}{\text{mp}} \rightarrow \subseteq \{0, \frac{1}{2}, 1\}^n \times \{0, \frac{1}{2}, 1\}^n$ is defined as:

$$x \xrightarrow[\text{mp}]{f} y \iff \exists i \in \{1, \dots, n\}, x' \in Approx(x) : \Delta(x, y) = \{i\} \wedge y_i = \frac{1}{2}(x_i + f_i(x')) .$$

We write $\frac{f}{\text{mp}} \rightarrow^*$ for the transitive closure of $\frac{f}{\text{mp}} \rightarrow$.

Similarly to the BN encoding of interval semantics presented in Sect. 6, the most permissive semantics of a BN f of dimension n can be encoded as

an asynchronous BN \tilde{f} of dimension $2n + 1$ where each node $i \in \{1, \dots, n\}$ is decoupled into an after-update value node $2i - 1$ and an before-update value node $2i$. As in Def. 17, the updating of this latter node consists in copying the after-update value node: $\tilde{f}_{2i}(z) \triangleq z_{2i-1}$. The definition of \tilde{f}_{2i-1} is a bit more complex as one has to rewrite $f_i(x)$ to use (non-deterministically) either the before-update or after-update value of input nodes. This non-deterministic choice can be encoded using an extra ‘‘coin flip’’ node $2n + 1$ with $\tilde{f}_{2n+1}(z) \triangleq \neg z_{2n+1}$. Then, assuming $f_i(x)$ is specified using propositional logic, the literals x_j appearing in $f_i(x)$ are replaced with $\tilde{x}_j \triangleq (z_{2n+1} \vee z_{2j}) \wedge (\neg z_{2n+1} \vee z_{2j-1})$. Also, contrary to the interval semantics, the most permissive semantics do not enforce the update application. Thus, $\tilde{f}_{2i-1}(z) \triangleq [f_i(x)]_{[\tilde{x}_j/x_j, j \in \{1, \dots, n\}]}(z)$.

7.3.2 Most permissive semantics simulates any multivalued refinement

Multivalued networks are generalization of Boolean networks where the nodes x_i can take values other than $\{0, 1\}$. Let us denote the possible values as $\mathbb{M} \triangleq \{0, \frac{1}{m}, \dots, \frac{m-1}{m}, 1\}$ for some integer m . For simplicity, we assume the same number of values for all the nodes.

Hence, a *configuration* is now a vector $x \in \mathbb{M}^n$. Given two configurations $x, y \in \mathbb{M}^n$, the components that differ are noted $\Delta(x, y) \triangleq \{i \in \{1, \dots, n\} \mid x_i \neq y_i\}$.

Definition 19 (Multivalued network) A *multivalued network* of dimension n over a value range $\mathbb{M} = \{0, \frac{1}{m}, \dots, \frac{m-1}{m}, 1\}$ is a collection of functions $f = \langle f_1, \dots, f_n \rangle$ where $\forall i \in \{1, \dots, n\}, f_i : \mathbb{M}^n \rightarrow \{\uparrow, \downarrow\}$.

Definition 20 (Asynchronous updating in multivalued networks)

Given a BN f , the binary irreflexive relation $\xrightarrow[\text{async}]{} \subseteq \mathbb{M}^n \times \mathbb{M}^n$ is defined as:

$$x \xrightarrow[\text{async}]{} y \iff \exists i \in \{1, \dots, n\} : \Delta(x, y) = \{i\} \wedge y_i = \begin{cases} \min\{0, x_i - \frac{1}{m}\} & \text{if } f_i(x) = \downarrow \\ \max\{1, x_i + \frac{1}{m}\} & \text{if } f_i(x) = \uparrow \end{cases}.$$

We write $\xrightarrow[\text{async}]{}^*$ for the transitive closure of $\xrightarrow[\text{async}]{}.$

We now define a notion of *multivalued refinement* of a Boolean network, which formalizes the intuition that the moves defined by the multivalued network are compatible with those of the Boolean network.

Definition 21 (Multivalued refinement) A multivalued network f of dimension n over a value range $\mathbb{M} = \{0, \frac{1}{m}, \dots, \frac{m-1}{m}, 1\}$ *refines* a Boolean network f' of equal dimension n iff for every configuration $x \in \mathbb{M}^n$ of f and every $i \in \{1, \dots, n\}$:

- $f_i(x) = \uparrow \implies \exists x' \in \text{Approx}(x) : f'_i(x') = 1$
- $f_i(x) = \downarrow \implies \exists x' \in \text{Approx}(x) : f'_i(x') = 0$

where $Approx$ is generalized to multi-valued networks by $Approx(x) \triangleq Approx(abstr(x))$.

Theorem 7 (Most permissive semantics simulates any multivalued refinement) *Let f' be a Boolean network of dimension n and f a multivalued refinement of f' . Then*

$$\forall x, y \in \mathbb{M}^n \quad x \xrightarrow[\text{async}]{f} y \implies abstr(x) \xrightarrow[\text{mp}]{f'}^* abstr(y).$$

where $abstr$ maps every configuration $x = x_1 \dots x_n \in \mathbb{M}^n$ of the multivalued network into a 3-valued configuration $abstr(x) \in \{0, \frac{1}{2}, 1\}^n$ defined as: for every $i \in \{1, \dots, n\}$,

- $abstr(x)_i \triangleq 0$ if $x_i = 0$,
- $abstr(x)_i \triangleq 1$ if $x_i = 1$,
- $abstr(x)_i \triangleq \frac{1}{2}$ otherwise.

Proof We assume for simplicity $m > 1$. By definition of $\xrightarrow[\text{async}]{f}$ for multivalued networks, there exists a unique i such that $\Delta(x, y) = \{i\}$. Then we have to study the different cases determined by the value of x_i and of $f_i(x)$.

The first case is $0 < x_i < \frac{m-1}{m}$ and $f_i(x) = \uparrow$. It implies $y_i = x_i + \frac{1}{m}$, and we observe that, in this case, $abstr(x) = abstr(y)$. Then trivially $abstr(x) \xrightarrow[\text{mp}]{f'}^* abstr(y)$. The case of $\frac{1}{m} < x_i < 1$ and $f_i(x) = \downarrow$ is symmetric.

The other cases are all similar; consider for instance $x_i = 0$ and $f_i(x) = \uparrow$, which imposes $y_i = \frac{1}{m}$. Notice first that $\Delta(abstr(x), abstr(y)) = \{i\}$ and $abstr(x)_i = 0$ and $abstr(y)_i = \frac{1}{2}$. Now, since f is a multivalued refinement of f' , then by Definition 21, there exists an $x' \in Approx(x) = Approx(abstr(x))$ such that $f'_i(x') = 1$. It remains to observe that $abstr(y)_i = \frac{1}{2}(abstr(x)_i + f'_i(x'))$ and we get $abstr(x) \xrightarrow[\text{mp}]{f'} abstr(y)$.

Example 2 The scenario pictured in Fig. 8 can be obtained as a behaviour of a 3-level refinement F of the BN f in Fig. 1, with the following update functions:

$$\begin{aligned} F_1(x) &\triangleq \uparrow \text{ if } x_2 < 1 \text{ else } \downarrow \\ F_2(x) &\triangleq \uparrow \text{ if } x_1 < 1 \text{ else } \downarrow \\ F_3(x) &\triangleq \uparrow \text{ if } x_1 \leq \frac{1}{2} \wedge x_2 \geq \frac{1}{2} \text{ else } \downarrow \end{aligned}$$

We get $000 \xrightarrow[\text{async}]{F} 0\frac{1}{2}0 \xrightarrow[\text{async}]{F} \frac{1}{2}\frac{1}{2}0 \xrightarrow[\text{async}]{F} \frac{1}{2}\frac{1}{2}\frac{1}{2} \xrightarrow[\text{async}]{F} \frac{1}{2}\frac{1}{2}1 \dots$

In particular, imagine that a fourth species would activate when x_1, x_2 and x_3 are all $\geq \frac{1}{2}$, then even the generalized asynchronous updating mode would not capture its activation, contrary to our interval semantics for BNs.

Example 3 Let us consider the BN f of dimension 3 defined as follows:

$$\begin{aligned} f_1(x) &\stackrel{\Delta}{=} 1 \\ f_2(x) &\stackrel{\Delta}{=} x_1 \\ f_3(x) &\stackrel{\Delta}{=} x_2 \wedge \neg x_1 \end{aligned}$$

Starting from configuration 000 the generalized asynchronous mode allow only the following iterations: $000 \xrightarrow[\text{gen}]{f} 100 \xrightarrow[\text{gen}]{f} 110$, where 110 is a fixpoint of f . The interval semantics lead to a very similar behaviour, with the following unique sequence of asynchronous iterations of the BN encoding of the interval semantics:

$$00\ 00\ 00 \xrightarrow[\text{async}]{\tilde{f}} 10\ 00\ 00 \xrightarrow[\text{async}]{\tilde{f}} 11\ 00\ 00 \xrightarrow[\text{async}]{\tilde{f}} 11\ 10\ 00 \xrightarrow[\text{async}]{\tilde{f}} 11\ 11\ 00$$

Indeed, in order to activate species 2, 1 has to be activated first as in the interval semantics species 2 only has access to the before-update value of 1. Then, once species 1 is active, it is impossible to activate species 3.

Now, let us consider the following 3-level refinement F of the BN f :

$$\begin{aligned} F_1(x) &\stackrel{\Delta}{=} \uparrow \\ F_2(x) &\stackrel{\Delta}{=} \uparrow \text{ if } x_1 \geq \frac{1}{2} \text{ else } \downarrow \\ F_3(x) &\stackrel{\Delta}{=} \uparrow \text{ if } x_2 \geq \frac{1}{2} \wedge x_1 \leq \frac{1}{2} \text{ else } \downarrow \end{aligned}$$

The following asynchronous iterations are possible from configuration 000: $000 \xrightarrow[\text{async}]{F} \frac{1}{2}00 \xrightarrow[\text{async}]{F} \frac{1}{2}\frac{1}{2}0 \xrightarrow[\text{async}]{F} \frac{1}{2}\frac{1}{2}\frac{1}{2}$. These iterations are also iterations of the most permissive semantics of f , $\xrightarrow[\text{mp}]{f}$. Essentially, as in this semantics species can have access to either the before-update or after-update value of other species, species 2 can be activated by reading the after-update value of 1, while species 3 can be activated by reading the before-update value of 1. An example of possible sequence of asynchronous iterations of the BN encoding of the most permissive semantics is the following:

$$\begin{aligned} 00\ 00\ 00 &\xrightarrow[\text{async}]{\tilde{\tilde{f}}} 10\ 00\ 00 \xrightarrow[\text{async}]{\tilde{\tilde{f}}} 10\ 10\ 00 \xrightarrow[\text{async}]{\tilde{\tilde{f}}} 10\ 11\ 00 \\ &\xrightarrow[\text{async}]{\tilde{\tilde{f}}} 10\ 11\ 10 \xrightarrow[\text{async}]{\tilde{\tilde{f}}} 10\ 11\ 11 \end{aligned}$$

As in the previous example, let us consider a fourth species activated when x_1 , x_2 , and x_3 are all greater or equal than $\frac{1}{2}$: such an activation is captured neither by the generalized asynchronous updating nor by the interval semantics of the abstract BN f , whereas it is captured by its most permissive semantics.

8 Discussion

With this paper, we detailed the link between Boolean Networks (BNs) and Contextual Petri Nets (CPNs) by focusing on the analysis of concurrency enabled by this latter framework. On the one hand, BNs have important structural properties between the components and their evolution, while on the other hand CPNs bring a fine-grained specification of the causality and effect of transitions. We show how we can take benefit of both approaches to first bring new updating modes to BNs by encoding CPN semantics, and, secondly, propose further extensions of these semantics aiming at obtaining correct Boolean abstractions of discrete dynamical systems.

To sum up, the contributions of this paper include:

- The encoding of BNs into CPNs, similar to other encoding already existing in the literature, here specialized for *contextual* Petri nets;
- The encoding of CPNs into BNs, which allows a brief proof by reduction of the PSPACE-completeness of the reachability decision in asynchronous BNs;
- A generic characterization of synchronism sensitivity in CPNs, which when instantiated to BN translations, allows to recover a recent result in BNs;
- The encoding of the interval semantics of CPNs as asynchronous BNs, enabling new behaviours missed by usual BN updating modes;
- An extension of the interval semantics for BNs which guarantees to include the behaviour of any multivalued refinement.

For practical applications, the thorough link between BNs and Petri nets enables the use of conceptual tools based on causality and concurrency, such as unfoldings offering more compact representation of behaviours [20, 7, 16, 27] and for which efficient software tools have been developed for CPNs [36], for problems arising in BNs.

The transitions enabled by the interval and most permissive semantics are due to nodes which update at different time scales. For instance with the interval semantics, whenever committed to a value change, in the meantime of the update application, the other nodes of the network still evolve subject to its before-update value. This time scale consideration brings an interesting feature when modeling biological networks which gathers processes of different nature and velocity. Our encodings can be applied only to a subset of nodes, offering a flexible modelling approach. Moreover, because the encodings rely on asynchronous BNs, they can be implemented using any software tools supporting the asynchronous updating mode.

The introduction of the most permissive semantics for BNs motivate future work to determine if it offers the smallest abstraction of any multivalued refinement (i.e., to any iterations of the most permissive semantics corresponds an asynchronous iteration of a multivalued refinement), and to assess the complexity of reachability decision. Finally, further work may explore links between BNs and CPNs with real-time semantics [6], aiming at tightening connections between the two hybrid frameworks.

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