# Combinatorics of block-parallel automata networks

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Abstract. Automata networks are finite collections of entities (the automata), each automaton having its own set of possible states, which interact with each other over discrete time, interactions being defined as local functions allowing the automata to change their state according to the states of their neighbourhoods. Inspired by natural phenomena, the studies on this very abstract and expressive model of computation have underlined the very importance of the way (*i.e.* the schedule) according to which the automata update their states, namely the update modes which can be deterministic, periodic, fair, or not. Indeed, a given network may admit numerous underlying dynamics, these latter depending highly on the update modes under which we let the former evolve. In this paper, we pay attention to a new kind of deterministic, periodic and fair update mode family introduced recently in a modelling framework, called the block-parallel update modes by duality with the well-known and studied block-sequential update modes. We compare block-parallel to block-sequential update modes, then count them: (1) in absolute terms, (2) by keeping only representatives leading to distinct dynamics, and (3) by keeping only representatives giving rise to non-isomorphic limit dynamics. Put together, this paper constitutes a first theoretical analysis of these update modes and their impact on automata networks dynamics.

### 1 Introduction

Automata networks were born at the beginning of modern computer science in the 1940s, notably through the seminal works of McCulloch and Pitts on neural networks, and von Neumann on cellular automata, which have become since then widely studied models of computation. The former is classically dived into a finite and heterogeneous structure (a graph) whereas the latter is dived into an infinite but regular structure (a lattice). Whilst there exist deep differences between them, they both belong to the family of automata networks, which groups together all distributed models of computation defined locally by means of automata which interact with each other over discrete time, so that the global computations they operate emerge from these local interactions governing them.

The end of the 1960s has underlined the prominent role of finite automata networks on which we focus in this paper, in the context of genetic regulation modelling [9,14]. The profiles of limit behaviours emerging from the system can

represent for instance phenotypes, cellular types, or even biological paces [10,2]. The update modes have decisive effects on the dynamics of automata networks, and acquiring a better understanding of their influence has become a hot topic in the domain since Robert's seminal works on discrete iterations [13], leading to numerous further studies in the last two decades [1,11,12]. Works addressing the role of periodic update modes focused on block-sequential update modes, namely modes in which automata are partitioned into a list of subsets such that the automata of a same subset update their state all at once in parallel while the subsets are iterated sequentially.

We still do not know which "natural schedules" govern gene expression and regulation, although chromatin dynamics seems to play a key role [8,6]. In [4] an unexplored family, dual to the block-sequential, is introduced and motivated, namely the block-parallel update modes. Rather than lists of sets, they are defined as sets of lists, or "partitioned orders", so that the automata of a list update their state sequentially according to the period of the list while the lists are triggered all in parallel at the initial time step. As highlighted by the authors, blockparallel update modes allow to capture endogenous biological timers/clocks of genetic or physiological origin, such as the aforementioned chromatin dynamics. Furthermore, they allow to break the property of fixed point set invariance (local update repetitions into a period are notably possible), letting automata networks have a richer range of dynamics. We give a first theoretical analysis of these modes, building a basis to further analyse their power of expressiveness.

Definitions are introduced in Section 2. Section 3 develops our main contributions and is divided into five parts. Section 3.1 characterises the update modes that are both block-sequential and block-parallel. We then address with closed formulas the counting of block-parallel modes: in absolute terms (Section 3.2), in terms of automata network dynamics (Section 3.3), up to isomorphic limit dynamics (Section 3.4). Numerical experiments are exposed in Section 3.5, suggesting that the search space may be drastically reduced, when one is specifically interested in the asymptotic (limit) behaviour of dynamical systems. Perspectives are discussed in Section 4. Omitted proofs can be found in Appendix A.

# 2 Definitions

Let  $\llbracket n \rrbracket = \{0, \ldots, n-1\}$ , let  $\mathbb{B} = \{0, 1\}$ , let  $x_i$  denote the *i*-th component of vector  $x \in \mathbb{B}^n$ , let  $x_I$  denote the projection of x onto an element of  $\mathbb{B}^{|I|}$  for some subset  $I \subseteq \llbracket n \rrbracket$ , let  $e_i$  be the *i*-th base vector, and  $\forall x, y \in \mathbb{B}^n$ , let x + y denote the bitwise addition modulo two. Let  $\sim$  denote the graph isomorphism, *i.e.* for G = (V, A) and G' = (V', A') we have  $G \sim G'$  if and only if there is a bijection  $\pi : V \to V'$  such that  $(u, v) \in A \iff (\pi(u), \pi(v)) \in A'$ .

Automata networks. An automata network (AN) of size n is a discrete dynamical system composed of a set of n automata [n], each holding a state within a finite alphabet  $X_i$  for  $i \in [n]$ . A configuration is an element of  $X = \prod_{i \in [n]} X_i$ . An AN is defined by a function  $f : X \to X$ , decomposed into n local functions  $f_i : X \to X_i$  for  $i \in [n]$ , where  $f_i$  is the *i*-th component of f. To let the system

evolve, one must define when the automata update their state using their local function, which can be done in multiple ways, called *update modes*.

Block-sequential update modes. A sequence  $(W_{\ell})_{\ell \in \llbracket p \rrbracket}$  with  $W_{\ell} \subseteq \llbracket n \rrbracket$  for all  $\ell \in \llbracket p \rrbracket$  is an ordered partition if and only if  $\bigcup_{\ell \in \llbracket p \rrbracket} W_{\ell} = \llbracket n \rrbracket$  and  $\forall i, j \in \llbracket p \rrbracket, i \neq j \implies W_i \cap W_j = \emptyset$ . An update mode  $\mu = (W_{\ell})_{\ell \in \llbracket p \rrbracket}$  is called *block-sequential* when  $\mu$  is an ordered partition, and the  $W_{\ell}$  are called *blocks*. The set of block-sequential update modes of size n is denoted  $\mathsf{BS}_n$ . The update of f under  $\mu \in \mathsf{BS}_n$  is given by  $f_{(\mu)} : X \to X$  as follows:

$$\begin{aligned} f_{(\mu)}(x) &= f_{(W_{p-1})} \circ \dots \circ f_{(W_1)} \circ f_{(W_0)}(x), \\ \text{where } \forall i \in \llbracket n \rrbracket, \ f_{(W_\ell)}(x)_i = \begin{cases} f_i(x) & \text{if } i \in W_\ell, \\ x_i & \text{otherwise} \end{cases} \end{aligned}$$

Block-parallel update modes. In a block-sequential update mode, the automata in a block are updated simultaneously while the blocks are updated sequentially. A block-parallel update mode is based on the dual principle: the automata in a block are updated sequentially while the blocks are updated simultaneously. Instead of being defined as a sequence of unordered blocks, a block-parallel update mode will thus be defined as a set of ordered blocks. A set  $\{S_k\}_{k \in [\![s]\!]}$ with  $S_k = (i_0^k, \ldots, i_{n_k-1}^k)$  a sequence of  $n_k > 0$  distinct elements of  $[\![n]\!]$  for all  $k \in [\![s]\!]$  is a partitioned order if and only if  $\bigcup_{k \in [\![s]\!]} S_k = [\![n]\!]$  and  $\forall i, j \in [\![s]\!], i \neq$  $j \implies S_i \cap S_j = \emptyset$ . An update mode  $\mu = \{S_k\}_{k \in [\![s]\!]}$  is called block-parallel when  $\mu$  is a partitioned order, and the sequences  $S_k$  are called o-blocks (for orderedblocks). The set of block-parallel update modes of size n is denoted BP<sub>n</sub>. With  $p = \operatorname{lcm}(n_1, \ldots, n_s)$ , the update of f under  $\mu \in \mathsf{BP}_n$  is given by  $f_{\{\mu\}} : X \to X$ as follows:  $f_{\{\mu\}}(x) = f_{(W_{p-1})} \circ \cdots \circ f_{(W_1)} \circ f_{(W_0)}(x)$ , where for all  $\ell \in [\![p]\!]$  we define  $W_\ell = \{i_\ell^k \mod n_k \mid k \in [\![s]\!]\}$ .

Basic considerations. There is a natural way to convert a block-parallel update mode  $\{S_k\}_{k \in [\![s]\!]}$  with  $S_k = (i_0^k, \ldots, i_{n_{k-1}}^k)$  into a sequence of blocks of length  $p = \operatorname{lcm}(n_1, \ldots, n_s)$ . We define it as  $\varphi$ :

$$\varphi(\{S_k\}_{k\in \llbracket s \rrbracket}) = (W_\ell)_{\ell \in \llbracket p \rrbracket} \text{ with } W_\ell = \{i_\ell^k \mod n_k \mid k \in \llbracket s \rrbracket\}.$$

In order to differentiate between sequences of blocks and sets of o-blocks, we denote by  $f_{(\mu)}$  (resp.  $f_{\{\mu\}}$ ) the dynamical system induced by f and  $\mu$  when  $\mu$  is a sequence of blocks (resp. a set of o-blocks), and simply  $f_{\mu}$  when it is clear from the context. Moreover, abusing notations, we denote by  $\varphi(\mathsf{BP}_n)$  the set of partitioned orders of [n] as sequences of blocks.

Block-sequential and block-parallel update modes are *periodic* (the same update procedure is repeated at each step), and *fair* (each automaton is updated at least once per step). We distinguish the concepts of *step* and *substep*. A step is the interval between x and  $f_{(\mu)}(x)$  (or  $f_{\{\mu\}}(x)$ ), and can be divided into  $p = |\mu|$  (or  $p = |\varphi(\mu)| = \operatorname{lcm}(n_1, \ldots, n_s)$ ) substeps, corresponding to the elementary intervals in which only one block of automata is updated. The most basic update mode is the parallel  $\mu_{par}$  which updates simultaneously all automata at each step. It is the element  $(\llbracket n \rrbracket) \in \mathsf{BS}_n$  and  $\{(i) \mid i \in \llbracket n \rrbracket\} \in \mathsf{BP}_n$ , with  $\varphi(\{(i) \mid i \in \llbracket n \rrbracket\}) = (\llbracket n \rrbracket)$ .

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Fig. 1: Illustration of the execution along time of local transition functions according to block-parallel updating mode  $\mu_{bp} = \{(0), (2, 1)\}$ . For the odd steps, we picture the blocks, and for the even steps, we picture the o-blocks.

Remark 1. Observe that in block-sequential update modes, each automaton is updated exactly once during a step, whereas in block-parallel update modes, some automata can be updated multiple times during a step. Update repetitions may have many consequences on the limit dynamics. For instance, the network of n = 3 automata such that  $f_i(x) = x_{i-1 \mod n}$  under the update mode  $\mu =$  $(\{1, 2\}, \{0, 2\}, \{0, 1\})$ , where each automaton is updated twice during a step, has 4 fixed points, among which 2, namely 010 and 101, cannot be obtained with block-sequential update modes (in this example,  $\mu \notin BP_n$ ).

Remark 2. Let  $\mu = \{S_k\}_{k \in [s]}$  be a block-parallel update mode. Each block of  $\varphi(\mu)$  is of the same size, namely s, and furthermore each block of  $\varphi(\mu)$  is unique.

Fixed points, limit cycles and attractors. Let  $f_{\mu}$  be the dynamical system defined by an AN f of size n and an update mode  $\mu$ . Let  $p \ge 1$ . A sequence of configurations  $x^0, \ldots, x^{p-1} \in X$  is a limit cycle of  $f_{\mu}$  if and only if  $\forall i \in [\![p]\!], f_{\mu}(x^i) = x^{i+1 \mod p}$ . A limit cycle of length p = 1 is a fixed point. The sequence of configurations  $x^0, x^1, \ldots, x^{p-1} \in X$  is an attractor if and only if it is a limit cycle and there exist  $x \in X$  and  $i \in [\![p]\!]$  such that  $f_{\mu}(x) = x^i$  but  $x \notin \{x^0, \ldots, x^{p-1}\}$ .

*Example 1.* Let  $f : [3] \times \mathbb{B} \times \mathbb{B} \to [3] \times \mathbb{B} \times \mathbb{B}$  the automata network defined as:

$$f(x) = \begin{pmatrix} f_0(x) = \begin{cases} 0 & \text{if } ((x_0 = 0) \land (x_1 = x_2)) \lor (x_0 = x_1 = x_2 = 1) \\ 1 & \text{if } x_1 + x_2 \mod 2 = 1 \\ 2 & \text{otherwise} \\ f_1(x) = (x_0 \neq 0) \lor x_1 \lor x_2 \\ f_2(x) = ((x_0 = 1) \land x_1) \lor (x_0 = 2) \end{cases} \end{pmatrix}.$$

Let  $\mu_{bs} = (\{1\}, \{0, 2\})$  and  $\mu_{bp} = \{(0), (2, 1)\}$ . The update mode  $\mu_{bs}$  is block-sequential and  $\mu_{bp}$  is block-parallel, with  $\varphi(\mu_{bp}) = (\{0, 2\}, \{0, 1\})$  as depicted in Figure 1. Systems  $f_{(\mu_{bs})}$  and  $f_{\{\mu_{bp}\}}$  have different dynamics, as depicted in Figure 2. They both have the same two fixed points and one limit cycle, but the similarities stop there. The limit cycle of  $f_{(\mu_{bs})}$  is of size 4, while that of  $f_{\{\mu_{bp}\}}$  is of size 2. Moreover, neither of the fixed points of  $f_{\{\mu_{bp}\}}$  is an attractor, while one of  $f_{(\mu_{bs})}$ , namely 211, is. Both of these update modes' dynamics are unique in  $\mathsf{BP}_3 \cup \mathsf{BS}_3$ .



Fig. 2: The dynamics of  $f_{(\mu_{bs})}$  (left) and  $f_{\{\mu_{bb}\}}$  (right) from 1.

# 3 Counting block-parallel update modes

For the rest of this section, let p(n) denote the number of integer partitions of n (multisets of integers summing to n), let d(i) be the maximal part size in the i-th partition of n, let m(i, j) be the multiplicity of the part of size j in the i-th partition of n. As an example, let n = 31 and assume the i-th partition is (2, 2, 3, 3, 3, 5, 5, 5), we have d(i) = 5 and m(i, 1) = 0, m(i, 2) = 2, m(i, 3) = 4, m(i, 4) = 0, m(i, 5) = 3. A partition will be the support of a partitioned order, where each part is an o-block. In our example, we can have:

 $\{(0,1), (2,3), (4,5,6), (7,8,9), (10,11,12), (13,14,15), (16,17,18,19,20), (21,22,23,24,25), (26,27,28,29,30)\},\$ 

and we picture it as the following *matrix-representation*:

$$\begin{pmatrix} 0 & 1 \\ 2 & 3 \end{pmatrix} \begin{pmatrix} 4 & 5 & 6 \\ 7 & 8 & 9 \\ 10 & 11 & 12 \\ 13 & 14 & 15 \end{pmatrix} \begin{pmatrix} 16 & 17 & 18 & 19 & 20 \\ 21 & 22 & 23 & 24 & 25 \\ 26 & 27 & 28 & 29 & 30 \end{pmatrix}.$$

We call matrices the elements of size  $j \cdot m(i, j)$  and denote them  $M_1, \ldots, M_{d(i)}$ , where  $M_j$  has m(i, j) rows and j columns  $(M_j$  is empty when m(i, j) = 0). The partition defines the dimensions of the matrices, and each row is an o-block.

For the comparison, the block-sequential update modes (ordered partitions of [n]) are given by the ordered Bell numbers, sequence OEIS A000670. A closed formula for it is:

$$|\mathsf{BS}_n| = \sum_{i=1}^{p(n)} \frac{n!}{\prod_{j=1}^{d(i)} (j!)^{m(i,j)}} \cdot \frac{\left(\sum_{j=1}^{d(i)} m(i,j)\right)!}{\prod_{j=1}^{d(i)} m(i,j)!}.$$

Intuitively, an ordered partition of n gives a support to construct a block-sequential update mode: place the elements of [n] up to permutation within

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the blocks. This is the left fraction: n! divided by j! for each block of size j, taking into account multiplicities. The right fraction corrects the count because we sum on p(n) the (unordered) partitions of n: each partition of n can give rise to different ordered partitions of n, by ordering all blocks (numerator, where the sum of multiplicities is the number of blocks) up to permutation within blocks of the same size which have no effect (denominator). The first ten terms are (n = 1 onward): 1, 3, 13, 75, 541, 4683, 47293, 545835, 7087261, 102247563.

#### 3.1 Intersection of block-sequential and block-parallel modes

In order to be able to compare block-sequential with block-parallel update modes, both of them will be written here under their sequence of blocks form (the usual form of block-sequential update modes and the rewritten form of block-parallel modes). First,  $\varphi(\mathsf{BP}_n) \cap \mathsf{BS}_n \neq \emptyset$ , since it contains at least  $\mu_{\mathsf{par}} = (\llbracket n \rrbracket) = \varphi(\{(0), (1), \ldots, (n-1)\})$ . However, neither  $\mathsf{BS}_n \subseteq \varphi(\mathsf{BP}_n)$  nor  $\varphi(\mathsf{BP}_n) \subseteq \mathsf{BS}_n$  are true. Indeed,  $\mu_s = (\{0, 1\}, \{2\}) \in \mathsf{BS}_3$  but  $\mu_s \notin \varphi(\mathsf{BP}_3)$  since a block-parallel cannot have blocks of different sizes in its sequential form. Symmetrically,  $\mu_p = \varphi(\{(1, 2), (0)\}) = (\{0, 1\}, \{0, 2\}) \in \mathsf{BP}_3$  but  $\mu_p \notin \mathsf{BS}_3$  since automaton 0 is updated twice. Nonetheless, we can precisely define their intersection.

**Lemma 1.**  $\mu \in (\mathsf{BS}_n \cap \varphi(\mathsf{BP}_n))$ , if and only if  $\mu$  is an ordered partition with p blocks of the same size s, if and only if there exists a partitioned order  $\mu'$  with s o-blocks of the same size p such that  $\varphi(\mu') = \mu$ .

*Proof.* Let  $n \in \mathbb{N}$ . We prove the first equivalence, the second follows directly.

 $(\Longrightarrow)$  Let  $\mu \in (\mathsf{BS}_n \cap \varphi(\mathsf{BP}_n))$ . Since  $\mu \in \mathsf{BS}_n$ ,  $\mu$  is an ordered partition. Furthermore,  $\mu \in \varphi(\mathsf{BP}_n)$  so all the  $\mu$ 's blocks are of the same size (Remark 2).

 $(\Leftarrow) \text{ Let } \mu = (W_{\ell})_{\ell \in \llbracket p \rrbracket} \text{ be an ordered partition of } \llbracket n \rrbracket \text{ with all its blocks} \\ \text{having the same size, denoted by } s. \text{ Since } \mu \text{ is an ordered partition, } \mu \in \mathsf{BS}_n. \\ \text{For each } \ell \in \llbracket p \rrbracket, \text{ we can number arbitrarily the elements of } W_{\ell} \text{ from 0 to } s - 1 \\ \text{as } W_{\ell} = \{W_{\ell}^0, \dots, W_{\ell}^{s-1}\}. \text{ Now, let us define the set of sequences } \{S_k\}_{k \in \llbracket s \rrbracket} \text{ the following way: } \forall k \in \llbracket s \rrbracket, S_k = \{W_{\ell}^k \mid \ell \in \llbracket p \rrbracket\}. \text{ It is a partitioned order such that } \\ \varphi(\{S_k\}_{k \in \llbracket s \rrbracket)} = \mu, \text{ which means that } \mu \in \varphi(\mathsf{BP}_n). \\ \Box$ 

As a consequence of Lemma 1, given  $n \in \mathbb{N}$ , the set  $SEQ_n$  of sequential update modes such that every automaton is updated exactly once by step and only one automaton is updated by substep, is a subset of  $(\mathsf{BS}_n \cap \varphi(\mathsf{BP}_n))$ . Moreover, we can count the number of sequences of blocks in the intersection.

**Proposition 1.** Given  $n \in \mathbb{N}$ , we have  $|\mathsf{BS}_n \cap \varphi(\mathsf{BP}_n)| = \sum_{d|n} \frac{n!}{\binom{n}{d}!^d}$ .

*Proof.* The proof derives directly from the sequence OEIS A061095, which counts the number of ways of dividing n labeled items into labeled boxes with an equal number of items in each box. In our context, the "items" are the automata, and the "labeled boxes" are the blocks of the ordered partitions.  $\Box$ 

#### 3.2 Partitioned orders

A block-parallel update mode is given as a partitioned order, *i.e.* an (unordered) set of (ordered) sequences. This concept is recorded as sequence OEIS A000262, described as the *number of "sets of lists"*. A nice closed formula for it is:

$$|\mathsf{BP}_n| = \sum_{i=1}^{p(n)} \frac{n!}{\prod_{j=1}^{d(i)} m(i,j)!}.$$

Intuitively, for each partition, fill all matrices (n! ways to place the elements of [n]) up to permutation of the rows within each matrix (matrix  $M_j$  has m(i, j) rows). Another closed formula is presented in Proposition 2, which is used as the basis of implementations in Section 3.5. The first ten terms are (n = 1 onward): 1, 3, 13, 73, 501, 4051, 37633, 394353, 4596553, 58941091.

**Proposition 2.** For any  $n \ge 1$  we have:

$$|\mathsf{BP}_{n}| = \sum_{i=1}^{p(n)} \prod_{j=1}^{d(i)} \binom{n - \sum_{k=1}^{j-1} k \cdot m(i,k)}{j \cdot m(i,j)} \cdot \frac{(j \cdot m(i,j))!}{m(i,j)!}.$$

*Proof.* Each partition is a support to generate different partitioned orders (sum on *i*), by considering all the combinations, for each matrix (product on *j*), of the ways to choose the  $j \cdot m(i, j)$  elements of [n] it contains (binomial coefficient, chosen among the remaining elements), and all the ways to order them up to permutation of the rows (ratio of factorials). Observe that developing the binomial coefficients with  $\binom{x}{y} = \frac{x!}{y!\cdot(x-y)!}$  gives

$$\prod_{j=1}^{d(i)} \binom{n-\sum_k}{j \cdot m(i,j)} \cdot (j \cdot m(i,j))! = \prod_{j=1}^{d(i)} \frac{(n-\sum_k)!}{(n-\sum_k -j \cdot m(i,j))!} = \frac{n!}{0!} = n!,$$

where  $\sum_{k}$  is a shorthand for  $\sum_{k=1}^{j-1} k \cdot m(i, k)$ , which leads to retrieve the OEIS formula.

#### 3.3 Partitioned orders up to dynamical equality

As for block-sequential update modes, given an AN f and two block-parallel update modes  $\mu$  and  $\mu'$ , the dynamics of f under  $\mu$  can be the same as that of f under  $\mu'$ . To go further, in the framework of block-parallel update modes, there exist pairs of update modes  $\mu, \mu'$  such that for any AN f, the dynamics  $f_{\{\mu\}}$  is the exact same as  $f_{\{\mu'\}}$ . As a consequence, in order to perform exhaustive searches among the possible dynamics, it is not necessary to generate all of them. We formalise this with the following equivalence relation.

**Definition 1.** For  $\mu, \mu' \in \mathsf{BP}_n$ , we denote  $\mu \equiv_0 \mu'$  when  $\varphi(\mu) = \varphi(\mu')$ .

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*Example 2.* Let  $\mu_1 = \{(0,1), (2,3)\}$  and  $\mu_2 = \{(2,1), (0,3)\}$ .  $\mu_1$  and  $\mu_2$  are different partitioned orders, but  $\varphi(\mu_1) = \varphi(\mu_2) = (\{0, 2\}, \{1, 3\})$ . Thus  $\mu_1 \equiv_0 \mu_2$ .

The following theorem shows that this equivalence relation is necessary and sufficient in the general case of ANs of size n, *i.e.*  $\equiv_0$  captures the dynamical equivalence among block-parallel update modes.

**Theorem 1.** For any  $\mu, \mu' \in \mathsf{BP}_n$ ,  $\mu \equiv_0 \mu' \iff \forall f : X \to X$ ,  $f_{\{\mu\}} = f_{\{\mu'\}}$ .

*Proof.* Let  $\mu$  and  $\mu'$  be two block-parallel update modes of  $\mathsf{BP}_n$ .

 $(\Longrightarrow)$  Let us consider that  $\mu \equiv_0 \mu'$ , and let  $f: X \to X$  be an AN. Then, we

have  $f_{\{\mu\}} = f_{(\varphi(\mu))} = f_{(\varphi(\mu'))} = f_{\{\mu'\}}$ . ( $\Leftarrow$ ) Let us consider that  $\forall f : X \to X, f_{\{\mu\}} = f_{\{\mu'\}}$ . Let us assume for the sake of contradiction that  $\varphi(\mu) \neq \varphi(\mu')$ . For ease of reading, we will denote as  $t_{\mu,i}$ the substep at which automaton i is updated for the first time with update mode  $\mu$ . Then, there is a pair of automata (i, j) such that  $t_{\mu,i} \leq t_{\mu,j}$ , but  $t_{\mu',i} > t_{\mu',j}$ . Let  $f: \mathbb{B}^n \to \mathbb{B}^n$  be a Boolean AN such that  $f(x)_i = x_i \lor x_j$  and  $f(x)_j = x_i$ , and  $x \in \mathbb{B}^n$  such that  $x_i = 0$  and  $x_j = 1$ . We will compare  $f_{\{\mu\}}(x)_i$  and  $f_{\{\mu'\}}(x)_i$ , in order to prove a contradiction. Let us apply  $f_{\{\mu\}}$  to x. Before step  $t_{\mu,i}$  the value of automaton i is still 0 and, most importantly, since  $t_{\mu,i} \leq t_{\mu,j}$ , the value of j is still 1. This means that right after step  $t_{\mu,i}$ , the value of automaton i is 1, and will not change afterwards. Thus, we have  $f_{\{\mu\}}(x)_i = 1$ . Let us now apply  $f_{\{\mu'\}}$ to x. This time,  $t_{\mu',i} > t_{\mu',j}$ , which means that automaton j is updated first and takes the value of automaton i at the time, which is 0 since it has not been updated yet. Afterwards, neither automata will change value since  $0 \vee 0$  is still 0. This means that  $f_{\{\mu'\}}(x)_i = 0$ . Thus, we have  $f_{\{\mu\}} \neq f_{\{\mu'\}}$ , which contradicts our earlier hypothesis. 

Let  $\mathsf{BP}_n^0 = \mathsf{BP}_n / \equiv_0$  denote the corresponding quotient set, *i.e.* the set of block-parallel update modes to generate for exhaustive computer analysis of the possible dynamics in the general case of ANs of size n.

**Theorem 2.** For any  $n \ge 1$ , we have:

$$|\mathsf{BP}_{n}^{0}| = \sum_{i=1}^{p(n)} \frac{n!}{\prod_{j=1}^{d(i)} (m(i,j)!)^{j}}$$
(1)

$$=\sum_{i=1}^{p(n)}\prod_{j=1}^{d(i)}\prod_{\ell=1}^{j}\binom{n-\sum_{k=1}^{j-1}k\cdot m(i,k)-(\ell-1)\cdot m(i,j)}{m(i,j)}$$
(2)

$$= \sum_{i=1}^{p(n)} \prod_{j=1}^{d(i)} \left( \binom{n - \sum_{k=1}^{j-1} k \cdot m(i,k)}{j \cdot m(i,j)} \cdot \prod_{\ell=1}^{j} \binom{(j-\ell+1) \cdot m(i,j)}{m(i,j)} \right).$$
(3)

*Proof.* Formula 1 is a sum for each partition of n (sum on i), of all the ways to fill all matrices up to permutation within each column (m(i, j)!) for each of the j columns of  $M_i$ ). Formula 2 is a sum for each partition of n (sum on i), of the product for each column of the matrices (products on i and  $\ell$ ), of the choice of elements (among the remaining ones) to fill the column (regardless of their order within the column). Formula 3 is a sum for each partition of n (sum on i), of the product for each matrix (product on j), of the choice of elements (among the remaining ones) to fill this matrix, multiplied by the number of ways to fill the columns of the matrix (product on  $\ell$ ) with these elements (regardless of their order within each column).

The equality of these three formulas is presented in Appendix A. To prove that they count  $|\mathsf{BP}_n^0|$ , we now argue that for any pair  $\mu, \mu' \in \mathsf{BP}_n$ , we have  $\mu \equiv_0 \mu'$  if and only if their matrix-representations are the same up to a permutation of the elements within columns (the number of equivalence classes is then counted by Formula 1). In the definition of  $\varphi$ , each block is a set constructed by taking one element from each o-block. Given that  $n_k$  in the definition of  $\varphi$  corresponds to j in the statement of the theorem, one matrix corresponds to all the o-blocks having the same size  $n_k$ . Hence, the  $\ell \mod n_k$  operations in the definition of  $\varphi$ amounts to considering the elements of these o-blocks which are in a common column in the matrix representation. Since blocks are sets, the result follows.  $\Box$ 

The first ten terms of the sequence  $(|\mathsf{BP}_n^0|)_{n\geq 1}$  are: 1, 3, 13, 67, 471, 3591, 33573, 329043, 3919387, 47827093. They match the sequence OEIS A182666 (defined by its exponential generating function), and we prove in Appendix B that they are indeed the same sequence.

#### 3.4 Partitioned orders up to isomorphism on the limit dynamics

The following equivalence relation defined over block-parallel update modes turns out to capture exactly the notion of having isomorphic limit dynamics. It is analogous to  $\equiv_0$ , except that a circular shift of order *i* may be applied on the sequences of blocks.

Let  $\sigma^i$  denote the circular-shift of order  $i \in \mathbb{Z}$  on sequences (shifting the element at position 0 towards position i).

**Definition 2.** For  $\mu, \mu' \in \mathsf{BP}_n$ , we denote  $\mu \equiv_{\star} \mu'$  when  $\varphi(\mu) = \sigma^i(\varphi(\mu'))$  for some  $i \in [\![|\varphi(\mu')|]\!]$  called the shift. Note that  $\mu \equiv_0 \mu' \implies \mu \equiv_{\star} \mu'$ .

**Notation 1** Given  $f_{\{\mu\}} : X \to X$ , let  $\Omega_{f_{\{\mu\}}} = \bigcap_{t \in \mathbb{N}} f^t_{\{\mu\}}(X)$  denote its limit set (abusing the notation of  $f_{\{\mu\}}$  to sets of configurations), and  $f^{\Omega}_{\{\mu\}} : \Omega_{f_{\{\mu\}}} \to \Omega_{f_{\{\mu\}}}$  its restriction to its limit set. Dynamics are deterministic, hence  $f^{\Omega}_{\{\mu\}}$  is bijective.

The next theorem shows that, if one is interested in the limit behaviour of ANs under block-parallel updates, then studying a representative from each equivalence class of the relation  $\equiv_{\star}$  is necessary and sufficient to get the full spectrum of possible limit dynamics (recall that ~ denotes graph isomorphism; thus in terms of dynamical systems they are conjugate).

**Theorem 3.** For any  $\mu, \mu' \in \mathsf{BP}_n$ ,  $\mu \equiv_{\star} \mu' \iff \forall f : X \to X, f_{\{\mu\}}^{\Omega} \sim f_{\{\mu'\}}^{\Omega}$ .

*Proof (sketch).* Let  $\mu$  and  $\mu'$  be two block-parallel update modes of  $\mathsf{BP}_n$ .

 $(\Longrightarrow) \text{ Let } \mu, \mu' \text{ be such that } \mu \equiv_{\star} \mu' \text{ of shift } \hat{i} \in \llbracket p \rrbracket, \text{ with } \varphi(\mu) = (W_{\ell})_{\ell \in \llbracket p \rrbracket}, \\ \varphi(\mu') = (W'_{\ell})_{\ell \in \llbracket p \rrbracket} \text{ and } p = |\varphi(\mu)| = |\varphi(\mu')|. \text{ It means that } \forall i \in \llbracket p \rrbracket, \text{ we have } W'_i = W_{i+\hat{i} \mod p}, \text{ and for any AN } f, \text{ we deduce that } \pi = f_{(W_0,\ldots,W_{i-1})} \text{ is the desired isomorphism from } \Omega_{f_{\{\mu\}}} \text{ to } \Omega_{f_{\{\mu'\}}}.$ 

( $\Leftarrow$ ) We prove the contrapositive, from  $\mu \not\equiv_{\star} \mu'$ , by case analysis. In each case we build an AN f such that  $f_{\{\mu\}}^{\Omega}$  is not isomorphic to  $f_{\{\mu'\}}^{\Omega}$ . In this sketch we detail only the simplest case.

- (1) If in  $\varphi(\mu)$  and  $\varphi(\mu')$ , there is an automaton  $\hat{\imath}$  which is not updated the same number of times  $\alpha$  and  $\alpha'$  in  $\mu$  and  $\mu'$  respectively, then we assume without loss of generality that  $\alpha > \alpha'$  and consider the AN f such that:
  - $X_{\hat{i}} = \llbracket \alpha \rrbracket$  and  $X_i = \{0\}$  for all  $i \neq \hat{i}$ ; and
  - $f_{\hat{\imath}}(x) = (x_{\hat{\imath}} + 1) \mod \alpha$  and  $f_i(x) = x_i$  for all  $i \neq \hat{\imath}$ .

It follows that  $f^{\Omega}_{\{\mu\}}$  has only fixed points since +1 mod  $\alpha$  is applied  $\alpha$  times, whereas  $f^{\Omega}_{\{\mu'\}}$  has no fixed point because  $\alpha' < \alpha$ .

(2) If in  $\varphi(\mu)$  and  $\varphi(\mu')$ , all the automata are updated the same number of times, then the transformation from  $\mu$  to  $\mu'$  is a permutation on [n] which preserves the matrices of their matrix representations. This case is harder and we tackle it in Appendix A through three subcases, in order to get extra hypotheses allowing to design specific ANs contradicting the isomorphism.

Let  $\mathsf{BP}_n^* = \mathsf{BP}_n / \equiv_*$  denote the corresponding quotient set.

**Theorem 4.** Let  $lcm(i) = lcm(\{j \in \{1, ..., d(i)\} | m(i, j) \ge 1\})$ . For any  $n \ge 1$ , we have:

$$|\mathsf{BP}_{n}^{\star}| = \sum_{i=1}^{p(n)} \frac{n!}{\prod_{j=1}^{d(i)} (m(i,j)!)^{j}} \cdot \frac{1}{lcm(i)}.$$
(4)

*Proof.* Let  $\mu, \mu' \in \mathsf{BP}_n$  two update modes such that  $\mu \equiv_{\star} \mu'$ . Then their sequential forms are of the same length, and each automaton appears the same number of times in both of them. This means that, if an automaton is in an o-block of size k in  $\mu$ 's partitioned order form, then it is also in an o-block of the same size in  $\mu$ 's. We deduce that two update modes of size n can only be equivalent as defined in Definition 2 if they are generated from the same partition of n.

Let  $\mu \in \mathsf{BP}_n^0$ , generated from partition i of n. Then  $\varphi(\mu)$  is of length lcm(i). Since no two elements of  $\mathsf{BP}_n^0$  have the same block-sequential form, the equivalence class of  $\mu$  in  $\mathsf{BP}_n^0$  contains exactly lcm(i) elements, all generated from the same partition i (all the blocks of  $\varphi(\mu)$  are different). Thus, the number of elements of  $\mathsf{BP}_n^n$  generated from a partition i is the number of elements of  $\mathsf{BP}_n^0$  generated from partition i, divided by the number of elements in its equivalence class for  $\mathsf{BP}_n^n$ , namely lcm(i).

*Remark 3.* Formula 4 can actually be obtained from any formula in Theorem 2 by multiplying by  $\frac{1}{\text{lcm}(i)}$  inside the sum on partitions (from i = 1 to p(n)).

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#### 3.5 Implementations

Proof-of-concept Python implementations of three underlying enumeration algorithms for  $\mathsf{BP}_n$ ,  $\mathsf{BP}_n^0$  and  $\mathsf{BP}_n^*$  are available on the following repository: https: //framagit.org/leah.tapin/blockpargen. We have conducted numerical experiments on a laptop, presented in Figure 3. Figure 3 shows the result of numerical experiments for n from 1 to 12.

In brief, enumerating  $\mathsf{BP}_n$ ,  $\mathsf{BP}_n^0$  and  $\mathsf{BP}_n^*$  up to n = 8 takes less than one second. Then we observe a significant time gain when enumerating only the elements of  $\mathsf{BP}_n^*$ , as depicted below.





Fig. 3: Numerical experiments of our Python implementations on a standard laptop (processor Intel-Core<sup>TM</sup> i7 @ 2.80 GHz). For n from 1 to 12, the table (left) presents the size of  $\mathsf{BP}_n$ ,  $\mathsf{BP}_n^0$  and  $\mathsf{BP}_n^*$  and running time to enumerate their elements (one representative of each equivalence class; a dash represents a time smaller than 0.1 second), and the graphics (right) depicts their respective sizes on a logarithmic scale. Observe that the sizes of  $\mathsf{BP}_n$  and  $\mathsf{BP}_n^0$  are comparable, whereas an order of magnitude is gained with  $\mathsf{BP}_n^*$ , which may be significant for advanced numerical experiments regarding limit dynamics under block-parallel udpate modes.

### 4 Conclusion and perspectives

This article settles the theoretical foundations to the study of block-parallel update modes in the AN setting. We first characterise their intersection with the classical block-sequential modes. Then, we provide closed formulas for counting: notably (1) a minimal set of representatives of block-parallel update modes that allow to generate the full spectrum of possible distinct dynamics, (2) a minimal set of representatives of block-parallel update modes that allow to generate the full spectrum of possible distinct dynamics, (2) a minimal set of representatives of block-parallel update modes that allow to generate the full spectrum of possible distinct limit dynamics up to isomorphism (*i.e.* the limit cycles lengths and distribution). Numerical experiments show that the computational gain is significant, in particular for the exhaustive study of how/when the fixed point invariance property is broken.

A major feature of block-parallel update modes is that they allow local update repetitions during a period. This is indeed the case for all block-parallel update modes which are not block-sequential (*i.e.* modes with at least two blocks (i)of distinct sizes when defined as a partitioned order, cf. Lemma 1). Since we know that local update repetitions can break the fixed point invariance property which holds in block-sequential ANs (cf. the example given in Remark 1), it would be interesting to characterise the conditions relating these repetitions to the architecture of interactions (so called interaction graph) giving rise to the existence of new fixed points. More generally, as a complement to the results of Section 3.4, the following problem can be studied: given an AN f, to which extent is f block-parallel sensitive/robust? In [1], the authors addressed this question on block-sequential Boolean ANs by developing the concept of update digraphs which allows to capture conditions of dynamical equivalence at the syntactical level. However, this concept does not apply as soon as local update repetitions are at stake. Hence, creating a new concept of update digraphs in the general context of periodic update modes would be an essential step forward to explain and understand updating sensitivity/robustness of ANs.

Another track of research would be to understand how basic interaction cycles of automata evolve under block-parallel updates. For instance, the authors of [7] have shown that such cycles in the Boolean setting are somehow very robust to block-sequential update modes variations: the number of their limit cycles of length p is the same as that of a smaller cycle (of same sign) evolving in parallel. Together with the combinatorial analysis of [3], this provides a complete analysis of the asymptotic dynamics of Boolean interaction cycles. This gives rise to the following question: do interaction cycles behave similarly under block-parallel update modes variations? The local update repetitions should again play an essential role. In this respect, the present work sets the foundations for theoretical developments and computer experiments (Theorems 3 and 4). Such a study could constitute a first approach of the more general problem raised above, since it is well known that cycles are the behavioural complexity engines of ANs [13].

Eventually, since block-parallel schedules form a new family of update modes of which the field of investigation is still largely open today, we think that a promising perspective of our work would consist in dealing with the computational complexity of classical decision problems for ANs, in the lines of [5] about reaction systems. The general question to be addressed here is: do local update repetitions induced by block-parallel update modes make such decision problems take place at a higher level in the polynomial hierarchy, or even reach polynomial space completeness? We have early evidence of the latter.

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# References

- J. Aracena, E. Goles, A. Moreira, and L. Salinas. On the robustness of update schedules in Boolean networks. *Biosystems*, 97:1–8, 2009.
- M. I. Davidich and S. Bornholdt. Boolean network model predicts cell cycle sequence of fission yeast. *PLoS One*, 3:e1672, 2008.
- J. Demongeot, M. Noual, and S. Sené. Combinatorics of Boolean automata circuits dynamics. Discrete Applied Mathematics, 160(4–5):398–415, 2012.
- J. Demongeot and S. Sené. About block-parallel Boolean networks: a position paper. Natural Computing, 19:5–13, 2020.
- A. Dennunzio, E. Formenti, L. Manzoni, and A. E. Porreca. Complexity of the dynamics of reaction systems. *Information and Computation*, 267:96–109, 2019.
- B. Fierz and M. G. Poirier. Biophysics of chromatin dynamics. Annual Review of Biophysics, 48:321–345, 2019.
- E. Goles and M. Noual. Block-sequential update schedules and Boolean automata circuits. In *Proceedings of AUTOMATA* '2010, pages 41–50. DMTCS, 2010.
- M. R. H
  übner and D. L. Spector. Chromatin dynamics. Annual Review of Biophysics, 39:471–489, 2010.
- S. A. Kauffman. Metabolic stability and epigenesis in randomly constructed genetic nets. Journal of Theoretical Biology, 22:437–467, 1969.
- L. Mendoza and E. R. Alvarez-Buylla. Dynamics of the genetic regulatory network for Arabidopsis thaliana flower morphogenesis. Journal of Theoretical Biology, 193:307–319, 1998.
- 11. M. Noual. *Updating automata networks*. PhD thesis, École normale supérieure de Lyon, 2012.
- L. Paulevé and S. Sené. Systems biology modelling and analysis: formal bioinformatics methods and tools, chapter Boolean networks and their dynamics: the impact of updates, pages 173–250. Wiley, 2022.
- 13. F. Robert. Discrete iterations: a metric study, volume 6 of Springer Series in Computational Mathematics. Springer, 1986.
- R. Thomas. Boolean formalization of genetic control circuits. Journal of Theoretical Biology, 42:563–585, 1973.

# A Full proofs

Proof (Proof of Theorem 2 for the equality between Formulas 1, 2 and 3). The equality between Formulas 1 and 2 is obtained by developing the binomial coefficients as follows:  $\binom{x}{y} = \frac{x!}{y! \cdot (x-y)!}$ , and by observing that the products of  $\frac{x!}{(x-y)!}$  telescope. Indeed, denoting  $a(j, \ell) = (n - \sum_{k=1}^{j-1} k \cdot m(i, k) - \ell \cdot m(i, j))!$ , we have

$$\prod_{j=1}^{d(i)} \prod_{\ell=1}^{j} \frac{(n - \sum_{k=1}^{j-1} k \cdot m(i,k) - (\ell-1) \cdot m(i,j))!}{(n - \sum_{k=1}^{j-1} k \cdot m(i,k) - \ell \cdot m(i,j))!} = \prod_{j=1}^{d(i)} \prod_{\ell=1}^{j} \frac{a(j,\ell-1)}{a(j,\ell)} = \frac{n!}{0!} = n!$$

because a(1,0) = n!, then a(1,j) = a(2,0), a(2,j) = a(3,0), ..., until a(d(i), j) = 0!.

The equality between Formulas 2 and 3 is obtained by repeated uses of the identity  $\binom{x}{z}\binom{x-z}{y} = \binom{x}{z+y}\binom{z+y}{y}$ , which gives by induction on j:

$$\prod_{\ell=1}^{j} \binom{x - (\ell - 1) \cdot y}{y} = \binom{x}{j \cdot y} \cdot \prod_{\ell=1}^{j} \binom{(j - \ell + 1) \cdot y}{y}.$$
(5)

Indeed, j = 1 is trivial and, using the induction hypothesis on j then the identity we get:

$$\begin{split} \prod_{\ell=1}^{j+1} \begin{pmatrix} x - (\ell-1) \cdot y \\ y \end{pmatrix} &= \begin{pmatrix} x - j \cdot y \\ y \end{pmatrix} \cdot \prod_{\ell=1}^{j} \begin{pmatrix} x - (\ell-1) \cdot y \\ y \end{pmatrix} \\ &= \begin{pmatrix} x - j \cdot y \\ y \end{pmatrix} \cdot \begin{pmatrix} x \\ j \cdot y \end{pmatrix} \cdot \prod_{\ell=1}^{j} \begin{pmatrix} (j - \ell + 1) \cdot y \\ y \end{pmatrix} \\ &= \begin{pmatrix} x \\ (j + 1) \cdot y \end{pmatrix} \cdot \begin{pmatrix} (j + 1) \cdot y \\ y \end{pmatrix} \cdot \prod_{\ell=1}^{j} \begin{pmatrix} (j - \ell + 1) \cdot y \\ y \end{pmatrix} \\ &= \begin{pmatrix} x \\ (j + 1) \cdot y \end{pmatrix} \cdot \prod_{\ell=0}^{j} \begin{pmatrix} (j - \ell + 1) \cdot y \\ y \end{pmatrix} \\ &= \begin{pmatrix} x \\ (j + 1) \cdot y \end{pmatrix} \cdot \prod_{\ell=1}^{j+1} \begin{pmatrix} (j - \ell + 1) \cdot y \\ y \end{pmatrix}. \end{split}$$

As a result, Formula 3 is obtained from Formula 2 by applying Equation 5 for each j with  $x = n - \sum_{k=1}^{j-1} k \cdot m(i,k)$  and y = m(i,j).

*Proof (Proof of Theorem 3).* Let  $\mu$  and  $\mu'$  be two block-parallel update modes of  $\mathsf{BP}_n$ .

 $(\Longrightarrow) \text{ Let } \mu, \mu' \text{ be such that } \mu \equiv_{\star} \mu' \text{ of shift } \hat{i} \in \llbracket p \rrbracket, \text{ with } \varphi(\mu) = (W_{\ell})_{\ell \in \llbracket p \rrbracket}, \\ \varphi(\mu') = (W'_{\ell})_{\ell \in \llbracket p \rrbracket} \text{ and } p = |\varphi(\mu)| = |\varphi(\mu')|. \text{ It means that } \forall i \in \llbracket p \rrbracket, \text{ we have } W'_i = W_{i+\hat{i} \mod p}, \text{ and for any AN } f, \text{ we deduce that } \pi = f_{(W_0, \dots, W_{i-1})} \text{ is the } H_i = (W_i)_{i+\hat{i} \mod p}$ 

desired isomorphism from  $\Omega_{f_{\{\mu\}}}$  to  $\Omega_{f_{\{\mu'\}}}$ . Indeed, we have  $f_{\{\mu\}}(x) = y$  if and only if  $f_{\{\mu'\}}(\pi(x)) = \pi(y)$  because

$$f_{\{\mu'\}} \circ \pi = f_{(W_0, \dots, W_{\hat{\imath}-1}, W'_0, \dots, W'_p)} = f_{(W'_{p-\hat{\imath}}, \dots, W'_p)} \circ f_{\{\mu\}} = \pi \circ f_{\{\mu\}}.$$

Note that  $\pi^{-1} = f_{\{\mu'\}}^{(q-1)} \circ f_{(W'_i \dots W'_{p-1})}$  with q the least common multiple of the limit cycle lengths, and  $\pi^{-1} \circ \pi$  (resp.  $\pi \circ \pi^{-1}$ ) is the identity on  $\Omega_{f_{\{\mu\}}}$  (resp.  $\Omega_{f_{\{\mu'\}}}).$ 

( $\Leftarrow$ ) We prove the contrapositive, from  $\mu \not\equiv_{\star} \mu'$ , by case analysis.

- (1) If in  $\varphi(\mu)$  and  $\varphi(\mu')$ , there is an automaton  $\hat{i}$  which is not updated the same number of times  $\alpha$  and  $\alpha'$  in  $\mu$  and  $\mu'$  respectively, then we assume without loss of generality that  $\alpha > \alpha'$  and consider the AN f such that:
  - $X_{\hat{i}} = \llbracket \alpha \rrbracket$  and  $X_i = \{0\}$  for all  $i \neq \hat{i}$ ; and

•  $f_{\hat{i}}(x) = (x_{\hat{i}} + 1) \mod \alpha$  and  $f_{i}(x) = x_{i}$  for all  $i \neq \hat{i}$ . It follows that  $f_{\{\mu\}}^{\Omega}$  has only fixed points since  $+1 \mod \alpha$  is applied  $\alpha$  times, whereas  $f^{\Omega}_{\{\mu'\}}$  has no fixed point because  $\alpha' < \alpha$ . We conclude that  $f^{\Omega}_{\{\mu\}} \not\sim$  $f^{\Omega}_{\{\mu'\}}.$ 

- (2) If in  $\varphi(\mu)$  and  $\varphi(\mu')$ , all the automata are updated the same number of times, then the transformation from  $\mu$  to  $\mu'$  is a permutation on [n] which preserves the matrices of their matrix representations (meaning that any  $i \in [n]$  is in an o-block of the same size in  $\mu$  and  $\mu'$ , which also implies that  $\mu$  and  $\mu'$  are constructed from the same partition of n). Then we consider subcases.
  - (2.1) If one matrix of  $\mu'$  is not obtained by a permutation of the columns from  $\mu$ , then there is a pair of automata  $\hat{i}, \hat{j}$  that appears in the k-th block of  $\varphi(\mu)$  for some k, and does not appear in any block of  $\varphi(\mu')$ . Indeed, one can take  $\hat{i}, \hat{j}$  to be in the same column in  $\mu$  but in different columns in  $\mu'$ . Let S be the o-block of  $\hat{i}$  and S' be the o-block of  $\hat{j}$ . Let p denote the least common multiple of o-blocks sizes in both  $\mu$  and  $\mu'$ . In this case we consider the AN f such that:
    - $X_{\hat{i}} = \mathbb{B} \times \left[\!\left[\frac{p}{|S|}\right]\!\right], X_{\hat{j}} = \mathbb{B} \times \left[\!\left[\frac{p}{|S'|}\right]\!\right], \text{ and } X_{\hat{i}} = \{0\} \text{ for all } \hat{i} \notin \{\hat{i}, \hat{j}\}.$  Given  $x \in X$ , we denote  $x_{\hat{i}} = (x_{\hat{i}}^b, x_{\hat{i}}^\ell)$  the state of  $\hat{i}$  (and analogously for  $\hat{j}$ ); and . . .

• 
$$f_{\hat{i}}(x) = \begin{cases} (x_{\hat{j}}^{b}, x_{\hat{i}}^{\ell} + 1 \mod \frac{p}{|S|}) & \text{if } x_{\hat{i}}^{\ell} = 0\\ (x_{\hat{i}}^{b}, x_{\hat{i}}^{\ell} + 1 \mod \frac{p}{|S|}) & \text{otherwise'} \end{cases}$$
  
 $f_{\hat{j}}(x) = \begin{cases} (x_{\hat{i}}^{b}, x_{\hat{j}}^{\ell} + 1 \mod \frac{p}{|S'|}) & \text{if } x_{\hat{j}}^{\ell} = 0\\ (x_{\hat{j}}^{b}, x_{\hat{j}}^{\ell} + 1 \mod \frac{p}{|S'|}) & \text{otherwise'} \end{cases}$ , and  $f_{\hat{i}}(x) = x_{\hat{i}} \text{ for all } i \notin \{\hat{i}, \hat{j}\}.$ 

Note that  $\hat{i}$  (resp.  $\hat{j}$ ) is updated  $\frac{p}{|S|}$  (resp.  $\frac{p}{|S'|}$ ) times during a step in both  $\mu$  and  $\mu'$ . Therefore for any  $x \in X$ , its two images under  $\mu$  and  $\mu'$  verify  $f_{\{\mu\}}(x)_{\hat{i}}^{\ell} = f_{\{\mu'\}}(x)_{\hat{i}}^{\ell} = x_{\hat{i}}^{\ell}$  (and analogously for  $\hat{j}$ ). Thus for the evolution of the states of  $\hat{i}$  and  $\hat{j}$  during a step, the second element

is fixed and only the first element (in  $\mathbb{B}$ ) may change. We split X into  $X^{=} = \{x \in X \mid x_{\hat{i}}^b = x_{\hat{j}}^b\}$  and  $X^{\neq} = \{x \in X \mid x_{\hat{i}}^b \neq x_{\hat{j}}^b\}$ , and observe the following facts by the definition of  $f_{\hat{i}}$  and  $f_{\hat{j}}$ :

- Under  $\mu$  and  $\mu'$ , all the elements of  $X^{=}$  are fixed points (indeed, only  $x_{\hat{i}}^{b}$  and  $x_{\hat{j}}^{b}$  may evolve by copying the other).
- Under  $\mu$ , let m, m' be the respective number of times  $\hat{i}, \hat{j}$  have been updated prior to the k-th block of  $\varphi(\mu)$  in which they are updated synchronously. Consider the configurations  $x, y \in X^{\neq}$  with  $x_{\hat{i}} = (0, -m \mod \frac{p}{|S|}), x_{\hat{j}} = (1, -m' \mod \frac{p}{|S'|}), y_{\hat{i}} = (1, -m \mod \frac{p}{|S|})$  and  $y_{\hat{j}} = (0, -m' \mod \frac{p}{|S'|})$ . It holds that  $f_{\{\mu\}}(x) = y$  and  $f_{\{\mu\}}(y) = x$ , because  $x_{\hat{i}}^b$  and  $x_{\hat{j}}^b$  are exchanged synchronously when  $x_{\hat{i}}^\ell = x_{\hat{j}}^\ell = 0$  during the k-th block of  $\varphi(\mu)$ , and are not exchanged again during that step by the choice of the modulo. Hence,  $f_{\{\mu\}}^{\Omega}$  has a limit cycle of length two.
- Under  $\mu'$ , for any  $x \in X^{\neq}$ , there is a substep with  $x_i^{\ell} = 0$  and there is a substep with  $x_j^{\ell} = 0$ , but they are not the same substep (because  $\hat{i}$  and  $\hat{j}$  are never synchronised in  $\mu'$ ). As a consequence,  $x_i^b$  and  $x_j^b$  will end up having the same value (the first to be updated copies the bit from the second, then the second copies its own bit), *i.e.*  $f_{\{\mu'\}}(x) \in X^=$ , and therefore  $f_{\{\mu'\}}^{2}$  has only fixed points.

*i.e.*  $f_{\{\mu'\}}(x) \in X^{=}$ , and therefore  $f_{\{\mu'\}}^{\Omega}$  has only fixed points. We conclude in this case that  $f_{\{\mu\}}^{\Omega} \not\sim f_{\{\mu'\}}^{\Omega}$ , because one has a limit cycle of length two, whereas the other has only fixed points.

- (2.2) If the permutation preserves the columns within the matrices (meaning that the automata within the same column in  $\mu$  are also in the same column in  $\mu'$ ), then we consider two last subcases:
  - (2.2.1) Moreover, if the permutation of some matrix is not circular (meaning that there are three columns which are not in the same relative order in  $\mu$  and  $\mu'$ ), then there are three automata  $\hat{\imath}$ ,  $\hat{\jmath}$  and  $\hat{k}$  in the same matrix such that in  $\mu$ , automaton  $\hat{\imath}$  is updated first, then  $\hat{\jmath}$ , then  $\hat{k}$ ; whereas in  $\mu'$ , automaton  $\hat{\imath}$  is updated first, then  $\hat{k}$ , then  $\hat{\jmath}$ . Let us consider the automata network f such that:
    - $X = \mathbb{B}^n;$
    - $f_{\hat{i}}(x) = x_{\hat{k}}, f_{\hat{j}}(x) = x_{\hat{i}} \text{ and } f_{\hat{k}}(x) = x_{\hat{j}}; \text{ and}$
    - $f_i(x) = x_i$  if  $i \notin \{\hat{i}, \hat{j}, \hat{k}\}.$

If the three automata are updated in the order  $\hat{i}$  then  $\hat{j}$  then  $\hat{k}$ , as it is the case with  $\mu$ , then after any update, they will all have taken the same value. It implies that  $f_{\{\mu\}}$  has only fixed points, precisely the set  $P = \{x \in \mathbb{B}^n \mid x_{\hat{i}} = x_{\hat{j}} = x_{\hat{k}}\}.$ 

If they are updated in the order  $\hat{i}$  then  $\hat{k}$  then  $\hat{j}$ , as with  $\mu'$ , however, the situation is a bit more complex. We consider two cases, according to the number of times they are updated during a period (recall that since they belong to the same matrix, they are updated repeatedly in the same order during the substeps):

• If they are updated an odd number of times each, then automata  $\hat{i}$  and  $\hat{j}$  will take the initial value of automaton  $\hat{k}$ , and automaton

 $\hat{k}$  will take the initial value of automaton  $\hat{j}$ . In this case,  $f^{\Omega}_{\{\mu'\}}$  has the fixed points P and limit cycles of length two.

• If they are updated an even number of times each, then the reverse will occur: automata  $\hat{i}$  and  $\hat{j}$  will take the initial value of automaton  $\hat{j}$ , and automaton  $\hat{k}$  will keep its initial value. In this case,  $f^{\Omega}_{\{\mu'\}}$  has the fixed points  $Q = \{x \in \mathbb{B}^n \mid x_i = x_j\}$  which strictly contains P (*i.e.*  $P \subseteq Q$  and  $Q \setminus P \neq \emptyset$ ).

In both cases  $f_{\{\mu'\}}^{\Omega}$  has more than the fixed points P in its limit set, hence we conclude that  $f_{\{\mu\}}^{\Omega} \not\sim f_{\{\mu'\}}^{\Omega}$ . (2.2.2) Moreover, if the permutation of all matrices is circular, then we

(2.2.2) Moreover, if the permutation of all matrices is circular, then we first observe that when  $\varphi(\mu)$  and  $\varphi(\mu')$  have one block in common, they have all blocks in common (because of the circular nature of permutations), *i.e.*  $\mu \equiv_{\star} \mu'$ . Thus, under our hypothesis, we deduce that  $\varphi(\mu)$  and  $\varphi(\mu')$  have no block in common. As a consequence, there exist automata  $\hat{i}, \hat{j}$  with the property from case (2.1), namely synchronised in a block of  $\varphi(\mu)$  but never synchronised in any block of  $\varphi(\mu')$ , and the same construction terminates this proof.

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# B Identification of Theorem 2 with sequence OEIS A182666

The exponential generating function of a sequence  $(a_n)_{n\in\mathbb{N}}$  is  $f(x) = \sum_{n\geq 0} a_n \frac{x^n}{n!}$ . **Lemma 2.** The exponential generating function of  $(|\mathsf{BP}_n^0|)_{n\in\mathbb{N}}$  is  $\prod_{j\geq 1} \sum_{k\geq 0} \left(\frac{x^k}{k!}\right)^j$ .

*Proof.* We will start from the exponential generating function by finding the coefficient of  $x^n$  and proving that it is equal to  $\frac{|\mathsf{BP}_n^0|}{n!}$ , and thus that the associated sequence is  $(|\mathsf{BP}_n^0|)_{n\in\mathbb{N}}$ .

$$\prod_{j\geq 1}\sum_{k\geq 0} \left(\frac{x^k}{k!}\right)^j = \left(\sum_{k\geq 0} \frac{x^k}{k!}\right) \times \left(\sum_{k\geq 0} \frac{x^{2k}}{(k!)^2}\right) \times \left(\sum_{k\geq 0} \frac{x^{3k}}{(k!)^3}\right) \times \cdots$$
$$= \underbrace{\left(1+x+\frac{x^2}{2!}+\cdots\right)}_{j=1} \times \underbrace{\left(1+x^2+\frac{x^4}{(2!)^2}+\cdots\right)}_{j=2} \times \underbrace{\left(1+x^3+\frac{x^6}{(2!)^3}+\cdots\right)}_{j=3} \times \cdots$$

Each term of the distributed sum is obtained by associating a  $k \in \mathbb{N}$  to each  $j \in \mathbb{N}_+$ , and by doing the product of the  $\frac{1}{(k!)^j} \cdot x^{jk}$ . Thus, if  $\mathbb{N}^{\mathbb{N}_+}$  is the set of maps from  $\mathbb{N}_+$  to  $\mathbb{N}$ , we have:

$$\prod_{j\geq 1}\sum_{k\geq 0} \left(\frac{x^k}{k!}\right)^j = \sum_{m\in\mathbb{N}^{\mathbb{N}_+}} \left(\prod_{j\geq 1}\frac{1}{(m(j)!)^j}\right) \cdot x^{\sum_{j\geq 1}j\cdot m(j)}.$$

From here, to get the coefficient of  $x^n$ , we need to do the sum only on the maps m such that  $\sum_{j\geq 1} j \cdot m(j) = n$ , which just so happen to be the partitions of n, with m(j) being the multiplicity of j in the partition. Thus, the coefficient of  $x^n$  is

$$\sum_{i=1}^{p(n)} \prod_{j \ge 1} \frac{1}{(m(i,j)!)^j} = \sum_{i=1}^{p(n)} \frac{1}{\prod_{j \ge 1}^{d(i)} (m(i,j)!)^j} = \frac{|\mathsf{BP}_n^0|}{n!}.$$

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