Soutenance d'Habilitation à Diriger des Recherches

Kévin Perrot

Études de la complexité algorithmique des réseaux d'automates

Le 25 janvier 2022 devant le jury composé de :

Julio Aracena*	PR, Univ. Concepción, Chili
Olivier Bournez	PR, LIX
Nadia Creignou	PR, LIS
Emmanuel Jeandel*	PR, LORIA
Jarkko Kari*	PR, Univ. Turku, Finlande
Loïc Paulevé	CR CNRS, LaBRI
Sylvain Sené	PR, LIS

*rapporteurs

talk and next slides in English

Intro. Computational complexity of automata networks

$$\begin{aligned} & f && : \{0,1\}^n \to \{0,1\}^n \\ \equiv\quad & f_i && : \{0,1\}^n \to \{0,1\} \text{ for } i \in [n] \end{aligned}$$

Local functions $(f_i)_{i\in[n]}$ **Interaction digraph** G_f **Dynamics** $\mathscr{G}_f$

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Local functions $(f_i)_{i\in[n]}$

$n = 4$

$f_1(x) = x_1$

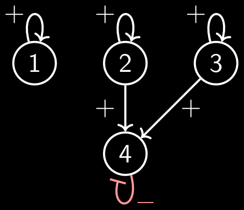
$f_2(x) = x_2$

$f_3(x) = x_3$

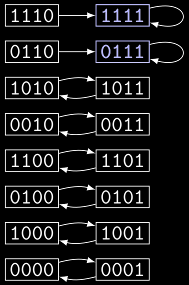
$f_4(x) = \varphi(x_1, x_2, x_3) \vee \neg x_4$

Interaction digraph G_f

$(i,j) \in G_f \iff \exists x : f_j(x + e_i) \neq f_j(x)$



Dynamics $\mathscr{G}_f$



$\varphi(x_1, x_2, x_3) = \neg[(x_1 \vee x_2) \Rightarrow \neg(x_2 \wedge x_3)] \equiv x_2 \wedge x_3$

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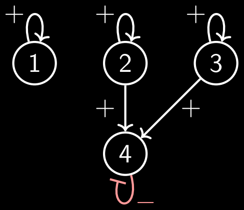

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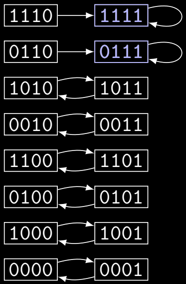

$\varphi(x_1, x_2, x_3) = \neg[(x_1 \vee x_2) \Rightarrow \neg(x_2 \wedge x_3)] \equiv x_2 \wedge x_3$

Theorem [Alon 1985]. It is NP-complete to decide whether a given f has at least one fixed point.

Theorem [Orponen 1992]. ...and counting them is #P-complete.

Remark. ...even under the promise $\Delta(G_f) \leq 2$.

Intro. Computational complexity of automata networks

Alphabets

- Boolean: $X = \{0,1\}^n$
- Uniform: $X = [\![q]\!]^n = \{0, 1, \ldots, q-1\}^n$
- Nonuniform: $X = [\![q_1]\!] \times [\![q_2]\!] \times \cdots \times [\![q_n]\!]$

Update modes

- Deterministic=Parallel: $f : X \to X$ with $\forall x, i :\ f(x)_i = f_i(x)$
- Sequential
- Block-sequential: ordered partition of $[n]$
- ...
- Asynchronous (perfect)
- Nondeterministic: $r : X \to \mathcal{P}(X)$

Gene regulation $P(G_f) \implies Q(\mathscr{G}_f)$

Outline

$[n] = \{1, 2, \ldots, n\}$
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Conclusion. Intuitive "complexity" of automata networks
Long-term perspectives

3. Encodings

An automata network as input: Boolean circuits.

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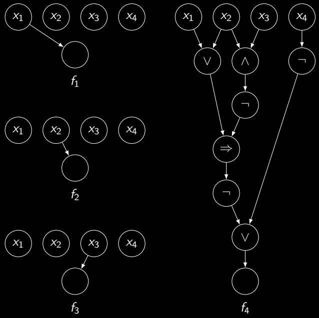
Circuits for $(f_i)_{i\in[n]}$



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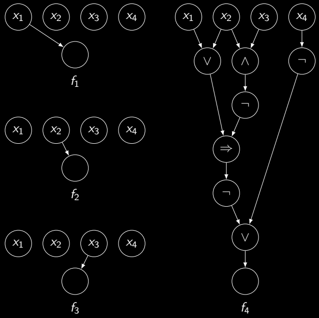

Theorem. Given f and G, does $G_f = G$? is DP-complete*,
and in P under the promise $\Delta(G_f) \leq d$ for some fixed $d \in \mathbb{N}$.
*$\mathrm{DP} = \{L_1 \cap L_2 \mid L_1 \in \mathrm{NP} \text{ and } L_2 \in \mathrm{coNP}\}$

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Local functions $(f_i)_{i\in[n]}$

$$n = 1$$

$$q = 16$$

denote x_i the bit of weight 2^{n-i} in integer $x \in [\![16]\!]$[1]

$$f_1(x) = 8 \cdot x_1 + 4 \cdot x_2 + 2 \cdot x_3 + (\varphi(x_1, x_2, x_3) \vee \neg x_4)$$

$$\varphi(x_1, x_2, x_3) = \neg[(x_1 \vee x_2) \Rightarrow \neg(x_2 \wedge x_3)] \equiv x_2 \wedge x_3$$

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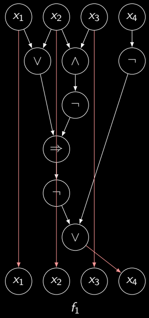

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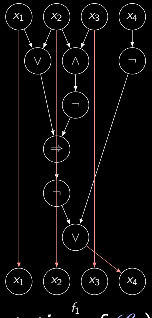

Remark. From n to 1 automaton quickly (*succinct graph representation* of $\mathscr{G}_f$).
$\implies$ Problems on fixed/bounded alphabets to enforce interactions.

Convention. If $\log_2(q) \notin \mathbb{N}$ then checking validity (of outputs) is coNP-complete $\implies$ consider outputs modulo q.

Outline

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6. First-Order questions on $\mathscr{G}_f$: given f

Metatheorem. Given f, any nontrivial property of $\mathscr{G}_f$ is hard to check.

Property "Graph FO".

Nontrivial.

Hard.

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Property "Graph FO". $\neg, \wedge, \vee, \Rightarrow, \exists, \forall$ on signature $\{=, \rightarrow\}$.

$$\exists x \forall y : y \rightarrow x$$

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$\exists x : x \to x$	Fixed point
$\exists x_1, x_2, x_3 : (x_1 \to x_2) \wedge (x_2 \to x_3) \wedge (x_3 \to x_1)$	3-cycle
$\forall x_1, x_2, y_1, y_2 : [(x_1 \to y_1) \wedge (x_2 \to y_2)] \Rightarrow (y_1 = y_2)$	Constant
$\forall x_1, x_2, y : [(x_1 \to y) \wedge (x_2 \to y)] \Rightarrow (x_1 = x_2)$	Injectivity

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ψ-dynamics
Input : the circuits of an automata network f.
Ouput : does $\mathscr{G}_f \models \psi$?

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1. Reduction from **SAT** requires N, S such that:

$$N \sqcup \cdots \sqcup \; N \; \sqcup \cdots \sqcup N \not\models \psi$$
$$N \sqcup \cdots \sqcup \; S \; \sqcup \cdots \sqcup N \models \psi$$

On each configuration the network evaluates φ, and:

- not satisfied: produces a copy of N,
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2. Model theory...
   - Finite $\equiv_m$ of structures ($\mathscr{G}_f$)
   - Ehrenfeucht-Fraïssé games
   - Hanf locality

   ...gives B, N, S and $\sqcup_1, \sqcup_2, \sqcup_3$ and $(\models, \not\models)$-symmetry.

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Extensions and perspectives.

$[\![q]\!]$

Nondet

MSO

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Extensions and perspectives.

$[\![q]\!]$ On fixed alphabet ?
Almost no control on $|B|, |N|, |S|$, but $\mathscr{G}_f$ has q^n configurations...
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MSO Monadic Second Order logic ?
Connectivity...

Enrich the signature $\{=, \rightarrow\}$ to distinguish configurations ?
Some P-complete problems...

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Results on deterministic Boolean automata networks $f : \{0,1\}^n \to \{0,1\}^n$

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$\mathfrak{P}^{\mathtt{max}}(G) =$ maximum number of fixed points on G

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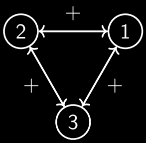
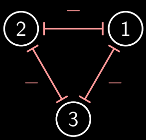


$\mathfrak{P}^{\mathtt{max}}(G) = 2$
$\mathfrak{P}^{\mathtt{min}}(G) = 2$
8 networks



$\mathfrak{P}^{\mathtt{max}}(G) = 3$
$\mathfrak{P}^{\mathtt{min}}(G) = 1$
8 networks

1 2 3	∧∧∧	∨∧∧	∨∨∧	∨∨∨
000	000	000	000	000
001	000	100	110	110
010	000	100	100	101
011	100	100	110	111
100	000	000	010	011
101	010	110	110	111
110	001	101	111	111
111	111	111	111	111

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000	111	111	111	111
001	001	101	111	111
010	010	110	110	111
011	000	000	010	011
100	100	100	110	111
101	000	100	100	101
110	000	100	110	110
111	000	000	000	000

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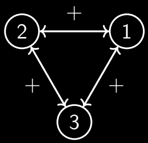

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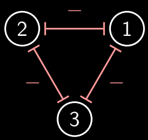

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8 networks

On n automata, there are 2^{n2^n} Boolean networks and $\underset{\{0,+,-,\pm\}}{\underset{\uparrow}{4}}{}^{n^2}$ signed digraph

7. Asymptotic dynamics $\mathscr{G}_f$ II: given G_f

Results on deterministic Boolean automata networks $f : \{0,1\}^n \to \{0,1\}^n$

$$\mathfrak{P}^{\texttt{max}}(G) = \text{maximum number of fixed points on } G$$
$$\mathfrak{P}^{\texttt{min}}(G) = \text{minimum number of fixed points on } G$$

Theorem [BDPR 2019 2022+]. Given a signed digraph G, deciding whether...

<table>
<tr><th>Problem</th><th>$k = 1$</th><th>$k \geq 2$</th><th>k given in input</th></tr>
<tr><td rowspan="2">$\mathfrak{P}^{\texttt{max}}(G) \geq k$</td><td rowspan="2">P</td><td rowspan="2">NP-complete</td><td>NEXPTIME-complete</td></tr>
<tr><td>$\mathrm{NP}^{\#\mathrm{P}}$-complete if $\Delta(G) \leq d$</td></tr>
<tr><td rowspan="2">$\mathfrak{P}^{\texttt{min}}(G) < k$</td><td colspan="3">NEXPTIME-complete</td></tr>
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</table>

7. Asymptotic dynamics $\mathscr{G}_f$ II: given G_f

Theorem. Given a signed digraph G, deciding whether $\mathfrak{P}^{\mathtt{max}}(G) \geq k$ is in P for $k = 1$, and NP-complete for any fixed $k \geq 2$.

Proof sketch. $k = 1$ $k = 2$

Fixed points

$\heartsuit$

Positive cycles
(even number of $-$ arcs)

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Proof sketch. $\boxed{k = 1}$ $k = 2$

- Lemma [$\Longrightarrow$ by Aracena 2008].
  $\mathfrak{P}^{\mathtt{max}}(G) \geq 1 \iff$ each initial strongly connected component of G has a positive cycle.

- Theorem [Robertson, Seymour, Thomas 1999; McCuaig 2004]. ⚠
  We can decide in polytime whether G has a positive cycle.

7. Asymptotic dynamics $\mathscr{G}_f$ II: given G_f

Theorem. Given a signed digraph G, deciding whether $\mathfrak{P}^{\mathtt{max}}(G) \geq k$ is in P for $k = 1$, and NP-complete for any fixed $k \geq 2$.

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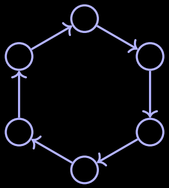
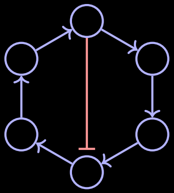
Basic observation.



2 fixed points



1 fixed point

The idea is to "neutralize" such negative chords by satisfying φ.

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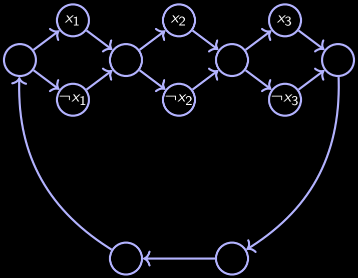

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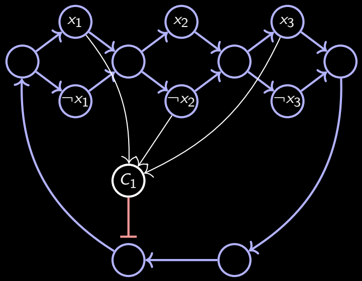

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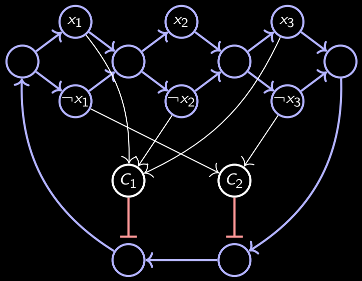

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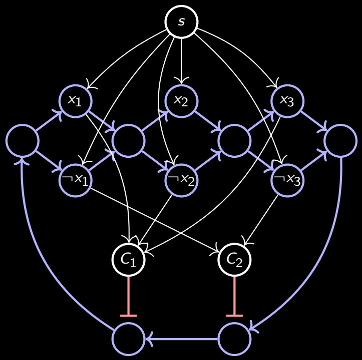

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In order to get two fixed points $x \neq y$:

1. Each clause must be "neutralized" by a literal equal in both fixed points.

But never $x_i = y_i$ and $\neg x_i = \neg y_i$ because:

2. Distinct fixed points must differ on a positive cycle.

7. Asymptotic dynamics $\mathscr{G}_f$ II: given G_f

Extensions and perspectives.

New...

7. Asymptotic dynamics $\mathscr{G}_f$ II: given G_f

Extensions and perspectives.

New... point of view on a classical direction $P(G_f) \implies Q(\mathscr{G}_f)$
Many further questions:

- Limit cycles ?
- $|\Omega_f|$?
- Unsigned G_f ?
- Alphabet $[\![q]\!]$?
- Other update modes ?

Outline

$[n] = \{1, 2, \ldots, n\}$
$[\![q]\!] = \{0, 1, \ldots, q-1\}$
$f_i : \{0,1\}^n \to \{0,1\}$ for $i \in [n]$
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8. Update modes

Block-sequential = ordered partition of $[n]$
(parallel within each block, and blocks sequentialy)

$f_1(x) = \neg x_2$
$f_2(x) = x_1 \vee \neg x_3$
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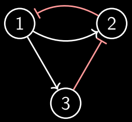
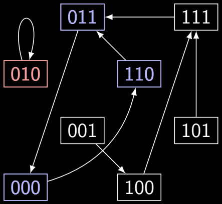
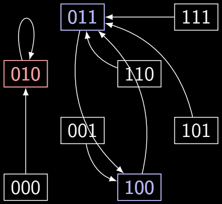


$\beta = (\{1, 2, 3\})$



$\beta' = (\{2\}, \{1, 3\})$



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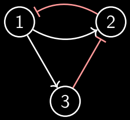

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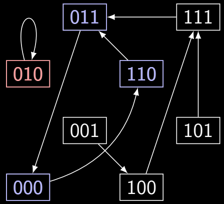

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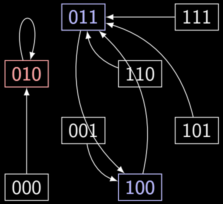

Remark. Block-seq.: fixed points are invariant, limit cycles are not.
Remark. From f and β we can compute $f' = f^{[\beta]}$ in polytime.

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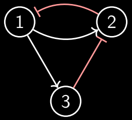

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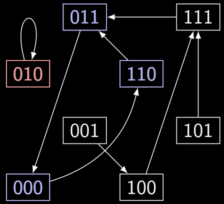

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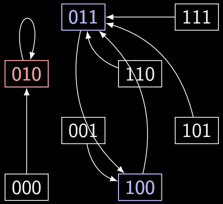

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Theorem [Aracena et al. 2013]. Fix $k \geq 2$. Given f, deciding whether $\exists \beta$ such $\mathscr{G}_{f^{[\beta]}}$ has a limit cycle of length k, is NP-complete.

Theorem [BGMPS 2021]. Fix $k \geq 2$. Given f, deciding whether $\exists \beta$ such $\mathscr{G}_{f^{[\beta]}}$ has no limit cycle of length k, is NP^{NP}-complete.

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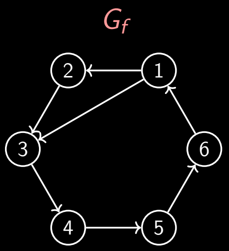

We have the same $\mathscr{G}_{f[\beta]}$ for any β among:

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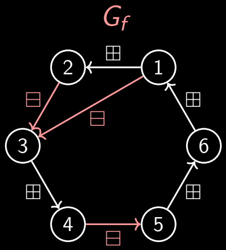

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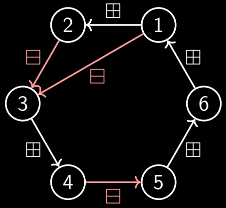

An update digraph is a $\{\boxplus, \boxminus\}$-edge-labeling of G_f.

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Same update digraph $\implies$ Same dynamics.

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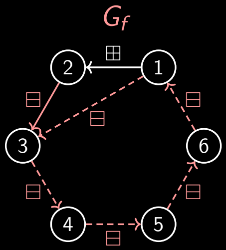

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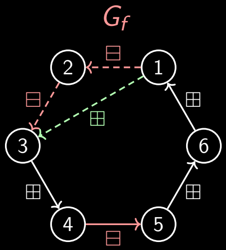

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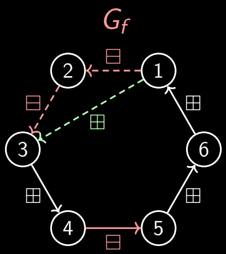

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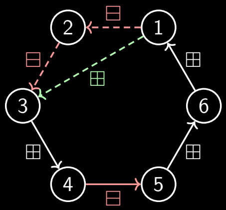

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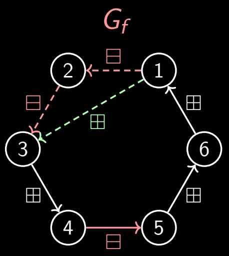

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A fun combinatorial problem:
- $n! \Leftrightarrow$ tournament
- $3^n - 2^{n+1} + 2$ on periodic ECAs
- $\mathcal{T}_{\bar{G}}(2, 0)$ on acyclic
- impossible to get 5 ?

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Long-term perspectives

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Intuitive "complexity" of automata networks

- Fixed or bounded alphabets to enforce interactions
  Succinct graph representation
- Bounded degree to enforce some locality
  May decrease the computational complexity
- Update modes offer a vast world (caution with encodings)

$\Longrightarrow$ A systematic study ? [Paulevé Sené] poset of update modes
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  on f_i from some h_i of domain $X' \subsetneq X$
  on G_f mandatory and/or forbidden arcs, graph families
  on $\mathscr{G}_f$ number of fixed points, structural properties
- Model theory to state metatheorems
  questions on $\clubsuit$ given $\spadesuit$ as input, with $\clubsuit, \spadesuit \in \{f, G_f, \mathscr{G}_f\}$

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Thank you !