# First-Order Logic with Reachability Predicates on Infinite Systems

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**Abstract**

This paper focuses on first-order logic (FO) extended by reachability predicates such that the expressiveness and hence decidability properties lie between FO and monadic second-order logic (MSO): in FO(R) one can demand that a node is reachably from another by some sequence of edges, whereas in FO(Reg) a regular set of allowed edge sequences can be given additionally. We study FO(Reg) logic in infinite grid-like structures which are important in verification. The decidability of logics between FO and MSO on those simple structures turns out to be sensitive to various parameters. Furthermore we introduce a transformation for infinite graphs called set-based unfolding which is based on an idea of Lohrey and Ondrusch. It allows to transfer the decidability of MSO to FO(Reg) onto the class of transformed structures. Finally we extend regular ground tree rewriting with a skeleton tree. We show that graphs specified in this way coincide with those expressible by vertex replacement and product operators. This allows to extend decidability results of Colcombet for FO(R) to those graphs.

**Keywords and phrases** First-Order Logic, Reachability, Infinite Grid, Structure Transformation, Unfolding, Ground Tree Rewriting, Vertex Replacement with Product

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## 1 Introduction

The general task in verification is to check whether an infinite graph structure satisfies a given specification, which is usually expressed by a logical formula in the fundamental first-order (FO) or monadic second-order (MSO) logic. These logics are well-studied and over the years many classes of infinite structures have been identified where the theory of one of these logics is decidable. The most prominent examples are automatic structures [13, 15, 2] like Presburger arithmetic $(\mathbb{N}, 0, 1, +)$ for FO, and natural numbers with successor $(\mathbb{N}, \mathrm{S})$ by Büchi [3] and the binary tree $(\{0,1\}^*, \mathrm{S}_1, \mathrm{S}_2)$ by Rabin [20] for MSO. In verification one often specifies properties dealing with reachability in graph structures. These cannot be expressed in FO logic. One could switch to MSO logic which comes at the expense of worse decidability properties. To overcome this problem we consider FO logic extended by reachability predicates. In FO(R) logic these predicates express that some element is reachable from another by using a subset of the available edge relations. In FO(Reg) logic one can express reachability by sequences of edge relations which form a regular language. Both logics lie strictly between FO and MSO according to their expressiveness and decidability.

In Section 3 we mainly study the decidability of FO(Reg) logic on infinite grids. Although they look simple one can express strong properties by formulas which makes them interesting for verification. Furthermore FO logic is known to be decidable whereas MSO logic is undecidable. We consider an $n$-dimensional grid to be a structure having $\mathbb{N}^n$ as domain and a successor and predecessor relation for each dimension. The decidability of FO(Reg) logic turns out to be sensitive to the various parameters, which is mostly inherited from important, closely related formalisms like Petri nets, vector addition systems, pushdown automata, register machines, and logic over arithmetic. Furthermore we extend studies of


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Wöhrle and Thomas [21] about FO logic extended by an operator for transitive closure, which reveals interesting parallels to the situation of FO(Reg) logic.

A generic way of generating structures having some particular decidable logic is by structure transformation. A standard transformation is interpretation where a new structure is defined by specifying its domain and relations by formulas. It preserves the decidability of FO or MSO logic, respectively, when the formulas come from this logic. Another approach for graph structures is unfolding where the new structure is the tree of all finite paths starting in a given initial vertex in the original structure. This transformation preserves the decidability of MSO logic [10]. In Section 4 we define set-based unfolding which is an abstraction of unfolding. It does not preserve the decidability of full MSO logic but FO(Reg) logic is decidable anyhow. The idea for this transformation goes back to a construction of Lohrey and Ondrusch [18]. Thus set-based unfolding is such a type of transformation, which maps the decidability of one particular logic to the decidability of a weaker logic. Another example of such a transformation is finite set interpretation by Colcombet and Löding [9] which maps decidability of weak MSO logic to FO logic in the resulting structure.

Lastly in Section 5 we extending an equivalence result for a class of graphs where FO(R) logic is decidable. The first way to describe this class is by regular ground tree rewriting (RGTR) systems, where the domain is given as a set of finite trees and edge relations are induced by rewriting rules which replace a subtree by another. The decidability of FO(R) logic on RGTR graphs was shown by a transformation to tree automata and tree transducers [11]. The second formalism is completely differently motivated and describes graphs by operations on colored graphs: the vertex replacement and product (VRP) operators. Usually those operators are aligned in a (possibly infinite) tree, called the VRP tree, and specify the graph which is its least fixed point. Colcombet [7, 8] showed RGTR graphs to be equivalent to graphs represented by regular VRP trees. He furthermore showed the FO(R) theory to be decidable for graphs of VRP trees with decidable MSO theory. With this motivation we extend RGTR to regular skeleton ground tree rewriting (RSGTR) by adding a usually infinite skeleton tree and obtain the equivalence to graphs of arbitrary VRP trees. The transformation furthermore preserves decidability of MSO logic of the VRP tree and skeleton tree, which makes the FO(R) theory of RSGTR graphs decidable if the skeleton has a decidable MSO theory.

## 2 Preliminaries

We use the following notations for intervals of integers: $\mathbb{Z} := (-\infty, \infty)$ and $\mathbb{N} := [0, \infty)$. By $\wp(S)$ we denote the powerset of a set $S$. Let $\Sigma$ be an alphabet, i.e., a finite set of symbols, then $\Sigma^*$ is the set of words over $\Sigma$, i.e., finite sequences of its symbols, and a language is a set of words. The number of occurrences of a symbol $\sigma \in \Sigma$ in a word $w$ is $|w|_\sigma \in \mathbb{N}$, the length of $w$ is $|w| \in \mathbb{N}$ and the empty word $\epsilon$ is the word of length $|\epsilon| = 0$. We assume the reader to be familiar with regular languages, i.e., the languages specified by regular expressions or equivalently by finite automata.

A structure $\mathcal{A} = \big(A, (f_i)_{i\in\mathfrak{f}}, (R_i)_{i\in\mathfrak{R}}\big)$ consists of a (possibly infinite) domain $A$, functions $f_i : A^{n_i} \to A$ and relations $R_i \subseteq A^{m_i}$ each of arity $n_i$ and $m_i$, respectively. A *relational* structure has only relations, and it is a *graph structure* if all relations are of arity 1 or 2. We consider only structures with finitely many functions and relations. An equivalence relation $\sim \subseteq A \times A$ is a congruence on a relational structure $\mathcal{A} = \big(A, (R_i)_{i\in\mathfrak{R}}\big)$ if $R_i(x_1, \dots, x_{m_i}) \Leftrightarrow R_i(y_1, \dots, y_{m_i})$ for all $R_i$ and $x_1 \sim y_1, \dots, x_{m_i} \sim y_{m_i}$. Its quotient $\mathcal{A}/\!\sim\; = \big(A', (R'_i)_{i\in\mathfrak{R}}\big)$ is defined as $A' := \big\{ [x] \;\big|\; x \in A \big\}$ and $\big([x_1], \dots, [x_{m_i}]\big) \in R'_i :\Leftrightarrow (x_1, \dots, x_{m_i}) \in R_i$ with

$[x] := \{ y \mid y \sim x \}$.

With first-order (FO) logic one can specify properties of a structure by using terms of variables $(x, y, z, \dots)$ and functions $(f_i)$, comparing terms $(=, R_i)$, quantifying elements $(\exists, \forall)$ and its boolean combinations $(\neg, \wedge, \vee, \rightarrow)$. Monadic second-order (MSO) logic additionally allows quantification over element sets $(X, Y, Z, \dots)$ and using them as unary relations. Weak MSO (WMSO) logic is a variant which only quantifies over finite sets. The theory of a logic and a structure is the set of formulas of that logic which have no free variables and hold in the structure. The property that an element can be reached from another in some graph structure can be expressed in MSO and WMSO logic but not in FO logic. For a graph structure $\mathcal{G} = \big(V, (P_\gamma)_{\gamma\in\Gamma}, (E_\sigma)_{\sigma\in\Sigma}\big)$ we define FO(Reg) logic to be the extension of FO logic by regular reachability predicates $\mathsf{reach}_L(x, y)$, for variables $x, y$ and a regular language $L \subseteq \Sigma^*$ (finitely represented by a regular expression or finite automaton), meaning that position $y$ can be reached from position $x$ by some sequence of edges $E_{\sigma_1}, \dots, E_{\sigma_n}$ such that $\sigma_1 \cdots \sigma_n \in L$. Let FO(R) logic be its restriction to simple reachability predicates $\mathsf{reach}_{\Sigma_0^*}(x, y)$ with $\Sigma_0 \subseteq \Sigma$. Reachability predicates can be expressed in MSO and WMSO logic by induction on the operators of a regular expression for the language of the predicate. It uses the fact that the transitive closure is expressible in MSO and WMSO. The expressiveness of the above logics increases as follows:

$$\text{FO} \quad \leq \quad \text{FO(R)} \quad \leq \quad \text{FO(Reg)} \quad \leq \quad \begin{cases} \text{MSO} \\ \text{WMSO} \end{cases}$$

Note that WMSO is usually a sublogic of MSO since finiteness is MSO-definable in most standard structures. FO(Reg) logic over $\mathcal{G}$ can furthermore be identified with FO logic over $\big(V, (P_\gamma)_{\gamma\in\Gamma}, (E_L)_{L\subseteq\Sigma^*, L \text{ regular}}\big)$, i.e., reachability is considered only with respect to the edge relations instead of arbitrary FO-definable relations (analogous for FO(R) logic).

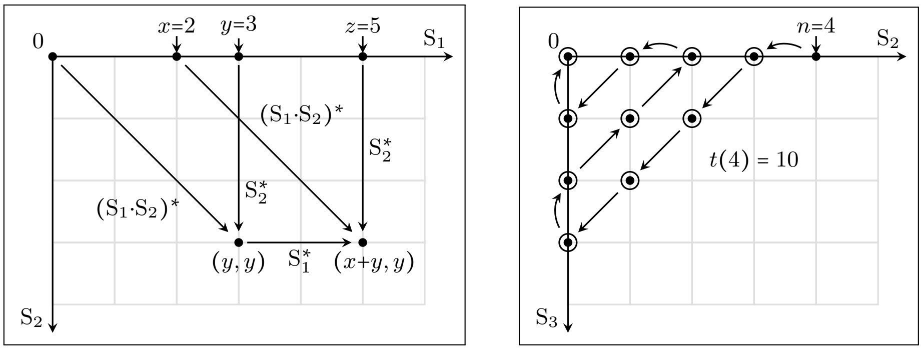
## 3 Reachability in Infinite Grids

We consider the $n$-dimensional infinite grid $\mathcal{N}^n := \big(\mathbb{N}^n, (\mathrm{S}_i, \bar{\mathrm{S}}_i)_{1\leq i\leq n}\big)$ to be the $n$-th product of the natural numbers $\mathcal{N} = (\mathbb{N}, \mathrm{S}, \bar{\mathrm{S}})$ with successor and predecessor, i.e., $\mathrm{S}_i$ and $\bar{\mathrm{S}}_i$ are the successor and predecessor relation of dimension $i$. The MSO theory is known to be decidable for $\mathcal{N}$ [3] but undecidable for its products. By using Büchi's result about the decidability of Presburger arithmetic, i.e., the FO theory of $(\mathbb{N}, 0, 1, +)$, one can easily see that the FO(R) theory is decidable for grids $\mathcal{N}^n$ of any dimension $n$. For this reason we study the situation for FO(Reg) logic, which reveals an interesting phenomenon.

▸ **Theorem 1.** *The FO(Reg) theory of $\mathcal{N}^2$ is decidable.*

**Proof.** We reduce this theory to Presburger arithmetic. To this end we transform a given FO(Reg) formula over $\mathcal{N}^2$ into an equivalent Presburger formula by interpreting each grid position $x = (x_1, x_2) \in \mathbb{N}^2$ as numbers $x_1, x_2 \in \mathbb{N}$. Then the standard FO operators can be transformed straightforward. It remains to express a reachability predicate $\mathsf{reach}_L(x, y)$ as Presburger formula, which we will do by use of vector addition systems with states (VASS).

A 2-dimensional VASS $\mathcal{V} = (Q, \Delta)$ consists of a finite state set $Q$ and a finite transition relation $\Delta \subseteq Q \times \mathbb{Z}^2 \times Q$. For states $p, q \in Q$ we define the reachability relation $R_{p,q} \subseteq (\mathbb{N}^2)^2$ consisting of all $(x, y) \in (\mathbb{N}^2)^2$ such that there exist sequences $z_0, \dots, z_k \in \mathbb{N}^2$ and $(q_0, d_0, q_1), \dots, (q_{k-1}, d_k, q_k) \in \Delta$ with $x = z_0$, $z_k = y$, $p = q_0$, $q_k = q$ and $z_i = z_{i-1} + d_i$ for all $i \in \{1, \dots, k\}$. For a reachability predicate $\mathsf{reach}_L(x, y)$ with language $L = L(\mathcal{A})$ of some automaton $\mathcal{A} = \big(Q, \{\mathrm{S}_1, \bar{\mathrm{S}}_1, \mathrm{S}_2, \bar{\mathrm{S}}_2\}, \delta, q_0, F\big)$ we define the VASS $(Q, \Delta)$ with $(p, e_i, q) \in \Delta$ iff




**(a)** Geometric addition $x + y = z$

**(b)** Geometric multiplication simulated by the function $t(n) \coloneqq n \cdot (n+1) \div 2$

**Figure 1** Arithmetic in the grid by: simulating addition and multiplication

$\delta(p, \mathrm{S}_i) = q$, and $(p, -e_i, q) \in \Delta$ iff $\delta(p, \bar{\mathrm{S}}_i) = q$ where $e_1 \coloneqq (1,0)$ and $e_2 \coloneqq (0,1)$. It is obvious from the construction, that for $x, y \in \mathbb{N}^2$ in the grid $\mathsf{reach}_L(x,y)$ holds iff $(x,y) \in R_{q_0,q_f}$ for some $q_f \in F$. Now we can make use of a result from Leroux and Sutre [16], stating that for any two states $p,q$ of a 2-dimensional VASS the reachability relation $R_{p,q} \subseteq (\mathbb{N}^2)^2$ is semi-linear (when identifying $(\mathbb{N}^2)^2$ with $\mathbb{N}^4$), i.e., a finite union of linear sets. Hence, $\bigcup_{q_f \in F} R_{q_0,q_f}$ is the relation defined by $\mathsf{reach}_L(x,y)$, which is still semi-linear (over $\mathbb{N}^4$). This finishes the proof since semi-linear sets are effectively equivalent to the sets definable in Presburger arithmetic [12]. ◂

If we consider the simpler model of the grid $\mathcal{N}_+^n = \left(\mathbb{N}^n, (\mathrm{S}_i)_{1 \le i \le n}\right)$ with only successor relations $S_i$, then the FO(Reg) theory is decidable for any dimension. This can be proven similarly to the above theorem by reducing a reachability predicate $\mathsf{reach}_L(x,y)$ to its Parikh image $\left\{ (|w|_{\mathrm{S}_1}, \dots, |w|_{\mathrm{S}_n}) \;\middle|\; w \in L \right\} \subseteq \mathbb{N}^n$, i.e., the tuples of occurrences of each symbol in words of $L$, which is effectively semi-linear for any $n$ [19]. On the other hand the proof of Theorem 1 cannot be extended to dimension 3 as in this case the semi-linearity is not present any longer [14]. The next result shows the sharpness of Theorem 1.

▸ **Theorem 2.** *The FO(Reg) theory of $\mathcal{N}^3$ is undecidable.*

**Proof.** We reduce the FO arithmetic, i.e., the FO theory of $(\mathbb{N}, 0, 1, +, \cdot)$, which is known to be undecidable, to the considered theory. Thus we transform a given FO formula over the arithmetic into an equivalent FO(Reg) formula over $\mathcal{N}^3$ by encoding a number $n \in \mathbb{N}$ as grid position $(n,0,0) \in \mathbb{N}^3$. W.l.o.g. we treat the arithmetic as relational, i.e., with relations $0, 1 \subseteq \mathbb{N}^1$ and $+, \cdot \subseteq \mathbb{N}^3$. It is easy to transform the standard FO operators as well as the relations 0 and 1. Thus only the relations + and $\cdot$ are remaining.

The addition $x + y = z$ can be defined geometrically in the grid as motivated in Fig. 1a by finding intersection points along horizontal, vertical and diagonal lines:

$$\begin{aligned}\psi_+(x,y,z) \;\coloneqq\; \exists y', z' \Big( & \mathsf{reach}_{(\mathrm{S}_1 \cdot \mathrm{S}_2)^*}(0, y') \wedge \mathsf{reach}_{\mathrm{S}_2^*}(y, y') \wedge \\ & \mathsf{reach}_{(\mathrm{S}_1 \cdot \mathrm{S}_2)^*}(x, z') \wedge \mathsf{reach}_{\mathrm{S}_2^*}(z, z') \wedge \mathsf{reach}_{\mathrm{S}_1^*}(y', z') \Big).\end{aligned}$$

We reduce the multiplication to addition and the triangle function $t(n) \coloneqq n \cdot (n+1) \div 2$ since $x \cdot y = z$ iff $t(x+y) = t(x) + t(y) + z$. Figure 1b geometrically motivates $t(n) = \left|\left\{ (i,j) \in \mathbb{N}^2 \mid i + j < n \right\}\right|$ as the number of positions in the triangle below $(n,0)$ in the plane. It further shows a path along the counterdiagonals with length exactly $t(n)$. To lift the input from $(n,0,0)$ to the starting point $(0,n,0)$ in the plane of the second and third dimension, we have to swap the position of the input $n \in \mathbb{N}$, which is done by a path of the language $L' \coloneqq (\bar{\mathrm{S}}_1 \cdot \mathrm{S}_2)^*$. Then the counterdiagonal path can be described by the language

$$L'' \coloneqq \Big( (\mathrm{S}_1 \cdot \bar{\mathrm{S}}_2) \cdot (\mathrm{S}_1 \cdot \bar{\mathrm{S}}_2 \cdot \mathrm{S}_3)^* + (\mathrm{S}_1 \cdot \bar{\mathrm{S}}_3) \cdot (\mathrm{S}_1 \cdot \mathrm{S}_2 \cdot \bar{\mathrm{S}}_3)^* \Big)^*$$

where the first dimension is used to count the length of the path. Now we can define $t(n)$ to be the maximal first component that is reachable by $L \coloneqq L' \cdot L''$ from $(n,0,0)$:

$$\psi_t(x,y) \;\coloneqq\; \mathsf{reach}_L(x,y) \wedge \forall y' \Big( \mathsf{reach}_L(x,y') \to \mathsf{reach}_{(\mathrm{S}_1 + \bar{\mathrm{S}}_2 + \bar{\mathrm{S}}_3)^*}(y',y) \Big).$$

This guarantees that the path turns only at border positions, i.e., from $x = (n,0,0)$ one reaches $(0,n,0)$ by $L'$ and then $y = \big(t(n),0,0\big)$ by $L''$. For the correctness it is obvious that $n \le t(n)$ for all $n \in \mathbb{N}$, and that taking a shortcut in $L'$ or $L''$ yields a smaller result. ◂

By a reduction to the FO arithmetic, we showed the FO(Reg) theory of $\mathcal{N}^3$ to be *highly undecidable* as well: each set of the arithmetical hierarchy (which consists of the sets definable in FO arithmetic) can be reduced to it. This fact makes it surprising that the same logic is decidable in the 2-dimensional case (cf. Theorem 1) anyhow. The hardness is introduced by the limitation of natural numbers, i.e., the boundedness in one direction. One can easily show the FO(Reg) theory of the grid $\mathcal{Z}^n \coloneqq \big(\mathbb{Z}^n, (\mathrm{S}_i, \bar{\mathrm{S}}_i)_{1 \le i \le n}\big)$ to be decidable by using Parikh images again.

We end this section with a digression on $\mathrm{FO(TC)}_{(1)}$, i.e., FO logic extended by an operator for the transitive closure (TC) of $\mathrm{FO(TC)}_{(1)}$-definable binary relations. Here we consider two variants which are powerful enough: $\mathrm{FO(TC)}^1_{(1)}$ is FO logic with TC only for FO-definable relations, and $\mathrm{FO(TC)}^2_{(1)}$ is FO logic with TC only for $\mathrm{FO(TC)}^1_{(1)}$-definable relations, i.e., the TC operator can not be nested, or at most once, respectively. Their expressiveness stays below MSO and WMSO on grid structures (without proof):

$$\mathrm{FO} \;\le\; \mathrm{FO(R)} \;\le\; \left\{ \begin{array}{c} \mathrm{FO(Reg)} \\ \mathrm{FO(TC)}^1_{(1)} \end{array} \right\} \;\le\; \mathrm{FO(TC)}^2_{(1)} \;\le\; \mathrm{FO(TC)}_{(1)} \;\le\; \left\{ \begin{array}{l} \mathrm{MSO} \\ \mathrm{WMSO} \end{array} \right.$$

Wöhrle and Thomas [21] studied the decidability of these logics on the 2-dimensional grid. They showed the $\mathrm{FO(TC)}^1_{(1)}$ theory of $\mathcal{N}^2$ to be decidable by a reduction to Presburger arithmetic, and the $\mathrm{FO(TC)}^2_{(1)}$ theory of $\mathcal{N}^2$ to be highly undecidable by reducing FO arithmetic. By copying the proof of Theorem 2 one can furthermore show the $\mathrm{FO(TC)}^1_{(1)}$ theory of $\mathcal{N}^3$ to be highly undecidable as well. It is interesting to observe the same phenomenon that the logic changes from being decidable to highly undecidable between dimension 2 and 3.

## 4 Set-Based Unfolding

The unfolding (or unraveling) $\mathsf{Unf}_{v_0}(\mathcal{G})$ of a graph structure $\mathcal{G}$ is a tree, the vertices of which are finite paths of $\mathcal{G}$ starting at the initial vertex $v_0$. The relations are inherited from $\mathcal{G}$: unary relations are set according to the last vertex of a path, and edge relations are used to extend paths, i.e., following an edge of the last vertex. Courcelle and Walukiewicz [10] have shown that $\mathsf{Unf}_{v_0}(\mathcal{G})$ preserves the decidability of MSO logic of $\mathcal{G}$ for any initial vertex $v_0$ that is MSO-definable in $\mathcal{G}$.

We present a model-theoretic structure transformation which is similar to the unfolding and preserves some logic decidability too. Instead of having finite paths as domain, we abstract each such path $v_0 E_{\sigma_1} v_1 \dots E_{\sigma_n} v_n$ to the *trace* $\big(v_n, \{v_0, v_1, \dots, v_n\}\big)$, in which $v_n$ is the last vertex and $\{v_0, v_1, \dots, v_n\}$ is the (finite) set of visited vertices of the path:

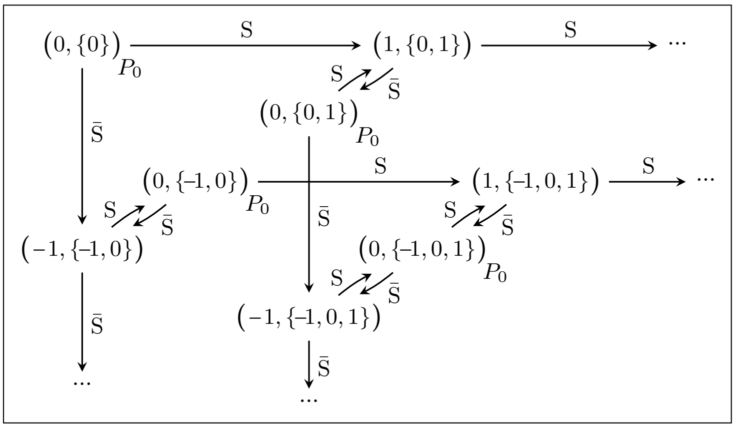



**Figure 2** Set-based unfolding $\mathsf{SetUnf}_0(\mathcal{Z})$ of the structure $\mathcal{Z} = (\mathbb{Z}, P_0, \mathrm{S}, \bar{\mathrm{S}})$

▸ **Definition 3.** Let $\mathcal{G} = \big(V, (P_\gamma)_{\gamma\in\Gamma}, (E_\sigma)_{\sigma\in\Sigma}\big)$ be a graph structure with unary and binary relations $P_\gamma$ and $E_\sigma$, respectively. For some set of initial traces $I \subseteq V \times \wp(V)$, i.e., for each $(v, V_0) \in I$: $V_0$ is finite and $v \in V_0$, the *set-based unfolding* $\mathsf{SetUnf}_I(\mathcal{G})$ *of* $\mathcal{G}$ *from* $I$ is the graph structure $\big(V', (P'_\gamma)_{\gamma\in\Gamma}, (E'_\sigma)_{\sigma\in\Sigma}\big)$ with

1. domain $V' \subseteq V \times \wp(V)$ being the smallest set of traces which contains $I$, and for all $\sigma, v, v', V_0$ if $(v, V_0) \in V'$ and $(v, v') \in E_\sigma$ then $\big(v, V_0 \cup \{v'\}\big) \in V'$,
2. predicates $(v, V_0) \in P'_\gamma$ iff $v \in P_\gamma$, and
3. edges $\big((v, V_0), (v', V'_0)\big) \in E'_\sigma$ iff $(v, v') \in E_\sigma$ and $V'_0 = V_0 \cup \{v'\}$.

We abbreviate $\mathsf{SetUnf}_{v_0}(\mathcal{G})$ for $\mathsf{SetUnf}_{\{(v_0,\{v_0\})\}}(\mathcal{G})$ with the initial trace $(v_0, \{v_0\})$ representing some $v_0$ in $\mathcal{G}$. Note that $\mathsf{SetUnf}_{v_0}(\mathcal{G})$ may not be a tree in contrast to $\mathsf{Unf}_{v_0}(\mathcal{G})$:

▸ **Example 4** (Free group and free inverse monoid)**.** Consider the graph structure $\mathcal{Z} = (\mathbb{Z}, P_0, \mathrm{S}, \bar{\mathrm{S}})$ with unary relation for 0, successor and predecessor relation, which is isomorphic to the free group $\mathrm{FG}(\{\mathrm{S}\})$ of the singleton alphabet $\{\mathrm{S}\}$. Its set-based unfolding $\mathsf{SetUnf}_0(\mathcal{Z})$ from vertex 0 yields the structure depicted in Fig. 2, which is isomorphic to the free inverse monoid $\mathrm{FIM}(\{\mathrm{S}\})$ of the same alphabet.

▸ **Theorem 5.** *The FO(Reg) theory of a quotient* $\mathsf{SetUnf}_I(\mathcal{G})/\!\sim$ *is decidable, if the MSO theory of the graph* $\mathcal{G}$ *is decidable and the set* $I$ *of initial traces, the congruence* $\sim$*, as well as finiteness are MSO-definable in* $\mathcal{G}$*.*

**Proof.** This proof is based on one from Lohrey and Ondrusch [18]. It goes by interpretation, i.e., each FO(Reg) formula $\varphi$ over $\mathsf{SetUnf}_I(\mathcal{G})/\!\sim$ can be transformed effectively into an equivalent MSO formula $\hat{\varphi}$ over $\mathcal{G}$. Thereby each trace of $\mathsf{SetUnf}_I(\mathcal{G})$ is encoded in $\mathcal{G}$ by a tuple $(x, X)$ of a position and a set variable. Given formulas $\psi_I(x, X)$ for the initial traces, and $\psi_\sim(x, X, y, Y)$ for the congruence, we define the transformation $\hat{\varphi}$ of $\varphi$ inductively:

$$\widehat{x = y} := \psi_\sim(x, X, y, Y) \qquad \widehat{\neg\varphi} := \neg\hat{\varphi}$$
$$\widehat{P_\gamma(x)} := P_\gamma(x) \qquad \widehat{\varphi \vee \psi} := \hat{\varphi} \vee \hat{\psi}$$
$$\widehat{E_\sigma(x,y)} := \widehat{\mathsf{reach}_\sigma(x,y)} \qquad \widehat{\exists x\, \varphi} := \exists x\, \exists X\, \big(\hat{\varphi} \wedge \psi_{\mathrm{dom}}(x, X)\big)$$
$$\widehat{\mathsf{reach}_L(x,y)} := \exists y'\, \exists Y', Z\, \big(\mathsf{Reach}_L(x, y', Z) \wedge (Y' = X \cup Z) \wedge \psi_\sim(y, Y, y', Y') \wedge \psi_{\mathrm{dom}}(y', Y')\big)$$

where $\psi_{\mathrm{dom}}(x,X) := \exists y\,\exists Y,Z\,\big(\psi_I(y,Y) \wedge \mathsf{Reach}_{\Sigma^*}(y,x,Z) \wedge (X = Y \cup Z)\big)$ is the domain formula, and $\mathsf{Reach}_L(x,y,Z)$ is an extended reachability predicate stating that $y$ is reachable from $x$ by a path labeled by some word in $L$ and exactly visiting the vertices $Z$, which was shown to be MSO-definable [18] since finiteness is MSO-definable in $\mathcal{G}$. The transformation of the reachability predicate is correct since the congruence $\sim$ also applies to finite paths, and hence reachability, i.e., $(x,X)$ reaches $(y,Y)$ by some edge sequence iff $(x',X')$ reaches $(y',Y')$ by the very same sequence for all traces $(x,X) \sim (x',X'), (y,Y) \sim (y',Y')$. ◂

The main result is a simpler version of this theorem with equality as trivial congruence:

▸ **Corollary 6.** *The FO(Reg) theory of* $\mathsf{SetUnf}_{v_0}(\mathcal{G})$ *is decidable if the MSO theory of the graph* $\mathcal{G}$ *is decidable and the vertex* $v_0$*, as well as finiteness are MSO-definable in* $\mathcal{G}$*.*

This reads similar to the preservation of MSO-decidability for unfolding [10] although it is a weaker result. On the other hand Example 4 demonstrates the sharpness of Corollary 6. The structure $\mathcal{Z} = (\mathbb{Z}, P_0, \mathrm{S}, \bar{\mathrm{S}})$ has a decidable MSO theory [3] and finiteness is MSO-definable in $\mathcal{Z}$. Thus $\mathsf{SetUnf}_0(\mathcal{Z})$ has a decidable FO(Reg) theory whereas the MSO theory is undecidable (by interpretation of the infinite grid [4]). Note that the results of this section also apply to WMSO, respectively. A good usage of set-based unfolding would be the Caucal hierarchy [6], which is a strict hierarchy of graph structures obtained by alternately unfolding and MSO-interpreting the class of finite graphs[1], since all such graphs have decidable MSO and WMSO theories [6, 17].

## 5 Regular Ground Tree Rewriting with Skeleton

We are dealing with trees over a *ranked alphabet* $\Sigma$, i.e., each symbol $f \in \Sigma$ has a certain arity or rank $|f| \in \mathbb{N}$. A tree $t = f(t_1,\dots,t_{|f|})$ has a symbol $f \in \Sigma$ at its root and each $t_i$ is a tree again. We can view $t$ as a (partial) function, which maps its domain $\mathrm{dom}(t) := \{\epsilon\} \cup \bigcup_{1\le i\le|f|}\big(i\cdot \mathrm{dom}(t_i)\big) \subseteq \mathbb{N}^*$ to $\Sigma$ with $t(\epsilon) := f$ and $t(i\cdot w) := t_i(w)$ for $1 \le i \le |f|$. The subtree $t|_v$ of $t$ at a position $v \in \mathrm{dom}(t)$ is defined as $t|_v(w) = t(v\cdot w)$. A tree is infinite if its domain is infinite, and it is furthermore *regular* if it has only finitely many different subtrees. We can view $t$ also as a graph structure $\big(\mathrm{dom}(t), (E_i)_{1\le i\le|f|, f\in\Sigma}, (P_f)_{f\in\Sigma}\big)$ with $E_i := \big\{ (w, w\cdot i) \bigm| w\cdot i \in \mathrm{dom}(t)\big\}$ and $P_f := \big\{ w \bigm| t(w) = f \big\}$. $T_\Sigma$ ($T_\Sigma^{\mathsf{fin}}$) denotes the set of (finite) trees over $\Sigma$. Subsets of $T_\Sigma$ are called tree languages. Analogous to words we use automata to specify languages of finite trees. A *tree automaton* $\mathcal{A} = \big(Q, \Sigma, (\Delta_f)_{f\in\Sigma}, F\big)$ consists of a finite state set $Q$ with some accepting states $F \subseteq Q$, a finite ranked alphabet $\Sigma$ and transition relations $\Delta_f \subseteq Q \times Q^{|f|}$ for each $f \in \Sigma$. A finite tree $t \in T_\Sigma^{\mathsf{fin}}$ is in the tree language $T(\mathcal{A})$ recognized by $\mathcal{A}$ if there exists a run $\rho : \mathrm{dom}(t) \to Q$, which is accepting, i.e., $\rho(\epsilon) \in F$, and which respects $\Delta$, i.e., $\big(\rho(r), \rho(r\cdot 1), \dots, \rho(r\cdot |f|)\big) \in \Delta_f$ for each position $r \in \mathrm{dom}(t)$ with $t(r) = f$. We call $\mathcal{A}$ *bottom-up deterministic* if for all $f \in \Sigma$, $(q_1,\dots,q_{|f|}) \in Q^{|f|}$ there is at most one $q \in Q$ with $(q, q_1, \dots, q_{|f|}) \in \Delta_f$. $\mathcal{A}$ is *top-down deterministic* if $|F| = 1$ and for all $f \in \Sigma$, $q \in Q$ there is at most one $(q_1,\dots,q_{|f|}) \in Q^{|f|}$ with $(q, q_1, \dots, q_{|f|}) \in \Delta_f$. Tree languages recognizable by a bottom-up deterministic (top-down deterministic) tree automata are called *regular* (*top-down deterministic recognizable*).

A regular ground tree rewriting (RGTR) system $(T, \Sigma, A, \to)$ consists of a top-down deterministic recognizable domain $T \subseteq T_\Sigma^{\mathsf{fin}}$ and finitely many rewriting rules $L \xrightarrow{a} R$ with

[1] In [6] Caucal actually defined the hierarchy with inverse rational mappings instead of MSO interpretation, which is shown to be equivalent [5].

regular tree languages $L, R \subseteq T_\Sigma^{\mathsf{fin}}$ and label $a \in A$. It defines a graph structure with $T$ as vertices, and $a$-labeled edges between trees $t, t' \in T$ if there is some rule $L \xrightarrow{a} R$ such that $t'$ is obtained by replacing one subtree $l \in L$ in $t$ by $r \in R$. Furthermore there is a constant for each tree. Dauchet and Tison [11] have shown that the FO(R) theory is decidable for RGTR graphs $(T, \Sigma, A, \rightarrow)$ with complete domain $T = T_\Sigma^{\mathsf{fin}}$ and rules of the form $\{l\} \xrightarrow{a} \{r\}$ with only singletons. The proof uses a translation to tree transducers and tree-automatic relations, such that one can actually extend the proof to general RGTR graphs. This result cannot be extended to higher logics like FO(Reg) or $\mathrm{FO(TC)}^1_{(1)}$ since we showed these theories to be undecidable on $\mathcal{N}^3$ and grids are some of the simplest structures representable by ground tree rewriting:

▸ **Example 7** (Infinite grid). Let $(T, \Sigma, A, \rightarrow)$ be an RGTR system over the ranked alphabet $\Sigma = \{2, 1, 0_L, 0_R\}$, each symbol having the arity according to its number, with $T = \left\{ 2(1^x(0_L), 1^y(0_R)) \mid x, y \in \mathbb{N} \right\}$, labels $A = \{\mathrm{S}_1, \mathrm{S}_2\}$, and rewriting rules $0_L \xrightarrow{\mathrm{S}_1} 1(0_L)$, $0_R \xrightarrow{\mathrm{S}_2} 1(0_R)$. Its graph is isomorphic to the infinite grid $\mathcal{N}_+^2 = (\mathbb{N}^2, \mathrm{S}_1, \mathrm{S}_2)$.

An algebraically motivated way of specifying infinite graphs is *vertex replacement with product* (VRP) [7, 8] where graphs are the least fixed point of equations of operations on colored graphs. These are structures $G = \big(V, (P_c)_{c \in C}, (E_a)_{a \in A}\big)$ with (possibly infinite) domain of colored vertices $V = \biguplus_{c \in C} P_c$ and edge relations $E_a$ for a finite set $C$ of colors and $A$ of actions. The family of those graphs is called $\mathcal{G}_{A,C}$. For the following let us fix some sets actions $A$ and colors $C$. The five VRP operators on colored graphs are

1. *Constant singleton graph*: $\dot{c} : {\mathcal{G}_{A,C}}^0 \rightarrow \mathcal{G}_{A,C}$, just one vertex having color $c \in C$,
2. *Recoloring*: $[\phi] : {\mathcal{G}_{A,C}}^1 \rightarrow \mathcal{G}_{A,C}$, for some color mapping $\phi : C \rightarrow C$,
3. *Adding edges*: $[c \overset{a}{\bowtie} d] : {\mathcal{G}_{A,C}}^1 \rightarrow \mathcal{G}_{A,C}$, labeled by $a \in A$ between colors $c, d \in C$,
4. *Disjoint union*: $\oplus : {\mathcal{G}_{A,C}}^2 \rightarrow \mathcal{G}_{A,C}$, and
5. *Asynchronous product*: $\otimes_\eta : {\mathcal{G}_{A,C}}^2 \rightarrow \mathcal{G}_{A,C}$, for a function $\eta : C^2 \rightarrow C$ merging the colors[2].

To specify an infinite graph we use a (possibly infinite) term of VRP operators called *VRP tree*, i.e., a tree over the ranked alphabet $\Omega_{A,C}$ consisting of the VRP operators $\dot{c}$, $[\phi]$, $[c \overset{a}{\bowtie} d]$, $\oplus$, $\otimes_\eta$ with arities 0, 1, 1, 2, 2, respectively. The *interpretation* $[\![t]\!]$ of a VRP tree $t \in T_{\Omega_{A,C}}$ is defined as its least fixed point according to the subgraph relation[3]. This is a complete partial order with the empty graph as least element, which guarantees the existence of a unique least fixed point $[\![t]\!]$ that furthermore is equal to the supremum of the chain $[\![t]\!]_0 \subseteq [\![t]\!]_1 \subseteq \cdots$ where $[\![t]\!]_d$ is the partial interpretation up to depth $d \in \mathbb{N}$, i.e., $[\![t]\!]_0 = \bot$ (the empty graph) and $[\![f(t_1, \ldots, t_n)]\!]_{d+1} = f([\![t_1]\!]_d, \ldots, [\![t_n]\!]_d)$ with VRP operator $f \in \Omega_{A,C}$.

▸ **Example 8** (Infinite grid). Let $A = \{\mathrm{S}_1, \mathrm{S}_2\}$, $C = \{0, 1, 2\}$, and the VRP tree $t$ as follows (depicted in Fig. 3):

$$t \;:=\; t_1 \otimes_{[(c,d) \mapsto 0]} t_2, \qquad t_i \;:=\; [0 \overset{\mathrm{S}_i}{\bowtie} 1]\Big(\dot{0} \oplus \left[\begin{smallmatrix} 0 \mapsto 1 \\ 1 \mapsto 2 \\ 2 \mapsto 2 \end{smallmatrix}\right] t_i\Big) \quad \text{for } i \in \{1, 2\}.$$

The interpretation $[\![t]\!]$ of $t$ is isomorphic to $\mathcal{N}_+^2 = (\mathbb{N}^2, \mathrm{S}_1, \mathrm{S}_2)$ when ignoring colors.

Colcombets main results are, that interpretations of regular VRP trees are effectively equivalent to RGTR graphs (up to isomorphism and color removal), and that the FO(R) theory of an interpretation is decidable if the VRP tree has a decidable MSO theory [7]. We

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[2] The asynchronous product $\otimes_\eta$ has a fixed function $\eta$ in [7]; and is called $\square_\eta$ in [8].

[3] $\big(V, (P_c)_{c \in C}, (E_a)_{a \in A}\big) \subseteq \big(V', (P'_c)_{c \in C}, (E'_a)_{a \in A}\big)$ if $V \subseteq V'$, $E_a \subseteq E'_a$, and $P_c \subseteq P'_c$ for each $a \in A, c \in C$.

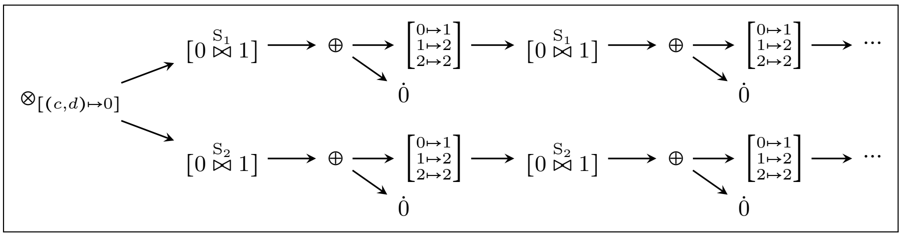


**Figure 3** VRP tree defining the infinite grid $\mathcal{N}_+^2 = (\mathbb{N}^2, \mathrm{S}_1, \mathrm{S}_2)$

are going to remove the regularity demand from the equivalence result by making RGTR as powerful as VRP trees in general. To this end we equip RGTR with a (usually infinite) tree, which functions as a skeleton for the specification of the domain and the rewriting rules. This concept is based on the *overlay* $t\|_s$ of trees $t : \mathrm{dom}(t) \to \Sigma$ and $s : \mathrm{dom}(s) \to \Gamma$ with

$$t\|_s : \ \mathrm{dom}(t) \to \Sigma\|_\Gamma, \qquad t\|_s(w) \ := \begin{cases} \big(t(w), s(w)\big) & \text{if } w \in \mathrm{dom}(s), \\ \big(t(w), \bot\big) & \text{otherwise} \end{cases}$$

with *overlay alphabet* $\Sigma\|_\Gamma := \Sigma \times \big(\Gamma \uplus \{\bot\}\big)$ of rank $|(f,g)| := |f|$. We write $T\|_s := \big\{\, t\|_s \;\big|\; t \in T \,\big\}$.

▸ **Definition 9.** A *regular skeleton ground tree rewriting* (RSGTR) system $(s, \Gamma, T, \Sigma, A, \to)$ consists of a *skeleton* $s \in T_\Gamma$, i.e., a tree over the ranked alphabet $\Gamma$, such that $(T, \Sigma\|_\Gamma, A, \to)$ forms an RGTR system. The graph structure it defines is the graph of the RGTR system $(T, \Sigma\|_\Gamma, A, \to)$ restricted to $T_\Sigma^{\mathsf{fin}}\|_s$, i.e., trees where the overlaid component corresponds to the skeleton tree $s \in T_\Gamma$.

▸ **Theorem 10.** *VRP interpretations are effectively equivalent to RSGTR graphs (up to isomorphism and color removal). Furthermore the conversion between the VRP tree and the skeleton tree preserves the decidability of MSO logic and regularity.*

**Proof.** The first part is the direction from VRP trees to RSGTR systems. Consider a given VRP tree $t \in T_{\Omega_{A,C}}$. We can simulate it by an RSGTR system (depending only on $A$ and $C$) with $t$ as skeleton. From the definition of the interpretation via chains, it follows that each node of the interpretation is represented by exactly one *finite prefix* of $t$. This is a part of $t$ starting from the root, such that for each vertex with label $f \in \Omega_{A,C}$ of the prefix:

1. if $f \in \big\{[\phi], [c \overset{a}{\bowtie} d]\big\}$ then the (unique) child has to belong to the prefix as well,
2. if $f = \oplus$ then either the left or the right child belongs to the prefix, and
3. if $f = \otimes_\eta$ then both children belong to the prefix.

Figure 4 depicts (when ignoring the numbers below the vertices) such a finite prefix of the infinite VRP tree of Fig. 3. Those prefixes form a deterministic top-down recognizable set when using the overlay alphabet $\Sigma\|_{\Omega_{A,C}}$ with $\Sigma := \{0, 1, 2, 2_L, 2_R\}$, each symbol having its number as rank. Then use 0 for constants, 1 for unary operators, 2 for products, and $2_L, 2_R$ for the left and right branches of disjoint unions, respectively.

To simulate the edges as introduced by the edge adding operators of $t$ we have to look at the coloring of vertices. The colors of a prefix can be computed easily in a bottom-up manner for each subtree such that the color of each subtree corresponds to the color of the vertex which is VRP-represented by that very subtree. Starting by copying the constant colors at the leaves, the computation simply merges at each subtree the colors of its children according to the semantic of the considered operator. In Fig. 4 the colors are written next to each vertex. If a subtree is labeled by an operator $[c \overset{a}{\bowtie} d]$ and has color $c$ assigned to it then

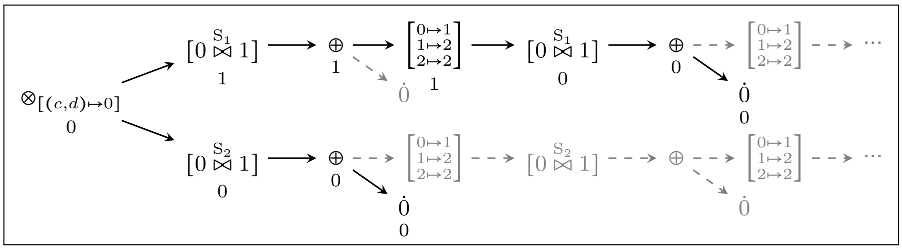

**Figure 4** A finite prefix of the VRP tree of Fig. 3 representing grid position $(1, 0)$

it can be rewritten to another one of color $d$. In Fig. 4 this means that there would be an $\mathrm{S}_2$-labeled transition from the subtree with operator $[0 \overset{\mathrm{S}_2}{\bowtie} 1]$ and color 0 to another subtree of color 1, which can only lead to the prefix where the paths at both children are of the same length, i.e., grid position $(1, 1)$. This can be implemented by regular rewriting rules over the overlay alphabet $\Sigma\|_{\Omega_{A,C}}$. We skip the exact definition, since it is easy but purely technical and does not bring any deeper insight than the explanation above. The MSO-decidability and regularity are preserved trivially since we chose $t$ itself to be the skeleton.

Showing the converse is a bit more challenging. Consider a given RSGTR system $(s, \Gamma, T, \Sigma, A, \Delta)$. To finish the proof we define a transformation of $s$ into a VRP tree $t$ whose structure mimics $s$ and $T$ in a top-down manner, whereas the definition of $\Delta$ is simulated bottom-up in its colors. Let $T$ be specified by a deterministic top-down tree automaton $\mathcal{A} = \big(Q, \Sigma\|_\Gamma, (\delta_f)_{f \in \Sigma\|_\Gamma}, q_0\big)$, and let $\Delta$ be represented by both the deterministic bottom-up tree automaton $\mathcal{A}'_q = \big(Q', \Sigma\|_\Gamma, (\delta'_f)_{f \in \Sigma\|_\Gamma}, \{q\}\big)$ and the relation $\Delta' \subseteq Q' \times A \times Q'$, such that $l \in L, r \in R$ for some rule $L \xrightarrow{a} R$ of $\Delta$ iff $l \in T(\mathcal{A}_p), r \in T(\mathcal{A}_q)$ for some $(p, a, q) \in \Delta'$. This alternative representation of the transitions can be obtained by a product construction of the automata in the rules of $\Delta$. The transformation mentioned above is the composition of the following tree transformations, each of which has the desired preservation properties:

1. For simplicity we first extend $s \in T_\Gamma$ to an infinite $m$-ary tree $s' \in T_{\Gamma'}$ where $m := \max\big\{ |f| \;\big|\; f \in \Sigma \big\}$ is the maximal rank of $\Sigma$, each symbol of $\Gamma' := \Gamma \uplus \{\bot\}$ has rank $m$, and $s'(w) := s(w)$ if $w \in \mathrm{dom}(s)$, or $s'(w) := \bot$ otherwise. Then $t\|_s = t\|_{s'}$ for each $t \in T_\Sigma$.
2. The actual work is done by transforming $s' \in T_{\Gamma'}$ into a *relaxed* VRP tree $t' \in T_{\Omega'_{A,C}}$ where $\Omega'_{A,C}$ is like $\Omega_{A,C}$ but the operators $\oplus$ and $\otimes_\eta$ are lifted to their $n$-ary correspondents $\bigoplus_{i \in \{1,\dots,n\}}$ and $\bigotimes_\eta$ with $\eta : C^n \to C$ for bounded $n \in \mathbb{N}$. We set actions $A$ as in $\mathcal{A}'$ and the colors $C := Q'$. We transform $s'$ into $t' := \lfloor s' \rfloor_{q_0}$ with $q_0 \in Q$ from $\mathcal{A}$ where $\lfloor s' \rfloor_q$ for each $q \in Q$ and tree $s' = g'(s'_1, \dots, s'_m) \in T_{\Omega'_{A,C}}$ is defined as the (unique) tree
$$\lfloor s' \rfloor_q \quad := \quad \underbrace{\cdots [p' \overset{a}{\bowtie} q'] \cdots}_{\substack{\text{for each} \\ (p', a, q') \in \Delta'}} \quad \bigoplus_{\substack{\delta_{(f, g')}(q) = \\ (p_1, \dots, p_{|f|})}} \left( \bigotimes\nolimits_{\delta'_{(f, g')}} \Big( \lfloor s'_1 \rfloor_{p_1}, \dots, \lfloor s'_{|f|} \rfloor_{p_{|f|}} \Big) \right).$$
When ignoring everything that deals with colors in this construction, one can verify that this defines just the domain $T$ by top-down simulating $\mathcal{A}$ with respect to the skeleton $s$. When just looking at the colors, then they exactly simulate The bottom-up behavior of $\mathcal{A}'$ is exactly simulated by the colors, where we use the relation $\Delta'$ to specified by transitions of $\mathcal{A}'$. The way the transformation is defined allows the preservance of regularity and MSO-decidability.
3. Finally we transform $t' \in T_{\Omega'_{A,C}}$ into $t \in T_{\Omega_{A,C'}}$ by simply reducing the $n$-ary operators $\bigoplus, \bigotimes_\eta$ to their binary versions $\oplus, \otimes_\eta$ or constants (for empty products). In general large products require the introduction of new colors $C'$ for $n$-tuples of old colors $C$. ◂

The restriction of Theorem 10 to regular trees, this yields exactly Colcombet's equivalence result [7], since a regular skeleton tree can already be simulated by the domain of an RGTR system. By combining Theorem 10 with the other main result of Colcombet we can lift the decidability of the FO(R) theory from RGTR to RSGTR:

▸ **Corollary 11.** *The FO(R) theory of an RSGTR graph is decidable if the skeleton tree has a decidable MSO theory.*

## 6 Conclusion

Let us summarize the main results of this work about FO logic extended by reachability. We have classified the decidability of FO(Reg) logic on infinite grids where the boundary of decidability turned out to be between dimension 2 and 3 (Theorems 1 and 2). By set-based unfolding we have introduced a new graph transformation which does not preserve the decidability of MSO logic but still transfers it to a decidable FO(Reg) logic on the unfolded graph (Corollary 6). By extending RGTR systems with a skeleton tree we have given an automaton-based formalism with the same expressive power as VRP trees (Theorem 10). One can furthermore reduce FO(Reg) logic on the graphs of those systems to MSO logic on its skeleton tree (Corollary 11).

Besides these results there still remain open questions. From graphs with decidable MSO theory we can generate members of the family of graphs having decidable FO(Reg) theories by set-based unfolding. Although not proven, we suppose that this family contains more graphs than obtainable in this way. And if so, how can this family be characterized? Furthermore it is known that interpretations of regular VRP trees are equivalent to RGTR graphs [7] whereas interpretations of regular VR trees (without the product operation) are equivalent to prefix recognizable graphs [1]. Which subclass of RSGTR graphs is described by interpretations of (possibly irregular) VR trees with decidable MSO theory?

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