Germán Vidal (Ed.)

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Preface

This book contains the papers presented at the 21st International Symposium on Logic-based Program Synthesis and Transformation, LOPSTR 2011, which is held July 18-20, 2011, co-located with PPDP 2011, the 13th International ACM SIGPLAN Symposium on Principles and Practice of Declarative Programming, AAIP 2011, the 4th International Workshop on Approaches and Applications of Inductive Programming, and WFLP 2011, the 20th International Workshop on Functional and (Constraint) Logic Programming. Previous LOPSTR symposia were held in Hagenberg (2010), Coimbra (2009), Valencia (2008), Lyngby (2007), Venice (2006 and 1999), London (2005 and 2000), Verona (2004), Uppsala (2003), Madrid (2002), Paphos (2001), Manchester (1998, 1992, and 1991), Leuven (1997), Stockholm (1996), Arnhem (1995), Pisa (1994), and Louvain-la-Neuve (1993). Information about the conference can be found at: `http://users.dsic.upv.es/~lopstr11/`.

The aim of the LOPSTR series is to stimulate and promote international research and collaboration in logic-based program development. LOPSTR traditionally solicits contributions, in any language paradigm, in the areas of specification, synthesis, verification, analysis, optimization, specialization, security, certification, applications and tools, program/model manipulation, and transformational techniques. LOPSTR has a reputation for being a lively, friendly forum for presenting and discussing work in progress. Formal proceedings are produced only after the symposium so that authors can incorporate this feedback in the published papers. The LOPSTR 2011 post-proceedings will be published in Springer's Lecture Notes in Computer Science series.

In response to the call for papers, 28 contributions were submitted from 13 different countries. The Programme Committee decided to accept fourteen full papers and four extended abstracts, basing this choice on their scientific quality, originality, and relevance to the symposium. Each paper was reviewed by at least three Program Committee members or external referees. In addition to the 18 contributed papers, this volume includes the abstracts of the invited talks by two outstanding speakers: John Gallagher (Roskilde University, Denmark) and Fritz Henglein (DIKU, University of Copenhagen, Denmark).

I want to thank the Program Committee members, who worked diligently to produce high-quality reviews for the submitted papers, as well as all the external reviewers involved in the paper selection. I am very grateful to the LOPSTR 2011 Symposium Chair, Peter Schneider-Kamp, and the local organizers for the great job they did in preparing the symposium. I would also like to thank Andrei Voronkov for his excellent EasyChair system that automates many of the tasks involved in chairing a conference.

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Program Analysis With Regular Tree Languages*

John P. Gallagher

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Abstract. Finite Tree Automata (FTAs) are mathematical "machines" that define recognisable sets of tree-structured terms; they provide a foundation for describing a variety of computational structures such as data, computation states and computation traces. The field of finite tree automata attracts growing attention from researchers in automatic program analysis and verification; there have been promising applications using FTAs in program specialisation, data flow analysis for a variety of languages, term-rewriting systems, shape analysis of pointer-based data structures, polymorphic type inference, binding time analysis, termination analysis, infinite state model checking and cryptographic protocol analysis. The study of FTAs originated in formal language theory and logic, but unlike string automata, which have been widely applied in computer science, especially in compiler theory, tree automata have not yet entered the mainstream of computing theory. In this talk, frameworks for designing static analyses based on tree automata are outlined. They can be used both prescriptively, for expressing and checking intended properties of programs, or descriptively, for capturing approximations of the actual states arising from computations. Computational techniques for handling FTAs efficiently are covered. Finally we look at extensions that go beyond the expressiveness of tree automata, as well as integrating arithmetic constraints.

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Dynamic Symbolic Computation for Domain-Specific Language Implementation*

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A domain-specific language (DSL) is a specification language designed to facilitate programming in a certain application domain. A well-designed DSL reflects the natural structure of the modeled domain, enforces abstraction, and its implementation exploits domain-specific properties for safety and performance.

Expounding on the latter, in this talk we describe a method for opportunistically adding symbolic computation at run-time to a base implementation that employs a general-purpose data structure, so as to improve asymptotic performance without changing the compositional structure of the language. Informally, it consists of repeatedly performing the following process:

1. Identify an operation with problematic performance characteristics, e.g. computation of Cartesian products.
2. Make the operation lazy by extending the data structure with a symbolic representation for the result of the operation.
3. Exploit domain-specific algebraic properties for transforming symbolic representations efficiently at run-time. (This may require adding additional symbolic representations.)

The resulting implementation is a hybrid of "concrete" computation steps from the base implementation and interleaved symbolic computation steps. Evaluation is lazy in a strong sense: It does not only delay evaluation by thunkifying a computation, but performs run-time inspection of symbolic representations.

We apply this method to a DSL for generic multiset programming, arriving at symbolic representations for multisets, predicates, and functions. Starting with a straightforward list representation, multisets are represented using formal (symbolic) products, unions, scaling, and maps in the final implementation. We show how the resulting implementation can be used in an efficient implementation of finite probability distributions with exact (rational) probabilities, avoiding the performance pitfalls of straightforward implementations when dealing with product probability spaces. Even though probability spaces have a natural monadic structure, we observe that a monadic *implementation* using the standard "black-box" computational function type, as in Haskell, forfeits the benefits of the exploiting run-time symbolic representation of functions for performance purposes as demonstrated here.

* This research has been partially supported by the Danish National Advanced Technology Foundation under Project *3d generation Enterprise Resource Planning Systems (3gERP)*.

A Linear Operational Semantics for Termination and Complexity Analysis of ISO Prolog*

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Abstract. We present a new operational semantics for Prolog which covers all constructs in the corresponding ISO standard (including "non-logical" concepts like cuts, meta-programming, "all solution" predicates, dynamic predicates, and exception handling). In contrast to the classical operational semantics for logic programming, our semantics is *linear* and not based on search trees. This has the advantage that it is particularly suitable for automated program analyses such as termination and complexity analysis. We prove that our new semantics is equivalent to the ISO Prolog semantics, i.e., it computes the same answer substitutions and the derivations in both semantics have essentially the same length.

1 Introduction

We introduce a new *state*-based semantics for Prolog. Any query Q corresponds to an initial state s_Q and we define a set of *inference rules* which transform a state s into another state s' (denoted $s \rightsquigarrow s'$). The evaluation of Q is modeled by repeatedly applying inference rules to s_Q (i.e., by the derivation $s_Q \rightsquigarrow s_1 \rightsquigarrow s_2 \rightsquigarrow \ldots$). Essentially, our states s represent the list of those goals that still have to be proved. But in contrast to most other semantics for Prolog, our semantics is *linear* (or *local*), since each state contains all information needed for the next evaluation step. So to extend a derivation $s_0 \rightsquigarrow \ldots \rightsquigarrow s_i$, one only has to consider the last state s_i. Thus, even the effect of cuts and other built-in predicates becomes local.

This is in contrast to the standard semantics of Prolog (as specified in the ISO standard [11, 13]), which is defined using a *search tree* built by SLD resolution with a depth-first left-to-right strategy. To construct the next node of the tree, it is not sufficient to regard the node that was constructed last, but due to backtracking, one may have to continue with ancestor goals that occurred much "earlier" in the tree. Advanced features like cuts or exceptions require even more sophisticated analyses of the current search tree. Even worse, "all solution" predicates like findall result in several search trees and the coordination of these trees is highly non-trivial, in particular in the presence of exceptions.

We show that our linear semantics is *equivalent* to the standard ISO seman-

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tics of Prolog. It does not only yield the same answer substitutions, but we also obtain the same *termination* behavior and even the same *complexity* (i.e., the length of the derivations in our semantics corresponds to the number of unifications performed in the standard semantics). Hence, instead of analyzing the termination or complexity of a Prolog program w.r.t. the standard semantics, one can also analyze it w.r.t. our semantics.

Compared to the ISO semantics, our semantics is much more suitable for such (possibly automated) analyses. In particular, our semantics can also be used for symbolic evaluation of *abstract* states (where the goals contain *abstract variables* representing arbitrary terms). Such abstract states can be generalized ("widened") and instantiated, and under certain conditions one may even *split up* the lists of goals in states [19, 20]. In this way, one can represent all possible evaluations of a program by a finite graph, which can then be used as the basis for e.g. termination analysis. In the standard Prolog semantics, such an abstraction of a query in a search tree would be problematic, since the remaining computation does not only depend on this query, but on the whole search tree.

In [19, 20] we already used a preliminary version of our semantics for termination analysis of a subset of Prolog containing definite logic programming and cuts. Most previous approaches for termination (or complexity [9]) analysis were restricted to definite programs. Our semantics was a key contribution to extend termination analysis to programs with cuts. The corresponding implementation in the prover AProVE resulted in the most powerful tool for automated termination analysis of logic programming so far, as shown at the *International Termination Competition*.[3] These experimental results are the main motivation for our work, since they indicate that such a semantics is indeed suitable for automated termination analysis. However, it was unclear how to extend the semantics of [19, 20] to full Prolog and how to prove that this semantics is really equivalent to the ISO semantics. These are the contributions of the current paper.

Hence, this paper forms the basis which will allow the extension of automated termination techniques to *full* Prolog. Moreover, many termination techniques can be adapted to infer upper bounds on the complexity [12, 18, 22]. Thus, the current paper is also the basis in order to adapt termination techniques such that they can be used for automated complexity analysis of full Prolog.

There exist several other alternative semantics for Prolog. However, most of them (e.g., [2, 4–8, 14, 15, 17]) only handle subsets of Prolog and it is not clear how to extend these semantics in a straightforward way to full Prolog.

Alternative semantics for *full* Prolog were proposed in [3, 10, 16]. However, these semantics seem less suitable for automated termination and complexity analysis than ours: The states used in [3] are considerably more complex than ours and it is unclear how to abstract the states of [3] for automated termination analysis as in [19, 20]. Moreover, [3] does not investigate whether their semantics also yields the same complexity as the ISO standard. The approach in [10] is close to the ISO standard and thus, it has similar drawbacks as the ISO semantics, since it also works on search trees. Finally, [16] specifies standard Prolog in rewriting logic. Similar to us, [16] uses a list representation for states. However,

[3] See `http://www.termination-portal.org/wiki/Termination_Competition`.

their approach cannot be used for complexity analysis, since their derivations can be substantially longer than the number of unifications needed to evaluate the query. Since [16] does not use explicit markers for the scope of constructs like the cut, it is also unclear how to use their approach for automated termination analysis, where one would have to abstract and to split states.

The full set of all inference rules of our semantics (for all 112 built-in predicates of ISO Prolog) can be found in [21]. Due to lack of space, in the paper we restrict ourselves to the inference rules for the most representative predicates. Sect. 2 shows the rules needed for definite logic programs. Sect. 3 extends them for predicates like the cut, negation-as-failure, and call. In Sect. 4 we handle "all solution" predicates and Sect. 5 shows how to deal with dynamic predicates like assertz and retract. Sect. 6 extends our semantics to handle exceptions (using catch and throw). Finally, Sect. 7 contains our theorems on the equivalence of our semantics to the ISO semantics. All proofs can be found in [21].

2 Definite Logic Programming

See e.g. [1] for the basics of logic programming. As in ISO Prolog, we do not distinguish between predicate and function symbols. For a term $t = f(t_1, \ldots, t_n)$, let $root(t) = f$. A *query* is a sequence of terms, where $\Box$ denotes the empty query. A *clause* is a pair $h :\!- B$ where the *head* h is a term and the *body* B is a query. If B is empty, then one writes just "h" instead of "$h :\!- \Box$".[4] A *Prolog program* $\mathcal{P}$ is a finite sequence of clauses.[5]

We often denote the application of a *substitution* σ by $t\sigma$ instead of $\sigma(t)$. A substitution σ is the *most general unifier* (mgu) of s and t iff $s\sigma = t\sigma$ and, whenever $s\gamma = t\gamma$ for some other unifier γ, there is a δ with $X\gamma = X\sigma\delta$ for all $X \in \mathcal{V}(s) \cup \mathcal{V}(t)$.[6] As usual, "$\sigma\delta$" is the composition of σ and δ, where $X\sigma\delta = (X\sigma)\delta$. If s and t have no mgu σ, we write $mgu(s,t) = \mathit{fail}$.

A Prolog program without built-in predicates is called a *definite* logic program. Our aim is to define a *linear* operational semantics where each state contains all information needed for backtracking steps. In addition, a state also contains a list of all *answer substitutions* that were found up to now. So a state has the form $\langle G_1 \mid \ldots \mid G_n \;;\; \delta_1 \mid \ldots \mid \delta_m \rangle$ where $G_1 \mid \ldots \mid G_n$ is a sequence of goals and $\delta_1 \mid \ldots \mid \delta_m$ is a sequence of answer substitutions. We do not include the clauses from $\mathcal{P}$ in the state since they remain static during the evaluation.

Essentially, a *goal* is just a *query*, i.e., a sequence of terms. However, to compute answer substitutions, a goal G is labeled by a substitution which collects

[4] In ISO Prolog, whenever an empty query $\Box$ is reached, this is replaced by the built-in predicate true. However, we also allow empty queries to ease the presentation.

[5] More precisely, $\mathcal{P}$ are just the program clauses for *static* predicates. In addition to $\mathcal{P}$, a Prolog program may also contain clauses for *dynamic* predicates and *directives* to specify which predicates are dynamic. As explained in Sect. 5, these directives and the clauses for dynamic predicates are treated separately by our semantics.

[6] While the ISO standard uses unification with occurs check, our semantics could also be defined in an analogous way when using unification without occurs check.

$$\frac{\Box_\delta \mid S \;;\; A}{S \;;\; A \mid \delta}\ (\textsc{Success}) \qquad \frac{(t,Q)_\delta \mid S \;;\; A}{(t,Q)_\delta^{c_1} \mid \cdots \mid (t,Q)_\delta^{c_a} \mid S \;;\; A}\ (\textsc{Case})\ \begin{array}{l}\text{if } \mathit{defined}_\mathcal{P}(t) \text{ and}\\ \mathit{Slice}_\mathcal{P}(t) =\\ (c_1,\ldots,c_a)\end{array}$$

$$\frac{(t,Q)_\delta^{h\,:\!-\,B} \mid S \;;\; A}{(B\sigma, Q\sigma)_{\delta\sigma} \mid S \;;\; A}\ (\textsc{Eval})\ \begin{array}{l}\text{if}\\ \sigma =\\ \mathit{mgu}(t,h)\end{array} \qquad \frac{(t,Q)_\delta^{h\,:\!-\,B} \mid S \;;\; A}{S \;;\; A}\ (\textsc{Backtrack})\ \begin{array}{l}\text{if}\\ \mathit{mgu}(t,h) =\\ \mathit{fail}.\end{array}$$

Fig. 1. Inference Rules for Definite Logic Programs

the effects of the unifiers that were used during the evaluation up to now. So if $(t_1,\ldots,t_k)$ is a query, then a goal has the form $(t_1,\ldots,t_k)_\delta$ for a substitution δ. In addition, a goal can also be labeled by a clause c, where the goal $(t_1,\ldots,t_k)_\delta^c$ means that the next resolution step has to be performed using the clause c.

The *initial state* for a query $(t_1,\ldots,t_k)$ is $\langle (t_1,\ldots,t_k)_\varnothing \;;\; \varepsilon\rangle$, i.e., the query is labeled by the identity substitution $\varnothing$ and the current list of answer substitutions is ε (i.e., it is empty). This initial state can be transformed by *inference rules* repeatedly. The inference rules needed for definite logic programs are given in Fig. 1. Here, Q is a query, S stands for a sequence of goals, A is a list of answer substitutions, and we omitted the delimiters "$\langle$" and "$\rangle$" for readability.

To illustrate these rules, we use the following program where $\mathsf{member}(t_1,t_2)$ holds whenever t_1 unifies with any member of the list t_2. Consider the query $\mathsf{member}(U,[1])$.[7] Then the corresponding initial state is $\langle \mathsf{member}(U,[1])_\varnothing \;;\; \varepsilon\rangle$.

$$\mathsf{member}(X,[X|\_]).\ \ (1) \qquad\qquad \mathsf{member}(X,[\_|XS]) \ :\!-\ \mathsf{member}(X,XS).\ \ (2)$$

When evaluating a goal $(t,Q)_\delta$ where $\mathit{root}(t) = p$, one tries all clauses $h :\!- B$ with $\mathit{root}(h) = p$ in the order they are given in the program. Let $\mathit{defined}_\mathcal{P}(t)$ indicate that $\mathit{root}(t)$ is a user-defined predicate and let $\mathit{Slice}_\mathcal{P}(t)$ be the list of all clauses from $\mathcal{P}$ whose head has the same root symbol as t. However, in the clauses returned by $\mathit{Slice}_\mathcal{P}(t)$, all occurring variables are renamed to fresh ones. Thus, if $\mathit{defined}_\mathcal{P}(t)$ and $\mathit{Slice}_\mathcal{P}(t) = (c_1,\ldots,c_a)$, then we use a (Case) rule which replaces the current goal $(t,Q)_\delta$ by the new list of goals $(t,Q)_\delta^{c_1} \mid \ldots \mid (t,Q)_\delta^{c_a}$. As mentioned, the label c_i in such a goal means that the next resolution step has to be performed using the clause c_i. So in our example, $\mathsf{member}(U,[1])_\varnothing$ is replaced by the list $\mathsf{member}(U,[1])_\varnothing^{(1)'} \mid \mathsf{member}(U,[1])_\varnothing^{(2)'}$, where $(1)'$ and $(2)'$ are freshly renamed variants of the clauses (1) and (2).

To evaluate a goal $(t,Q)_\delta^{h\,:\!-\,B}$, one has to check whether there is a $\sigma = \mathit{mgu}(t,h)$. In this case, the (Eval) rule replaces t by B and σ is applied to the whole goal. Moreover, σ will contribute to the answer substitution, i.e., we replace δ by $\delta\sigma$. Otherwise, if t and h are not unifiable, then the goal $(t,Q)_\delta^{h\,:\!-\,B}$ is removed from the state and the next goal is tried (Backtrack). An empty goal $\Box_\delta$ corresponds to a successful leaf in the SLD tree. Thus, the (Success) rule removes such an empty goal and adds the substitution δ to the list A of answer substitutions (we denote this by "$A \mid \delta$"). Fig. 2 shows the full evaluation of the initial state $\langle \mathsf{member}(U,[1])_\varnothing \;;\; \varepsilon\rangle$. Here, $(1)'$ and $(1)''$ (resp. $(2)'$ and $(2)''$)

[7] As usual, $[t_1,\ldots,t_n]$ abbreviates $.(t_1,.(\ldots,.(t_n,[\,])\ldots))$ and $[t \mid ts]$ stands for $.(t,ts)$.

	$\mathsf{member}(U, [1])_{\varnothing}\ ;\ \varepsilon$
CASE	$\mathsf{member}(U, [1])_{\varnothing}^{(1)'} \mid \mathsf{member}(U, [1])_{\varnothing}^{(2)'}\ ;\ \varepsilon$
EVAL	$\square_{\{U/1,\, X'/1\}} \mid \mathsf{member}(U, [1])_{\varnothing}^{(2)'}\ ;\ \varepsilon$
SUCCESS	$\mathsf{member}(U, [1])_{\varnothing}^{(2)'}\ ;\ \{U/1,\, X'/1\}$
EVAL	$\mathsf{member}(U, [])_{\{X'/U,\, XS'/[]\}}\ ;\ \{U/1,\, X'/1\}$
CASE	$\mathsf{member}(U, [])_{\{X'/U,\, XS'/[]\}}^{(1)''} \mid \mathsf{member}(U, [])_{\{X'/U,\, XS'/[]\}}^{(2)''}\ ;\ \{U/1,\, X'/1\}$
BACKTRACK	$\mathsf{member}(U, [])_{\{X'/U,\, XS'/[]\}}^{(2)''}\ ;\ \{U/1,\, X'/1\}$
BACKTRACK	$\varepsilon\ ;\ \{U/1,\, X'/1\}$

Fig. 2. Evaluation for the Query $\mathsf{member}(U, [1])$

are fresh variants of (1) (resp. (2)) that are pairwise variable disjoint. So for example, X and XS were renamed to X' and XS' in $(2)'$.

3 Logic and Control

In Fig. 3, we present inference rules to handle some of the most commonly used pre-defined predicates of Prolog: the cut (!), negation-as-failure (\+), the predicates call, true, and fail, and the Boolean connectives *Conn* for conjunction (',') , disjunction (';'), and implication ('->').[8] As in the ISO standard, we require that in any *clause* $h :- B$, the term h and the terms in B may not contain variables at *predication positions*. A position is a *predication position* iff the only function symbols that may occur above it are the Boolean connectives from *Conn*. So instead of a clause $\mathsf{q}(X) :- X$ one would have to use $\mathsf{q}(X) :- \mathsf{call}(X)$.

The effect of the cut is to remove certain backtracking possibilities. When a cut in a clause $h :- B_1, !, B_2$ with $root(h) = p$ is reached, then one does not backtrack to the remaining clauses of the predicate p. Moreover, the remaining backtracking possibilities for the terms in B_1 are also disregarded. As an example, we consider a modified member program.

$$\mathsf{member}(X, [X|\_]) \ :-\ !. \quad (3) \qquad \mathsf{member}(X, [\_|XS]) \ :-\ \mathsf{member}(X, XS). \quad (4)$$

In our semantics, the elimination of backtracking steps due to a cut is accomplished by removing goals from the state. Thus, we re-define the (CASE) rule in Fig. 3. To evaluate $p(\ldots)$, one again considers all program clauses $h :- B$ where $root(h) = p$. However, every cut in B is labeled by a fresh natural number m. For any clause c, let $c[!/!_m]$ result from c by replacing all (possibly labeled) cuts ! on *predication positions* by $!_m$. Moreover, we add a *scope delimiter* $?_m$ to make the end of their scope explicit. As the initial query Q might also contain cuts, we also label them and construct the corresponding initial state $\langle (Q\,[!/!_0])_{\varnothing} \mid ?_0\ ;\ \varepsilon \rangle$.

In our example, consider the query $\mathsf{member}(U, [1, 1])$. Its corresponding initial state is $\langle \mathsf{member}(U, [1, 1])_{\varnothing} \mid ?_0\ ;\ \varepsilon \rangle$. Now the (CASE) rule replaces the goal

[8] The inference rules for true and the connectives from *Conn* are straightforward and thus, we only present the rule for ',' in Fig. 3. See [21] for the set of all rules.

$$\frac{(t,Q)_\delta \mid S \;;\; A}{(t,Q)_\delta^{c_1[!/!_m]} \mid \cdots \mid (t,Q)_\delta^{c_a[!/!_m]} \mid ?_m \mid S \;;\; A}\ (\textsc{Case})\ \text{if } \mathit{defined}_\mathcal{P}(t),\ \mathit{Slice}_\mathcal{P}(t) = (c_1,\ldots,c_a), \text{ and } m \text{ is fresh}$$

$$\frac{(!_m,Q)_\delta \mid S' \mid ?_m \mid S \;;\; A}{Q_\delta \mid ?_m \mid S \;;\; A}\ (\textsc{Cut}) \qquad \frac{(',' (t_1,t_2),Q)_\delta \mid S \;;\; A}{(t_1,t_2,Q)_\delta \mid S \;;\; A}\ (\textsc{Conj})$$

$$\frac{?_m \mid S \;;\; A}{S \;;\; A}\ (\textsc{Failure}) \qquad \frac{(\mathsf{call}(t),Q)_\delta \mid S \;;\; A}{(t[\mathcal{V}/\mathsf{call}(\mathcal{V}),\ !/!_m],Q)_\delta \mid ?_m \mid S \;;\; A}\ (\textsc{Call})\ \begin{array}{l}\text{if } t \notin \mathcal{V}\\ \text{and } m \text{ is}\\ \text{fresh.}\end{array}$$

$$\frac{(\mathsf{fail},Q)_\delta \mid S \;;\; A}{S \;;\; A}\ (\textsc{Fail}) \qquad \frac{(\backslash+(t),Q)_\delta \mid S \;;\; A}{(\mathsf{call}(t),!_m,\mathsf{fail})_\delta \mid Q_\delta \mid ?_m \mid S \;;\; A}\ (\textsc{Not})\ \begin{array}{l}\text{where } m \text{ is}\\ \text{fresh.}\end{array}$$

Fig. 3. Inference Rules for Programs with Pre-defined Predicates for Logic and Control

$\mathsf{member}(U,[1,1])_\varnothing$ by $\mathsf{member}(U,[1,1])_\varnothing^{(3)'[!/!_1]} \mid \mathsf{member}(U,[1,1])_\varnothing^{(4)'[!/!_1]} \mid ?_1$. Here, $(3)'$ is a fresh variant of the rule (3) and $(3)'[!/!_1]$ results from $(3)'$ by labeling all cuts with 1, i.e., $(3)'[!/!_1]$ is the rule $\mathsf{member}(X',[X'|\_]) :- !_1$.

Whenever a cut $!_m$ is evaluated in the current goal, the (Cut) rule removes all backtracking goals up to the delimiter $?_m$ from the state. The delimiter itself must not be removed, since the current goal might still contain more occurrences of $!_m$. So after evaluating the goal $\mathsf{member}(U,[1,1])_\varnothing^{(3)'[!/!_1]}$ to $(!_1)_{\{U/1,\,X'/1\}}$, the (Cut) rule removes all remaining goals in the list up to $?_1$.

When a predicate has been evaluated completely (i.e., when $?_m$ becomes the current goal), then this delimiter is removed. This corresponds to a failure in the evaluation, since it only occurs when all solutions have been computed. Fig. 4 shows the full evaluation of the initial state $\langle \mathsf{member}(U,[1,1])_\varnothing \mid ?_0 \;;\; \varepsilon\rangle$.

The built-in predicate call allows meta-programming. To evaluate a term $\mathsf{call}(t)$ (where $t \notin \mathcal{V}$, but t may contain connectives from *Conn*), the (Call) rule replaces $\mathsf{call}(t)$ by $t[\mathcal{V}/\mathsf{call}(\mathcal{V}),\ !/!_m]$. Here, $t[\mathcal{V}/\mathsf{call}(\mathcal{V}),\ !/!_m]$ results from t by replacing all variables X on predication positions by $\mathsf{call}(X)$ and all (possibly labeled) cuts on predication positions by $!_m$. Moreover, a delimiter $?_m$ is added to mark the scope of the cuts in t.

Another simple built-in predicate is fail, whose effect is to remove the current goal. By the cut, call, and fail, we can now also handle the "negation-as-failure"

	$\mathsf{member}(U,[1,1])_\varnothing \mid ?_0 \;;\; \varepsilon$
Case	$\mathsf{member}(U,[1,1])_\varnothing^{(3)'[!/!_1]} \mid \mathsf{member}(U,[1,1])_\varnothing^{(4)'[!/!_1]} \mid ?_1 \mid ?_0 \;;\; \varepsilon$
Eval	$(!_1)_{\{U/1,\,X'/1\}} \mid \mathsf{member}(U,[1,1])_\varnothing^{(4)'[!/!_1]} \mid ?_1 \mid ?_0 \;;\; \varepsilon$
Cut	$\square_{\{U/1,\,X'/1\}} \mid ?_1 \mid ?_0 \;;\; \varepsilon$
Success	$?_1 \mid ?_0 \;;\; \{U/1,\ X'/1\}$
Failure	$?_0 \;;\; \{U/1,\ X'/1\}$
Failure	$\varepsilon \;;\; \{U/1,\ X'/1\}$

Fig. 4. Evaluation for the Query $\mathsf{member}(U,[1,1])$

operator \+: the (Not) rule replaces the goal $(\backslash+(t), Q)_\delta$ by the list $(\mathsf{call}(t), !_m, \mathsf{fail})_\delta \mid Q_\delta \mid ?_m$. Thus, Q_δ is only executed if $\mathsf{call}(t)$ fails.

As an example, consider a program with the fact a and the rule $\mathsf{a} :- \mathsf{a}$. We regard the query $\backslash+(',' (\mathsf{a}, !))$. The evaluation in Fig. 5 shows that the query terminates and fails (since we do not obtain any answer substitution).

	$\backslash+(',' (\mathsf{a}, !))_\varnothing \mid ?_0 \;;\; \varepsilon$
Not	$(\mathsf{call}(',' (\mathsf{a}, !)), !_1, \mathsf{fail})_\varnothing \mid ?_1 \mid ?_0 \;;\; \varepsilon$
Call	$(',' (\mathsf{a}, !_2), !_1, \mathsf{fail})_\varnothing \mid ?_2 \mid ?_1 \mid ?_0 \;;\; \varepsilon$
Conj	$(\mathsf{a}, !_2, !_1, \mathsf{fail})_\varnothing \mid ?_2 \mid ?_1 \mid ?_0 \;;\; \varepsilon$
Case	$(\mathsf{a}, !_2, !_1, \mathsf{fail})^{\mathsf{a}}_\varnothing \mid (\mathsf{a}, !_2, !_1, \mathsf{fail})^{\mathsf{a} :- \mathsf{a}}_\varnothing \mid ?_2 \mid ?_1 \mid ?_0 \;;\; \varepsilon$
Eval	$(!_2, !_1, \mathsf{fail})_\varnothing \mid (\mathsf{a}, !_2, !_1, \mathsf{fail})^{\mathsf{a} :- \mathsf{a}}_\varnothing \mid ?_2 \mid ?_1 \mid ?_0 \;;\; \varepsilon$
Cut	$(!_1, \mathsf{fail})_\varnothing \mid ?_2 \mid ?_1 \mid ?_0 \;;\; \varepsilon$
Cut	$\mathsf{fail}_\varnothing \mid ?_1 \mid ?_0 \;;\; \varepsilon$
Fail	$?_1 \mid ?_0 \;;\; \varepsilon$
Failure	$?_0 \;;\; \varepsilon$
Failure	$\varepsilon \;;\; \varepsilon$

Fig. 5. Evaluation for the Query $\backslash+(',' (\mathsf{a}, !))$

4 "All Solution" Predicates

We now consider the unification predicate = and the predicates findall, bagof, and setof, which enumerate all solutions to a query. Fig. 6 gives the inference rules for = and findall (bagof and setof can be modeled in a similar way, cf. [21]).

We extend our semantics in such a way that the collection process of such "all solution" predicates is performed just like ordinary evaluation steps of a program. Moreover, we modify our concept of *states* as little as possible.

A call of $\mathsf{findall}(r, t, s)$ executes the query $\mathsf{call}(t)$. If $\sigma_1, \ldots, \sigma_n$ are the resulting answer substitutions, then finally the list $[r\sigma_1, \ldots, r\sigma_n]$ is unified with s.

We model this behavior by replacing a goal $(\mathsf{findall}(r, t, s), Q)_\delta$ with the list $\mathsf{call}(t) \mid \%^{r,[],s}_{Q,\delta}$. Here, $\%^{r,\ell,s}_{Q,\delta}$ is a findall-*suspension* which marks the "scope" of findall-statements, similar to the markers $?_m$ for cuts in Sect. 3. The findall-suspension fulfills two tasks: it collects all answer terms (r instantiated with an

$$\frac{(\mathsf{findall}(r,t,s), Q)_\delta \mid S \;;\; A}{\mathsf{call}(t)_\varnothing \mid \%^{r,[],s}_{Q,\delta} \mid S \;;\; A}\ (\textsc{FindAll}) \qquad \frac{\%^{r,\ell,s}_{Q,\delta} \mid S \;;\; A}{(\ell{=}s, Q)_\delta \mid S \;;\; A}\ (\textsc{FoundAll})$$

$$\frac{\Box_\theta \mid S' \mid \%^{r,\ell,s}_{Q,\delta} \mid S \;;\; A}{S' \mid \%^{r,\ell|r\theta,s}_{Q,\delta} \mid S \;;\; A}\ (\textsc{FindNext})\ \text{if } S' \text{ contains no findall-suspensions}$$

$$\frac{(t_1 = t_2, Q)_\delta \mid S \;;\; A}{(Q\sigma)_{\delta\sigma} \mid S \;;\; A}\ (\textsc{UnifySuccess}) \quad \text{if } \sigma = mgu(t_1, t_2)$$

$$\frac{(t_1 = t_2, Q)_\delta \mid S \;;\; A}{S \;;\; A}\ (\textsc{UnifyFail})\ \text{if } mgu(t_1, t_2) = \mathit{fail} \qquad \frac{\Box_\delta \mid S \;;\; A}{S \;;\; A \mid \delta}\ (\textsc{Success})\ \text{if } S \text{ contains no findall-suspensions}$$

Fig. 6. Additional Inference Rules for Prolog Programs with findall

	$\mathsf{findall}(U, \mathsf{member}(U, [\mathsf{1}]), L)_{\varnothing} \mid ?_0 \;;\; \varepsilon$
FINDALL	$\mathsf{call}(\mathsf{member}(U, [\mathsf{1}]))_{\varnothing} \mid \%_{\square,\varnothing}^{U,[],L} \mid ?_0 \;;\; \varepsilon$
CALL	$\mathsf{member}(U, [\mathsf{1}])_{\varnothing} \mid ?_1 \mid \%_{\square,\varnothing}^{U,[],L} \mid ?_0 \;;\; \varepsilon$
CASE	$\mathsf{member}(U, [\mathsf{1}])_{\varnothing}^{(3)'[!/!_2]} \mid \mathsf{member}(U, [\mathsf{1}])_{\varnothing}^{(4)'[!/!_2]} \mid ?_2 \mid ?_1 \mid \%_{\square,\varnothing}^{U,[],L} \mid ?_0 \;;\; \varepsilon$
EVAL	$(!_2)_{\{U/1,\, X'/1\}} \mid \mathsf{member}(U, [\mathsf{1}])_{\varnothing}^{(4)'[!/!_2]} \mid ?_2 \mid ?_1 \mid \%_{\square,\varnothing}^{U,[],L} \mid ?_0 \;;\; \varepsilon$
CUT	$\square_{\{U/1,\, X'/1\}} \mid ?_2 \mid ?_1 \mid \%_{\square,\varnothing}^{U,[],L} \mid ?_0 \;;\; \varepsilon$
FINDNEXT	$?_2 \mid ?_1 \mid \%_{\square,\varnothing}^{U,[\mathsf{1}],L} \mid ?_0 \;;\; \varepsilon$
FAILURE	$?_1 \mid \%_{\square,\varnothing}^{U,[\mathsf{1}],L} \mid ?_0 \;;\; \varepsilon$
FAILURE	$\%_{\square,\varnothing}^{U,[\mathsf{1}],L} \mid ?_0 \;;\; \varepsilon$
FOUNDALL	$([\mathsf{1}]{=}L)_{\varnothing} \mid ?_0 \;;\; \varepsilon$
UNIFYSUCCESS	$\square_{\{L/[\mathsf{1}]\}} \mid ?_0 \;;\; \varepsilon$
SUCCESS	$?_0 \;;\; \{L/[\mathsf{1}]\}$
FAILURE	$\varepsilon \;;\; \{L/[\mathsf{1}]\}$

Fig. 7. Evaluation for the Query $\mathsf{findall}(U, \mathsf{member}(U, [\mathsf{1}]), L)$

answer substitution of t) in its list ℓ and it contains all information needed to continue the execution of the program after all solutions have been found.

If a goal is evaluated to $\square_\theta$, its substitution θ would usually be added to the list of answer substitutions of the state. However, if the goals contain a findall-suspension $\%_{Q,\delta}^{r,\ell,s}$, we instead insert $r\theta$ at the end of the list of answers ℓ using the (FINDNEXT) rule (denoted by "$\ell \mid r\theta$").[9] To avoid overlapping inference rules, we modify the (SUCCESS) rule such that it is only applicable if (FINDNEXT) is not.

When $\mathsf{call}(t)$ has been fully evaluated, the first element of the list of goals is a findall-suspension $\%_{Q,\delta}^{r,\ell,s}$. Before continuing the evaluation of Q, we unify the list of collected solutions ℓ with the expected list s (using the built-in predicate $=$).

As an example, for the Prolog program defined by the clauses (3) and (4), an evaluation of the query $\mathsf{findall}(U, \mathsf{member}(U, [\mathsf{1}]), L)$ is given in Fig. 7.

5 Dynamic Predicates

Now we also consider built-in predicates which modify the program clauses for some predicate p at runtime. This is only possible for "new" predicates which were not defined in the program and for predicates where the program contains a dynamic directive before their first clause (e.g., ":− dynamic p/1"). Thus, we consider a program to consist of two parts: a static part $\mathcal{P}$ containing all program clauses for static predicates and a dynamic part, which can be modified at runtime and initially contains all program clauses for dynamic predicates.

Therefore, we extend our states by a list $\mathcal{D}$ which stores all clauses of dynamic predicates, where each of these clauses is labeled by a natural number. We now denote a state as $\langle S \;;\; \mathcal{D} \;;\; A \rangle$ where S is a list of goals and A is a list of answer

[9] As there may be nested findall calls, we use the first findall-suspension in the list.

$$\frac{(t,Q)_\delta \mid S \;;\; \mathcal{D} \;;\; A}{(t,Q)_\delta^{c_1[!/!_m]} \mid \cdots \mid (t,Q)_\delta^{c_a[!/!_m]} \mid ?_m \mid S \;;\; \mathcal{D} \;;\; A}\ (\textsc{Case})\ \begin{array}{l}\text{if } \mathit{defined}_\mathcal{P}(t),\\ \mathit{Slice}_{(\mathcal{P}\mid\overline{\mathcal{D}})}(t) = (c_1,\ldots,c_a),\\ \overline{\mathcal{D}} \text{ is } \mathcal{D} \text{ without clause labels,}\\ \text{and } m \text{ is fresh}\end{array}$$

$$\frac{(\mathsf{asserta}(c),Q)_\delta \mid S \;;\; \mathcal{D} \;;\; A}{Q_\delta \mid S \;;\; (c,m) \mid \mathcal{D} \;;\; A}\ (\textsc{AssA})\ \begin{array}{l}\text{if } m\in\mathbb{N}\\ \text{is fresh}\end{array} \qquad \frac{(\mathsf{assertz}(c),Q)_\delta \mid S \;;\; \mathcal{D} \;;\; A}{Q_\delta \mid S \;;\; \mathcal{D} \mid (c,m) \;;\; A}\ (\textsc{AssZ})\ \begin{array}{l}\text{if } m\in\mathbb{N}\\ \text{is fresh}\end{array}$$

$$\frac{(\mathsf{retract}(c),Q)_\delta \mid S \;;\; \mathcal{D} \;;\; A}{:\!\neq_{Q,\delta}^{c,(c_1,m_1)} \mid \cdots \mid :\!\neq_{Q,\delta}^{c,(c_a,m_a)} \mid S \;;\; \mathcal{D} \;;\; A}\ (\textsc{Retract})\ \begin{array}{l}\text{if } \mathit{Slice}_\mathcal{D}(c) =\\ ((c_1,m_1),\ldots,(c_a,m_a))\end{array}$$

$$\frac{:\!\neq_{Q,\delta}^{c,(c',m)} \mid S \;;\; \mathcal{D} \;;\; A}{(Q\sigma)_{\delta\sigma} \mid S \;;\; \mathcal{D}\setminus(c',m) \;;\; A}\ (\textsc{RetSuc})\ \begin{array}{l}\text{if } \sigma =\\ mgu(c,c')\end{array} \qquad \frac{:\!\neq_{Q,\delta}^{c,(c',m)} \mid S \;;\; \mathcal{D} \;;\; A}{S \;;\; \mathcal{D} \;;\; A}\ (\textsc{RetFail})\ \begin{array}{l}\text{if}\\ mgu(c,c')\\ = \mathit{fail}\end{array}$$

Fig. 8. Additional Inference Rules for Prolog Programs with Dynamic Predicates

substitutions. The inference rules for the built-in predicates asserta, assertz, and retract in Fig. 8 modify the list $\mathcal{D}$.[10] Of course, the (Case) rule also needs to be adapted to take the clauses from $\mathcal{D}$ into account (here, "$\mathcal{P} \mid \overline{\mathcal{D}}$" stands for appending the lists $\mathcal{P}$ and $\overline{\mathcal{D}}$). All other previous inference rules do not depend on the new component $\mathcal{D}$ of the states.

For a clause[11] c, the effect of $\mathsf{asserta}(c)$ resp. $\mathsf{assertz}(c)$ is modeled by inserting (c,m) at the beginning resp. the end of the list $\mathcal{D}$, where m is a fresh number, cf. the rules (AssA) and (AssZ). The labels in $\mathcal{D}$ are needed to uniquely identify each clause as demonstrated by the following query for a dynamic predicate p.

$$\mathsf{assertz(p(a))},\ \mathsf{assertz(p(b))},\ \mathsf{retract(p}(X)\mathsf{)},\ \underbrace{X\mathsf{=\ a},\ \mathsf{retract(p(b))},\ \mathsf{assertz(p(b))},\ \mathsf{fail}}_{Q}$$

So first the two clauses p(a) and p(b) are asserted, i.e., $\mathcal{D}$ contains $(\mathsf{p(a)},1)$ and $(\mathsf{p(b)},2)$. When $\mathsf{retract(p}(X)\mathsf{)}$ is executed, one collects all p-clauses from $\mathcal{D}$, since these are the only clauses which might be removed by this retract-statement.

To this end, we extend the function *Slice* such that $\mathit{Slice}_\mathcal{D}(c)$ returns fresh variants of all labeled clauses c' from $\mathcal{D}$ where $\mathit{root}(\mathit{head}(c)) = \mathit{root}(\mathit{head}(c'))$. An execution of $(\mathsf{retract}(c),Q)_\delta$ then creates a new *retract marker* for every clause in $\mathit{Slice}_\mathcal{D}(c) = ((c_1,m_1),\ldots,(c_a,m_a))$, cf. the (Retract) inference rule in Fig. 8. Such a retract marker $:\!\neq_{Q,\delta}^{c,(c_i,m_i)}$ denotes that the clause with label m_i should be removed from $\mathcal{D}$ if c unifies with c_i by some mgu σ. Moreover, then the computation continues with the goal $(Q\sigma)_{\delta\sigma}$, cf. (RetSuc). If c does not unify with c_i, then the retract marker is simply dropped by the rule (RetFail).

So in our example, we create the two retract markers $:\!\neq_{Q,\varnothing}^{\mathsf{p}(X),(\mathsf{p(a)},1)}$ and $:\!\neq_{Q,\varnothing}^{\mathsf{p}(X),(\mathsf{p(b)},2)}$, where Q are the last four terms of the query. Since $\mathsf{p}(X)$ unifies

[10] The inference rules for the related predicate abolish are analogous, cf. [21].

[11] For $\mathsf{asserta}(c)$, $\mathsf{assertz}(c)$, and $\mathsf{retract}(c)$, we require that the body of the clause c may not be empty (i.e., instead of a fact $\mathsf{p}(X)$ one would have to use $\mathsf{p}(X) :\!-\mathsf{true}$). Moreover, c may not have variables on predication positions.

$$
\begin{array}{ll}
 & \underline{(\mathsf{assertz}(\mathsf{p}(\mathsf{a})), \mathsf{assertz}(\mathsf{p}(\mathsf{b})), \mathsf{retract}(\mathsf{p}(X)), Q)_{\varnothing} \mid ?_0 \;;\; \varepsilon \;;\; \varepsilon} \\
\textsc{AssZ} & \underline{(\mathsf{assertz}(\mathsf{p}(\mathsf{b})), \mathsf{retract}(\mathsf{p}(X)), Q)_{\varnothing} \mid ?_0 \;;\; (\mathsf{p}(\mathsf{a}), 1) \;;\; \varepsilon} \\
\textsc{AssZ} & \underline{(\mathsf{retract}(\mathsf{p}(X)), Q)_{\varnothing} \mid ?_0 \;;\; (\mathsf{p}(\mathsf{a}), 1) \mid (\mathsf{p}(\mathsf{b}), 2) \;;\; \varepsilon} \\
\textsc{Retract} & \underline{:\!\neq_{Q,\varnothing}^{\mathsf{p}(X),(\mathsf{p}(\mathsf{a}),1)} \mid :\!\neq_{Q,\varnothing}^{\mathsf{p}(X),(\mathsf{p}(\mathsf{b}),2)} \mid ?_0 \;;\; (\mathsf{p}(\mathsf{a}), 1) \mid (\mathsf{p}(\mathsf{b}), 2) \;;\; \varepsilon} \\
\textsc{RetSuc} & \underline{(Q[X/\mathsf{a}])_{\{X/\mathsf{a}\}} \mid :\!\neq_{Q,\varnothing}^{\mathsf{p}(X),(\mathsf{p}(\mathsf{b}),2)} \mid ?_0 \;;\; (\mathsf{p}(\mathsf{b}), 2) \;;\; \varepsilon} \\
\vdots & \\
\textsc{RetSuc} & \underline{(\mathsf{assertz}(\mathsf{p}(\mathsf{b})), \mathsf{fail})_{\{X/\mathsf{a}\}} \mid :\!\neq_{Q,\varnothing}^{\mathsf{p}(X),(\mathsf{p}(\mathsf{b}),2)} \mid ?_0 \;;\; \varepsilon \;;\; \varepsilon} \\
\textsc{AssZ} & \underline{\mathsf{fail}_{\{X/\mathsf{a}\}} \mid :\!\neq_{Q,\varnothing}^{\mathsf{p}(X),(\mathsf{p}(\mathsf{b}),2)} \mid ?_0 \;;\; (\mathsf{p}(\mathsf{b}), 3) \;;\; \varepsilon} \\
\textsc{Fail} & \underline{:\!\neq_{Q,\varnothing}^{\mathsf{p}(X),(\mathsf{p}(\mathsf{b}),2)} \mid ?_0 \;;\; (\mathsf{p}(\mathsf{b}), 3) \;;\; \varepsilon} \\
\textsc{RetSuc} & \underline{(Q[X/\mathsf{b}])_{\{X/\mathsf{b}\}} \mid ?_0 \;;\; (\mathsf{p}(\mathsf{b}), 3) \;;\; \varepsilon} \\
\vdots & \\
\textsc{Failure} & \varepsilon \;;\; (\mathsf{p}(\mathsf{b}), 3) \;;\; \varepsilon
\end{array}
$$

Fig. 9. Evaluation for a Query using assertz and retract

with $\mathsf{p}(\mathsf{a})$, the first clause $(\mathsf{p}(\mathsf{a}), 1)$ is retracted from $\mathcal{D}$. Due to the unifier $\{X/\mathsf{a}\}$, the term $(X{=}\mathsf{a})[X/\mathsf{a}]$ is satisfied. Hence, $\mathsf{retract}(\mathsf{p}(\mathsf{b}))$ and $\mathsf{assertz}(\mathsf{p}(\mathsf{b}))$ are executed, i.e., the clause $(\mathsf{p}(\mathsf{b}), 2)$ is removed from $\mathcal{D}$ and a new clause $(\mathsf{p}(\mathsf{b}), 3)$ is added to $\mathcal{D}$. When backtracking due to the term fail at the end of the query, the execution of $\mathsf{retract}(\mathsf{p}(X))$ is again successful, i.e., the retraction described by the marker $:\!\neq_{Q,\varnothing}^{\mathsf{p}(X),(\mathsf{p}(\mathsf{b}),2)}$ succeeds since $\mathsf{p}(X)$ also unifies with the clause $(\mathsf{p}(\mathsf{b}), 2)$. However, this retract-statement does not modify $\mathcal{D}$ anymore, since $(\mathsf{p}(\mathsf{b}), 2)$ is no longer contained in $\mathcal{D}$. Due to the unifier $\{X/\mathsf{b}\}$, the next term $(X{=}\,\mathsf{a})[X/\mathsf{b}]$ is not satisfiable and the whole query fails. However, then $\mathcal{D}$ still contains $(\mathsf{p}(\mathsf{b}), 3)$. Hence, afterwards a query like $\mathsf{p}(X)$ would yield the answer substitution $\{X/\mathsf{b}\}$. See Fig. 9 for the evaluation of this example using our inference rules.

6 Exception Handling

Prolog provides an *exception handling mechanism* by means of two built-in predicates throw and catch. The unary predicate throw is used to "throw" exception terms and the predicate catch can react on thrown exceptions.

When reaching a term $\mathsf{catch}(t, c, r)$, the term t is called. During this call, an exception term e might be thrown. If e and c unify with the mgu σ, the recover term r is instantiated by σ and called. Otherwise, the effect of the catch-call is the same as a call to $\mathsf{throw}(e)$. If no exception is thrown during the execution of $\mathsf{call}(t)$, the catch has no other effect than this call.

To model the behavior of catch and throw, we augment each goal in our states by context information for every catch-term that led to this goal. Such a catch-*context* is a 5-tuple (m, c, r, Q, δ), consisting of a natural number m which marks the scope of the corresponding catch-term, a catcher term c describing which exception terms to catch, a recover term r which is evaluated in case of a caught

$$\frac{(\mathsf{catch}(t,c,r),Q)_{\delta,C} \mid S \;;\; \mathcal{D} \;;\; A}{\mathsf{call}(t)_{\varnothing,\, C|(m,c,r,Q,\delta)} \mid ?_m \mid S \;;\; \mathcal{D} \;;\; A}\ (\textsc{Catch})\ \text{where } m \text{ is fresh}$$

$$\frac{(\mathsf{throw}(e),Q)_{\theta,\, C|(m,c,r,Q',\delta)} \mid S' \mid ?_m \mid S \;;\; \mathcal{D} \;;\; A}{(\mathsf{call}(r\sigma),Q'\sigma)_{\delta\sigma,\, C} \mid S \;;\; \mathcal{D} \;;\; A}\ (\textsc{ThrowSuccess})\ \begin{array}{l}\text{if } e \notin \mathcal{V} \text{ and } \sigma = \\ mgu(c,e') \text{ for a} \\ \text{fresh variant } e' \text{ of } e\end{array}$$

$$\frac{(\mathsf{throw}(e),Q)_{\theta,\, C|(m,c,r,Q',\delta)} \mid S' \mid ?_m \mid S \;;\; \mathcal{D} \;;\; A}{(\mathsf{throw}(e),Q)_{\theta,\, C} \mid S \;;\; \mathcal{D} \;;\; A}\ (\textsc{ThrowNext})\ \begin{array}{l}\text{if } e \notin \mathcal{V} \text{ and} \\ mgu(c,e') = \mathit{fail} \\ \text{for a fresh variant} \\ e' \text{ of } e\end{array}$$

$$\frac{(\mathsf{throw}(e),Q)_{\theta,\varepsilon} \,|\, S\,;\, \mathcal{D};\, A}{\mathsf{ERROR}}\ (\textsc{ThrowErr})\ \text{if } e \notin \mathcal{V} \qquad \frac{\square_{\theta,\varepsilon} \,|\, S\,;\, \mathcal{D};\, A}{S\,;\, \mathcal{D};\, A \,|\, \theta}\ (\textsc{Success})\ \begin{array}{l}\text{if } S \text{ contains} \\ \text{no } \mathsf{findall}\text{-} \\ \text{suspensions}\end{array}$$

$$\frac{\square_{\theta,\, C|(m,c,r,Q,\delta)} \mid S' \mid ?_m \mid S \;;\; \mathcal{D} \;;\; A}{(Q\theta)_{\delta\theta,\, C} \mid S' \mid ?_m \mid S \;;\; \mathcal{D} \;;\; A}\ (\textsc{CatchNext})\ \begin{array}{l}\text{if } S' \text{ contains no} \\ \mathsf{findall}\text{-suspensions}\end{array}$$

$$\frac{\square_{\theta,C} \mid S' \mid \%^{r,\ell,s}_{Q',\delta',C'} \mid S \;;\; \mathcal{D} \;;\; A}{S' \mid \%^{r,\ell|r\theta,s}_{Q',\delta',C'} \mid S \;;\; \mathcal{D} \;;\; A}\ (\textsc{FindNext})\ \begin{array}{l}\text{if } S' \text{ contains no } \mathsf{findall}\text{-suspensions and} \\ (\, C \text{ is either empty or else its last element} \\ \text{is } (m,c,r,Q,\delta) \text{ and } S' \text{ contains no } ?_m\,)\end{array}$$

Fig. 10. Additional Inference Rules for Prolog Programs with Error Handling

exception, as well as a query Q and a substitution δ describing the remainder of the goal after the catch-term. In general, we denote a list of catch-contexts by C and write $Q_{\delta,C}$ for a goal with the query Q and the annotations δ and C.

To evaluate $(\mathsf{catch}(t,c,r),Q)_{\delta,C}$, we append the catch-context (m,c,r,Q,δ) (where m is a fresh number) to C (denoted by "$C \mid (m,c,r,Q,\delta)$") and replace the catch-term by $\mathsf{call}(t)$, cf. (Catch) in Fig. 10. To identify the part of the list of goals that is caused by the evaluation of this call, we add a scope marker $?_m$.

When a goal $(\mathsf{throw}(e),Q)_{\theta,\, C|(m,c,r,Q',\delta)}$ is reached, we drop all goals up to the marker $?_m$. If c unifies with a fresh variant e' of e using an mgu σ, we replace the current goal by the instantiated recover goal $(\mathsf{call}(r\sigma),Q'\sigma)_{\delta\sigma,\, C}$ using the rule (ThrowSuccess). Otherwise, in the rule (ThrowNext), we just drop the last catch-context and continue with the goal $(\mathsf{throw}(e),Q)_{\theta,C}$. If an exception is thrown without a catch-context, then this corresponds to a program error. To this end, we extend the set of states by an additional element ERROR.

Since we extended goals by a list of catch-contexts, we also need to adapt all previous inference rules slightly. Except for (Success) and (FindNext), this is straightforward[12] since the previous rules neither use nor modify the catch-contexts. As catch-contexts can be converted into goals, findall-suspensions $\%$ and retract-markers $:\!\neq$ have to be annotated with lists of catch-contexts, too.

An interesting aspect is the interplay of nested catch- and findall-calls. When

[12] However, several built-in predicates (e.g., call and findall) impose "error conditions". If their arguments do not have the required form, an exception is thrown. Thus, the rules for these predicates must also be extended appropriately, cf. [21].

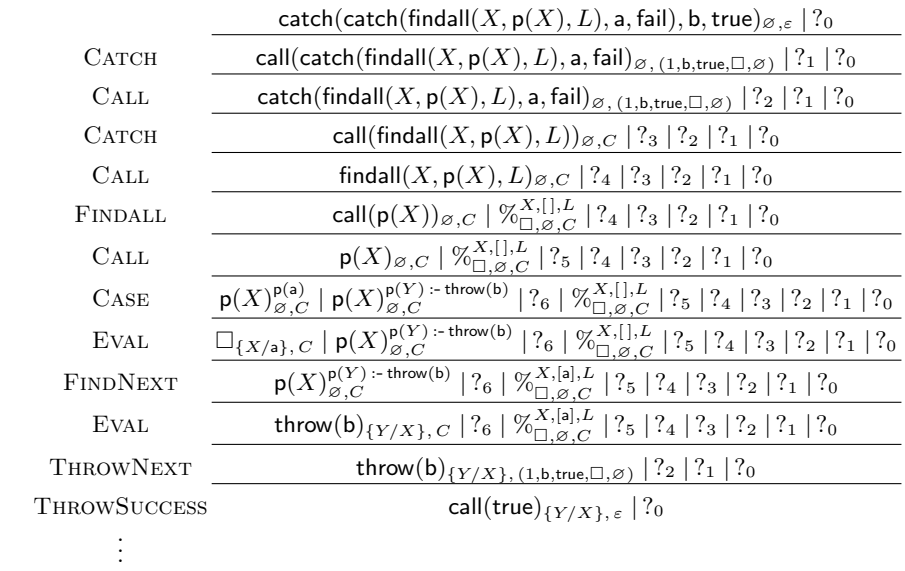

Fig. 11. Evaluation for a Query of Nested catch- and findall-Calls

reaching a goal $\square_{\theta,\,C|(m,c,r,Q,\delta)}$ which results from the evaluation of a catch-term, it is not necessarily correct to continue the evaluation with the goal $(Q\theta)_{\delta\theta,\,C}$ as in the rule (CatchNext). This is because the evaluation of the catch-term may have led to a findall-call and the current "success" goal $\square_{\theta,\,C|(m,c,r,Q,\delta)}$ resulted from this findall-call. Then one first has to compute the remaining solutions to this findall-call and one has to keep the catch-context (m, c, r, Q, δ) since these computations may still lead to exceptions that have to be caught by this context. Thus, then we only add the computed answer substitution θ to its corresponding findall-suspension, cf. the modified (FindNext) rule.

For the program with the fact $\mathsf{p}(\mathsf{a})$ and the rule $\mathsf{p}(Y) :- \mathsf{throw}(\mathsf{b})$, an evaluation of a query with catch and findall is given in Fig. 11. Here, the clauses $\mathcal{D}$ for dynamic predicates and the list A of answer substitutions were omitted for readability. Moreover, C stands for the list $(1, \mathsf{b}, \mathsf{true}, \square, \varnothing) \mid (3, \mathsf{a}, \mathsf{fail}, \square, \varnothing)$.

7 Equivalence to the ISO Semantics

In this section, we formally define our new semantics for Prolog and show that it is equivalent to the semantics defined in the ISO standard [11, 13]. All definitions and theorems refer to the *full* set of inference rules (handling full Prolog). As mentioned, all inference rules and all proofs can be found in [21].

Theorem 1 ("Mutual Exclusion" of Inference Rules). *For each state, there is at most one inference rule applicable and the result of applying this rule is unique up to renaming of variables and of fresh numbers used for markers.*

Let $s_0 \rightsquigarrow s_1$ denote that the state s_0 was transformed to the state s_1 by one of our inference rules. Any finite or infinite sequence $s_0 \rightsquigarrow s_1 \rightsquigarrow s_2 \rightsquigarrow \ldots$ is

called a *derivation* of s_0. Thm. 1 implies that any state has a unique maximal derivation (which may be infinite). Now we can define our semantics for Prolog.

Definition 2 (Linear Semantics for Prolog). *Consider a Prolog program with the clauses $\mathcal{P}$ for static predicates and the clauses $\overline{\mathcal{D}}$ for dynamic predicates. Let $\mathcal{D}$ result from $\overline{\mathcal{D}}$ by labeling each clause in $\overline{\mathcal{D}}$ by a fresh natural number. Let Q be a query and let $s_Q = \langle S_Q; \mathcal{D}; \varepsilon \rangle$ be the* corresponding initial state*, where $S_Q = (Q[!/!_0])_{\varnothing,\varepsilon} \mid ?_0$.*

(a) We say that the execution of Q has length $\ell \in \mathbb{N} \cup \{\infty\}$ *iff the maximal derivation of s_Q has length ℓ. In particular, Q is called* terminating *iff $\ell \neq \infty$.*
(b) We say that Q leads to a program error *iff the maximal derivation of s_Q is finite and ends with the state* ERROR*.*
(c) We say that Q leads to the (finite or infinite) list of answer substitutions *A iff either the maximal derivation of s_Q is finite and ends with a state $\langle \varepsilon; \mathcal{D}'; A \rangle$, or the maximal derivation of s_Q is infinite and for every finite prefix A' of A, there exists some S and $\mathcal{D}'$ with $s_Q \rightsquigarrow^* \langle S; \mathcal{D}', A' \rangle$. As usual, $\rightsquigarrow^*$ denotes the transitive and reflexive closure of $\rightsquigarrow$.*

In contrast to Def. 2, the ISO standard [11, 13] defines the semantics of Prolog using search trees. These search trees are constructed by a depth-first search from left to right, where of course one avoids the construction of parts of the tree that are not needed (e.g., because of cuts). In the ISO semantics, we have the following for a Prolog program $\mathcal{P}$ and a query Q:[13]

(a) The execution of Q has *length* $k \in \mathbb{N} \cup \{\infty\}$ iff k unifications are needed to construct the search tree (where the execution of a built-in predicate also counts as at least one unification step).[14] Of course, here every unification attempt is counted, no matter whether it succeeds or not. So in the program with the fact p(a), the execution of the query p(b) has length 1, since there is one (failing) unification attempt.
(b) Q leads to a *program error* iff during the construction of the search tree one reaches a goal $(\mathsf{throw}(e), Q)$ and the thrown exception is not caught.
(c) Q leads to the list of *answer substitutions* A iff Q does not lead to a program error and A is the list of answer substitutions obtained when traversing the (possibly infinite) search tree by depth-first search from left to right.

Thm. 3 (a) shows that our semantics and the ISO semantics result in the same termination behavior. Moreover, the computations according to the ISO semantics and our maximal derivations have the same length up to a constant factor. Thus, our semantics can be used for termination and complexity analysis of Prolog. Thm. 3 (b) states that our semantics and the ISO semantics lead to the same program errors and in (c), we show that the two semantics compute

[13] See [21] for a more formal definition.
[14] In other words, even for built-in predicates p, the evaluation of an atom $p(t_1, \ldots, t_n)$ counts as at least one unification step. For example, this is needed to ensure that the execution of queries like "repeat, fail" has length ∞.

the same answer substitutions (up to variable renaming).[15]

Theorem 3 (Equivalence of Our Semantics and the ISO Semantics). *Consider a a Prolog program and a query Q.*

(a) Let ℓ be the length *of Q's execution according to our semantics in Def. 2 and let k be the* length *of Q's execution according to the ISO semantics. Then we have $k \leq \ell \leq 3 \cdot k + 1$. So in particular we also obtain $\ell = \infty$ iff $k = \infty$ (i.e., the two semantics have the same termination behavior).*

(b) Q leads to a program error *according to our semantics in Def. 2 iff Q leads to a* program error *according to the ISO semantics.*

(c) Q leads to a (finite or infinite) list of answer substitutions $\delta_0, \delta_1, \ldots$ *according to our semantics in Def. 2 iff Q leads to a list of* answer substitutions $\theta_0, \theta_1, \ldots$ *according to the ISO semantics, where the two lists have the same length $n \in \mathbb{N} \cup \{\infty\}$ and for each $i < n$, there exists a variable renaming τ_i such that for all variables X in the query Q, we have $X\theta_i = X\delta_i\,\tau_i$.*

To see why we do not have $\ell = k$ in Thm. 3(a), consider again the program with the fact $\mathsf{p(a)}$ and the query $\mathsf{p(b)}$. While the ISO semantics only needs $k = 1$ unification attempt, our semantics uses 3 steps to model the failure of this proof. Moreover, in the end we need one additional step to remove the marker $?_0$ constructed in the initial state. The evaluation is shown in Fig. 12, where we omitted the catch-contexts and the components for dynamic predicates and answer substitutions for readability. So in this example, we have $\ell = 3 \cdot k + 1 = 4$.

$$\begin{array}{rc} & (\mathsf{p(b)})_{\varnothing} \mid ?_0 \\ \textsc{Case} & \hline (\mathsf{p(b)})_{\varnothing}^{\mathsf{p(a)}} \mid ?_1 \mid ?_0 \\ \textsc{Backtrack} & \hline ?_1 \mid ?_0 \\ \textsc{Failure} & \hline ?_0 \\ \textsc{Failure} & \hline \varepsilon \end{array}$$

Fig. 12. Evaluation for $\mathsf{p(b)}$

8 Conclusion

We have presented a new operational semantics for full Prolog (as defined in the corresponding ISO standard [11, 13]) including the cut, "all solution" predicates like findall, dynamic predicates, and exception handling. Our semantics is *modular* (i.e., easy to adapt to subsets of Prolog) and *linear* resp. *local* (i.e., derivations are lists instead of trees and even the cut and exceptions are local operations where the next state in a derivation only depends on the previous state).

We have proved that our semantics is equivalent to the semantics based on search trees defined in the ISO standard w.r.t. both termination behavior and computed answer substitutions. Furthermore, the number of derivation steps in our semantics is equal to the number of unifications needed for the ISO semantics (up to a constant factor). Hence, our semantics is suitable for (possibly automated) analysis of Prolog programs, for example for static analysis of termination and complexity using an abstraction of the states in our semantics as in [19, 20].

In [19, 20], we already successfully used a subset of our new semantics for automated termination analysis of definite logic programs with cuts. In future work, we will extend termination analysis to deal with all our inference rules in

[15] Moreover, the semantics are also equivalent w.r.t. the side effects of a program (like the changes of the dynamic clauses, input and output, etc.).

order to handle full Prolog as well as to use the new semantics for asymptotic worst-case complexity analysis. We further plan to investigate uses of our semantics for debugging and tracing applications exploiting linearity and locality.

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A Strategy Language for Graph Rewriting

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Abstract. We give a formal semantics for a graph-based programming language, where a program consists of a collection of graph rewriting rules, a user-defined strategy to control the application of rules, and an initial graph to be rewritten. The traditional operators found in strategy languages for term rewriting have been adapted to deal with the more general setting of graph rewriting, and some new constructs have been included in the language to deal with graph traversal and management of rewriting positions in the graph. This language is part of the graph transformation and visualisation environment PORGY.
Keywords: port graph, graph rewriting, strategies, visual environment

1 Introduction

Rewriting [5, 36] is a transformation process based on the use of rules that are applied to syntactic objects (words, terms, programs, proofs, graphs, etc.). It has a variety of applications; for instance, it is used to simplify algebraic expressions in computer algebra, to perform syntactic analysis of programs or natural language expressions, to define the operational semantics of a programming language, to study the structure of a group or a monoid, or to express the computational content of a mathematical proof. Other practical applications include program refactoring, code optimisation in compilers, specification of security policies, or the modelling of complex systems in biology.

To model complex systems, graphical formalisms have clear advantages, in particular in the earlier phases of the specification: graphical formalisms are more intuitive and make it easier to visualise a system and convey intuitions or ideas about it. Graph rewriting rules can be used to model their dynamic evolution. Computing by graph rewriting is also a fundamental concept in concurrency. From a theoretical point of view, graph rewriting comes with solid logic, algebraic and categorical foundations [14, 16], and from a practical point of view, graph transformations have many applications in specification, programming, and simulation tools [16]. In this paper, we focus on *port graph rewriting systems* [3], a general class of graph rewriting systems that have been successfully used to model biochemical systems and interaction net systems [25].

When the graphs are large or growing along transformations, or when the number of graph rewriting rules is big, visualisation becomes crucial to under-

stand the evolution of the system. PORGY [2] is a visual environment that allows users to define graphs and graph rewriting rules, and to experiment with a graph rewriting system in an interactive way. To control the application of graph rewriting rules, PORGY uses a *strategy language*, which is the main subject of this paper.

Reduction strategies define which (sub)expression(s) should be selected for evaluation and which rule(s) should be applied (see [24, 12] for general definitions). These choices affect fundamental properties of computations such as laziness, strictness, completeness, termination and efficiency, to name a few (see, e.g.,[39, 37, 26]). Used for a long time in λ-calculus [8], strategies are present in programming languages such as Clean [29], Curry [22], and Haskell [23] and can be explicitely defined to rewrite terms in languages such as ELAN [11], Stratego [38], Maude [27] or Tom [7]. They are also present in graph transformation tools such as PROGRES [35], AGG [17], Fujaba [28], GROOVE [33], GrGen [19] and GP [32]. PORGY's strategy language draws inspiration from these previous works, but a distinctive feature of PORGY's language is that it allows users to define strategies including not only operators to combine graph rewriting rules but also operators to define the location in the target graph where rules should, or should not, apply. The latter is useful to specify graph traversal algorithms, and in general when programming on graphs, as shown in [18].

The PORGY environment is described in [2], and [18] illustrates various programming techniques through detailed examples. In this paper, we focus on the design and implementation of the strategy language. Our main contribution is a precise description and formal semantics for the language, which allows users to analyse programs and reason about computations. The formal semantics has also been used as a basis for the implementation of the language.

The strategy language is used to control PORGY's rewrite engine: it allows users to *create rewriting derivations* and *specify graph traversals and graph transformations in a modular way*. To achieve the latter, the language offers a set of primitives to select rewriting rules and a set of primitives to select the *position* where the rules apply. Users can select subgraphs to use as focusing positions for rewriting interactively (in a direct and visual way) or intensionally (using a focusing expression). Alternatively, positions could be encoded in the rewrite rules using labels or markers (as done in other languages based on graph rewriting which do not have focusing primitives). We prefer to separate the two notions (positions and rules) to make programs more readable (the rewrite rules are not cluttered with encodings), and easier to maintain and adapt. In this sense, the language is modular: for example, to change the traversal algorithm it is sufficient to change the strategy and not the whole rewriting system.

The paper is organised as follows. In Section 2, we recall the concept of port graph. Section 3 is the core of the paper: we present the syntax of the strategy language and formally define its semantics. Section 4 illustrates the language with examples, and Section 5 states properties. Section 6 briefly describes its implementation in PORGY. Section 7 discusses related languages before concluding and giving directions for future work.

2 Background: Port Graph Rewriting

There are several definitions of graph rewriting, using different kinds of graphs and rewriting rules (see, for instance, [13, 20, 9, 31, 10, 25]). In this paper we consider port graph rewriting systems, of which interaction nets [25] are a particular case. We recall below the main notions of port graph rewriting, and refer to [3, 4] for more details and examples of port graphs.

Port graphs. Intuitively, a port graph is a graph where nodes have explicit connection points called *ports*; edges are attached to ports.

Let $\mathscr{N}$ and $\mathscr{P}$ be two disjoint sets of node names and port names respectively. A *p-signature* over $\mathscr{N}$ and $\mathscr{P}$ is a mapping $\nabla : \mathscr{N} \to 2^{\mathscr{P}}$ which associates a finite set of port names to a node name. A p-signature can be extended with variables: $\nabla^{\mathcal{X}} : \mathscr{N} \cup \mathcal{X}_{\mathscr{N}} \to 2^{\mathscr{P} \cup \mathcal{X}_{\mathscr{P}}}$, where $\mathcal{X}_{\mathscr{P}}$ and $\mathcal{X}_{\mathscr{N}}$ are two disjoint sets of port name variables and node name variables respectively. A *labelled port graph* over a *p-signature* $\nabla^{\mathcal{X}}$ is a tuple $G = \langle V_G, lv_G, E_G, le_G \rangle$ where: V_G is a finite set of nodes; $lv_G : V_G \to \mathscr{N} \cup \mathcal{X}_{\mathscr{N}}$ is an injective labelling function for nodes; $E_G \subseteq \{\langle (v_1, p_1), (v_2, p_2) \rangle \mid v_i \in V_G, p_i \in \nabla^{\mathcal{X}}(lv_G(v_i)) \cup \mathcal{X}_{\mathscr{P}}\}$ is a finite multiset of edges; $le_G : E_G \to (\mathscr{P} \cup \mathcal{X}_{\mathscr{P}}) \times (\mathscr{P} \cup \mathcal{X}_{\mathscr{P}})$ is an injective labelling function for edges such that $le_G(\langle (v_1, p_1), (v_2, p_2) \rangle) = (p_1, p_2)$. A port may be associated to a state (for instance, active/inactive or principal/auxiliary); this is formalised using a mapping from ports to port states. Similarly, nodes can also have associated properties (like colour or shape that are used for visualisation properties and for the `Property()` operator shown in 3).

It is worth noticing that a port graph can be considered as a labelled graph where: (1) each node v with ports $p_1, \ldots, p_n$ translates to a graph consisting of a *center*-labelled node v, n *port*-labelled nodes $p_1, \ldots, p_n$, and edges connecting the center to each of the ports; (2) the edges between two ports in a port graph are translated as edges between the two corresponding port-labelled nodes. Conversely, any labelled graph is a port graph in which each (port graph) node has a number of ports equal to the arity of its label.

As a consequence of this remark, expressivity results, computational power, as well as correctness and completeness results on labelled graphs and rewriting can be translated to port graphs. This is the approach taken here for defining the concepts of rewriting on port graphs.

Let G and H be two port graphs over the same p-signature $\nabla^{\mathcal{X}}$. A *port graph morphism* $f : G \to H$ maps elements of G to elements of H preserving sources and targets of edges, constant node names and associated port name sets, up to variable renaming. We say that G and H are *isomorphic* if $f : V_G \times \nabla(lv_G(V_G)) \to V_H \times \nabla(lv_H(V_H))$ is bijective.

A *port graph rewrite rule* $L \Rightarrow R$ is itself represented as a port graph consisting of two port graphs L and R over the same p-signature and one special node $\Rightarrow$, called *arrow node*. L and R are called the *left-* and *right-hand side* respectively. The arrow node describes the interface of the rule as follows. For each port p in L, to which corresponds a non-empty set of ports $\{p_1, \ldots, p_n\}$ in R, the arrow node has a unique port r and the incident directed edges (p, r) and

(r, p_i), for all $i = 1, \ldots, n$; all ports from L that are deleted in R are connected to the *black hole* port of the arrow node. When the correspondence between ports in the left- and right-hand sides of the rule is obvious we omit the ports and edges involving the arrow node. The arrow node is used to avoid dangling edges during rewriting (see [20, 13]). Full details can be found in [1].

Port Graph Rewriting. Let $L \Rightarrow R$ be a port graph rewrite rule and G a port graph such that there is an injective port graph morphism g from L to G; hence $g(L)$ is a subgraph of G. A *rewriting step* on G using $L \Rightarrow R$, written $G \rightarrow_{L \Rightarrow R} G'$, transforms G into a new graph G' obtained from G by replacing the subgraph $g(L)$ of G by $g(R)$, and connecting $g(R)$ to the rest of the graph as specified in the arrow node of the rule. We call $g(L)$ a redex, and say that G rewrites to G' using $L \Rightarrow R$ at the position defined by $g(L)$, or that G' is a *result* of applying $L \Rightarrow R$ on G at $g(L)$. Several injective morphisms g from L to G may exist (leading to different rewriting steps); they are computed as solutions of a *matching* problem from L to (a subgraph of) G. If there is no such injective morphism, we say that G is *irreducible* by $L \Rightarrow R$. Given a finite set $\mathcal{R}$ of rules, a port graph G *rewrites* to G', denoted by $G \rightarrow_{\mathcal{R}} G'$, if there is a rule r in $\mathcal{R}$ such that $G \rightarrow_r G'$. This induces a transitive relation on port graphs, denoted by $\rightarrow^*_{\mathcal{R}}$. Each *rule application* is a rewriting step and a *derivation*, or computation, is a sequence of rewriting steps. A port graph on which no rule is applicable is in *normal form*. Rewriting is intrinsically non-deterministic since it may be possible to rewrite several subgraphs of a port graph with different rules or use the same one at different places, possibly getting different results.

3 Strategy Language

We introduce the concept of graph program and give the syntax and semantics of the strategy language. In addition to the well-known constructs to select rewrite rules, the language provides primitives to focus on specific positions on the graph that are selected or banned for rewriting. Focusing is useful to program graph traversals, for instance, and is a distinctive feature of the language.

Definition 1. *A* located graph G^Q_P *consists of a port graph G and two distinguished subgraphs P and Q of G, called respectively the* position subgraph*, or simply position, and the* banned subgraph*.*

In a located graph G^Q_P, P represents the subgraph of G where rewriting steps may take place (i.e., P is the focus of the rewriting) and Q represents the subgraph of G where rewriting steps are forbidden. We give a precise definition below; the intuition is that subgraphs of G that overlap with P may be rewritten, if they are outside Q. When applying a port graph rewrite rule, not only the underlying graph G but also the position and banned subgraphs may change. A *located port graph rewrite rule*, defined below, specifies two disjoint subgraphs M and N of the right-hand side R that are used to update the position and banned subgraphs, respectively. If M (resp. N) is not specified, R (resp. the

empty graph $\emptyset$) is used as default. Below, the set operators union, intersection and complement (denoted respectively $\cup, \cap, \setminus$) apply to graphs considered as sets of nodes and edges.

Definition 2. *A* located port graph rewrite rule *is given by a port graph rewrite rule $L \Rightarrow R$ and two disjoint subgraphs M and N of R. It is denoted $(L \Rightarrow R)^N_M$. A located graph G^Q_P is rewritten to $G'^{Q'}_{P'}$ using $(L \Rightarrow R)^N_M$ if $G \rightarrow_{L \Rightarrow R} G'$ by choosing a morphism g such that $g(L) \cap P$ is not empty and $g(L) \cap Q$ is empty; the new position P' is then defined as $P' = (P \setminus g(L)) \cup g(M)$; the new banned subgraph Q' is then defined as $Q' = Q \cup g(N)$.*

In general, for a given rule $(L \Rightarrow R)^N_M$ and located graph G^Q_P, more than one morphism g, such that $g(L) \cap P$ is not empty and $g(L) \cap Q$ is empty, might exist (i.e., several rewriting steps at P avoiding Q might be possible). Thus, the application of the rule at the position P avoiding Q produces a *set of results*. In practice, when several results are possible, one is computed (non-deterministically), *backtracking* to try another one if later the strategy fails.

Definition 3. *A* graph program *is given by a set of located port graph rewrite rules $\mathcal{R}$, a strategy expression S (built from $\mathcal{R}$ using the grammar below) and a located graph G^Q_P. It is denoted by $\left[S_{\mathcal{R}}, G^Q_P\right]$, or simply $\left[S, G^Q_P\right]$ when $\mathcal{R}$ is clear from the context.*

The formal semantics of the language will be given below, using an Abstract Reduction System [36, 24, 12]. Given a graph program $\left[S_{\mathcal{R}}, G^Q_P\right]$, derivations are built according to the strategy $S_{\mathcal{R}}$, resulting in a *derivation tree*. Irreducible graph programs have the form $\left[\mathsf{Id}, G^Q_P\right]$ or $\left[\mathsf{Fail}, G^Q_P\right]$, depending on whether the strategy on the initial graph program is successful or not. A graph program may define a non-terminating computation (if there is an infinite derivation) or may produce several results (if there are several finite branches). The *result set* for a graph program is the set of leaves in the derivation tree.

3.1 Syntax and Informal Description

The syntax of the strategy language is given in Figure 1. The *strategy expressions* used in graph programs are generated by the non-terminal S. A strategy expression combines rule applications, generated by A, and focusing operations, generated by F. The application constructs and some of the strategy constructs in the language are strongly inspired from existing rewriting strategy languages such as ELAN [11], Stratego [38] and Tom [7]. The following syntax is a revised and simplified version of the one found in [2, 18]; the main difference is that we now have an explicit notion of banned subgraph and a more concise syntax for iterative commands.

Focusing. These constructs are functions from graph programs to port graphs: they apply on a graph program $\left[S_{\mathcal{R}}, G^Q_P\right]$ and return a subgraph of G. They are

Let L, R be port graphs, M, N positions, ρ a property, m, n integers, $p_i \in [0, 1]$.

$$\begin{aligned}
\textbf{(Focusing)}\quad & F := \texttt{CrtGraph} \mid \texttt{CrtPos} \mid \texttt{CrtBan} \mid \texttt{AllSuc}(F) \mid \texttt{OneSuc}(F) \\
& \mid \texttt{NextSuc}(F) \mid \texttt{Property}(\rho, F) \mid F \cup F \mid F \cap F \mid F \setminus F \mid \emptyset \\
\textbf{(Applications)}\quad & A := \mathsf{Id} \mid \mathsf{Fail} \mid (L \Rightarrow R)^N_M \mid (A \parallel A) \\
\textbf{(Strategies)}\quad & S := A \mid S; S \mid \texttt{ppick}(S_1, p_1, \ldots, S_i, p_i) \\
& \mid \texttt{while}(S)\texttt{do}(S) \mid (S)\texttt{orelse}(S) \\
& \mid \texttt{if}(S)\texttt{then}(S)\texttt{else}(S) \mid \texttt{isEmpty}(F) \\
& \mid \texttt{setPos}(F) \mid \texttt{setBan}(F)
\end{aligned}$$

Fig. 1. Syntax of the strategy language.

used in strategy expressions to change the positions P and Q where rules apply and to specify different types of graph traversals.

- `CrtGraph` returns the whole graph G, `CrtPos` returns the current position subgraph P in the located graph, and `CrtBan` returns the current banned subgraph Q in the located graph.
- `AllSuc`(F) returns the subgraph consisting of all the immediate successors of the nodes in F, where an immediate successor of a node v is a node that has a port connected to a port of v. `OneSuc`(F) returns a subgraph consisting of one immediate successor of a node in F, chosen non-deterministically. `NextSuc`(F) computes successors of nodes in F using for each node only a subset of its ports; we call the ports in this distinguished subset the *next* ports (so `NextSuc`(F) returns a subset of the nodes in `AllSuc`(F)).
- `Property`(ρ, F) is a filtering construct, that returns a subgraph of G containing only the nodes from F that satisfy the decidable property ρ. It typically tests a property on nodes or ports, allowing us for instance to select the subgraph of red nodes or nodes with active ports (as mentioned in Section 2, ports and nodes in port graphs may have associated properties).
- The set theory operators compute new expressions from the previous constructs.

Applications. The focusing subgraphs P and Q in the target graph and the distinguished graphs M and N in a located port graph rewrite rule are original features of the language. A rule can only be applied if at least a part of the redex is in P and cannot be applied on Q.

- Id is a basic strategy that never fails and leaves the graph unchanged whereas Fail leaves the graph unchanged and returns failure.
- $(L \Rightarrow R)^N_M$ represents the application of the rule $L \Rightarrow R$ at the current position P and avoiding Q in G^Q_P.
- $A \parallel A'$ represents simultaneous application of A and A' on disjoint subgraphs of G and returns Id only if both applications are possible and Fail otherwise.

Strategies.

- The expression $S; S'$ represents sequential application of S followed by S', as usual.
- When probabilities $p_1, \ldots, p_n \in [0, 1]$ are associated to strategies $S_1, \ldots, S_n$ such that $p_1 + \ldots + p_n = 1$, the strategy $\texttt{ppick}(S_1, p_1, \ldots, S_n, p_n)$ non-deterministically picks one of the strategies for application, according to the given probabilities.
- $\texttt{while}(S)\texttt{do}(S')$ keeps on sequentially applying S' while the expression S rewrites to Id. If it returns Fail, then Id is returned.
- $(S)\texttt{orelse}(S')$ applies S if possible, otherwise applies S' and fails if both fail.
- $\texttt{if}(S)\texttt{then}(S')\texttt{else}(S'')$ checks if the application of S to (a copy of) G_P^Q returns Id, in which case S' is applied to G_P^Q, otherwise S'' is applied.
- $\texttt{isEmpty}(F)$ returns Id if F returns an empty graph and Fail otherwise. This can be used for instance inside the condition of an `if` or `while`, to check if the strategy makes P empty or not.
- $\texttt{setPos}(F)$ (resp. $\texttt{setBan}(F)$) takes the graph resulting from a focusing expression and sets the current position subgraph P (resp. the current banned subgraph Q) to that graph.

3.2 Semantics

The focusing operators defined by the grammar for F in Fig. 1 have a functional semantics. They apply to the current located graph, and compute a subgraph (i.e., they return a subgraph of G). For instance, `CrtGraph` applied to G_P^Q returns G. We define below the result of each focusing operation on a given located graph.

$\texttt{CrtGraph}(G_P^Q)$	$= G$	$\texttt{CrtPos}(G_P^Q) = P$ $\texttt{CrtBan}(G_P^Q) = Q$
$\texttt{AllSuc}(F)(G_P^Q)$	$= G'$	where G' consists of all immediate successors of nodes in F
$\texttt{OneSuc}(F)(G_P^Q)$	$= G'$	where G' consists of one immediate successor of a node in F, chosen non-deterministically
$\texttt{NextSuc}(F)(G_P^Q)$	$= G'$	where G' consists of the immediate successors, via ports labelled "next", of nodes in F
$\texttt{Property}(\rho, F)(G_P^Q)$	$= G'$	where G' consists of all nodes in F satisfying ρ

The constructs in the grammars for A and S in Fig. 1 are defined by semantic rules given below, which are applied to graph programs $\left[S, G_P^Q\right]$ (see Definition 3). We follow a *small step* style of operational semantics [30]. The semantic rules define computation steps on configurations (graph programs or intermediate objects, denoted by angular brackets, that use auxiliary operators). We type variables in rules by naming them as the initial symbol of the corresponding grammar with an index number if needed (for example: A_1 is a variable of application type, representing a rule application or a parallel application of rules; S_3 represents a strategy expression; F_2 represents a focusing expression).

– Graph rewrite rules are themselves strategy operators.

$$[(L \Rightarrow R)^N_M, G^Q_P] \to [\mathsf{Id}, {G'}^{Q'}_{P'}] \text{ if } G^Q_P \to_{(L\Rightarrow R)^N_M} {G'}^{Q'}_{P'}$$
$$[(L \Rightarrow R)^N_M, G^Q_P] \to [\mathsf{Fail}, G^Q_P] \text{ if the rule is } \textit{not} \text{ applicable}$$

– Position definition:

$$[\mathtt{setPos}(F), G^Q_P] \to [\mathsf{Id}, G^Q_{P'}] \text{ where } P' \text{ is the result of } F$$
$$[\mathtt{setBan}(F), G^Q_P] \to [\mathsf{Id}, G^{Q'}_P] \text{ where } Q' \text{ is the result of } F$$

$$[\mathtt{isEmpty}(F), G^Q_P] \to [\mathsf{Id}, G^Q_P] \text{ if } F \text{ is an empty graph}$$
$$[\mathtt{isEmpty}(F), G^Q_P] \to [\mathsf{Fail}, G^Q_P] \text{ if } F \text{ is not an empty graph}$$

– Sequential application:

$$[S_1; S_2, G^Q_P] \to \langle [S_1, G^Q_P];_2 S_2, G^Q_P\rangle$$
$$\langle [\mathsf{Id}, {G'}^{Q'}_{P'}];_2 S_2, G^Q_P\rangle \to [S_2, {G'}^{Q'}_{P'}]$$
$$\langle [\mathsf{Fail}, {G'}^{Q'}_{P'}];_2 S_2, G^Q_P\rangle \to [\mathsf{Fail}, {G'}^{Q'}_{P'}]$$

– Conditional :

$$[\mathtt{if}(S_1)\mathtt{then}(S_2)\mathtt{else}(S_3), G^Q_P] \to \langle \mathtt{if}_2([S_1, G_P])\mathtt{then}(S_2)\mathtt{else}(S_3), G^Q_P\rangle$$
$$\langle \mathtt{if}_2([\mathsf{Id}, {G'}^{Q'}_{P'}])\mathtt{then}(S_2)\mathtt{else}(S_3), G^Q_P\rangle \to [S_2, G^Q_P]$$
$$\langle \mathtt{if}_2([\mathsf{Fail}, {G'}^{Q'}_{P'}])\mathtt{then}(S_2)\mathtt{else}(S_3), G^Q_P\rangle \to [S_3, G^Q_P]$$

– Iteration:

$$[\mathtt{while}(S_1)\mathtt{do}(S_2), G^Q_P] \to [\mathtt{if}(S_1)\mathtt{then}(\mathtt{while}(S_1)\mathtt{do}(S_2))\mathtt{else}(\mathsf{Id}), G^Q_P]$$

– Priority choice:

$$[(S_1)\mathtt{orelse}(S_2), G^Q_P] \to \langle ([S_1, G^Q_P])\mathtt{orelse}_2(S_2), G^Q_P\rangle$$
$$\langle ([\mathsf{Id}, {G'}^{Q'}_{P'}])\mathtt{orelse}_2(S_2), G^Q_P\rangle \to [\mathsf{Id}, {G'}^{Q'}_{P'}]$$
$$\langle ([\mathsf{Fail}, {G'}^{Q'}_{P'}])\mathtt{orelse}_2(S_2), G^Q_P\rangle \to [S_2, G^Q_P]$$

– Probabilistic choice:

$$[\mathtt{ppick}(S_1, p_1, \ldots, S_i, p_i), G^Q_P] \to [S_j, G^Q_P] \quad \text{if } \textit{prob}(p_1, \ldots, p_i) = j$$

where $\textit{prob}(p_1, \ldots, p_i)$ returns the element $j \in \{1 \ldots n\}$ with probability p_j.

– Parallelism is allowed through the operator $||$ which works on applications only (not on general strategies). It implements simultaneous application of rules at disjoint redexes (we profit of the ability to specify subgraphs as banned for rewriting, to ensure that the redexes are disjoint).

$$[(L \Rightarrow R)^N_M || A_2, G^Q_P] \to \langle [(L \Rightarrow R)^N_M, G^Q_P]||_2 A_2, G^Q_P\rangle$$
$$\langle [\mathsf{Id}, {G'}^{Q'}_{P'}]||_2 A, G^Q_P\rangle \to [\mathtt{setBan}(\mathtt{CrtBan} \cup (G' \setminus G)); A; \mathtt{setBan}(F), {G'}^{Q'}_{P'}]$$
where $F = \mathtt{CrtBan} \setminus ((G' \setminus G) \setminus (Q' \setminus Q))$
Here we add new elements after a rewrite into Q, do the next application and then restore Q to what it should have been using F.
$$\langle [\mathsf{Fail}, {G'}^{Q'}_{P'}]||_2 A, G^Q_P\rangle \to [\mathsf{Fail}, {G'}^{Q'}_{P'}]$$

4 Examples

In this section we give examples to illustrate the expressivity of the language. The `not` and `try` operators, well-known in strategy languages for term rewriting, are not primitive operators in our language but can also be derived. The expression `repeat`(S) that applies the strategy S as long as possible. We can also define bounded iteration and a for-loop; $|||$ is a weaker version of $\|$.

- `not`$(S) \triangleq$ `if`(S)`then`(Fail)`else`(Id) fails if S succeeds and succeeds if S fails; the graph is unchanged.
- `try`$(S) \triangleq (S)$`orelse`(Id) is a strategy that behaves like S if S succeeds, but if S fails then it behaves like Id.
- `repeat`$(S) \triangleq$ `while`(S)`do`(S) applies S as long as possible and returns Id with the graph on which S has failed.
- `while`(S_1)`do`(S_2)`max`$(n) \triangleq$ `if`(S_1)`then`$(S_2;$ `if`(S_1)`then`$(S_2; \dots)$`else`(Id)$)$`else`(Id) where $\dots$ is n times.
- `for`(n)`do`$(S) \triangleq S; \dots; S$ where S is repeated n times.
- $A \,|||\, A'$ is similar to $A||A'$ except that it returns Id if at least one application of A or A' is possible.

$$A_1|||A_2 \triangleq \texttt{if}(A_1)\texttt{then}(\texttt{if}(A_1||A_2)\texttt{then}(A_1||A_2)\texttt{else}(A_1))\texttt{else}(A_2)$$

Using focusing (specifically the `Property` construct) we can create concise strategies that perform traversals. In this way, we can define outermost or innermost rewriting on trees without needing to change the rewrite rules. This is standard in term-based languages such as ELAN or Stratego; here we can also define traversals in graphs.

- Outermost rewriting on trees: we begin by defining the starting position $start \triangleq$ `Property`$(root, G)$, which selects the subgraph containing just the root of the tree. If we define the next ports for each node in the tree to be the ones that connect with their children, then the strategy for outermost rewriting with a rule R is:
  `setPos`$(start)$;
  `repeat`$($`if`(R)`then`$(R;$ `setPos`$(start))$`else`$($`setPos`$($`NextSuc`$($`CrtPos`$))))$
- Innermost rewriting on trees: assuming the rules have no superpositions, this can be written, as for the outermost strategy, by using a strategy $start \triangleq$ `Property`$(leaf, G)$ that selects the leaves of the tree, and by defining, for each node, the "next" port to be the one that connects with the parent node.
- Interface Normal Form: this is a generalisation of the outermost strategy for graphs (not necessarily trees). We define the *interface* of a port graph G as the set of nodes of G that have a free port. They can be selected by defining the position $Int \triangleq$ `Property`$(interface, G)$. The idea is to rewrite as near as possible to the interface (i.e., outermost). For each port node, we define its next port to be the principal port of the node and compute the Interface Normal Form with respect to the rule R as follows:
  `setPos`(Int);
  `repeat`$($`if`(R)`then`$(R;$ `setPos`$(Int))$`else`$($`setPos`$($`NextSuc`$($`CrtPos`$))))$

Finally, the following example shows how a non-ordered list of three colours (Blue, Red and White) can be sorted to represent the French flag (Blue first, then White and finally Red). We have three port nodes representing each colour (shown in Figure 2) that have two ports each: a *previous* port (to the left of the node) and a *next* port (to the right of the node). We also have a $Mast$ port node at the beginning of the list.

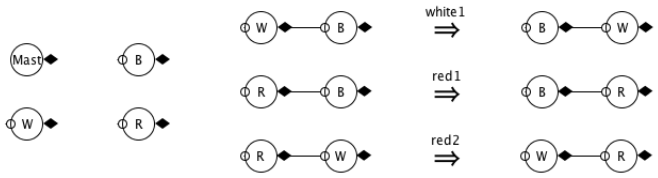

Fig. 2. The four port node types and the 3 flag sorting rules.

Using the three rules in Figure 2, we can swap two colours if they are in the wrong order. Using the ||| operator we can also attempt to apply as many of these rules as we can in parallel. Our overall strategy would then be:

$$\texttt{repeat}(\texttt{setPos}(\texttt{CrtGraph}); ((\mathit{white1}|||\mathit{red1})|||\mathit{red2}))$$

We can also program a sorting algorithm that starts from the mast. The initial P contains only the *Mast* port node. If no rule can be applied, we move P one position across the list and try again. After a rule is applied we reset P to be just *Mast*. When we reach the end of the list, the program terminates and the list is correctly ordered. By defining: $\mathit{swap} \triangleq ((\mathit{white}1)\texttt{orelse}(\mathit{red}1))\texttt{orelse}(\mathit{red}2)$ and $\mathit{backToMast} \triangleq \texttt{Property}(\mathit{mast}, \texttt{CrtGraph})$, the strategy is:

```
setPos(backToMast);
while(not(isEmpty(CrtPos)))do
(if(swap)then(swap; setPos(backToMast))else(setPos(NextSuc(CrtGraph)\CrtPos)
```

This example illustrates the modularity of programs in the language: to program a flag-sorting algorithm that proceeds from the mast onwards we do not need to change the rewrite rules (in contrast with other graph rewriting languages where focusing constructs are not available).

We give more examples of use of the language in [18], including a program to play pacman and another to create a fractal, taking advantage of the visual features of PORGY.

5 Properties

Graph programs are not terminating in general, however we can characterise a terminating sublanguage and characterise the normal forms of terminating graph programs.

Proposition 1 (Termination). *The sublanguage that excludes the* while *construct is terminating.*

Proof. (Sketch) We use an interpretation of the strategy expressions and located graphs and show that this interpretation strictly decreases with each application of a rewrite rule within the semantics. The interpretation is a lexicographic combination of the number of $||$ and $||_2$ operators, the size of the strategy expression and the rank of the root operator for the strategy expression. We define *rank 1* for all the original operators and *rank 0* for the auxiliary ones. □

Proposition 2 (Normal Forms). *A graph program* $\left[S, G_P^Q\right]$ *either rewrites indefinitely (when the strategy* S *does not terminate) or rewrites to an expression of the form* $\left[E, G_P^Q\right]$*, where* E *is* Id *or* Fail*.*

Proof. (Sketch) By inspection of the semantic rules, every graph program $[S, G_P^Q]$ different from $[\mathsf{Id}, G_P^Q]$ or $[\mathsf{Fail}, G_P^Q]$ can be matched by a left-hand side of a rule. This is true because S has a top operator which is one of the syntactic constructions and there is a semantic rule which applies to it. Moreover every expression of the form $\langle X, G_P^Q\rangle$ is reducible, because X either contains a graph program $[S, G_P^Q]$ different from $[\mathsf{Id}, G_P^Q]$ or $[\mathsf{Fail}, G_P^Q]$ that so can be matched by a left-hand side of a rule as above, or X contains $[\mathsf{Id}, G_P^Q]$ or $[\mathsf{Fail}, G_P^Q]$ and one of the auxiliary rules can apply. □

If for a given port graph rewrite rule and located graph, several redexes exist, one is arbitrarily chosen and if it leads to a failure then another one is taken. This kind of non-determinism is an inherent feature of graph rewriting systems. Beyond this, the operators `OneSuc()` and `ppick()` make graph programs non-deterministic (and do not give rise to backtracking). For the sublanguage that excludes them, we have the following unicity property for the result set:

Proposition 3 (Result Set). *Each graph program in the sublanguage that excludes* `OneSuc()` *and* `ppick()`*, has at most one set of results. In other words, the sets of leaves for all possible derivation trees associated to one graph program are identical.*

Proof. (Sketch) For the sublanguage that excludes `OneSuc()`, `ppick()` and rule applications, the semantic rules define a deterministic transition system on configurations, that is, for each configuration, at most one rule may apply. This is a consequence of the fact that there are no superpositions between rules.

The rules defining application of a port graph rewrite rule $(L \Rightarrow R)_M^N$ are non-deterministic: for a given configuration, several redexes may exist (in the case where a rule can be applied in more than one position in G_P^Q) and each of them gives rise to a branch in the tree. Although there may be more than one derivation, the set of leaves is uniquely defined. □

Proposition 4 (Completeness). *The set of graph programs* $\left[S, G_P^Q\right]$ *is Turing complete.*

Proof. (Sketch) Consequence of Theorem 1 in [21], which shows that sequence, iteration and the ability to apply a rule from a set is sufficient to simulate a Turing machine. Iteration (while) and sequence (;) are primitives in our language. The application of a rule from a set can be defined using the orelse operator. □

It is also interesting to consider which sublanguages of our language are Turing complete.

Proposition 5 (Complete sublanguage). *The sublanguage consisting of graph programs where $S_{\mathcal{R}}$ is built from* Id, Fail, *rules $(L \Rightarrow R)_M^N$ in $\mathcal{R}$, sequential composition (;), iteration (*while*), and* orelse *is Turing complete.*

Proof. (Sketch) Since Turing machine computations can be simulated using ;, while and orelse, the result follows. □

The same result could be obtained by replacing orelse with the conditional construct if then else. Perhaps more surprising is the fact that we can simulate Turing machine computations using the sublanguage consisting of sequential composition (;), iteration (while) and rule application $(L \Rightarrow R)_M^N$ together with Id, Fail and `setPos()`. This result follows from [15], where it is proved that the computations of any Turing machine can be simulated by a term rewriting system consisting of just one rule, using a strategy that forces the reduction steps to take place at specific positions (called S-deep-only derivations in [15]). We omit the details of the proof, but highlight the fact that, given a sequence of transitions in the Turing machine, Dauchet [15] shows how to build a rewrite rule to simulate the transitions, using a strategy to select the position for rewriting according to the instruction used by the machine. The `setPos()` construct can be used to simulate Dauchet's strategy directly, by moving the focus of rewriting to the corresponding subterm after each rewrite step.

6 Implementation

The strategy language defined in this paper is part of the PORGY system [2], an environment for visual modelling of complex systems through port graphs and port graph rewrite rules. PORGY provides tools to visualise traces of rewriting, and the strategy language is used in particular to guide the construction of the derivation tree.

A graph program $\left[S_{\mathcal{R}}, G_P^Q\right]$ is created in PORGY by drawing a set of rules $\mathcal{R}$ and a graph G directly in PORGY, or by importing them from a file. The positions P and Q are selected visually on the initial port graph and the strategy S is typed into a text-box where a button is available to launch the computation.

The strategy expression is first parsed to create a *strategy tree*. A *strategy engine* then takes the tree and applies a series of rewrites, according to the small-step operational semantics given above. Some of these rules call for an application or a focusing to be performed on the graph, and some of the rules require a copy of the graph to be made. This is done efficiently in PORGY thanks to the cloning functionalities of the underlying TULIP system.

7 Related Work and Conclusion

Graph rewriting is implemented in a variety of tools. Below we review some of the strategy languages used in graph rewriting tools and compare them with PORGY's language. In AGG [17], application of rules can be controlled by defining *layers* and then iterating through and across layers. PROGRES [35] allows users to define the way rules are applied and includes non-deterministic constructs, sequence, conditional and loops. The Fujaba [28] Tool Suite offers a basic strategy language, including conditionals, sequence and method calls, but no parallelism. GROOVE [33] permits to control the application of rules, via a control language with sequence, loop, random choice, try()else() and simple function calls. In GReAT [6] the pattern-matching algorithm always starts from specific nodes called "pivot nodes"; rule execution is sequential and there are conditional and looping structures. GrGen.NET [19] uses the concept of search plans to represent different matching strategies. GP [32] is a rule-based, non-deterministic programming language, where programs are defined by sets of graph rewrite rules and a textual strategy expression. The strategy language has three main control constructs: sequence, repetition and conditional, and uses a Prolog-like backtracking technique.

None of the languages above has focusing constructs; compared to these systems, the PORGY strategy language follows a more modular design, with primitives for focusing as well as traditional strategy constructs. PORGY also emphasises visualisation and scale, thanks to the TULIP back-end which can handle large graphs with millions of elements and comes with powerful visualisation and interaction features.

The strategy language defined in this paper, including the backtracking mechanism, is strongly inspired by the work on GP and PROGRES, and by the strategy languages developed for term rewriting. It can be applied to terms as a particular case (since terms are just trees). When applied to trees, the constructs dealing with applications and strategies are similar to those found in ELAN or Stratego, where users can also define strategies to apply rules in sequence, to iterate rules, etc. The focusing sublanguage on the other hand can be seen as a lower level version of these languages, because term traversals are not directly available in our language but can be programmed using focusing constructs.

The PORGY environment is still evolving. The strategy language could be enhanced by allowing, for instance, more parallelism (using techniques from the K semantic framework [34]). Verification and debugging tools for avoiding conflicting rules or non-termination for instance are planned for future work.

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Clones in logic programs and how to detect them

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Abstract. In this paper, we propose a theoretical framework that allows to capture, by program analysis, the notion of code clone in the context of logic programming. Informally, two code fragments are considered as cloned if they implement the same functionality. Clone detection can be advantageous from a software engineering viewpoint, as the presence of code clones inside a program reveals redundancy, broadly considered a "bad smell". In the paper, we present a detailed definition of a clone in a logic program and provide an efficient detection algorithm able to identify an important subclass of code clones that could be used for various applications such as program refactoring and plagiarism recognition. Our clone detection algorithm is not tied to a particular logic programming language, and can easily be instantiated for different such languages.

Keywords: logic programming languages, code clone, code duplication, clone detection algorithm

1 Introduction

Certain characteristics of a source code are usually recognized as constituting a "bad smell", meaning an indication for poor design quality [6]. Among these, an important place is taken by *code duplication*, also called *code cloning* [6]. Intuitively, two code fragments can be considered cloned if they implement an identical or sufficiently similar functionality, independent of them being textually equal or not. An example of the latter case would be two sorting procedures, the one based on a bubble-sort algorithm, the other on a quick-sort algorithm. Even if the scientific community is divided about the need of suppressing code clones (they are not always considered harmful), it is generally accepted that they should, at least, be detected [12] and techniques for clone detection can be applied in various domains like program refactoring [6], plagiarism detection [9], source code provenance analysis [7] and virus recognition [19]. Since duplication is intrinsically linked to semantic equivalence, its detection is an undecidable problem that can however be approximated by automatic program analysis.

Clone detection has received a substantial amount of attention during recent years, mainly in the context of the imperative and object-oriented programming paradigms. Several overviews systematically synthesizing the state-of-the-art of

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this research field can be found in [12, 13]. As it is pointed out in [12], there is no generally accepted definition for what constitutes a clone and the latter's definition is often bound to a particular detection technique. However, only few works consider code cloning for declarative programming languages. Two recent papers have focused on the functional programming paradigm by presenting an abstract syntax tree (AST)-based approach dedicated to Erlang [10] and Haskell programs [3]. In the context of logic programming, [16] essentially motivates the need for clone detection in logic programs, while [17] outlines a basic code duplication analysis of logic programs. Dealing with refactorings for Prolog programs, [14] proposes transformations handling two particular cases of duplication and is, as such, related to our own work. Some language-independent detection techniques were developed too but, as it was reported in [13], they suffer from an important loss in precision since they cannot be tuned for the target language.

This paper proposes a detailed study of code cloning in logic programs by expanding and formalizing the general ideas that were present in [17]. In the remainder of this paper, we first establish the notion of code clone in a logic program. Fundamentally, we consider two predicate definitions cloned if one is a (partial) renaming of the other modulo a permutation of the arguments, clauses and body atoms. We secondly present an efficient algorithm for detecting an important subclass of these code clones.

2 Theory of duplication

2.1 Preliminaries

In what follows, we assume the reader to be familiar with the basic logic programming concepts as they are found, for example, in [1]. To simplify the presentation of the different concepts, we restrict ourselves to *definite programs*, i.e. programs without negation. In particular, we consider a logic program to be defined as a set of *predicates*, representing relations between data objects manipulated by the program. Each predicate p/m, with name p and arity m, is defined by a set of *clauses* of the form $H \leftarrow B_1, \ldots, B_s$ with H, an *atom*, i.e. a predicate name followed by its corresponding number of arguments, *head* of the clause, and $B_1, \ldots, B_s$, a conjunction of atoms, *body* of the clause.

Without loss of generality, we make the hypothesis that clauses are converted to a flattened form such that each atom is of the form $q(X_1, \ldots, X_n)$, $X = Y$ or $X = f(X_1, \ldots, X_n)$ (with $X, Y, X_1, \ldots, X_n$ different variables, q a predicate name and f a functor name). This can easily be done by replacing the terms in the original clauses by new variables and creating (and simplifying) explicit unifications for variables in the body of the clause. We suppose that in this flattened form all clauses defining a predicate share the same identical head and that all other variables are uniquely renamed. For example, the definition of `append/2` in flattened form would be as follows:

```
append(X,Y,Z) ← X=[], Z=Y
append(X,Y,Z) ← X=[Xh|Xt], append(Xt,Y,Zt), Z=[Xh|Zt]
```

In our definitions, we will formally refer to a predicate definition by a couple $(H, \langle C_1, \ldots, C_k \rangle)$ where H is the head shared by all clauses of the predicate and $\langle C_1, \ldots, C_k \rangle$ the sequence of clause bodies as they occur in the definition. Likewise, the body of a clause or, more generally, any conjunction, will be represented as a sequence of atoms $\langle B_1, \ldots, B_s \rangle$. For any conjunction of atoms C (possibly a single atom), we use $vars(C)$ to denote the set of variables occurring in C. For any *finite mapping* $m = \{(e_1, e'_1), \ldots, (e_n, e'_n)\}$[1], we use $dom(m)$ and $img(m)$ to represent, respectively, the *domain* and *image* of the mapping, and for an element $e \in dom(m)$ we use $m(e)$ to represent the element associated to e in the mapping. A *variable renaming* ρ is a finite bijective mapping from a set of variables onto another set of variables, distinct from the original ones. Given a conjunction of atoms C, $C\rho$ represents the result of simultaneously replacing in C every occurrence of a variable $X \in dom(\rho)$ by $\rho(X)$.

2.2 Definition of a clone

In order to ease the definition of a clone in a logic program, we first define a *predicate mapping* as a way of expressing a link between the syntactical constructs of two predicate definitions.

Definition 1. *Given two predicates p/m and q/n defined by $p = (p(X_1, \ldots, X_m), \langle C_1, \ldots, C_k \rangle)$ and $q = (q(Y_1, \ldots, Y_n), \langle C'_1, \ldots, C'_l \rangle)$, a* predicate mapping from p to q *is defined as a triple $\langle \phi, \chi, \{\psi^{i,j} \mid (i,j) \in \chi\} \rangle$ where ϕ, χ are bijective mappings between subsets of, respectively, the argument and clause positions of p and q, and each $\psi^{i,j}$ a bijective mapping between subsets of the atom positions of C_i and C'_j. Given a predicate mapping $\langle \phi, \chi, \{\psi^{i,j} \mid (i,j) \in \chi\} \rangle$, we will call its components ϕ, χ, and each of the $\psi^{i,j}$ respectively an* argument mapping, clause mapping *and* body mapping.

A predicate mapping merely defines a possibly incomplete correspondence between the arguments and clauses of two predicate definitions and – for each pair of associated clauses – the body atoms. Note that a predicate mapping is a purely structural concept, with no meaning attached.

Informally, a *clone* in a logic program refers to a mapping between two predicate definitions such that the parts of the definitions that participate in the mapping are syntactically identical modulo a variable renaming.

Definition 2. *Given two predicates p/m and q/n defined by $p = (p(X_1, \ldots, X_m), \langle C_1, \ldots, C_k \rangle)$ and $q = (q(Y_1, \ldots, Y_n), \langle C'_1, \ldots, C'_l \rangle)$, a* clone from p to q *is a predicate mapping $\langle \phi, \chi, \{\psi^{i,j} \mid (i,j) \in \chi\} \rangle$ from p to q such that $\chi \neq \emptyset$ and, for each pair of clauses $C_i = \langle B_1, \ldots, B_s \rangle$ and $C'_j = \langle B'_1, \ldots, B'_t \rangle$ with $(i,j) \in \chi$, $\psi^{i,j} \neq \emptyset$ and there exists a renaming ρ with $dom(\rho) \subseteq vars(C_i) \cup \{X_u | 1 \leq u \leq m\}$ and $img(\rho) \subseteq vars(C'_j) \cup \{Y_v | 1 \leq v \leq n\}$ such that:*

[1] We will sometimes use the equal notation $m = \{e_1/e'_1, \ldots, e_n/e'_n\}$ for a mapping.

1. $(u, v) \in \phi \Leftrightarrow (X_u, Y_v) \in \rho$
2. *for each atom* $B_w \in C_i$ *with* $w \in dom(\psi^{i,j})$*:*
   - *if* B_w *is an atom other than a recursive call, then* $B_w\rho = B'_{\psi^{i,j}(w)}$
   - *if* B_w *is a recursive call, say* $p(Z_1, \ldots, Z_m)$*, then* $B'_{\psi^{i,j}(w)}$ *is a recursive call, say* $q(Z'_1, \ldots, Z'_n)$*, and* $(u, v) \in \phi \Leftrightarrow (Z_u, Z'_v) \in \rho$.

The renaming ρ *will be called* induced by ϕ and $\psi^{i,j}$.

The duplication relation embodied by our concept of clone from the predicate p to the predicate q is such that at least one atom from a clause of p has to present some similarity with an atom from a clause of q. However, there is no constraint on the minimal size of the argument mapping. Two body atoms are considered similar if they differ only in a variable renaming. Concerning recursive calls, their mapping is conditioned by a permutation of their arguments guided by the argument mapping. If the latter is empty, recursive calls are mapped unconditionally, regardless of their arguments.

Example 1. Let us consider the following predicate definitions, in which the body atoms of each clause are indexed by their position, to facilitate later reference:

```
abs_list(A,B) ← A=[]1, B=[]2
abs_list(A,B) ← A=[Ah|At]1, abs(Ah,Bh)2, abs_list(At,Bt)3, B=[Bh|Bt]4

add1&sqr_list(Y,X) ← X=[]1, Y=[]2
add1&sqr_list(Y,X) ← X=[Xh|Xt]1, N is Xh+12, Yh is N*N3,
       add1&sqr_list(Yt,Xt)4, Y=[Yh|Yt]5
```

The predicates `abs_list` and `add1&sqr_list` generate, from a given list, the list where each element is, respectively, the absolute value of the original element and the original element added to 1 and then squared. The predicate mapping $c = \langle \phi, \chi, \{\psi^{1,1}, \psi^{2,2}\}\rangle$ with $\phi = \{(1,2),(2,1)\}$, $\chi = \{(1,1),(2,2)\}$, $\psi^{1,1} = \{(1,1),(2,2)\}$ and $\psi^{2,2} = \{(1,1),(3,4),(4,5)\}$ is a clone according to our definition. The induced renamings associated to ϕ and $\psi^{1,1}$ and $\psi^{2,2}$ are, respectively, $\rho_1 = \{A/X, B/Y\}$ and $\rho_2 = \{A/X, B/Y, Ah/Xh, At/Xt, Bh/Yh, Bt/Yt\}$. This clone reflects a partial correspondence between both predicates and, in a perspective of refactoring, this common functionality could be generalized in a higher-order predicate *maplist*/3, performing a certain operation (given as third argument) on each element of an input list.

As shown by Example 1, the renamings induced by the argument mapping and each body mapping share a common part, i.e. the renaming induced by the argument mapping. Furthermore, if a body mapping induces a match between two arguments, then the latter have to be mapped by the argument mapping. But two arguments may be linked by the argument mapping without being involved in any body mapping. As a consequence, two clones may vary due to the argument mapping alone. Note that our definition of a clone is general enough

to represent duplication between two different predicate definitions, as well as duplication within a single predicate definition ($p = q$), as well as duplication within a single clause of a single definition ($p = q$, $\chi = \{(i, i)\}$ for some i).

2.3 Hierarchy of clones

Given two predicates p and q, we use $Clones(p, q)$ to denote the finite set of all distinct clones from p to q. We can define the following natural partial order relation over $Clones(p, q)$.

Definition 3. *Given two predicates p and q and two clones $c_1 = \langle \phi_1, \chi_1, \{\psi_1^{i,j} | (i, j) \in \chi_1\} \rangle$ and $c_2 = \langle \phi_2, \chi_2, \{\psi_2^{i,j} | (i, j) \in \chi_2\} \rangle$ in $Clones(p, q)$, c_1 is a* subclone of c_2, *denoted $c_1 \subseteq c_2$, iff $(\phi_1 \subseteq \phi_2) \wedge (\chi_1 \subseteq \chi_2) \wedge (\forall (i, j) \in \chi_1 : \psi_1^{i,j} \subseteq \psi_2^{i,j})$.*

Although stating a preference relation over the set of clones is difficult since this notion is intrinsically linked to the programmer's assessment [18], the order relation defined above allows us to focus on the *maximal* clones in the sense that none of these can be extended into another valid clone. For two predicates p and q, we denote by $\mathcal{C}(p, q)$ the finite unique set of maximal elements of $Clones(p, q)$.

Example 2. The mapping c from Example 1 is a maximal element of the set $Clones($`abs_list`$,$ `add1&sqr_list`$)$. One can verify that the only other maximal element of this set is $\langle \phi, \chi, \{\psi^{1,1}, \psi^{2,2}\} \rangle$ with $\phi = \{(1, 1), (2, 2)\}$, $\chi = \{(1, 1), (2, 2)\}$, $\psi^{1,1} = \{(1, 2), (2, 1)\}$ and $\psi^{2,2} = \{(1, 5), (3, 4), (4, 1)\}$.

How clones can be further classified, most probably in function of the desired application, is a topic for further research. We will now present how we can compute the set of maximal clones between two predicate definitions.

3 Analysis of duplication

3.1 Preliminaries

The analysis we propose focuses on a subset of the maximal clones that may exist between two predicates. Indeed, our clone detection algorithm is parameterized with respect to a given clause mapping and only computes clones involving monotonically increasing body mappings. This choice is justified as follows.

First, since clauses can be seen as isolated rules or computation units, finding clones involving different clause mappings boils down to iterating the search algorithm over these different clause mappings, which can be easily implemented. Moreover, practical logic programming languages or systems may or may not consider clause order as part of the definition of a predicate. Hence, the clause mappings that should be considered for finding valid clones will depend on the language or system under consideration.

Second, practical logic languages - an example being Prolog [4] - often consider the order of the individual atoms in a rule as part of the definition. For such languages, it makes sense to restrict the search for clones to monotonically

increasing body mappings as they will consider the conjunction `a,b` to be semantically different from `b,a`. Even for more declarative languages that abstract from the order of the atoms – an example being Mercury [15] – the atoms in a conjunction can often be rearranged in some standardized and semantics preserving way such that if two conjunctions `a,b` and `b,a` have the same semantics, they will be reordered in the same way [5].

3.2 Clone detection algorithm

A body mapping ψ whose $dom(\psi)$ and $img(\psi)$ are intervals, i.e. sets composed only of successive values, will be called a *block mapping*. As a special case, a block mapping ψ whose $|dom(\psi)| = |img(\psi)| = 1$ will be called an *atomic block mapping*. A block mapping, respectively a body mapping, ψ between two conjunctions is maximal if there does not exist a block mapping, respectively a body mapping, ψ' between the two conjunctions with $\psi \subset \psi'$. Obviously, a body mapping can be seen as constructed from individual block mappings and a block mapping from individual atomic block mappings. The converse is not necessarily true: not all sets of (atomic) block mappings can be combined into a valid body mapping. This principle is the basis of our algorithm: from two conjunctions, the set of maximal block mappings is generated by combining the atomic block mappings, and the set of maximal body mappings is generated by combining the maximal block mappings. This combination operation will be refined later.

Given an argument mapping ϕ concerning two argument sets $\{X_1, \ldots, X_m\}$ and $\{Y_1, \ldots, Y_n\}$, and a body mapping ψ between two conjunctions that do not contain recursive calls, if ρ_1 is the renaming induced by ϕ and ρ_2 by ψ, ψ is said *conform to* ϕ if $\rho_1 \cup \rho_2$ is a renaming such that $(u, v) \in \phi \Leftrightarrow (X_u, Y_v) \in \rho_1 \cup \rho_2$. This is denoted by ψ_ϕ and corresponds to the first condition of the definition of a clone. By extension, a *set of body mappings* S, not involving recursive calls, is said *conform to* ϕ if each of its elements is conform to ϕ. This is denoted by S_ϕ.

Finally, two special union operators are used by our algorithm: $\biguplus$, whose goal is to create a set where each element is the union between two elements of the two original sets : $A \biguplus B = \{a \cup b \mid a \in A,\ b \in B\}$, and $\bigsqcup$, whose goal is to keep only the maximal elements among all elements of the two original sets: $A \bigsqcup B = (A \cup B) \setminus \{x | \exists x' \in (A \cup B) \setminus \{x\} : x \subseteq x'\}$.

Figure 1 gives an overview of our clone detection algorithm, which takes as input two predicates p/m and q/n and a clause mapping χ. The algorithm performs the following operations for each argument mapping ϕ (of size from 0 to m, if we suppose, without loss of generality, $m \leq n$):

The first operation consists in comparing each pair (C_i, C'_j) of clauses associated by the clause mapping χ. This comparison will be performed by three successive procedures. First, the recursive calls of the clauses are transformed to make it possible for them to be treated just like the other atoms of the clause bodies. Concretely, the procedure $transform\_recursive\_calls$ replaces each recursive call in C_i, say $p(Z_1, \ldots, Z_m)$, respectively in C'_j, say $q(Z'_1, \ldots, Z'_n)$, by an atom whose predicate name is rec, where "rec" is a special name, different from

ALGORITHM($LoClo(p, q, \chi)$)
Input: predicates p and q, clause mapping χ
Output: set Res of maximal clones from p to q with a clause mapping subset of χ and monotonically increasing body mappings

1 $Res = \emptyset$
2 $\forall \phi$:
3 $\quad \chi' = W = \emptyset$
4 $\quad \forall (i, j) \in \chi$, with C_i in p and C'_j in q:
5 $\quad\quad (Cr_i, Cr'_j) = transform\_recursive\_calls(\phi, C_i, C'_j)$
6 $\quad\quad \mathcal{BM}_\phi^{i,j} = compute\_block\_mappings(\phi, Cr_i, Cr'_j)$
7 $\quad\quad \mathcal{M}_\phi^{i,j} = compute\_body\_mappings(\mathcal{BM}_\phi^{i,j})$
8 $\quad\quad$ **If** $\mathcal{M}_\phi^{i,j} \neq \emptyset$
$\quad\quad$ **Then**
9 $\quad\quad\quad \chi' = \chi' \bigcup \{(i, j)\}$
10 $\quad\quad\quad W = W \biguplus \{\{\psi_\phi^{i,j}\} | \psi_\phi^{i,j} \in \mathcal{M}_\phi^{i,j}\}$
11 $\quad$ **If** $\chi' \neq \emptyset$
$\quad$ **Then**
12 $\quad\quad Res = Res \bigsqcup \{< \phi, \chi', w > | w \in W\}$
13 **Return** Res

Fig. 1. Clone detection algorithm.

all other predicate names occurring in the program, and where the arguments are a subset of the actual arguments, determined as $\{Z_u | u \in dom(\phi)\}$, respectively $\{Z'_v | v \in img(\phi)\}$. The positions of the new arguments are also modified: in the recursive calls of C_i, they are written in increasing order with respect to their index u, while in the recursive calls of C'_j, the new position of the argument Z'_v with $(u, v) \in \phi$ is equal to $|\{(x, y) | (x, y) \in \phi \wedge x \leq u\}|$. The result of transforming the clauses C_i and C'_j in this way is denoted by Cr_i and Cr'_j.

Example 3. The predicates `abs_list` and `add1&sqr_list` from Example 1 allow for seven different argument mappings. In case $\phi = \{(1, 2)\}$, their recursive calls are transformed into, respectively, $rec(At)$ and $rec(Xt)$. We see that the variable Xt, which was originally the second argument, is now the first one. In case $\phi = \emptyset$, both recursive calls will simply become rec.

Then, a second procedure computes, from the given pair of transformed clauses, its set of all maximal monotonically increasing block mappings conform to ϕ, denoted by $\mathcal{BM}_\phi^{i,j}$. This operation, which will not be detailed due to lack of space, may be performed by a dynamic programming algorithm with an upper bound for the running time of $S \times T \times L$ where S and T are the lengths of the clause bodies in terms of number of atoms and L is the length of the longest block mapping. Thirdly, this set $\mathcal{BM}_\phi^{i,j}$ serves as a basis to generate the set of all maximal monotonically increasing body mappings conform to ϕ, denoted by $\mathcal{M}_\phi^{i,j}$. This important operation will be refined later. If $\mathcal{M}_\phi^{i,j}$ is not empty, i.e. if the clauses i and j share some similarity in accordance with ϕ, then the sets χ'

and W are updated. These sets, both initialized as empty sets before the loop examining the pairs of clauses, represent, respectively, all the pairs of clauses which share some similarity in accordance with ϕ (thus $\chi' \subseteq \chi$) and all the sets of body mappings that will belong to a different clone.

Finally, once all pairs of clauses have been considered, if χ' is not empty, i.e. if at least one pair of clauses presents some similarity in accordance with ϕ, the clones containing ϕ are build from χ' and W. They are placed in the set *Res*, from which all subclones are suppressed.

Example 4. Let us reconsider the predicates `abs_list` and `add1&sqr_list` from Example 1 and, for the sake of illustration, we fix $\chi = \{(1,1),(2,2)\}$ and $\phi = \emptyset$. It follows that $\mathcal{BM}_\phi^{1,1} = \mathcal{M}_\phi^{1,1} = \emptyset$ and $\mathcal{BM}_\phi^{2,2} = \mathcal{M}_\phi^{2,2} = \{\psi_\phi^{2,2}\}$, where $\psi_\phi^{2,2} = \{(3,4)\}$. Only the recursive calls are mapped by the body mapping since the latter is forbidden to create a link between one of the arguments A and B and one of the arguments Y and X, because of the empty argument mapping. After having compared all pairs of clauses, it results that $\chi' = \{(2,2)\}$ and $W = \{\{\psi_\phi^{2,2}\}\}$. This allows to generate the clone $< \emptyset, \chi', \{\psi_\phi^{2,2}\} >$. For the same χ and $\phi = \{(1,2),(2,1)\}$, we obtain $\mathcal{BM}_\phi^{1,1} = \mathcal{M}_\phi^{1,1} = \{\psi_\phi^{1,1}\}$, where $\psi_\phi^{1,1} = \{(1,1),(2,2)\}$, and $\mathcal{BM}_\phi^{2,2} = \{\{(1,1)\},\{(3,4),(4,5)\}\}$. These two block mappings will be combined to give $\mathcal{M}_\phi^{2,2} = \{\psi_\phi^{2,2}\}$, where $\psi_\phi^{2,2} = \{(1,1),(3,4),(4,5)\}$. In this case, we have $\chi' = \chi$ and $W = \{\{\psi_\phi^{1,1}, \psi_\phi^{2,2}\}\}$. Finally, the clone $< \phi, \chi, \{\psi_\phi^{1,1}, \psi_\phi^{2,2}\} >$ is created. It is a maximal clone between both predicates, as stated in Example 1. As the first clone of this example is a subclone of the second one, only the latter will be kept in the solution set *Res*.

The hard part of the algorithm consists in combining the block mappings of $\mathcal{BM}_\phi^{i,j}$ in order to construct $\mathcal{M}_\phi^{i,j}$. This set can be computed by an iterative process as follows. The process starts with a single arbitrary block mapping from $\mathcal{BM}_\phi^{i,j}$. Then, the following instructions are repeated until $\mathcal{BM}_\phi^{i,j} = \emptyset$: one of the remaining block mappings is selected from $\mathcal{BM}_\phi^{i,j}$ and successively combined with each body mapping currently in $\mathcal{M}_\phi^{i,j}$. As we will detail below, such a combination operation may result in several new body mappings. The latter replace the original body mapping that was used for combination in $\mathcal{M}_\phi^{i,j}$, at the same time keeping only the maximal ones in the set. The order in which the block mappings are selected from $\mathcal{BM}_\phi^{i,j}$ does not influence the result nor the complexity of the algorithm.

Let us discuss now how a block and a body mappings – or in general, any two body mappings – can be combined to obtain a (set of) new body mapping(s). We first introduce the concept of conflict between atomic block mappings.

Definition 4. *Given two atomic block mappings $\psi = \{(i,j)\}$ and $\psi' = \{(k,l)\}$ from the conjunctions $C = B_1, ..., B_s$ and $C' = B'_1, ..., B'_t$, there exists an* atomic conflict between ψ and ψ' *if at least one of the following conditions holds:*

- $(i = k \wedge j \neq l) \vee (i \neq k \wedge j = l)$*: ψ and ψ' overlap and combining them would not respect the bijection constraint*

- $(i < k \wedge j > l) \vee (i > k \wedge j < l)$: *$\psi$ and ψ' cross and combining them would not respect the monotonic increase constraint*
- *there does not exist a renaming ρ such that $(B_i, B_k)\rho = (B'_j, B'_l)$: the conjunctions targeted by the combination of ψ and ψ' are not syntactically equal modulo a variable renaming*

Based on this definition, we define the unique undirected *conflict graph of two body mappings* ψ and ψ' as the graph $CG(\psi, \psi') = (V, E)$ where the set of vertices $V = \{\{a\}|a \in \psi \vee a \in \psi'\}$ and the set of edges $E = \{\{v, v'\}|v, v' \in V \wedge \exists$ an atomic conflict between v and $v'\}$. Each vertex represents thus an atomic block mapping and each edge an atomic conflict between the atomic block mappings corresponding to the vertices. Slightly abusing notation, we introduce the following terminology. Given a conflict graph $CG = (V, E)$ and an atomic block mapping $v \in V$, a *direct conflict of* v is an edge $e = \{v, v'\} \in E$ while an *indirect conflict of* v is an edge $e = \{v', v''\} \in E$ such that $\exists\{v, v'\} \in E$ or $\exists\{v, v''\} \in E$.

Our algorithm combines two body mappings by first organizing all their atomic conflicts into a conflict graph. Then, this graph is partitioned into connected components, each of them representing a conflict (sub)graph that contains atomic conflicts that are mutually dependent in the sense that they involve the same atomic block mappings. Each connected component will then progressively be pruned by exploring how each conflict can be resolved until one obtains a set of conflict graphs with an empty edge set, i.e. a set of body mappings that are valid combinations of (sub)mappings of the two original body mappings represented by the initial connected component. The principle of pruning requires two special operators over a conflict graph. The operator **.** serves at fixing one atomic block mapping and eliminating from the graph the parts conflicting with it. Formally, given a conflict graph $CG = (V, E)$ and an atomic block mapping $v \in V$, $CG.v = (V', E')$, where $V' = V \setminus \{x|\{v, x\} \in E\}$ and $E' = E \setminus \{\{x, y\}|\{x, y\}$ is a direct or indirect conflict of $v\}$. The second operator **-** serves at eliminating two conflicting atomic block mappings from the graph. Formally, given a conflict graph $CG = (V, E)$ and an atomic conflict $e = \{v, v'\} \in E$, $CG\text{-}e = (V', E')$, where $V' = V \setminus \{v, v'\}$ and $E' = E \setminus \{\{x, y\}|\{x, y\}$ is a direct conflict of v or $v'\}$.

The algorithm transforming a connected component G of a conflict graph is presented in Figure 2. In the algorithm, we use $d(v)$ to refer to the *degree of a vertex* v, i.e. the number of incident edges in the graph. As base case, an input graph containing no atomic conflict corresponds to a body mapping. As general case, we select in the graph an atomic conflict between atomic block mappings, ideally both but if not, one of them, characterized by a degree of value 1. If such an edge does not exist, the atomic conflict between the two atomic block mappings with the maximal sum of degrees is selected. This manner of selecting atomic conflicts according to the degree of their associated vertices aims at minimizing the running time of the algorithm, since the number of recursion calls may vary from 1 to 3 as it will be explained below.

The solution set *Res* will be computed differently depending on the type of the selected atomic conflict. In the first case (steps 3 and 4), the atomic conflict

ALGORITHM($resolve(G)$)
Input: conflict graph $G = (V, E)$
Output: set Res of maximal monotonically increasing body mappings constructed from non-conflicting atomic block mappings of G

1 **If** $E = \emptyset$
2 **Then** $Res = \{ \bigcup_{v \in V} v \}$
Else
3 **If** $\exists e = \{v, v'\} \in E : d(v) = 1 \wedge d(v') = 1$
4 **Then** $Res = e \biguplus resolve(G\text{-}e)$
Else
5 **If** $\exists e = \{v, v'\} \in E : d(v) = 1 \vee d(v') = 1$
6 **Then** $Res = resolve(G.v) \bigcup resolve(G.v')$
Else
7 **Select** $e = \{v, v'\} \in E : d(v) + d(v')$ maximal
8 $Res = resolve(G.v) \bigcup resolve(G.v') \bigcup resolve(G\text{-}e)$
9 **Return** Res

Fig. 2. Conflict graph resolution algorithm.

$e = \{v, v'\}$ is isolated from the others since both its atomic block mappings are not involved in any other conflict. To resolve e, we will thus separate the conflicting atomic block mappings and construct on the one hand, the set of solution body mappings containing v and the other hand, the set of solution body mappings containing v'. Concretely, v and v' are added separately to each element that will be found by continuing the search with the resolution of the initial conflict graph G without e. In the second case (steps 5 and 6), one of both atomic block mappings forming the atomic conflict e is involved in other atomic conflicts. Again, resolving e means keeping either v or v' but the rest of the graph can no more be resolved independently of them. For that reason, the procedure *resolve* is called recursively, on the one hand, on the initial conflict graph G where v is fixed so that it will be part of all the subsequently found solution body mappings, and on the other hand, on G where v' is fixed, which ensures that none solution from one recursion branch will be subset of a solution from the other one. The set Res is the union of both solution sets. Finally, the third case (steps 7 and 8) is identical to the second one, except that a third recursion branch is needed, where none of the atomic block mappings v and v' is kept in the solution body mappings. This avoids loosing some solutions. Indeed, it is possible that a certain atomic block mapping conflicting with v and another one conflicting with v' are not conflicting when put together. This third recursion branch allows them to be joined in at least one solution body mapping.

To combine two body mappings ψ and ψ', we thus compute $\biguplus_{g \in S} resolve(g)$, where S is the set of connected components of $CG(\psi, \psi')$. Each resulting body mapping is thus a union between $|S|$ smaller mutually non-conflicting body mappings, each from one solution set of a different connected component. The union operator ensures that no doubles are present in the resulting set.

Example 5. From the following two generic conjunctions of atoms `p(W)`$_1$`,q(X)`$_2$`, r(Y)`$_3$`, r(Z)`$_4$`,s(X,Y,Z)`$_5$ and `p(A)`$_1$`,q(B)`$_2$`,r(C)`$_3$`,s(A,B,C)`$_4$, two block mappings can be extracted: $\psi = \{(1,1),(2,2),(3,3)\}$ and $\psi' = \{(4,3),(5,4)\}$. Trying to combine them leads to the conflict graph $CG(\psi,\psi') = (V,E)$, with $V = \{\{(1,1)\},\{(2,2)\},\ \{(3,3)\},\{(4,3)\},\{(5,4)\}\}$ (to ease the reading, we will reference each atomic block mapping constituting a vertex by $v_i, 1 \leq i \leq 5$, respecting the order in which they are written) and $E = \{\{v_1,v_5\},\{v_2,v_5\},\{v_3,v_4\},\{v_3,v_5\}\}$. Let us abbreviate $CG(\psi,\psi')$ to CG. This graph contains only one connected component, i.e. itself. To resolve it, the first atomic conflict $\{v_1,v_5\}$ can be selected since $d(v_1) = 1$ and $d(v_5) = 3$. It is the second recursive case of our procedure *resolve*. Two atomic (sub)graphs have thus to be treaten: $CG.v_1 = (\{v_1,v_2,v_3,v_4\},\{\{v_3,v_4\}\})$ and $CG.v_5 = (\{v_4,v_5\},\emptyset)$. $CG.v_1$ contains only one atomic conflict in which both atomic block mappings are of degree 1. It is the first recursion case, where the graph $(CG.v_1)$-$\{v_3,v_4\} = (\{v_1,v_2\},\emptyset)$ has to be resolved. As its set of edges is empty, we fall in the base case of the procedure: there is no more atomic conflict and the graph represents the body mapping $\{(1,1),(2,2)\}$. The latter will be united with the vertices v_3 and v_4 separately to give the set of body mappings $\{\{(1,1),(2,2),(3,3)\},\{(1,1),(2,2),(4,3)\}\}$, solution set of $CG.v_1$. The resolution of the graph $CG.v_5$ is direct, since its set of atomic conflicts is empty, and produces the singleton set of body mappings $\{\{(4,3),(5,4)\}\}$. Finally, the solution set of the conflict graph CG is the union between $resolve(CG.v_1)$ and $resolve(CG.v_5)$ which gives three body mappings corresponding to the following non-conflicting subconjunction pairs: `p(W)`$_1$`,q(X)`$_2$`,r(Y)`$_3$ and `p(A)`$_1$`,q(B)`$_2$`,r(C)`$_3$; `p(W)`$_1$`,q(X)`$_2$`,r(Z)`$_4$ and `p(A)`$_1$`,q(B)`$_2$`, r(C)`$_3$; `r(Z)`$_4$`,s(X,Y,Z)`$_5$ and `r(C)`$_3$`,s(A,B,C)`$_4$.

3.3 Complexity

The complexity of the algorithm is determined by the computation of all argument mappings. Then, the examination of all pairs of clauses depends on the size of the clause mapping given as input. The time consuming operations consist in the computation of the block mappings between two clause bodies and, especially, in the resolution of a conflict graph. The latter operation is exponential in nature given the multiple ways in which conflicts may be resolved. While this complexity did not turn out to be problematic in our preliminary evaluation (see Section 3.4), it remains to be studied whether it is still manageable in practice.

We will now define some supplementary notions closely linked to the complexity of our algorithm. Our definition of a clone in a logic program allows us to highlight a particular kind of clone.

Definition 5. *Given two predicates p/m and q/n defined respectively by k and l clauses, an* exact clone from p to q *is a clone $\langle \phi, \chi, \{\psi^{i,j} | (i,j) \in \chi\}\rangle$ such that $|\phi| = m = n$, $|\chi| = k = l$, and $\forall (i,j) \in \chi$, with $C_i = B_1,\ldots,B_s$ in p and $C'_j = B'_1,\ldots,B'_t$ in q, $|\psi^{i,j}| = s = t$. A clone which is not exact is called* partial.

An exact clone occurs typically when q is a "copy-pasted" instance of p, possibly renamed but without any other modification. Partial clones are of course much more frequent than exact clones.

Thanks to these notions, we may characterize the duplication relation between two predicates p and q by discerning three main classes of duplication (according to our algorithm, we consider only clones with monotonically increasing body mappings):

1. *Empty duplication*: $\mathcal{C}(p,q) = \emptyset$

2. *Exact duplication*: $\mathcal{C}(p,q) = \{c|c \text{ is an exact clone from } p \text{ to } q\}$
   $\cup\{c|c \text{ is a partial clone from } p \text{ to } q\}$
   In this class of duplication, it is possible that several different exact clones exist between both predicates (at least one is required). When $\mathcal{C}(p,q)$ contains only one exact clone, the relation is called *perfect exact duplication*.

3. *Partial duplication*: $\mathcal{C}(p,q) = \{c|c \text{ is a partial clone from } p \text{ to } q\}$
   When $\mathcal{C}(p,q)$ is a singleton, the relation is called *perfect partial duplication*.

Clones representing empty or perfect duplication are detected faster than the others since these particular cases do not involve any atomic conflict to be resolved. An interesting topic of research would be to investigate the relative frequency of the different kinds of duplication relations in a logic program.

3.4 Tests

To test the feasibility of our approach, as a proof of concept, we created five test cases, each corresponding to a different class, or subclass, of duplication between two predicates. All test cases are composed of 2 generic predicates of arity 3, defined by 3 clauses of 10 atoms. We aimed at testing the core of the algorithm, i.e. the computation of the block and body mappings. For every test case, all possible pairs of clauses, each from a different predicate definition, were examined and all maximal monotonically increasing block and body mappings were detected, without requiring the conformity to any argument mapping. In other words, this simplified computation is an overvalued worst case approximation of the computation given an argument mapping. Moreover, the algorithm was run 100 times per test case in order to obtain a fair average runtime estimation, on a Intel Dual Core 2.5GHz 4Go DDR3 computer. To reflect the complexity of our approach, we give the total number of found body mappings and the total number of atomic conflicts that the algorithm had to resolve.

The results are reported in Figure 3, the last column showing the average runtimes for a given clause mapping. First of all, we should note that the detected block and body mappings were the expected ones. We can then observe a clear division between the average runtimes. Indeed, the test cases 1, 3 and 5 were analyzed in a time interval from 14 ms to 17 ms, while the test cases 2 and 4 in about 29 ms. This illustrates the efficiency of the algorithm, which performs

better when there is no atomic conflict. However, it is interesting to note that the test case 4 faced 56% more atomic conflicts than the test case 2, which did not prevent the algorithm to perform as well in both cases. Finally, we can see that the number of body mappings is linked to the number of atomic conflicts. More numerous the conflicts, the more the clause bodies are split up into smaller body mappings.

# Test	Body mappings nb	Atomic conflicts nb	Average runtime (ms)
1	0	0	14
2	21	93	29
3	3	0	17
4	25	145	28
5	2	0	16

Fig. 3. Results of tests on the algorithm.

4 Discussion and future work

The definition of a clone and the clone detection algorithm we propose are, to our best knowledge, the most general and the first to be fully formalized in logic programming literature. As proof of concept, we made an implementation of the algorithm that we ran on a limited series of tests. This illustrates the feasibility of our technique and the obtained results are encouraging. All clones between two predicates are detected in a non-naive way. It can be noted that our algorithm is generic. Indeed, it could easily be adapted to a particular logic programming language. Besides, it could be tuned and optimized by introducing parameters guiding the search process. For example, one could want to impose a minimal size to the detected clones (according to some appropriate notion of size) in order to avoid small and potentially meaningless clones. Or, in a typed and moded context, the variable renamings induced by the argument and body mappings could be restricted to pairs of variables of the same type and/or mode.

As it is based on syntactic equality, our clone definition may be related to the notion of *structural clone* [12], which depends on the design structures of a certain language and is particularly suited for refactoring. This way of approximating semantic similarity is expedient in logic programming. Indeed, contrary to an imperative program which represents a step-by-step algorithm manipulating data objects, a logic program basically specifies a number of relations that hold between the data objects. In this sense, its arguably simple syntax is closely linked to its semantics. Following from our clone definition, our clone detection technique may be considered AST-based-like. Indeed, it corresponds to a search of two (possibly partially) isomorphic subgraphs in the AST of the given predicates, where leaves representing variable names are discarded but respecting however the constraint of a consistent variable renaming. This guarantees better precision compared to naive comparison for subtree equality. Some existing

AST-based tools take also renamings into account, like CReN [8], CloneDR [2], Wrangler [10], HaRe [3]. Except for the first one, these tools are able to find exact and partial clones. Regarding logic programming, this is a crucial concern and our algorithm is dedicated to detecting partial clones.

In the context of logic programming, [14] presents two refactorings to remove code duplication. The first one aims at identifying identical subsequences of goals in different predicate bodies, in order to extract them into a new predicate. The detection phase is said to be comparable to the problem of determining longest common subsequences and seems as such much more limited than our approach. The second refactoring aims at eliminating copy-pasted predicates, with identical definitions. However, to limit the search complexity, only predicates with identical names in different modules are considered duplicated. Both refactorings are implemented in the tool ViPReSS.

Among the topics we see for further work, we cite a more thorough evaluation of our approach. Our algorithm could be compared to other existing AST-based techniques, including those mentioned above, and to ViPReSS. A detailed formal study of the different classes of duplication spotted by our algorithm could also be undertaken. Besides, our current definition of a clone in a logic program could be generalized to accept an abstraction of constants and data structures. Another way to extend the definition concerns its granularity. Currently, the range of the duplication relation is two predicates. Instead, it could be valuable to consider a set of duplicated predicates, forming then a *class of clones* [11], possibly with a certain threshold of similarity to be defined. In a perspective of refactoring, this would allow to refactor all predicates inside a family at the same time instead of separately. Furthermore, in [20] is exposed the concept of *chained clone* which involves several procedures linked by a caller-callee relation, and the concept of *chained clone set* which is an equivalent class of chained clone. These notions could be applied to our case, by combining "basic" clones, formed by a pair of predicates, into more complex clones, formed by a pair of sets of predicates. Finally, it could be interesting to characterize as precisely as possible the link between our structural definition of a clone and semantic similarity, which could lead to improve the definition for capturing duplicates partly, or even non, syntactically equal.

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Meta-Predicate Semantics

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Abstract. We describe and compare design choices for meta-predicate semantics, as found in representative Prolog predicate-based module systems and in Logtalk. We look at the consequences of these design choices from a pragmatic perspective, discussing explicit qualification semantics, computational reflection support, expressiveness of meta-predicate declarations, portability of meta-predicate definitions, and meta-predicate performance. We also describe how to extend the usefulness of meta-predicate definitions. Our aim is to provide useful insights to discuss meta-predicate semantics and portability issues based on actual implementations and common usage patterns.

Keywords: meta-predicates, predicate-based module systems, objects.

1 Introduction

Prolog and Logtalk [1, 2] meta-predicates are predicates with one or more arguments that are either goals or closures[1] used for constructing goals, which are called in the body of a predicate clause. Common examples are all-solutions meta-predicates such as `setof/3` and list mapping predicates. Prolog implementations may also classify predicates as meta-predicates whenever the predicate arguments need to be module-aware. Examples include built-in database predicates such as `assertz/1` and `retract/1` and built-in reflection predicates such as `current_predicate/1` and `predicate_property/2`.

Meta-predicates provide a mechanism for reusing programming patterns. By encapsulating meta-predicate definitions in library modules and library objects, exported and public meta-predicates allow client modules and client objects to reuse these patterns, customized by calls to local predicates.

In order to compare meta-predicate support, as found in representative Prolog predicate-based module systems and in Logtalk, a number of design choices can be considered. These include explicit qualification semantics, computational reflection support, expressiveness of meta-predicate declarations, safety of meta-predicate definitions, portability of meta-predicate definitions, and meta-predicate performance. When discussing meta-predicate semantics, it is useful to define the contexts where a meta-predicate is defined, called, and executed. The following definitions extend those found on [3] and will be used in this paper:

[1] In Prolog and Logtalk, a closure is defined as a callable term used to construct a goal by appending one or more additional arguments.

Definition context This is the object or module containing the meta-predicate definition.

Calling context This is the object or module from which a meta-predicate is called. This can be the object or module where the meta-predicate is defined in the case of a local call or another object or module assuming that the meta-predicate is within scope.

Execution context This includes both the calling context and the definition context. It is comprised by all the information required by the language runtime to correctly execute a meta-predicate call.

Lookup context This is the object or module where we start looking for the meta-predicate definition (the definition can always be reexported from another module or inherited from another object).

This paper is organized as follows. Section 2 describes meta-predicate directives. Section 3 discusses the consequences of using explicit qualified meta-predicate calls and the transparency of control constructs when using explicit qualification. Section 4 describes the support for computational reflection for meta-predicates. Section 5 discusses the portability of meta-predicate directives and meta-predicate definitions. Section 6 describes how lambda expressions can be used to extend the usefulness of meta-predicate definitions. Section 7 presents some remarks on meta-predicate performance. Section 8 summarizes our conclusions and discusses future work. For a discussion on the safety of meta-predicate definitions, we refer the reader to [3].

2 Meta-Predicate Directives

Meta-predicate directives are required for proper compilation of meta-predicates in both Logtalk and Prolog predicate-based module systems in order to avoid forcing the programmer to explicitly qualify all meta-arguments. Meta-predicate directives are also useful for compilers to optimize meta-predicate calls (e.g. when using lambda expressions as meta-arguments) and to be able to check meta-predicate calls for errors (e.g. using a non-callable term in place of a meta-argument) and potential errors (e.g. arity mismatches when working with closures). The design choices behind the current variations of meta-predicate directives translate to different trade-offs between simplicity and expressiveness. The meta-predicate template information declared via meta-predicate directives can usually be programmatically retrieved using built-in reflection predicates such as `predicate_property/2`, as we will discuss in Section 4.

2.1 The ISO Prolog Standard `metapredicate/1` Directive

The ISO Prolog standard for Modules [4] specifies a `metapredicate/1` directive that allows us to describe which meta-predicate arguments are normal arguments and which are meta-arguments using a predicate template. In this template, the atom `*` represents a normal argument while the atom `:` represents

a meta-argument. We are not aware of any Prolog module system implementing this directive. The standard does allow for alternative meta-predicate directives, providing solely as an example a `meta/1` directive that takes a predicate indicator as argument. This alternative directive is similar to the `tool/2` and `module_transparent/1` directives discussed below. However, from the point-of-view of standardization and code portability, allowing for alternative directives is harmful, not helpful.

2.2 The Prolog `meta_predicate/1` Directive

The ISO Prolog specification of a meta-predicate directive suffers from one major shortcoming [5]: it doesn't distinguish between goals and closures. The de facto standard solution for specifying closures is to use a non-negative integer representing the required number of additional arguments [6]. By interpreting a goal as a closure requiring zero additional arguments, we can reserve the atom `:` to represent arguments that need to be module-aware without necessarily referring to a predicate. This convention is found in recent GNU Prolog, Qu-Prolog, SICStus Prolog, SWI-Prolog, and YAP versions and is being adopted by B-Prolog, XSB, and other Prolog compilers. In Prolog compilers without a module system, or with a module system where module expansion only needs to distinguish between normal arguments and meta-arguments, using an integer for representing closures can still be useful for cross-reference tools.

Despite being able to specify closure meta-arguments, there is still a known representation shortcoming. Some predicates accept a list of options where one or more options are module-aware. For example, the third argument of the predicate `thread_create/3` [7] is a list of options that can include an `at_exit/1` option. This option specifies a goal to be executed when a thread terminates. In this case, the argument is not a meta-argument but may *contain* a sub-term that will be used as a meta-argument. Although we could devise (a most likely cumbersome) syntax for these cases, the elegant solution for this representation problem is provided by the `tool/2` and `module_transparent/1` directives discussed below.

A minor limitation with the ISO Prolog `metapredicate/1` directive, which is solved by the `meta_predicate/1` directive, is the representation of the instantiation mode of the normal arguments. For representing the instantiation mode of normal arguments, the atoms `+`, `?`, `@`, and `-` are commonly used, as specified in the ISO Prolog standard [8]. However, using mode indicators in `meta_predicate/1` directives is no replacement for a *mode* directive. Consider the following two `meta_predicate/1` directives:

```
:- meta_predicate(forall(0, 0)).
:- meta_predicate(setof(@, 0, -)).
```

For `forall/2`, `0` means `@`. For `setof/3`, `0` means `+`. Thus, using mode indicators in meta-predicate directives is inherently ambiguous (but still common practice).

2.3 The Logtalk `meta_predicate/1` Directive

Logtalk uses a `meta_predicate/1` directive, based on the Prolog `meta_predicate/1` directive described above, extended with meta-predicate mode indicators for representing a predicate indicator, `(/)`, a list of predicate indicators, `[/]`, and a list of goals, `[0]`. In addition, the atom `:` is replaced by `::` for consistency with the message sending operator. Logtalk uses this information to verify meta-predicate definitions, as discussed in [3]. Logtalk also supports a `mode/2` predicate directive[2] for specifying the instantiation mode and the type of predicate arguments (plus the predicate determinism). Therefore, the atom `*` is used to indicate normal arguments in `meta_predicate/1` directives.

The extended set of meta-predicate mode indicators allows Logtalk to specify accurate meta-predicate templates for virtually all proprietary built-in meta-predicates found on all compatible Prolog compilers. This allows Logtalk to cope with the absence, limitations, differences, and sometimes ambiguity of meta-predicate templates in those Prolog compilers. In fact, some Prolog compilers still don't implement the `meta_predicate/1` predicate property, while some other Prolog compilers return ambiguous meta-predicate templates due to the use of the `:` meta-predicate mode indicator for any type of meta-argument.

2.4 The Ciao Prolog `meta_predicate/1` Directive

Ciao Prolog uses a `meta_predicate/1` directive that supports an extensive set of meta-predicate mode indicators [9] that, although apparently not adopted elsewhere, subsumes in expressive power the sets of meta-predicate mode indicators found on other Prolog compilers and in Logtalk. For example, it is possible to specify that a meta-argument should be a clause or, more specifically, a fact, using the mode indicators `clause` and `fact`. Moreover, a `list(Meta)` mode indicator, where `Meta` is itself a mode indicator, allows easy specification of lists of e.g. goals, predicate-indicators, or clauses.

2.5 The `tool/2` and `module_transparent/1` Directives

An alternative to the `meta_predicate/1` directive, used in ECLiPSe [10] and in earlier SWI-Prolog versions [11], is to simply declare meta-predicates as *module transparent*, forgoing the specification of which arguments are normal arguments and which arguments are meta-arguments. For this purpose, ECLiPSe provides a `tool/2` directive and SWI-Prolog provides a (apparently deprecated) `module_transparent/1` directive. These directives take predicate indicators as arguments and thus support a simpler and user-friendlier solution when compared with the `meta_predicate/1` directive. However, we have shown in [3] that distinguishing between goals and closures and specifying the exact number of closure additional arguments is necessary to avoid misusing meta-predicate definitions to break module and object encapsulation.

[2] `http://logtalk.org/manuals/refman/directives/mode2.html`

3 Explicit Qualification Semantics

The semantics of explicit qualification is the most significant design decision on meta-predicate semantics. This section compares two different semantics, found on actual implementations, for the explicit qualification of meta-predicates and control constructs.

3.1 Explicit Qualification of Meta-Predicate Calls

Given an explicit qualified meta-predicate call, we have two choices for the corresponding semantics:

1. The explicit qualification sets only the initial lookup context for the meta-predicate definition. Therefore, all meta-arguments that are not explicitly-qualified are called in the meta-predicate calling context.
2. The explicit qualification sets both the initial lookup context for the meta-predicate definition and the meta-predicate calling context. Therefore, all meta-arguments that are not explicitly-qualified are called in the meta-predicate lookup context (usually the same as the meta-predicate definition context).

These two choices for explicit qualification semantics are also described in the ISO Prolog standard for modules. This standard specifies a read-only flag, `colon_sets_calling_context`, which would allow a programmer to query the semantics of a particular module implementation.

Logtalk and the ECLiPSe module system implement the first choice. Prolog module systems derived from the Quintus Prolog module system [6], including those found on SICStus Prolog, SWI-Prolog, and YAP implement the second choice (the native XSB module system is atom-based, not predicate-based).

In order to illustrate the differences between the two choices above, consider the following example, running on Prolog module systems implementing the second choice. First, we define a meta-predicate library module:

```
:- module(library, [my_call/1]).

:- meta_predicate(my_call(0)).
my_call(Goal) :-
    write('Calling: '), writeq(Goal), nl,
    call(Goal).

me(library).
```

The `my_call/1` meta-predicate simply prints a message before calling its argument (which is a goal, as declared in its meta-predicate directive). Second, we define a simple client module that imports and calls our meta-predicate using a local predicate, `me/1`, as its argument:

```
:- module(client, [test/1]).

:- use_module(library, [my_call/1]).

test(Me) :-
    my_call(me(Me)).

me(client).
```

To test our code, we use the following query:

```
| ?- client:test(Me).
Calling: client:me(_)
Me = client
yes
```

This query provides the expected result: the meta-predicate argument is called in the context of the client, not in the context of the meta-predicate definition. But consider the following seemingly innocuous changes to the client module:

```
:- module(client, [test/1]).

test(Me) :-
    library:my_call(me(Me)).

me(client).
```

In this second version, instead of importing the `my_goal/1` meta-predicate, we use explicit qualification in order to call it. Repeating our test query now gives[3]:

```
| ?- client:test(Me).
Calling: library:me(_)
Me = library
yes
```

In order for a programmer to understand this result, he/she needs to be aware that the `:/2` operator both calls a predicate in another module and changes the calling context of the predicate to that module. The first use is expected. The second use is not intuitive, is not useful, and often not properly documented. First, in other programming languages, the choice between implicitly-qualified calls and explicitly-qualified calls is one of typing convenience to the programmer, not one of semantics. Second, in the most common case where a client is reusing a library meta-predicate, the client wants to customize the meta-predicate call with its own local predicate. Different clients will customize the call to the library meta-predicate using different local predicates. In those cases where the

[3] The test could not be performed using Ciao Prolog, which reports a bad module qualification error in the explicit qualified call, complaining that the meta-predicate is not imported, despite the library module being loaded. Importing the predicate eliminates the error but also makes the interpretation of the test result ambiguous.

meta-predicate is defined and used locally, explicit qualification is seldom necessary. We can, however, conclude that the meta-predicate definition still works as expected as the calling context is set to the library module. If we still want the `me/1` predicate to be called in the context of the client module instead, we need to explicitly qualify the meta-argument by writing:

```
test(Me) :-
    library:my_call(client:me(Me)).
```

This is an awkward solution but it works as expected in the cases where explicit qualification is required. It should be noted, however, that the idea of the `meta_predicate/1` directive is to avoid the need for explicit qualifications in the first place. But that requires using `use_module/1-2` directives for importing the meta-predicates and implicit qualification when calling them. This explicit qualification of meta-arguments is not necessary in Logtalk or in the ECLiPSe module system, where explicit qualification of a meta-predicate call sets where to start looking for the meta-predicate definition, not where to look for the meta-arguments definitions.

The semantics of the `:/2` operator in Prolog module systems derived from the Quintus Prolog module system is rooted in optimization goals. When a directive `use_module/1` is used, most (if not all) Prolog compilers require the definition of the imported module to be available, thus resolving the call at compilation time. However, that does not seem to be required when compiling an explicitly qualified module call. For example, using recent versions of SICStus Prolog, SWI-Prolog, and YAP, the following code compiles without errors or warnings (despite the fact that the module `fictitious` does not exist):

```
:- module(client, [test/1]).

test(X) :-
    fictitious:predicate(X).
```

Thus, in this case, the `fictitious:predicate/1` call is resolved at runtime. In our example above with the explicit call to the `my_call/1` meta-predicate, the implementation of the `:/2` operator propagates the module prefix to the meta-arguments that are not explicitly qualified at runtime. This runtime propagation results in a performance penalty. Therefore, and not surprisingly, the use of explicit qualification is discouraged by the Prolog implementers. In fact, until recently, most Prolog implementations provided poor performance for `:/2` calls even when the necessary module information was available at compile time.

Logtalk and ECLiPSe illustrate the first choice for the semantics of explicitly-qualified meta-predicate calls. Consequently, both systems provide the same semantics for implicitly and explicitly qualified meta-predicate calls. Consider the following objects, corresponding to a Logtalk version of the Prolog module example used in the previous section:

```
:- object(library).

    :- public(my_call/1).
    :- meta_predicate(my_call(::)).
    my_call(Goal) :-
        write('Calling: '), writeq(Goal), nl,
        call(Goal),
        sender(Sender), write('Sender:  '), writeq(Sender).

    me(library).

:- end_object.


:- object(client).

    :- public(test/1).
    test(Me) :-
        library::my_call(me(Me)).

    me(client).

:- end_object.
```

Our test query becomes:

```
| ?- client::test(Me).
Calling: me(_G216)
Sender:  client
Me = client.
yes
```

That is, meta-arguments are always called in the context of the meta-predicate call. Logtalk also implements common built-in meta-predicates such as `call/1-N`, `\+/1`, `findall/3`, and `phrase/3` with the same semantics as user-defined meta-predicates. In order to avoid misinterpretations, these built-in meta-predicates are implemented as private predicates.[4] Thus, the following call is illegal and results in a permission error:

```
| ?- an_object::findall(T, g(T), L).
error(permission_error(access, private_predicate, findall(T,g(T),L)),
      an_object::findall(T, g(T), L),
      user)
```

The correct call would be:

```
| ?- findall(T, an_object::g(T), L).
```

[4] Logtalk supports *private*, *protected*, and *public* predicates. A predicate may also be *local* if no scope directive is present, making the predicate invisible to the built-in reflection predicates (`current_predicate/1` and `predicate_property/2`).

3.2 Transparency of Control Constructs

One of the design choices regarding meta-predicate semantics is the transparency of control constructs to explicit qualification. The relevance of this topic is that most control constructs can also be regarded as meta-predicates. In fact, there is a lack of agreement in the Prolog community on which language elements are control constructs and which language elements are predicates. For the purposes of our discussion, we use the classification found on the ISO Prolog standard, which specifies the following control constructs: `call/1`, *conjunction*, *disjunction*, *if-then*, *if-then-else*, and `catch/3`. The standard also specifies `true/0`, `fail/0`, `!/0`, and `throw/1` as control constructs but none of these can be interpreted as a meta-predicate.

When a control construct is transparent to explicit qualification, the qualification propagates to all the control constructs arguments that are not explicitly qualified. For example, the following equivalences hold for most Prolog module systems[5] (left column) and Logtalk (right column):[6]

```
M:(A, B)      ⇔ (M:A, M:B)        O::(A, B)      ⇔ (O::A, O::B)
M:(A; B)      ⇔ (M:A; M:B)        O::(A; B)      ⇔ (O::A; O::B)
M:(A -> B; C) ⇔ (M:A -> M:B; M:C) O::(A -> B; C) ⇔ (O::A -> O::B; O::C)
```

In Prolog module systems where the `:/1` operator sets both the meta-predicate lookup context and the meta-arguments calling context, the above equivalences are consistent with the explicit qualification semantics of meta-predicates described in the previous section. For example:

```
M:findall(T, G, L) ⇔ findall(T, M:G, L)
M:assertz(A)       ⇔ assertz(M:A)
```

This is also true for user-defined meta-predicates. For the example presented in the previous section, the following equivalence holds:

```
library:my_call(me(Me)) ⇔ my_call(library:me(Me))
```

Thus, the different semantics of implicitly and explicitly qualified meta-predicate calls allows the semantics of explicitly qualified control constructs to be consistent with the semantics of explicitly qualified meta-predicate calls.

In Logtalk, where explicit qualification of meta-predicates calls only sets the lookup context, the semantics of control constructs are different: the above equivalences are handy, supported, and can be interpreted as a shorthand notation for sending a set of messages to the same object. ECLiPSe implements a simpler design choice, disallowing the above shorthands, and thus treating control constructs and meta-predicates uniformly. We can conclude that ensuring the same

[5] Note, however, that some Prolog compilers, such as Ciao and ECLiPSe, don't support explicit qualification of control constructs.

[6] Although both columns seem similar, the `::/2` Logtalk operator is a *message-sending* operator whose semantics differ from the module `:/2` explicit-qualification operator.

semantics for implicitly and explicitly qualified meta-predicate calls requires either disallowing explicit qualification of control constructs (as found on e.g. Ciao and ECLiPSe) or different semantics for explicitly qualified control constructs, and thus a clear distinction between control constructs and predicates.

4 Computational Reflection Support

Computational reflection allows us to perform computations about the *structure* and the *behavior* of an application. For meta-predicates, structural reflection allows us to find where the meta-predicate is defined and about the meta-predicate template, while behavioral reflection allows us to access the meta-predicate execution context. As described in Section 1, a meta-predicate execution context includes information about from where the meta-predicate is called. This is only meaningful, however, in the presence of a predicate encapsulation mechanism such as modules or objects. Access to the execution-context is usually not required for common user-level meta-predicate definitions but can be necessary when meta-predicates are used to extend sytem meta-call features. In Logtalk, full access to predicate execution context is provided by the `sender/1`, `self/1`, `this/1`, and `parameter/2` built-in predicates. For Prolog compilers supporting predicate-based module systems, the following table provides an overview of the available reflection built-in predicates:

Prolog compiler	**Built-in reflection predicates**
Ciao 1.10	`predicate_property/2` (in library `prolog_sys`)
ECLiPSe 6.1	`get_flag/3`
SICStus Prolog 4.2	`predicate_property/2`
SWI-Prolog 5.10.4	`context_module/1`, `predicate_property/2`, `strip_module/3`
YAP 6.2	`context_module/1`, `predicate_property/2`, `strip_module/3`

From this table we conclude that the most common built-in predicate is `predicate_property/2`. Together with the ECLiPSe `get_flag/3` and the SWI-Prolog and YAP `context_module/1` predicates, these built-ins only provide *structural* reflection. Specifically, information about the meta-predicate template and the definition context of the meta-predicate. SWI-Prolog and YAP are the only systems that provide *built-in* access to the meta-predicate calling context using the predicate `strip_module/3`. As a simple example of using this predicate consider the following module:

```
:- module(m, [mp/2]).

:- meta_predicate(mp(0, -)).
mp(Goal, Caller) :-
    strip_module(Goal, Caller, _),
    call(Goal).
```

After compiling and loading this module, the following queries illustrate both the functionality of the `strip_module/3` predicate and the consequences of explicit qualification of the meta-predicate call:

```
| ?- mp(true, Caller).
Caller = user
yes

| ?- m:mp(true, Caller).
Caller = m
yes
```

For Prolog compiler module systems descending from the Quintus Prolog module system, it is possible to access the meta-predicate calling context by looking into the implicit qualification of a meta-argument:

```
:- module(m, [mp/2]).

:- meta_predicate(mp(0, -)).
mp(Goal, Caller) :-
    Goal = Caller:_,
    call(Goal).
```

After compiling and loading this module, we can reproduce the results illustrated by the queries above for the SWI-Prolog/YAP version of this module. One possible caveat would be if the Prolog compiler fails to ensure that there is always a single qualifier for a goal. That is, that terms such as `M1:(M2:(M3:G))` are never generated internally when propagating module qualifications.

In the case of ECLiPSe, a built-in predicate for accessing the meta-predicate calling context is not necessary as the `tool/2` directive works by connecting a meta-predicate interface with its implementation:

```
:- module(m).

:- export(mp/2).
:- tool(mp/2, mp/3).
mp(Goal, Caller, Caller) :-
    call(Goal).
```

After loading this module, repeating the above queries illustrates the difference in explicit qualification semantics between ECLiPSe and the other compilers:

```
[eclipse 16]: mp(true, Caller).
Caller = eclipse
Yes (0.00s cpu)

[eclipse 17]: m:mp(true, Caller).
Caller = eclipse
Yes (0.00s cpu)
```

Note that the module `eclipse` is the equivalent of the module `user` in other Prolog compilers.

5 Portability of Meta-Predicate Definitions

The portability of meta-predicate definitions depends on three main factors: the use of implicit qualification when calling meta-predicates in order to avoid the different semantics for explicitly qualified calls discussed in Section 3, the portability of the meta-predicate directives, and the portability of the meta-call primitives used when implementing the meta-predicates. Other factors that may impact portability are the preprocessing solutions for improving meta-predicate performance, described in Section 7, and the mechanisms for computational reflection about meta-predicate definition and execution, discussed in Section 4.

5.1 The call/1-N Control Constructs

The `call/1` control construct is specified in the ISO Prolog standard [8]. This control construct is implemented by virtually all Prolog compilers. The `call/2-N` control constructs, whose use is strongly recommended for meta-predicates working with closures [3], is included in the latest revision of the ISO Prolog Core standard. A growing number of Prolog compilers implement these control constructs but with different maximum values for `N`, which can raise some portability problems. Ideally, the `call/1-N` control constructs would support `N` up to the maximum predicate arity. That depends, however, on the design decisions of a Prolog compiler implementation. For example, in some compilers, such as SWI-Prolog and YAP, the maximum predicate arity of a Prolog predicate is limited only by the available memory. From a pragmatic point-of-view, it is unlikely that user written code (but not necessarily user *generated* code) would require a large upper limit of `N`. Despite the apparent lack of agreement, the more significant portability issues here are Prolog compilers only supporting `call/1` or an arguably small value of `N`. The following table summarizes the implementations of the `call/2-N` control construct on selected Prolog compilers:

System	N	Notes
B-Prolog 7.4	10/65535	(interpreted/compiled i.e. maximum arity)
Ciao 1.10	255	(maximum arity using the `hiord` library)
CxProlog 0.95.0	9	—
ECLiPSe 6.1#68	255	(maximum arity)
GNU Prolog 1.3.1	11	—
JIProlog 3.0.2	5	—
K-Prolog 6.0.4	9	—
Qu-Prolog 8.12	1	(supports a `call_predicate/1-5` predicate)
SICStus Prolog 4.2	255	(maximum arity)
SWI-Prolog 5.10.4	8/1024	(interpreted/compiled i.e. maximum arity)
XSB 3.3	11	—
YAP 6.2	12	—

This table only lists *built-in* support for `call/2-N` control construct. While this control construct can be defined by the programmer using the built-in pred-

icate `=../2` and an `append/3` predicate, such definitions provide relative poor performance due to the construction and appending of temporary lists.

5.2 Specification of Closures and Instantiation Modes in Meta-Predicate Directives

The main portability issue of meta-predicate directives is the use of non-negative integers to specify closures and the atoms used to specify the instantiation mode of normal arguments. Although the use of non-negative integers comes from Quintus Prolog, it was historically regarded as a way to provide information to cross-reference and documentation tools, with Prolog compilers accepting this notation only for backward-compatibility with existing code. Other Prolog compilers such as Ciao define alternative but incompatible syntaxes for specifying closures. There is also some variation in the atoms used for representing the instantiation modes of normal arguments. Some Prolog compilers use an extended set of atoms for documenting argument instantiation modes compared to the basic set (`+`, `?`, `@`, and `-`) found in the ISO Prolog standard. It is therefore tempting to use these extended sets in meta-predicate directives, which will likely raise portability issues. Hopefully, recent Prolog standardization initiatives, specially the development of portable libraries, will lead to a de facto standard meta-predicate directive derived from the extended directive described in Section 2.2.

6 Extending Meta-Predicate Definitions Usefulness

The usefulness of meta-predicate definitions can be extended by adding support for lambda expressions. In the same way meta-predicates avoid the repeated coding of common programming patterns, lambda expressions avoid the definition of auxiliary predicates whose sole purpose is to be used as arguments in meta-predicate calls. Consider the following example (using Logtalk lambda expression syntax[7]):

```
| ?- meta::map([(X,Y),Z]>>(Z is sqrt(X*X+Y*Y)),[(1,4),(2,5),(8,3)],Ds).
Ds = [4.1231056256176606,5.3851648071345037,8.5440037453175304]
yes
```

Without lambda expressions, it would be necessary to define an auxiliary predicate to compute the distance from a point to the origin. This example also illustrates an additional issue when using meta-predicates: the `map/3` list mapping meta-predicate accepts as first argument a closure that is extended by *appending* two arguments. Thus, an existing predicate for calculating the distance, e.g. `distance(X, Y, Distance)`, cannot not be used without writing an auxiliary predicate for the sole purpose of packing the first two arguments.

Native support for lambda expressions can be found in e.g. λProlog [12], Qu-Prolog, and Logtalk. For Prolog compilers supporting a module system, a library is available [13] that adds lambda expressions support. There is, however, a lack of community agreement on lambda expression syntax.

[7] `http://logtalk.org/manuals/refman/grammar.html#grammar_lambdas`

7 Meta-Predicate Performance

Considering that meta-programming is often touted as a major feature of Prolog, the relative poor performance of meta-calls can drive programmers to avoid using meta-predicates in production code where performance is crucial. A common solution is to interpret meta-predicate definitions as high-level macros and to preprocess meta-predicate calls in order to replace them with calls to auxiliary predicate definitions that do not contain meta-calls. This preprocessing is usually only performed on stable code as the automatically generated auxiliary predicates often complicate debugging. The preprocessing code is often implemented in optional libraries, which can be found on Logtalk and several Prolog compilers such as ECLiPSe, SWI-Prolog, and YAP. These libraries, however, require custom code for each meta-predicate. Therefore, user-defined meta-predicates will fail to match the performance of library-supported meta-predicates unless the user also writes its own custom preprocessing code. A more generic solution for pre-processing meta-predicate definitions is needed to make these programming patterns more appealing for performance-critical applications.

8 Conclusions and Future Work

We presented and discussed a comprehensive set of meta-predicate design decisions based on current practice in Logtalk and in Prolog predicate-based module systems. An interesting result is that none of the two commonly implemented semantics for explicitly qualified calls provides an ideal solution that both meets user expectations and allows the distinction between meta-predicates and control constructs to be waived. By describing the consequences of these design decisions we provided useful insight to discuss meta-predicate semantics, often a difficult subject for inexperienced programmers and a source of misunderstandings when porting applications and discussing Prolog standardization. From the point-of-view of writing portable code (including portable libraries), the current state of meta-predicate syntax and semantics across Prolog compilers is still a challenge, despite recent community efforts. We hope that this paper contributes to a convergence of meta-predicate directive syntax, meta-predicate semantics, and meta-predicate related reflection built-in predicates among Prolog compilers.

Future work will include comparing Logtalk and Prolog predicate-based module systems with Prolog atom-based module system and derived object-oriented extensions. The most prominent example of a Prolog compiler featuring an atom-based module system is XSB [14] (which is used in the implementation of the object-oriented extension Flora [15]). XSB does not support a meta-predicate directive. Explicit-qualification of meta-arguments is used whenever the atom-based semantics fail to provide the desired behavior for the implementation of a specific meta-predicate. Interestingly, although atom-based module systems appear to solve or avoid some the issues discussed along this paper, predicate-based module systems are the most common implementation choice. This may be due to historical reasons but a deep understanding of the pros and cons of atom-based

systems, at both the conceptual and implementation levels, will be required to perform a detailed comparison with the better known predicate-based systems.

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Modular Extensions for Modular (Logic) Languages

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Abstract. We address the problem of developing mechanisms for easily implementing modular extensions to modular (logic) languages. By (language) extensions we refer to different groups of syntactic definitions and translation rules that extend a language. Our use of the concept of modularity in this context is twofold. We would like these extensions to be modular, in the sense above, i.e., we should be able to develop different extensions mostly separately. At the same time, the sources and targets for the extensions are modular languages, i.e., such extensions may take as input separate pieces of code and also produce separate pieces of code. Dealing with this double requirement involves interesting challenges to ensure that modularity is not broken: first, combinations of extensions (as if they were a single extension) must be given a precise meaning. Also, the separate translation of multiple sources (as if they were a single source) must be feasible. We present a detailed description of a code expansion-based framework that proposes novel solutions for these problems. We argue that the approach, while implemented for Ciao, can be adapted for other Prolog-based systems and languages.

Keywords: Compilation; Modules; Modular Program Processing; Separate Compilation; Prolog; Ciao; Language Extensions; Domain Specific Languages.

1 Introduction

The choice of a good notation and adequate semantics when encoding a particular problem can dramatically affect the final outcome. Extreme examples are programming pearls, whose beauty is often completely lost when translated to a distant language. In practice, large projects are bigger than pearls and often no single language fulfills all expectations (which can include many aspects, such as development time or execution performance). The programmer is forced to make a commitment to one language —and accept sub-optimal encoding— or more than one language —at the expense of interoperability costs.

An alternative is to provide new features and idioms as syntactic and semantic extensions of a language, thus achieving notational convenience while avoiding inter-language communication costs. In the case of Prolog, language extension through term-expansion systems (combined with operator definitions) has traditionally offered a quick way to develop variants of logic languages and semantics (e.g., experimental domain-specific languages, constraint systems, optimizations, debugging tools, etc.). Some systems, and in particular Ciao [10],

have placed special attention on these capabilities, extending them [1] and exploiting them as the base for many language extensions.

Once a good mechanism is available for writing extensions and a number of them are available, it is natural to consider whether combining a number of them following modular design principles is feasible. For example, consider embedding a simple handy *functional notation* [3] (syntactic sugar to write goals, marked with `~`, in term positions), into a more complex extension, such as the Prolog-based implementation of CHR [8]. In this new dialect, the CHR rule (see Sect. 6.2.1 in Frühwirth's book [8]):

```
T eq and(T1, T2), T1 eq 1, T2 eq X <=> T eq X.
```

can be written more concisely as:

```
T eq and(~eq(1), ~eq(X)) <=> T eq X.
```

Intuitively, expansions are applied one after the other. This already points out that at least a mechanism to determine application order is needed. This is already undesirable because it requires users to be aware of the valid orderings. Furthermore, just ordering may not be enough. In our example, if functional syntax is applied first, it must normalize the `~eq(_)` terms before CHR translation happens, but there is no simple way to indicate to the functional expansion that the CHR constraints have to be treated syntactically as goals. If CHR translation is done first, it will not recognize that `~eq(_)` corresponds to a constraint, and incorrect code will be generated before the functional expansion takes place. Thus, the second rule cannot be translated into the first one by simply composing the two expansions, without tweaking the translation code, which is undesirable.

Moreover, current extension mechanisms have difficulties dealing with the module system. An example is the Typed Prolog extension of [13], which elegantly implements gradually typed Prolog in the style of Hindley-Milner, but needs to treat programs as monolitic, non-modular, units. Even if extensions are made module-aware, the *dynamic* features of traditional Prolog systems present an additional hurdle: programs can change dynamically, and modules may be loaded at runtime, with no clear distinction between program code and translation code, and with no limits on what data is available to the expansion (e.g., consulting the predicates compiled in other arbitrary modules). In the worst case, this leads to a chaotic scenario, where reasoning about language translations is an impossible task.

The previous examples illustrate the limitations of the current extension mechanisms for Prolog and motivate the goals of this work:

- **Predictable Combination of Fine-grained Extensions**: The extension mechanisms must be fine-grained enough to allow rich combinations, but also provide a simple interface for users of extensions. Namely, programmers should be able to write modules using several extensions (e.g., functional notation, DCGs, and profiling), without being required to know the application order of rules or the compatibility of extensions. Obviously, the result of the combination of such extensions must be predictable. That indirectly leads us to the necessity of describing a precise compilation model that includes compilation and loading of the extension code.
- **Integration with Module Systems**: It is thus necessary to make the extensions module-aware, while at the same time constraining them to respect

the module system. For example, it must be possible to determine during expansion to what module a goal being expanded belongs, if that information is available, or to export new declarations. It is well known that modularity, if not designed carefully, can make static analysis impossible [2]. A flexible extension system that however allows breaking modularity renders any efforts towards static transformations useless.

This paper presents a number of novel contributions aimed at addressing these problems. We take as starting point the module and extension system implemented in Ciao [1,10], which is more elaborate than the one offered by traditional Prolog systems. We provide in this paper a refined formal description of the compilation model, and use it to propose and justify the definition of a number of distinct translation phases as well as the information that is available at each one. Then, we propose a set of rule-based extension mechanisms that we argue generalize previous approaches and allows us to provide better solutions for a good number of the problems mentioned earlier.

The paper is structured as follows. Section 2 gives a detailed description of the core translation process for extensions. Section 3 defines a compilation model that integrates the extensions. Section 4 and Section 5 illustrate the rules defined in the previous section by defining several (real-life) language features and extensions. We close with a discussion of related and future work in Section 6, and conclusions in Section 7.

2 Language Extensions as Translation Rules

By language extensions we refer to translations that manipulate a symbolic representation of a given program. For simplicity we will use *terms* representing abstract syntax trees, denoted by $\mathcal{T}$, following the usual definition of *ground* terms in *first order logic*. To simplify notation, we include sequences of terms ($Seq(\mathcal{T})$) as part of $\mathcal{T}$.[3] We also assume some standard definitions and operations on terms: $\mathsf{termFn}(x)$ denotes the $(name, arity)$ of the term, $\mathsf{args} : \mathcal{T} \rightarrow Seq(\mathcal{T})$ obtains the term arguments (i.e., the sequence of children), and $\mathsf{setArgs} : \mathcal{T} \times Seq(\mathcal{T}) \rightarrow \mathcal{T}$ replaces the arguments of a term.

We use a homogeneous term representation for the program, but terms may represent a variety of language elements. The meaning of each term is often given by its surrounding context. In order to reflect this, each input term is labeled with a symbolic *kind* annotation. That annotation determines which transformation to apply to each term.

We define the main transformation algorithm $\mathbf{tr}[\![x : \kappa]\!] = x'$ in Fig. 1. Given a term x of *kind* κ, it obtains a term x' by applying the available rules. Translation ends for a term when the *final* kind is found. The transformation is driven by rules (defined in *compilation modules*). Note that the rules may contain guards in order to make them conditional on the term. Rule $x : \kappa \Longrightarrow x' : \kappa'$ denotes that when a term x of kind κ is found, it is replaced by x' of kind κ'. Rule $\kappa \succ \kappa'$ is the same, but the term is unmodified. Finally, rules $x : \kappa_x \overset{\mathsf{decons}}{\Longrightarrow} \vec{a} : \vec{\kappa}$ and $(\vec{a} : \vec{\kappa},\ x) \overset{\mathsf{recons}}{\Longrightarrow} \kappa_x : x'$ allow the deconstruction (*decons*) of a term into

[3] We will assume –for simplicity and contrary to common practice– that when compiling a program variables are read as special ground terms.

$$
\begin{aligned}
\mathbf{tr}[\![x : \mathit{final}]\!] &= x \\
\mathbf{tr}[\![x : \kappa]\!] &= \mathbf{tr}[\![x : \kappa']\!] \quad (\text{if } \kappa \succ \kappa') \\
\mathbf{tr}[\![x : \kappa]\!] &= \mathbf{tr}[\![x' : \kappa']\!] \quad (\text{if } x : \kappa \Longrightarrow x' : \kappa') \\
\mathbf{tr}[\![x : \kappa_x]\!] &= \mathbf{tr}[\![x' : \kappa'_x]\!] \quad (\text{if } x : \kappa_x \overset{\mathsf{decons}}{\Longrightarrow} \vec{a} : \vec{\kappa}) \\
&\quad \text{where} \\
&\qquad a'_i = \mathbf{tr}[\![a_i : \kappa_i]\!] \quad \forall i.1 < i < |\vec{a}| \\
&\qquad (x : \kappa_x,\ \vec{a'}) \overset{\mathsf{recons}}{\Longrightarrow} x' : \kappa'_x \\
\mathbf{tr}[\![x : \mathit{try}(t, \kappa_1, \kappa_2)]\!] &= \begin{cases} \mathbf{tr}[\![x' : \kappa_1]\!] & \text{if } t(x, x') \\ \mathbf{tr}[\![x : \kappa_2]\!] & \text{otherwise} \end{cases} \\
\mathbf{tr}[\![x_1 \ldots x_n : \mathit{seq}(\kappa)]\!] &= (\mathbf{tr}[\![x_1 : \kappa]\!] \ldots \mathbf{tr}[\![x_n : \kappa]\!])
\end{aligned}
$$

Fig. 1. The Transformation Algorithm

smaller parts, which are translated and then put together by reconstruction of the term (*recons*). Intuitively, this pair of rules allows performing a complex expansion that reuses other rules (which may be defined elsewhere). We will see examples of all these rules later. We divided expansions into finer-grained translations because we want to be able to combine them and to allow them to be interleaved with other rules in such combinations. Monolithic expansions would render their combination infeasible in many cases.

Additionally, there are some rules for *special kinds*, which are provided here for programmer convenience, even if they can be defined in terms of the previous rules. Their meaning is the following: the $\mathit{try}(t, \kappa_1, \kappa_2)$ kind tries to transform the input with the relation t. If it is possible, the resulting term is transformed with kind κ_1. Otherwise, the untransformed input is retried with kind κ_2. This is useful to compose translations. The $\mathit{seq}(\kappa)$ kind indicates that the input term is a sequence of elements of kind κ.[4]

Composition of Transformations Note that the transformation algorithm does not make any assumption regarding the order in which rules are defined in the program, given that the rules define a fixed order relation between kinds. We will see in Section 5 how to give an unambiguous meaning to conflicting rules targeting the same kind.

Example 1 (Combining Transformations). Consider the example about merging CHR and *functional syntax* presented in the introduction. It can be solved in our framework by introducing rules such as:

$$
\begin{aligned}
(a \setminus b \texttt{ <=> } c) : \mathit{chrclause}_1 &\overset{\mathsf{decons}}{\Longrightarrow} (a\ b\ c) : (\mathit{goal}_1\ \mathit{goal}_1\ \mathit{goal}_1) \\
(\_ : \mathit{chrclause}_1,\ (a\ b\ c)) &\overset{\mathsf{recons}}{\Longrightarrow} (a \setminus b \texttt{ <=> } c) : \mathit{chrclause}_2
\end{aligned}
$$

Those rules expose the internal structure of some constructs to allow the cooperation between translations. That is, those rules mean that in the middle of

[4] In the Prolog implementation sequences are replaced by lists.

the translation from the kinds $\mathit{chrclause}_1$ and $\mathit{chrclause}_2$ we allow treatment of a kind goal_1, which could be treated, e.g., by the functional syntax package. Note that neither the CHR nor the functional package are required to know about the existence of each other.

3 Integration in the Compilation Model

In our compilation model programs are separated into modules. Modules can import and use code from other modules. Additionally, modules may load language extensions through special *compilation modules*. For the sake of simplicity, we will show here the compilation passes required for a simplified language with exported symbols (e.g., predicates) and imported modules. Extending it to support more features is straightforward.

We assume that compilation is performed on a single module at a time, in two phases.[5] Let us also assume that each phase reads and writes a series of initial (sources), temporal, and final compilation results (linkable/executable binaries). We will call those elements *nodes*, since clearly there is a dependency relation between them. In practice, nodes are read and written from a (persistent) memory, that we will abstract here as a mapping V. We denote as $V(n)$ the value of a node. We denote as $V(n) \leftarrow v$ the destructive assignment of v to n in V, and $V(n)$ the value of n in V.

Given a module i, the first phase ($\mathsf{strPass}$) performs the source code (denoted for conciseness as $\mathsf{src}[i]$) parsing and additional processing to obtain the *abstract syntax tree* ($\mathsf{ast}[i]$) and module interface ($\mathsf{itf}[i]$). In order to extend the compilation, we introduce a call to strTr. This will be defined herein in terms of the translation algorithm $\mathbf{tr}[\![\cdot : \tau]\!]$ (Fig. 1), working on the program definitions. We will see actual example definitions for them in Section 5. We call this the *structural* pass, since we can change arbitrarily the structure of the syntax tree, but we are not yet able to fully provide a semantics for the program, which may depend on external definitions from imported modules.[6] Indeed, the information about local definitions (e.g., defined predicates) and the module *interface* (defined below) is available only at the end of this pass. Note that we load compilation modules dynamically during compilation. We will show later how this is done.

Once the first phase finishes, the module interfaces are available. In the second phase ($\mathsf{semPass}$), the interface of the imported modules are collected and processed alongside with the module abstract syntax tree ($\mathsf{ast}[i]$) and interface ($\mathsf{itf}[i]$). The output of this phase (denoted as $\mathsf{bin}[i]$), can be either in an executable form (e.g., bytecode), or in a suitable *kernel* language treatable by other tools (e.g., like program analysis). As in the previous phase, we introduce an extensible translation pass called semTr, similar to strTr. However, this time it can access the interface of imported modules. We name this the *semantic* pass.

[5] This is common in many languages, since at least two passes are required to allow identifiers in arbitrary order in the program text.

[6] It is important not to confuse *importing* a module with *including* a file. The latter is purely syntactic and can be performed during program reading. For the sake of clarity, we omit dependencies to included files in further sections.

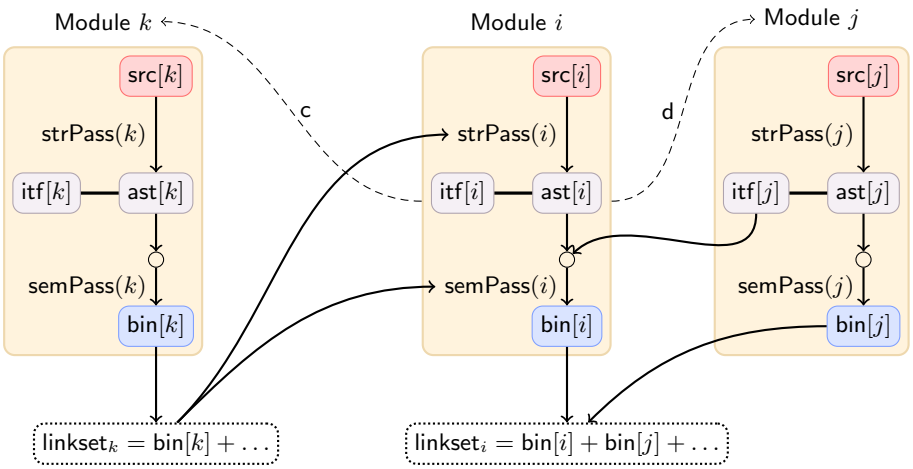

Fig. 2. Example of compilation dependencies for module i, which imports module j (d arrow), and requires compilation module k (c arrow).

For loading compilation modules (or any other module) dynamically, we need to compute the *link-set* (the reflexive transitive closure of the *import* relation between modules), or the minimum set of modules required during execution of a module.

Compilation Order In general, determining the order in which compilation must occur, and which recompilations have to take place whenever some source changes is not a straightforward task. For example, see Figure 2 which shows the dependencies for the incremental compilation of a module i depending on module j and compilation module k. We need an algorithm that automatically schedules compilation of modules (both program and translation modules) and which is incremental in order to reduce compilation times. Both of these requirements are necessary in a scalable, useful, dynamic environment. I.e., when developing, the user should not have to do anything special in order to ensure that all modules are compiled and up to date. However, since dependencies are dynamic we cannot (and would not want to) rely on traditional tools like `Makefiles`.

3.1 Incremental Compilation

We solve the problems of determining the compilation order, and making the algorithm incremental, with minor changes. The idea is to invoke the necessary compilation passes before each $V(n)$ is read, in order to access up-to-date values. For that, we define the UpdateNode(n) in Algorithm 1.

The algorithm works with *time-stamps*. We extend the V mapping with an (also persistent) mapping T between nodes and time-stamps, so that: $T(x) = \bot$ if the node does not have any value, and for each $V(n) \leftarrow v$, $T(n)$ is updated with a recent time-stamp. We need another mapping S, that relates a node with

```
   data: mappings V, T, and S
 1 def UpdateNode(n):
 2     r = RulingNode(n) ; CheckNode(r)
 3     if S(r) = invalid then
 4         S(r) ← working
 5         if GenNode(r) then S(r) ← valid(T(r)) else S(r) ← error
 6 def CheckNode(r):
 7     if S(r) = ⊥ then
 8         if UpToDate(T(r), NodeInputs(r)) then S(r) ← valid(T(r))
 9         else S(r) ← invalid
10 def UpToDate(t, oldin):
11     if t = ⊥ ∨ oldin = ⊥ then return False
12     foreach n_in ∈ oldin do
13         r_in = RulingNode(n_in) ; CheckNode(r_in)
14         if ¬((S(r_in) = valid(t_in)) ∧ (t_in ≤ t)) then return False
15     return True
```

Algorithm 1: UpdateNode

its *status*, and is non-persistent and monotonous during a *compilation session* (during which compilation of a set of modules takes place, with no allowed changes in source code). When a *compilation session* starts, we begin with the empty status for all nodes. Finally, we assume that for passes that produce more than one output node (e.g., the interface and the syntax tree), we can choose a fixed one of them as the *ruling node* (e.g., the interface). We denote by RulingNode(n) the ruling node of n.

UpdateNode works by obtaining the ruling node, invoking CheckNode to update its status, and, depending on it, invoking GenNode to (re)generate the outputs if necessary. CheckNode (line 6) examines the node and updates its status. If the node was visited before, the status will be different from $\bot$, and it will exit. If not, it will check that r is up to date (UpToDate($t, oldin$), line 10) w.r.t. all the dynamic input dependencies ($oldin$ = NodeInputs(r)). In our case, for strPass(i) the input nodes are src[i] and the *link-set* of all compilation modules specified in the (old) itf[i]. For semPass(i) the input nodes are itf[i] and itf[j], for each imported module j specified in itf[i], in addition to the nodes for compilation modules. The input nodes are $\bot$ if it was not possible to obtain them (i.e., no itf[i] is found). If the node is up-to-date, its status is marked as valid(t), indicating that it needs no recompilation. If not, it is marked as invalid. This may mark the status of other dependent nodes, but no action is performed on them.

For terminal nodes (e.g., source code src[i] for some module i), GenNode(r) will simply check that the node r exists, and NodeInputs(r) is empty. CheckNode will mark existing terminal nodes as *valid*. Non-existing nodes will be marked as *invalid*, and later UpdateNode will try to generate them. Since they do not exist, they will be marked as *error*. For computable nodes, GenNode(r) invokes the compilation pass that generates the corresponding output ruling node (based on

static output dependencies, i.e., $\mathsf{strPass}(i)$ generates $\mathsf{itf}[i]$, $\mathsf{semPass}(i)$ generates $\mathsf{bin}[i]$). If compilation was successful, the status is updated with $\mathsf{valid}(T(r))$ (indicating that it was successfully generated within this *compilation session*). On error, error is used as mark. An additional $\mathsf{working}$ status is used to mark nodes being computed and detect compilation loops (i.e., compilation modules depending on themselves). Note that for nodes whose value is assumed to be always up to date (*frozen nodes*, e.g., precompiled system libraries or static modules that cannot be updated) we make $S(n) = \mathsf{valid}(0)$ by definition (denoting the oldest possible time-stamp).

Correctness and Optimality of Time-stamp Approximation The algorithm is based on, given a node, knowing if it needs to be recomputed. Based on the fact that each compilation pass only depends on its inputs, we can determine this by checking if the contents of a node have changed w.r.t. the contents used for the pass. For that, we could keep all the versions of each node, and number them in increasing order. Instead of local version numbers, we can use *time-stamps*, as a global version counter updated each time a node is written. This has the property that for each generated node n, $T(n) \geq T(m)$ for each m being an input dependency of n. If we can reason on time-stamps, then keeping the contents of each node version is unnecessary.[7] So if we find an input dependency with a time-stamp greater than $T(n)$, then it is possible that it may have changed. We may have false positives (time changed but the value is the same), which will result in more work than necessary, but not incorrect results. If the time-stamp is less or equal then we can be assured that it has not changed since n was generated. Unless time-stamps are artificially changed by hand, we will not have false negatives (whenever a node needs to be computed, it will be).

We only need to keep for each node its dependencies (the name of the nodes, not their value), or provide a way of inferring them from other stored values.[8]

Handling Compilation Module Loops When a compilation module depends on modules that depend on it, a *deadlock* situation occurs. The compilation module cannot be compiled because it requires some modules that cannot be compiled yet. However, it is common to have languages that compile themselves. We solve the issue by distinguishing between normal and static modules. Static modules have been compiled previously and their $\mathsf{bin}[i]$ and $\mathsf{itf}[i]$ are kept for following compilations (say $\mathsf{bin}[i]^S$ and $\mathsf{itf}[i]^S$ respectively). In that case, $(\mathsf{itf}[i] = \mathsf{itf}[i]^S \wedge \mathsf{bin}[i] = \mathsf{bin}[i]^S)$. The set of all static modules for the compiler constitutes the *bootstrap* system. Note that *self-compiling* modules require caution, since accidentally losing the bootstrap will make the source code useless (our source, only understood by our compilation module, may be written in a language for which there exists no working compiler).

[7] When dealing with large dependencies, this seems inpractical, both in terms of time and space. We want this operation to be as fast as possible and not consume much additional space.

[8] That is of course not necessary for static dependencies (e.g., that each $\mathsf{ast}[i]$ depends on $\mathsf{src}[i]$).

$$\begin{aligned}
\mathit{sents} &\succ \mathit{sents}_{\vec{\mathcal{E}_s}} & \mathit{term} &\succ \mathit{term}_{\vec{\mathcal{E}_t}}\\
\mathit{sents}_{ts} &\succ \mathit{seq}(\mathit{sent}_{ts}) & \mathit{term}_{[t|ts]} &\succ \mathit{try}(t, \mathit{term}_{ts}, \mathit{term}_{ts})\\
\mathit{sent}_{[t|ts]} &\succ \mathit{try}(t, \mathit{sents}_{ts}, \mathit{sent}_{ts}) & \mathit{term}_{[]} &\succ \mathit{rterm}\\
\mathit{sent}_{[]} &\succ \mathit{term} & x : \mathit{rterm} &\overset{\text{decons}}{\Longrightarrow} \mathsf{args}(x) : (\mathit{term} \ldots \mathit{term})\\
& & (x : \mathit{rterm},\ \vec{a}) &\overset{\text{recons}}{\Longrightarrow} \mathsf{setArgs}(x, \vec{a}) : \mathit{final}
\end{aligned}$$

$$\begin{aligned}
\mathit{clauses} &\succ \mathit{seq}(\mathit{clause}) & \mathit{body} &\succ \mathit{try}(f, \mathit{control}, \mathit{goal})\\
\mathit{clause} &\succ \mathit{clause}_{\vec{\mathcal{E}_c}} & f(x, x) &\equiv x \in \{\texttt{,/2}, \texttt{;/2}, \ldots\}\\
\mathit{clause}_{[t|ts]} &\succ \mathit{try}(t, \mathit{clause}_{ts}, \mathit{clause}_{ts}) & x : \mathit{control} &\overset{\text{decons}}{\Longrightarrow} \mathsf{args}(x) : (\mathit{body} \ldots \mathit{body})\\
\mathit{clause}_{[]} &\succ \mathit{hb} & (x : \mathit{control},\ \vec{a}) &\overset{\text{recons}}{\Longrightarrow} \mathsf{setArgs}(x, \vec{a}) : \mathit{final}\\
(h \texttt{:-} b) : \mathit{hb} &\overset{\text{decons}}{\Longrightarrow} (h\ b) : (\mathit{head}\ \mathit{body}) & \mathit{goal} &\succ \mathit{goal}_{\vec{\mathcal{E}_g}}\\
(_ : \mathit{hb},\ (h\ b)) &\overset{\text{recons}}{\Longrightarrow} (h \texttt{:-} b) : \mathit{final} & \mathit{goal}_{[t|ts]} &\succ \mathit{try}(t, \mathit{body}, \mathit{goal}_{ts})\\
& & \mathit{goal}_{[]} &\succ \mathit{resolv}
\end{aligned}$$

Fig. 3. Emulating Ciao translation rules

Module Invariants and Extensions Although the kernel language may provide low-level pathways if necessary (e.g., to implement debuggers, code inspection tools, or advanced transformation tools), it is important not to break the module *invariants*. One invariant is the module interface ($\mathsf{itf}[j]$), which once computed cannot be changed without invalidating the compilation of any module i that imports it j. For this reason, a *semantic* expansion cannot modify the module interface.

4 Backward Compatibility

We now illustrate how the Ciao expansion primitives [1] can be easily emulated within the proposed approach. Ciao extensions are defined in special libraries called *packages*. They contain lexical and syntactic definitions (such as new operators), and hooks for language extension, defined in *compilation modules*. The available hooks can be seen as partial functional relations (or predicates that given an input have at least one solution) that translate different program parts: *term*, *sentence*, *clause*, and *goal translations*. For conciseness, we will denote them as $\mathcal{E}_t$, $\mathcal{E}_s$, $\mathcal{E}_c$, $\mathcal{E}_g \subseteq \mathcal{T} \times \mathcal{T}$, respectively. The transformations in a single package will be the tuple $\mathcal{E} = (\mathcal{E}_t, \mathcal{E}_s, \mathcal{E}_c, \mathcal{E}_g)$. We will denote with $\vec{\mathcal{E}} = (\mathcal{E}_1 \ldots \mathcal{E}_n)$ all the transformation specifications that are local and used in module, and by $\vec{\mathcal{E}_k}$ the sequence of translations $(\mathcal{E}_{1_k} \ldots \mathcal{E}_{n_k})$, for a particular $k \in \{t, s, c, g\}$. Fig. 3 shows the emulation of these translations.

The translations made during the strTr phase start with $\mathbf{tr}[\![\cdot : \mathit{sents}]\!]$. A term of kind *sents* represents a sequence of sentences, that is translated as a $\mathit{sents}_{\vec{\mathcal{E}_s}}$. Subscripts are used here to represent families of *kinds*. The kind sents_{ts} represents a sequence of sentences that require the translation sent_{ts}. The third rule indicates that a sentence of kind $\mathit{sent}_{[t|ts]}$ (we extract the first element of the

list of transformations) will be transformed by t, yielding a term of kind sents_{ts} (i.e., a sequence of sentences) on success.[9] In case of failure, the untransformed term will be treated as a sent_{ts}. In this way, all transformations in $\vec{\mathcal{E}_s}$ (i.e., all `sentence_trans`) will be applied. Once ts is empty, the result is translated as kind *term*, equivalent to $\mathit{term}_{\vec{\mathcal{E}_t}}$. Similarly to the previous case, all transformations in ts (i.e., all `term_trans`) are tried and removed from the list of pending transformations. When ts is empty, the datum is treated as an *rterm*, which divides the problem into the translation of arguments as kind *term* and reuniting them as a final (non-suitable for further translations) result. Both transformations are applied in the same order as specified in Ciao.

The translations made during the semTr phase start with $\mathbf{tr}[\![\cdot : \mathit{clauses}]\!]$. Sequences of clauses are treated in a similar way as sentences, with the difference that the translation of a clause always returns one clause (not a sequence). When all translations in $\vec{\mathcal{E}_c}$ (all `clause_trans`) have been performed, the head and body are treated. In this figure, we do not show any successor for the *head* kind, since this will be done in the following examples (we could add $\mathit{head} \succ \mathit{final}$ to mark the end of the translation). For *body*, we apply the same body translation on the arguments of control constructs (e.g. `,/2`, `;/2`, etc.). If we are not treating a control structure, the translations in $\vec{\mathcal{E}_g}$ are applied (all `goal_trans`). Note that the first kind in the *try* kind of goals is *goal*. In contrast with other translations, when a goal translation is successfully applied, it is not removed from the list; all translations are tried again until none is applicable.[10] In such case, the term is translated as a *resolve* kind (for the same reason as for *head*, we leave it open for later translations).

Note the flexibility of the base framework: for instance, introducing changes in the expansion rules at fundamental levels can be done, even modularly.

Priority-based Ordering of Transformations The rules presented in this section establish a precise and fixed application order. However, when more than one sentence, term, clause, or goal translation is used in the same module the ordering among them also needs to be specified. The standard solution for this problem in Ciao is to use the order in which the packages which contain the expansion code are stated (e.g., in `:- use_package([dcg, fsyntax])` the `dcg` transformations precede those of `fsyntax`. We propose an arguably better solution for this problem: to introduce a priority in each hook, so that all transformations in $\vec{\mathcal{E}}$ can be ordered beforehand. With this solution (now implemented in Ciao) directives such as `:- use_package([dcg, fsyntax])` and `:- use_package([fsyntax, dcg])` are fully equivalent, and both would apply the transformations in the right order. Of course, this moves the responsibility from the user of the extension to the extension developer. However, in practice this represents a huge advantage for users of packages.

[9] We assume that concatenation of sequences is implicit. We can adapt all the discussion to work with lists of sentences, but that would obscure the exposition.

[10] This preserves the semantics of the original translation hooks, where termination is up to the writter of translation rules. Detecting those problems is out of the scope of this paper.

5 Examples and Applications

We show the expressivity of the rules with fragments of two translations that deal with the module system and meta-predicates. Each of them is presented separately, but their combination results in a transformation equivalent to that hardwired in the Ciao compiler (and which was not expressible in the old transformation hooks). For the sake of clarity, we continue using the formal notation in all the following sections. Writing the Prolog equivalent of both the rules and the driver algorithm presented here is straightforward. As implemented in the Ciao compiler, Prolog terms can be used to represent the abstract syntax tree. The different stages of compilation can be kept in memory as facts in the dynamic database, with extra arguments to identify the module.

We indicate the current module as cm. We will assume that we have access to the information visible during the translation, such as parsed module code, declarations, interfaces, etc.

Example 2 (Predicate-based Module System). The following rules perform the module resolution and symbol replacement in all the clause goals to implement a predicate-based module system via a language extension. Instead of duplicating the logic to locate goal positions, the translations are *inserted* in the right place just after goal expansions are performed (Fig. 3).

We denote that a predicate symbol f is defined in the current module by $\mathsf{localdef}(f) \equiv \mathsf{defined}(f) \in \mathsf{ast}[\mathsf{cm}]$, and that f is exported by an imported module m by $\mathsf{importdef}(f,m) \equiv (\mathsf{exported}(f) \in \mathsf{itf}[m] \wedge \mathsf{imported}(m) \in \mathsf{ast}[\mathsf{cm}])$. Let $\mathsf{modlocal}(m,t)$ be a term operation that replaces the principal functor of term t by another one that is private to module m (e.g., by a special representation, not directly accessible from user code, that concatenates the name of the current module cm with the symbol). The translation of *head* transforms the term using that operation. The rule for *resolv* does the same, but uses the module obtained from lookup (that indicates where the predicate is defined).[11]

$$
\begin{aligned}
x : \mathit{head} &\Longrightarrow \mathsf{modlocal}(\mathsf{cm}, x) : \mathit{final} && \\
x : \mathit{resolv} &\Longrightarrow \mathsf{modlocal}(m, x') : \mathit{meta} && (\text{if } \mathsf{lookup}(x, m, x')) \\
x : \mathit{resolv} &\Longrightarrow \mathsf{error}(\text{"}\mathit{module\ error}\text{"}) : \mathit{final} && (\text{if } \neg\mathsf{lookup}(x, \_, \_))
\end{aligned}
$$

$$
\begin{aligned}
\mathsf{lookup}(a, m, a') \equiv\ & (\neg\mathsf{qual}(a, \_, \_) \ \wedge a' = a \wedge \mathsf{localdef}(f) \wedge m = \mathsf{cm}) \vee \\
& (\neg\mathsf{qual}(a, \_, \_) \ \wedge a' = a \wedge \mathsf{importdef}(f, m) \wedge m = \mathsf{cm}) \vee \\
& (\mathsf{qual}(a, m, a') \wedge m = \mathsf{cm} \wedge \mathsf{localdef}(f)) \vee \\
& (\mathsf{qual}(a, m, a') \wedge m \neq \mathsf{cm} \wedge \mathsf{importdef}(f, m)) \\
& \text{where } f = \mathsf{termFn}(a')
\end{aligned}
$$

The complete specification is lengthy, but not more complicated. E.g., it would require more elaborate error handling, which checks for ambiguity on import (e.g., m in lookup must be unique, etc.).

[11] $\mathsf{qual}(mg, m, g)$ is true iff the term mg is the qualification of term g with term m (e.g., `lists:append([1],[2],[1,2])`). We use it to avoid ambiguity with the colon symbol used elsewhere in rules.

Example 3 (Rules for Meta-predicates). Goals that call meta-predicates in Prolog require special handling of their arguments. We specify the translation of such goals though a kind *meta*. The translation rule decomposes the term into meta-arguments, each of kind $\mathit{marg}(\tau)$, where τ is the meta-type for the predicate, e.g., `goal`). Note that we assume that $\mathsf{ast}[\mathsf{cm}]$ includes a term $\mathsf{metaPred}(f, \vec{\tau})$ for each `:- meta_predicate` declaration. That relates the module-local symbol f of the predicate with each of the *meta-types* of the goal arguments. The translation of $\mathit{marg}(\tau)$ returns a pair of the transformed term and an optional goal. Then, the composition rule rebuilds the goal by placing the transformed terms as arguments, collecting the optional goals in front of it:

$$
\begin{aligned}
g : \mathit{meta} &\overset{\mathsf{decons}}{\Longrightarrow} \vec{x} : \vec{\kappa} \quad \text{where} \\
&\quad \vec{x} = \mathsf{args}(g) \\
&\quad \mathsf{metaPred}(\mathsf{termFn}(g), \vec{\tau}) \in \mathsf{ast}[\mathsf{cm}] \\
&\quad \kappa_i = \mathit{marg}(\tau_i) \quad \forall i. 1 < i < |\vec{\tau}| \\
(g : \mathit{meta},\ \vec{a}) &\overset{\mathsf{recons}}{\Longrightarrow} g' : \mathit{final} \quad \text{where} \\
&\quad a_i = (x_i, s_i) \quad \forall i. 1 < i < l, \quad l = |\vec{a}|, \\
&\quad g' = \mathsf{toConj}((s_1\ s_2\ \ldots\ s_l\ \mathsf{setArgs}(g, \vec{x})))
\end{aligned}
$$

The toConj function transforms the input sequence into a conjunction of literals. We list below the rules for arguments. In the cases where the arguments do not need any treatment, we use ϵ as the second element in the pair, which denotes the empty sequence. The case where the argument represents a goal, but is not known at compile time (e.g., x is a variable, or $x = qm : \_$, where qm is not an atom), is captured by $\mathsf{needsRt}(x)$. In such case the rule emits code that will perform an expansion at run time (which however may share code with those rules). Finally, if the argument represents a goal, we use a deconstruction rule to expose an argument of kind *body*, which once translated is put back in a pair, as required by $\mathit{marg}(\_)$.[12]

$$
\begin{aligned}
x : \mathit{marg}(\tau) &\Longrightarrow (x, \epsilon) : \mathit{final} && (\text{if } \tau \neq \mathsf{goal}) \\
x : \mathit{marg}(\tau) &\Longrightarrow (x', (\mathtt{rtexp}(x, \tau, \mathsf{cm}, x'))) : \mathit{final} && (\text{if } \tau = \mathsf{goal} \wedge \mathsf{needsRt}(x)) \\
&\quad \text{where } x' \text{ is a new variable} \\
x : \mathit{marg}(\tau) &\overset{\mathsf{decons}}{\Longrightarrow} x : \mathit{body} && (\text{if } \tau = \mathsf{goal} \wedge \neg\mathsf{needsRt}(x)) \\
(\_ : \mathit{marg}(\tau),\ x) &\overset{\mathsf{recons}}{\Longrightarrow} (x, \epsilon) : \mathit{final}
\end{aligned}
$$

Example 4 (Combined Transformation). The previous transformations can be combined to translate goals involving meta-predicate calls into plain module-qualified goals. The rules defined in this section and in Section 4 can be used to transform the input goal:

$$G = \texttt{findall(X,member(X,[1,2,3]),Xs)}$$

[12] This allows applying rules treating *bodies*, such as symbol renaming for the module system.

as G' by evaluating **tr**$[\![G : goal]\!]$ so that:

$$G' = \texttt{'aggregates:findall'(X,'lists:member'(X,[1,2,3]),Xs)}$$

assuming that `findall/3` is imported from the module `aggregates`, that `member/2` is imported from `lists`, and that the meta-predicate declaration of `findall/3` specifies that its second argument is a goal.

6 Related Work

In addition to the classic examples for imperative languages, such as the `C` preprocessor, or more semantic approaches like `C++` *templates* and Java *generics*, much work has been carried out in the field of extensible syntax and semantics in the context of functional programming. Modern template systems such as the one implemented in the Glasgow Haskell compiler [14] generally provide syntax extension mechanisms in addition to static metaprogramming. The Objective Caml preprocessor, Camlp4 [4], provides similar features but focuses more on the syntax extension aspects. Both systems allow the combination of different syntax within the host language by using explicit mechanisms of quotations/antiquotations.

Another elegant approach consists on defining language extensions based on interpreters. In [11] a methodology for building domain-specific languages is shown, which combines the use of modular monad interpreters with a partial evaluation stage to reduce or eliminate the interpretation overhead. Although this approach provides a clean semantics for the extension, it has the disadvantage of requiring the (not always automatable) partial evaluation phase for efficiency, and its integration with the rest of the language and with the compilation architecture is more complex.

Another solution explored has been to expose the abstract syntax tree, through a reasonable interface, to the extensions. Racket (formerly PLT Scheme) [7] has an open macro system providing a flexible mechanism for writing language extensions. It allowed the design of domain-specific languages (including syntax), but also language features such as, e.g., the class and component systems, which in Racket are written using this framework. To the extent of our knowledge, there is no formal description of the framework nor whether and how multiple language extensions interact when specified simultaneously. However, it is interesting to note that despite growing independently, Ciao and Racket, both dynamic languages, have developed similar ideas, like separation of compile-time and run-time affairs and the necessity of expansions at different phases.

Finally, extensibility has also been achieved by making use of rewriting rules. For instance, by mixing such features with compilation inlining, the Glasgow Haskell compiler provides a powerful tool for purely functional code optimization [12]. It seems however that the result of the application of such rules can quickly become unpredictable [6]. In the context of constraint programming, a successful language transformation tool is Cadmium [5], which compiles solver-independent constraint models.

7 Conclusions

We have described an extensible compilation framework for dynamic programming languages that is amenable to performing separate, incremental compilation. Extensibility is ensured by a language of rewrite rules, defined in *pluggable* compilation modules. Although the work is mainly focused on Prolog-like languages, most of the presentation deals with common concepts (modules, interfaces, declarations, identifiers), and thus we believe that it can be adapted to other paradigms with minor effort.

In general, the availability of a rich and expressive extension system is a large asset for language design. One obvious advantage is that it helps accommodate the programmer's need for syntactic sugar, while keeping changes in the kernel language at a minimum. It also offers benefits for portability, since it makes it possible to keep a common front end (or a set of language features) and *plug in* different kernel engines (e.g., Prolog systems) at the back end, as long as they provide access to the same kernel language (or one that is rich enough) [15].

Beyond the obvious usefulness of the framework as a separation of concerns during the design of extensions (the support for extension composition and separate compilation, etc.), the translation rules can also be seen as a complementary specification mechanism for the language features designed. If such rules are succinct and clear enough, which is not that hard in practice, they can actually be exposed to programmers alongside standard documentation. We plan to modify the lpdoc tool [9] to provide support for this.

We believe that the model proposed makes it easier to provide unambiguous, composable specifications of language extensions, that should not only make reasoning about correctness easier, but also avoid causing and propagating erroneous language design decisions (such as, e.g., unintended compilation dependencies between modules that would ruin any *parallel* compilation or analysis efforts) that are normally hard to detect and correct. We also hope that our contribution will contribute, in the context of logic programming, towards setting a basis for interoperability and portability of language extensions among different systems.

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Work in progress: A prototype refactoring tool based on a mechanically-verified core

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Abstract. This is a brief experience report on implementing a tiny refactoring tool around a verified core which has been generated using a theorem prover. This forms part of ongoing work which seeks to experiment with this setup to find a workable arrangement. It is based on earlier work on verifying refactorings and generating their definitions from theorem-prover scripts.

Keywords: program refactoring, theorem proving, code generation, functional programming

1 Introduction

Verifying the correctness of a specification is often difficult enough, but it feels all the more rewarding when a little more work could yield a readily executable artefact from a specification. This article describes the adaptation of a theorem-prover script to generate code, and the integration of this code with supporting code[1]. The composite code implements a refactoring tool for a tiny functional language, the core of which comprises the program-transformation component (and which has been verified to be semantics-preserving). The tool described is small, and this account is anecdotal at best, but this work was carried out to find out about what kind of challenges one faces when building a tool around a verified core. It was hoped that working on a small prototype would reveal some of the pitfalls to watch out for before endeavouring to work on a larger-scale project of this kind.

These pitfalls may arise both on the theorem-proving side as well as in the non-verified part of the program. This article describes the experimental refactoring tool 'prefactor' and the article's contribution is twofold: in section 4 it extends earlier work [6] to build a prototype refactoring tool, and in section 6.1 it outlines a different approach to obtain code from a refactoring's correctness proof, as an alternative to the approach taken earlier [6]. Earlier work tended to be more theoretically-motivated; this time round the objective is to study how the theoretical element could be adapted to better suit the generation of code for use in programming tools.

[1] The Isabelle and ML source code related to this article can be downloaded from the author's webpage.

2 Background

This account builds on two earlier articles: the first [7] describes a set of refactoring specifications which were verified using Isabelle/HOL [5]; the second article [6] takes one of these specifications, verifies an implementation against it, and describes the generation of code for the implementation. Since the refactoring involved injecting a new subterm into an existing term one of the pre-conditions to its application was that the subterm was of the right type. This necessitated including an executable definition of a type-checker in the proof script and verifying it against the language's static semantics. The type-checking code was then generated together with the refactoring. This used Isabelle/HOL's code-generation facility developed by Florian Haftmann [2]. Program generation worked by translating (necessarily terminating) recursive definitions made in Isabelle into a target language; for this reason we call this *generation* rather than *extraction* (which usually means mining a program out of a proof). Extraction of refactorings has also been explored and this is described in section 6.1.

2.1 Refactoring

Program refactoring involves making alterations to a program such that its external behaviour is unchanged. This is done to improve the code's clarity and maintainability, or to adapt it before adding new functionality. What constitutes a refactoring cannot entirely be formalised, but it is often possible to formalise and prove a refactoring's behaviour-preservation property. Refactorings are often applied manually but it is desirable to automate the application of refactorings since not only do they tend to be bureaucratic but, for this reason, they are very easy to get wrong. In order to be useful, automatic applications of refactorings must not only preserve the external behaviour of a program but they must also preserve its appearance – whitespace, bracketing, and comments.

Let us look at a small example of refactoring. The illustration on the next page shows the effect of refactoring a program, and attention is drawn to the type of `f`: this refactoring broadens the function's return type into the a disjoint union. For example, one could use this refactoring to adapt the program to model partial functions in this way. Note that other parts of the program are changed selectively by the refactoring to adapt to this change. The symbol F represents a metavariable ranging over expressions denoting functions over natural numbers. The syntax of the 'case' expression means the following: if `(f y)` is a left-injection then the left arm of the expression is used: `x` is bound to the value of `(f y)` and used in the body of the expression (which lies to the left of '$\Leftarrow$'). The behaviour for right-injections is symmetric. Note that the expression-bodies in both arms of the case-expression are of type `nat`: the changes made to the program by the refactoring are constrained to occurrences of `f` – the function

we refactored. Once refactored, more functionality can be added to the program to benefit from its new structure.

```
fun f : nat → nat
fun f x = F

fun m : nat → nat
fun m y =
  (f y)
```

Original program

→

```
fun f : nat → nat⊕unit
fun f x = left nat⊕unit F

fun m : nat → nat
fun m y =
 case [x ⇐x] (f y) [v⇒ zero]
```

Refactored program

Refactorings are gathered into a *catalogue* which contains their descriptions in a uniform style. Such a description includes an informal specification of a refactoring's *side-conditions*, i.e. criteria which must be satisfied before applying the program transformation. These criteria should be sufficient to preserve a program's behaviour. A refactoring tool can be regarded as a mechanised catalogue together with supporting functions (for parsing and printing the program, for example). Refactoring tools are never used directly, they are used through an IDE as illustrated in Figure 1. The prototype described in this article follows this mode of use, as described in section 3. This article is concerned with refactoring programs in a tiny functional language based on PCF, and the syntax of which is similar to that of ML. The refactoring implemented in this tool, over programs in this language, is described on the next page.

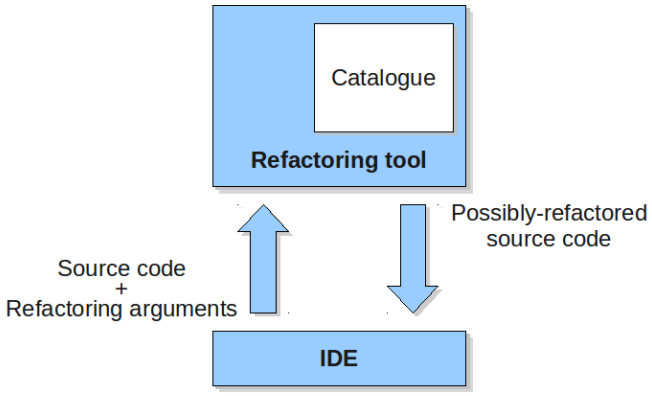

Fig. 1. A refactoring tool usually interfaces with an IDE through which the user indicates the code they wish to refactor, chooses the refactoring they wish to apply, and supplies any additional arguments required by that refactoring. The refactoring tool then attempts to apply the refactoring and returns the refactored source code to the IDE. If the refactoring does not take place (because, for example, the program failed to parse, or one of the side-conditions was not satisfied) then the source code is unchanged.

The refactoring implemented in this tool serves to broaden the type of a variable into a disjoint union with an arbitrary type supplied by the user. Symbols A and B are metavariables ranging over types; M_1, M_2 and N are metavariables ranging over terms. The substitution operation on terms is implicit (this operation is highlighted in the scheme below). The variable identifiers `v1` and `v2`, the term N, and the type B are user-supplied parameters to the refactoring.
The refactoring takes expressions having the following shape:

$$(\textbf{fn}\ \ x\ \ :\ \ A\ \Rightarrow\ M_1\ )\ \ M_2$$

... and transforms them as shown below.

$$(\textbf{fn}\ \ x\ \ :\ \ A \oplus B\ \Rightarrow$$
$$\quad M_1\,[\,(\textbf{case}\ \ [\mathrm{v1} \Leftarrow \mathrm{v1}]\ \ x\ \ [\mathrm{v2} \Rightarrow N\,])\,/x]$$
$$)\ \ (\textbf{left}\ \ A \oplus B\ \ M_2\ )$$

3 Design

The plan was to adapt previous work [6] to form a basis for a tool. The proof script had to be modified slightly so that the generated code would work with the data structure used to represent programs (described in the next section). Once this code had been generated it was interfaced with supporting code which implemented the other features needed by the tool: the parser, printer, and interface with the outside world. The intended behaviour of the tool is outlined in Figure 2.

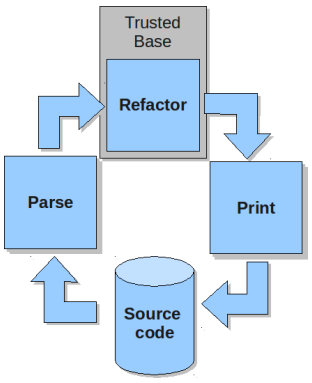

Fig. 2. Stages in automated refactoring. Since the refactoring code described here was generated from a verified specification it is considered to form the trusted core of the refactoring tool.

3.1 Program representation

As previously mentioned, a refactoring must preserve all features of concrete syntax – such as whitespace and bracketing – and must not discard comments from the refactored code. Various approaches have been tried by existing tools to ensure this. Li et al. [3] describe the process used in HaRe, a refactoring tool for Haskell. The first approach described, outlined in [3, Fig.8], is very close to Figure 2. This architecture was refined to use two representations of a program (as a token stream and a syntax tree) as shown in [3, Fig.9]. In [4] they contrast this approach with that taken in Wrangler, a refactoring tool for Erlang.

The approach taken in this work appears to be similar to that taken in Wrangler: the AST was augmented to include more information (relating to concrete syntax). In particular, each node of the abstract syntax tree was augmented with an element of type `string list` inside which the parser stores the whitespace and bracketing surrounding, and occurring within (in case of mixfix), an expression. This information is called *filling* here. The Wrangler approach is conceptually simpler than that taken in HaRe because it uses a single program representation.

3.2 Checks

Checks are applied to ensure the correct application of a refactoring. There are two categories of checks: *general* checks include parsing and type-checking – these are applied uniformly to all programs; *side-condition* checks are applied specifically by different refactorings. All the checks apart from the parser are encoded in the proof script and their code is generated by Isabelle.

3.3 Tool interface

Refactoring tools are usually used via an IDE as suggested by Figure 1. Prefactor was designed with this interface in mind, though it is currently only usable through the command line. The user indicates which part of the program they wish to refactor by providing two integers: an *index* indicating the position of the first character of the segment to be refactored and the *range* indicating the width, in characters, of the subterm to be refactored. A function called *point* was implemented that accepts a term, index, and range, and returns the largest well-formed subterm if one such could be identified in the specified segment.

4 Method

This section describes the implementation of supporting code and the adaptation of the Isabelle proof script to generate the code on which the refactoring tool is based. The combined code was compiled using Standard ML of New Jersey (version 110.69).

4.1 Generating the refactoring

Apart from the refactoring, the generated code also included its dependencies: the side-condition predicates, the type-checker, and the associated data structures. The type-checker is called after a program is parsed to ensure that the refactoring behaves as intended: it preserves the behaviour of meaningful programs. Recall from section 3.1 that the syntax tree was defined to store whitespace and bracketing. The definition of the language's syntax in Isabelle was purely abstract, and this produced a choice: either extending Isabelle's definition to include filling, or writing more supporting functions to interface with the definitions used in Isabelle. The former would result in more work, since changing Isabelle definitions was bound to require altering the dependent proofs, but the latter would increase the 'untrusted code base' and hence go against the spirit of this work. The decision was taken to compromise but lean towards the former option: the definitions inside Isabelle were changed to include filling, but filling there was not defined as a list of strings but as a singleton type. The rationale was that since the filling has no logical significance it would simplify matters to regard it, within the theorem-prover, as being the simplest kind of data possible. Despite the orthogonality of this change to the logical content, the proofs still required modification. At least this was alleviated by the simple definition of filling (because as far as the theorem-prover was concerned all filling is equivalent). Another alternative would have been to make the type of filling a parameter to the datatype specifying the language's abstract syntax. This would have required a modification to the program logic to reflect that expressions are equivalent modulo filling. In retrospect this would have been a better choice.

After code generation, the definition of filling in the generated code was changed from `datatype filling = Filling` to the pair of declarations consisting of `type filling = string list` and `val Filling = []`. Four other changes were made to the generated code:

- As a result of the above change the equality predicate over fillings needed to be adapted to work over its new type.
- In Isabelle/HOL sets and predicates are identified, but the target language distinguishes between, say, `string Set` and `string -> bool`. This slipped past the code generator and an instance of the latter had to be manually changed into the other form.
- Some ML structures generated from Isabelle theories (`String`, `List`, and `Option`) had to be renamed because they clashed with Basis definitions in Standard ML.
- A few lines of code to print status messages were added to instrument the tool.

4.2 Supporting code

The parser was generated using ml-yacc and ml-lex, both distributed with Standard ML of New Jersey. The printer was straightforward to write since the filling

information was local to each expression. The code to extract subterms given an index and range (section 3.1) required more careful handling and would have been laborious to write for a larger language. However, like the parser, other parts of the supporting code may be amenable to automatic generation from a specification – perhaps from the same specification as the parser's.

4.3 Testing

The parsing and printing phases of the process can be tested by running them in sequence and checking the output for any deviation from the original source-code. The tool can be instructed to do this, and to additionally run the `diff` tool to spot any differences. The tool can also be instructed to type-check a program and to extract a subterm occurring at a particular segment (using the point function described in section 3.1).

It came as something of a surprise that it was possible to cause the refactoring to malfunction, but this goes to highlight how subtle it is to build such tools. Consider the following candidate for refactoring – the plan being to change the type of `x` to `nat⊕unit`:

```
((fn x : nat ⇒
 (succ (succ x))
  zero
)
```

Recall from page 81 that the refactoring is given strings `v1` and `v2` as variable identifiers to inject into the refactored program. Now if one of these is set to be a reserved word such as `if` and the refactoring is effected, then the resulting program would be malformed, as shown below:

```
((fn x : (nat⊕unit) ⇒
  (succ (succ (case [ if ⇐ if ] x [ var2 ⇒ zero ] )))
  (left (nat⊕unit) zero)
)
```

This problem isn't detected by the refactoring's checks. In Isabelle such a confusion could not take place owing to the abstract nature of the syntax. The problem could be solved in different ways: for instance, one could check that identifiers are not reserved words – this could become an additional side-condition. More generally, one could parse the refactoring's output to determine whether the refactoring had undesired effects such as this.

5 Discussion

The most laborious part of the work was the Isabelle development. The code/proof ratio underscores this: the Isabelle script consisted of almost 3000 lines. From

this a little over 400 lines of Standard ML were generated, thus providing the tool's verified core. The support and interface code amounted to around 1000 lines, and the lexing and parsing code produced by ml-lex and ml-yacc amounted to around 1300 lines. The theorem-proving component makes this approach expensive and possibly even discouraging, but this is balanced against the degree of safety it yields. As the previous section showed however, this may not be sufficient to trump all possible failure cases.

Most of the Isabelle/HOL script contained proofs of foundational results related to the type system, and are therefore entirely reusable by further verifications of refactorings. This suggests that, through reuse, the effort needed to formalise refactorings could be amortised against further development.

6 Future work

It would be useful to experiment with different data structures for representing programs in a theorem-prover in such a manner that would lighten the proof burden. It would also be interesting to explore the facility with which refactorings formalised in this manner can be composed. Integration with an IDE needs to be explored, as well as enabling refactorings to return error messages (explaining which side-condition failed to fire).

6.1 Extracting refactorings

Instead of generating a refactoring's code as done here (based on [6]) one could extract it from a formal proof – this is 'program extraction' in a more orthodox sense. This has been experimented with for the refactoring used in this article, making use of Stefan Berghofer's implementation [1] of modified realizability in Isabelle/HOL. This required rephrasing the statement of the refactoring's correctness (cf. [6]) as follows:

> Let C_R be a proposition encoding the side-conditions of the refactoring described on page 81. (These side-conditions are explained in detail in [6, Theorem 11.7].) All the symbols appearing below have the expected denotations (e.g. Γ ranges over type contexts; p, M, N, L over expressions; x over variables; σ over types; etc) and all, except for R and C_R, are $\forall$-quantified. (The $\forall$-quantified variables correspond with parameters to the refactoring.) For all $\Gamma, p, \sigma, \tau, \ldots$ values there exists a function R such that the following properties hold together:
>
> 1. If $\Gamma \rhd p : \sigma$ then $\Gamma \rhd R\,p = p : \sigma$
> 2. If $p = (\lambda x^T N)M$ and C_R holds, then
> $R\,p \;=\; (\lambda x^{\tau+\tau'} N[\langle x' \Leftarrow x' \rangle x \langle y \Rightarrow L \rangle / x])(\mathrm{inL}_{\tau+\tau'} M)$
> 3. If $p \neq (\lambda x^T N)M$ or $\neg C_R$ holds, then $R\,p \;=\; p$

Property (1) states that R preserves the behaviour of all (well-typed) programs. Property (2) states that it effects the desired transformation on programs for which the refactoring is defined, and property (3) states that the refactoring leaves other programs unchanged.

The computational witness of the refactoring was extracted from the correctness proof after proving the decidability of the predicates involved. Compared to the approach taken in [6] one is not verifying an explicitly-defined function encoded in a theorem-prover's syntax, and the specification of the refactoring is higher-level.

7 Conclusion

Earlier work sought primarily to verify the correctness of refactorings' specifications, and only to generate implementations of refactorings as an afterthought. This article described a tiny tool built around a core which has been generated by a theorem-prover. This was exploratory work to observe some of the difficulties faced before working on a more ambitious scale.

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On the partial deduction of non-ground meta-interpreters
(Extended abstract)

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Abstract. In this extended abstract we investigate to what extent known partial deduction techniques can be used in order to successfully specialise non-ground meta interpreters. We formalise the notion of a successful specialisation for such a meta interpreter, and we disucss under what condition such a successful specialisation can be achieved by well-known control techniques, but we also show that interpreters exist for which this condition cannot be met by a specialiser, independently of the control strategy employed by the specialiser.

Keywords: partial deduction, meta interpreters, logic programming

1 Introduction

Writing meta interpreters is a well-known technique to enhance the expressive power of logic programs [9]. Essentially, a meta interpreter is a program that handles another program as data. Following standard terminology, we refer to the program that is handled as data by the term *object program*, and to the program that is handling (or "interpreting") the object program, by the term *meta program*. One way of writing meta interpeters in logic programming is to use the so-called *nonground representation*. Using this representation, a term of the object program is represented by a term in the meta program having the same syntax. Variables at the object level are represented by variables at the meta level. The major advantage of this representation (over the alternative, so-called *ground* representation) is that SLD-resolution of the object program is immediate, while performing unification and backtracking on the meta program, and that the answer substitutions of the object program are available through the answer substitutions of the meta program [1]. A simple and classic example of a non-ground meta interpreter for pure Prolog that returns, for each computed answer, the number of derivation steps, is depicted in the top part of Figure 1 (the `solve/2` predicate). The bottom part of the figure gives an explicit definition of the `clause` predicate defining the well-known `reverse` and `append` predicates as object program. For the given interpreter this explicit representation is not necessary as one could provide the standard definition of these predicates and use the Prolog-builtin `clause/2`. Using an explicit representation allows, however,

to represent the structure of the object program in an alternative way, e.g. using lists to represent conjunctions.

```
solve(true,0).
solve((A,B),D):- solve(A,D1), solve(B,D2), D is D1+D2.
solve(A,D):-clause(A,B), solve(B,DP), D is DP+1.

clause(reverse([],[]),true).
clause(reverse([X|Xs],Y),(reverse(Xs,Ys), append(Ys,[X],Y))).
clause(append([],Y,Y),true).
clause(append([X|Xs],Y,[X|Z]), append(Xs,Y,Z)).
```

Fig. 1. A simple non-ground meta interpreter counting derivation steps.

Although appealing as a programming technique, the execution of an object program through a meta interpreter usually is less efficient (typically an order of magnitude slower) than the execution of an equivalent program in the meta language [18]. A natural approach to solving the efficiency problem consists in specialising the interpreter with respect to a set of given object program queries [17, 6, 19]. As such, the overhead could be removed by performing interpretation of the object program (essentially *parsing* the object program) during specialisation. The idea is that the residual program combines the functionality of the object program with those offered by the interpreter, whereas it can be directly executed, without requiring the meta interpreter. For example, the result of specialising the meta interpreter of Figure 1 with respect to a query `solve(append(X,Y,Z),D)` could be the program represented in Figure 2 representing the `append` predicate adorned with the extra functionality of counting the number of derivation steps in a query.

```
append([],L,L,0).
append([X|Xs],Y,[X|Z],D):- append(Xs,Y,Z,DP), D is DP+1.
```

Fig. 2. Result of specialising for the query `solve(append(X,Y,Z),D)`

In this work we explore the key issues in achieving this kind of specialistion with a generic algorithm for partial deduction. While the problem of specialising meta interpreters has received a lot of attention in the past (see e.g. [19, 17, 6, 11, 15, 3]), we believe that a systematic exploration adds understanding both to the problem of meta interpreter specialisation and to the possibilities and limits of partial deduction as a transformation technique in general.

2 Partially deducing a non-ground meta interpreter

2.1 Preliminaries

In what follows we assume the reader to be familiar with the basic concepts and techniques in partial deduction [7] and we refer to [13] for a comprehensive overview of the current state of the art. Following the literature on the subject, we define a partial deduction of a program with respect to a set of atomic queries as the resultants obtained from a set of partial SLD(NF)-trees,[1] one for each atom in the set.

Definition 1. *Let P be a logic program, $\mathcal{A} = \{A_1, \ldots, A_n\}$ a set of atoms, and $\mathcal{T} = \{\tau_1, \ldots, \tau_n\}$ a set of partial SLD(NF)-trees for the atoms in $\mathcal{A}$. If we denote by $res(\tau)$ the set of* resultants *associated to τ, i.e. the set of clauses of the form*

$$A\theta \leftarrow B_1, \ldots, B_k$$

where $A \in \mathcal{A}$ is the root of τ, $\leftarrow B_1, \ldots, B_k$ is the query comprising the leaf of a non-failing branch in τ, and θ the composition of the mgu's computed along the branch, then $\bigcup res(\tau_i)$ for all $\tau_i \in \mathcal{T}$ is called a partial deduction for $\mathcal{A}$ in P.

It is well-known that in order for a partial deduction for $\mathcal{A}$ in P to represent a correctly specialised program (i.e. a program with the same semantics as P as far as the atomic queries in $\mathcal{A}$ are concerned), it is sufficient that no two atoms in $\mathcal{A}$ have a common instance and that each atom in the bodies of the clauses constituting the partial deduction is an instance of some atom in $\mathcal{A}$. These conditions are referred to as, respectively, the *independence* and *closedness* conditions [14]. A generic algorithm for computing a partial deduction of a given program P with respect to a set of atoms of interest S is given in Figure 3 [13].

Starting from an initial set of atoms of interest, the algorithm constructs a finite partial SLD(NF)-tree for each atom in the set, and adds the atoms in the leaves of the tree to the set of atoms under consideration. The construction of such a partial SLD(NF)-tree is guided by a so-called *local control* mechanism, represented by the *unfold* operation. Then the process is basically repeated, computing a series of subsequent sets of atoms $\mathcal{A}_1$, $\mathcal{A}_2$,... until a fixed point is reached. In each step, the set $\mathcal{A}_i$ is carefully abstracted such that a fixed point is guaranteed to be reached while guaranteeing the independence and closedness conditions to hold. The abstraction process constitutes the *global control* mechanism, represented by the *revise* procedure. A myriad of techniques to instantiate the *unfold* and *revise* operations exist (see [13] for an overview), some of which will be discussed briefly further down the text.

Example 1. Figures 4 and 5 represent, respectively, a set of partial SLD-trees and the associated partial deduction as they could be produced by an instantiation of the generic partial deduction algorithm for an initial atom of interest

[1] A *partial* SLD(NF)-tree is an SLD(NF)-tree in which leafs can be queries with no selected atom. This is a generalisation of the standard notion of SLD(NF)-tree in which leafs can only be the queries `true` or `fail`.

Input: A program P and a set S of atoms of interest
Output: A specialised program P' and a set of atoms $\mathcal{A}$

let $i = 0$; $\mathcal{A}_0 = S$
repeat
  for each $A_k \in \mathcal{A}_i$ let $\tau_k = \mathit{unfold}(P, A_k)$
  let $\mathcal{A}'_i = \mathcal{A}_i \cup \{B | B \in \mathit{leaves}(\tau_k)\}$
  let $\mathcal{A}_{i+1} = \mathit{revise}(\mathcal{A}'_i)$
  let $i = i + 1$
until $\mathcal{A}_i = \mathcal{A}_{i-1}$
let $\mathcal{A} = \mathcal{A}_i$
let $P' = \bigcup_{A_k \in \mathcal{A}} \mathit{resultants}(\tau_k)$

Fig. 3. A generic algorithm for partial deduction

`solve(reverse(X,Y),D)` and constructing the set $\mathcal{A} = \{$`solve(reverse(X,Y),D)`, `solve(append(Ys,[X'],Y),D2)`$\}$. To ease the representation, we did not depict

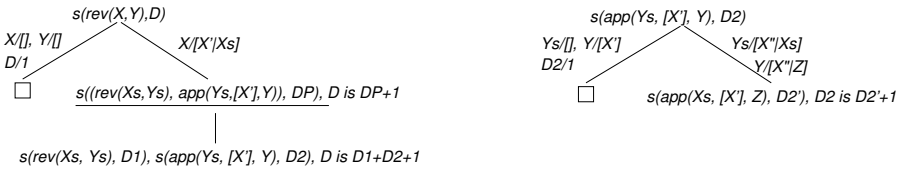

Fig. 4. Partial SLD-trees

the intermediate unfolding steps for atoms involving `clause/2` and `is/2`, and we abbreviate `solve`, `reverse` and `append` to, respectively, `s`, `rev` and `app`.

```
s(rev([],[]),1).
s(rev([X'|Xs],Y),D):- s(rev(Xs,Ys),D1), s(app(Ys,[X'],Y),D2),D is D1+D2+1.

s(app([],[X'],[X']),1).
s(app([X"|Xs],[X'],[X"|Z]),D2):- s(app(Xs,[X'],Z),D2'), D2 is D2'+1.
```

Fig. 5. The partial deduction resulting from the SLD-trees of Fig. 4.

2.2 Partially deducing the non-ground meta interpreter

In order to formally capture the desired result from specialising a meta interpreter, let us introduce the following notions. For a program P we use Π_P and F_P to denote, respectively, the set of predicate and function symbols used in P. If we use V to represent a meta interpreter then we use V_P to represent V augmented with a definition of the `clause` predicate representing P as an object program. For any combination V_P we suppose that $\Pi_P \cap F_V = \emptyset$, that is,

there is no confusion possible between the function symbols employed by the interpreter and the predicate symbols of the object program. For a given V_P, we call *object-structure* the set of predicates from the object program, that is Π_P. Consequently, for a given V_P, we will say that a term, substitution, atom, or program is *object-structure free* if and only if it does not contain any predicate from Π_P. For the result of partially deducing a meta interpreter and object program combination V_P to be successful, we require that the result of specialisation must be object-structure free. The choice for this characterisation is justified as follows. First, the fact that the predicates from the object program are no longer present as functors in the specialised meta program is the most direct and visible indication that the specialiser has removed the layer of interpretation introduced by the interpreter. Moreover, it is a perfectly measurable characteristic which, as we will show, translates directly to a verifyable condition during the partial deduction process.

In its basic form, the partial deduction algorithm does not remove any functors from the program it is specialising. However, in practice, partial deduction is usually combined with some form of structure filtering [8, 2]. The latter transformation consists in renaming a resultant of the form $A_0\theta_0 \leftarrow A_1\theta_1, \ldots, A_n\theta_n$ (where the A_i are atoms in $\mathcal{A}$) by transforming each $A_i\theta_i$ into an atom $p_i(t_1, \ldots, t_k)$ where p_i is a new predicate name associated to A_i, and $t_1, \ldots, t_k$ are the terms occuring in the image of θ_i. As such, only the functors and terms occurring in the substitutions θ_i are present in the residual program, whereas the functors and terms occuring in the atoms from $\mathcal{A}$ are not. This observation allows us to formulate a sufficient condition under which the result of partially deducing a combination V_P can be transformed into an object-structure free program.

Definition 2. *Given a meta interpreter V and an object program P. Let P' denote the set of resultants from a partial deduction of V_P with respect to a set of atomic queries $\mathcal{A}$. We say that P' is* object-structure closed w.r.t. $\mathcal{A}$ *if and only if for each atom B_i of a clause $B_0 \leftarrow B_1, \ldots, B_n \in P'$ there exist $A \in \mathcal{A}$ such that $B_i = A\theta$ for some substitution θ, and θ is object-structure free.*

Reconsidering Example 1, since every (non-builtin) atom in the body of the resultant clauses in Fig. 5 is a variant of some atom in $\mathcal{A}$, the set of resultants is obviously object-structure closed w.r.t. $\mathcal{A}$. The definition of object-structure closedness captures the fact that no object-structure is passed from one partial SLD(NF)-tree to another, nor propagated to any of the atoms of interest in $\mathcal{A}$. Consequently, it can be transformed into an object-structure free program such as the one depicted in Figure 6. This result is generalised in Proposition 1.

Proposition 1. *Given a meta interpreter V and an object program P. Let P' denote the set of resultants comprising a partial deduction of V_P with respect to a set of atomic queries $\mathcal{A}$. If P' is object-structure closed w.r.t $\mathcal{A}$, then P' can be transformed into an object-structure free program.*

Returning to the partial deduction algorithm, it is not hard to see that in order for the condition of Definition 2 to hold, the following must be true. First, the

```
s_rev([],[],1).
s_rev([X'|Xs],Y,D):- s_rev(Xs,Ys,D1), s_app(Ys,[X'],Y,D2),D is D1+D2+1.

s_app([],[X'],[X'],1).
s_app([X"|Xs],[X'],[X"|Z],D2):- s_app(Xs,[X'],Z,D2'), D2 is D2'+1.
```

Fig. 6. The program from Fig. 5 after structure filtering.

partial deduction must start from a set of queries that are sufficiently instantiated such that the computed answers do not contain object-structure. For the example interpreter and object program from Figure 1, this means that queries must be instances of `solve(append(X,Y,Z))` or `solve(reverse(X,Y))`. This is rather obvious, as specialisation w.r.t a query such as `solve(X)` cannot, in general, lead to a object-structure free specialised program. Secondly, and more importantly, the interplay between local and global control (the *unfold* and *revise* operations) must be such that the *revise* operation does not abstract object-structure away from the atoms in order to obtain a finite set $\mathcal{A}$. In case of the example from Figure 1, this means – again – that no atoms of the form `solve(X)` should be introduced in $\mathcal{A}$ by generalisation.

Observation 1. There exist meta interpreters V such that, for *any* object program P and set of initial queries S, there exist a set of atoms $\mathcal{A}$ and a partial deduction of V_P w.r.t. $\mathcal{A}$, say P', such that $S \subseteq \mathcal{A}$ and P' object-structure closed w.r.t. $\mathcal{A}$.

Among the observations we would like to discuss, Observation 1 is by far the most positive as it claims there are meta interpreters for which a program specialiser *could* get rid of the interpretation overhead, independently of the object program under consideration. This, of course, is no surprise, as it simply generalises several results that can be found in the literature. For example, Sterling and Beer [18] declare a number of rules that are sufficient to specialise a certain class of meta interpreters. In [11], Lakhotia and Sterling follow a somewhat more general approach, defining – independently of a particular interpreter – *what* knowledge should be gathered about an interpreter that is to be specialised and how this knowledge should be coded in unfolding rules. Another example is given in [3], in which the authors provide a specialiser capable of satisfactorily specialising a vanilla-like meta interpreter dealing with program compositions. Important as these results are, they do not, however, imply that a satisfactory degree of specialisation can be achieved by a *general* partial deduction system, i.e. a system that has not been tuned for dealing with a particular interpreter.

Observation 2. Let V be a meta interpreter, P an object program and P' an object-structure closed partial deduction of V_P with respect to a set of atoms $\mathcal{A}$ including the atoms of interest S. Then P' may be relatively hard to construct by generally well-performing control techniques for partial deduction.

The reason why it can be hard for a general partial deduction system to obtain an object-structure closed partial deduction is due to the way in which local

(and global) control are generally implemented. Nearly all somewhat sophisticated control techniques for unfolding are based on well-founded or well-quasi orders (see [13] for an overview) in order to be able to stop the construction of a partial SLD(NF)-tree as soon as either a series of related selected atoms along a branch cannot be shown to decrease in size (case of well-founded orders) or when some kind of embedding is detected between two such related atoms along the branch (case of well-quasi orders). While this makes perfect sense from a termination point of view, it can be noted that data structures that are fluctuating in size are an essential characteristic of practically any meta interpreter.

Example 2. Reconsidering the partial SLD-tree on the left of Fig. 4, Most unfolding techniques, such as those based on homeomorphic embedding [13] would not have unfolded the atom `s((rev(Xs,Ys),app(Ys,[X'],Y)),D2)` as it is embedding the root of the tree. Still, unfolding this atom is a key ingredient for achieving an object-structure free partial deduction.

Control techniques have been developed that try to deal with this kind of fluctuating structures, such as our own work [20] which provides a local control strategy based on homeomorphic embedding allowing a structure to grow during unfolding as long as it gets smaller in a subsequent derivation step. While this strategy is able to handle automatic specialisation of the classical vanilla meta interpreter, it is an ad-hoc strategy which is hard to generalise to other meta interpreters. It is as yet unclear whether binding-time analysis [4, 12] allows for a more systematic solution to the problem. Not unfolding deep enough would not be a problem if the atoms that are not unfolded, and hence are brought into the set $\mathcal{A}$, would become the roots of new SLD(NF)-trees without alteration. However, most global control techniques also use well-quasi orders like the homeomorphic embedding relation in order to decide what atoms in $\mathcal{A}$ must be replaced by a more general atom in order to guarantee finiteness of the set. Generalising two embedded atoms of which at least one contains an object-level conjunction (which will most probably be the case since the atom was not unfolded) will most likely result in a loss of object-structure. Continuing Example 2, the most specific generalisation of the atoms `s(rev(X,Y),D)` and `s((rev(Xs,Ys),app(Ys,[X'],Y)),D2)` results in `solve(X,D)` being added to $\mathcal{A}$ implying the partial deduction no longer being object-structure closed.

While the previous observation shows that it may be hard – but not impossible – to construct a partial deduction that is object-structure closed, the following observation shows that combinations of a meta interpreter and object program exist for which no object-structure closed partial deduction can be constructed, and this independently of the control strategies used by the partial deduction algorithm.

Observation 3. There exist meta interpreters V such that, for *some* object programs P and set of initial queries S, there does not exist a set of atoms $\mathcal{A}$ and a partial deduction of V_P w.r.t. $\mathcal{A}$, say P', such that $S \subseteq \mathcal{A}$ and P' object-structure closed w.r.t. $\mathcal{A}$.

Consider the variant of a simple vanilla meta interpreter depicted in Figure 7. The difference with the classical vanilla interpreter resides in the fact that it uses lists to represent object-level conjunctions, and that it performs list concatenation before further processing the query under consideration.

```
solve([]).
solve([X|Xs]):- clause(X,B), append(B,Xs,R), solve(R).
```

Fig. 7. A simple meta interpreter using lists.

Albeit it can be argued that the interpreter presented in Figure 7 is not a well-written interpreter – e.g. w.r.t. the guidelines given in [11] and [10] – it is nevertheless a correctly functioning meta interpreter. However, together with the (dummy) object program, consisting of a single clause `clause(a,[a,a])` it presents a problem for the partial deduction algorithm, in the sense that it is impossible to constuct an object-structure closed partial deduction. The problem is due to the fact that the interpreter never explicitly breaks the conjunctions it handles into smaller parts. Indeed, assuming that the local control strategy unfolds calls to the `append` and `clause` predicates, all atoms in the set $\mathcal{A}$ will be of the form `solve([a,...,a])`, each such atom having a different number of `a`'s in the list. Consequently, at some point the *revise* operation will generalise two or more of these atoms into an atom such as `solve([a,a|X])`, thereby loosing the property of the partial deduction being object-structure closed.

3 Discussion

In this work in progress, we aim at examining to what extent (non-ground) meta interpreters can be successfully specialised by a general partial deduction algorithm. We have formalised what we take as a successful specialisation, and made a number of observations on what is (im)possible to achieve by partial deduction, and this independently of a concrete control strategy. Ongoing work includes further elaborating the observations that are described informally in this extended abstract, and investigating whether and how the partial deduction algorithm can possibly be enriched in order to elegantly deal with a broader class of (meta)programs than currently handled. The link with abstract partial deduction [16] and contextual specialisation [5] will also be explored.

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Using Real Relaxations During Program Specialization

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Abstract. We propose a program specialization technique for locally stratified CLP($\mathbb{Z}$) programs, that is, logic programs with linear constraints over the set $\mathbb{Z}$ of the integer numbers. For reasons of efficiency our technique makes use of a relaxation from integers to reals. We reformulate the familiar unfold/fold transformation rules for CLP programs so that: (i) the applicability conditions of the rules are based on the satisfiability or entailment of constraints over the set $\mathbb{R}$ of the real numbers, and (ii) every application of the rules transforms a given program into a new program with the same perfect model constructed over $\mathbb{Z}$. Then, we introduce a strategy which applies the transformation rules for specializing CLP($\mathbb{Z}$) programs with respect to a given query. Finally, we show that our specialization strategy can be applied for verifying properties of infinite state reactive systems specified by constraints over $\mathbb{Z}$.

1 Introduction

Reactive systems are often composed of processes that make use of possibly unbounded data structures. In order to specify and reason about this type of systems, several formalisms have been proposed, such as unbounded counter automata [27] and vector addition systems [26]. These formalisms are based on linear constraints over variables ranging over the set $\mathbb{Z}$ of the integer numbers.

Several tools for the verification of properties of systems with unbounded integer variables have been developed in recent years. Among these we would like to mention ALV [36], FAST [6], LASH [25], and TReX [1]. These tools use sophisticated solvers for constraints over the integers which are based on automata-theoretic techniques [22] or techniques for proving formulas of Presburger Arithmetic [32].

Also constraint logic programming is a very powerful formalism for specifying and reasoning about reactive systems [20]. In fact, many properties of counter

automata and vector addition systems, such as *safety* properties and, more generally, temporal properties, can be easily translated into constraint logic programs with linear constraints over the integers, called CLP($\mathbb{Z}$) programs. [21].

Unfortunately, dealing with constraints over the integers is often a source of inefficiency and, in order to overcome this limitation, many verification techniques are based on the interpretation of the constraints over the set $\mathbb{R}$ of the real numbers, instead of the set $\mathbb{Z}$ of the integer numbers [7,13]. This extension of the domain of interpretation is sometimes called *relaxation*.

The relaxation from integers to reals, also called the *real relaxation*, has several advantages: (i) many constraint solving problems (in particular, the satisfiability problem) have lower complexity if considered in the reals, rather than in the integers [33], (ii) the class of linear constraints over the reals is closed under *projection*, which is an operation often used during program verification, while the class of linear constraints over the integers is not, and (iii) many highly optimized libraries are actually available for performing various operations on constraints over the reals, such as satisfiability testing, projection, widening, and convex hull, which are often used in the field of static program analysis [10,11] (see, for instance, the Parma Polyhedral Library [3]).

Relaxation techniques can be viewed as *approximation* techniques. Indeed, if a property holds for all real values of a given variable then it holds for all integer values, but not vice versa. This approximation technique can be applied to the verification of reactive systems. For instance, if a safety property $\varphi =_{def} \forall x \in \mathbb{R}$ $(\mathit{reachable}(x) \rightarrow \mathit{safe}(x))$ holds, then it also holds when replacing the set $\mathbb{R}$ by the set $\mathbb{Z}$. However, if $\neg\varphi =_{def} \exists x \in \mathbb{R}$ $(\mathit{reachable}(x) \wedge \neg \mathit{safe}(x))$ holds, then we cannot conclude that $\exists x \in \mathbb{Z}$ $(\mathit{reachable}(x) \wedge \neg \mathit{safe}(x))$ holds.

Now, as indicated in the literature (see, for instance, [17,19,29,30,31]) the verification of infinite state reactive systems can be done via program specialization and, in particular, in [19] we proposed a technique consisting of the following two steps: (*Step* 1) the specialization of the constraint logic program that encodes the given system, with respect to the query that encodes the property to be verified, and (*Step* 2) the construction of the *perfect model* of the specialized program.

In this paper we propose a variant of the verification technique introduced in [19]. This variant is based on the specialization of locally stratified CLP($\mathbb{Z}$) programs and uses a relaxation from the integers to the reals.

In order to do so, we need: (i) a suitable reformulation of the familiar unfold/fold transformation rules for CLP programs [14,18] so that: (i.1) the applicability conditions of the rules are based on the satisfiability or entailment of constraints over the reals $\mathbb{R}$, and (i.2) every application of the rules transforms a given program into a new program with the same perfect model constructed over the integers $\mathbb{Z}$, called *perfect* $\mathbb{Z}$*-model*, and then (ii) the introduction of a transformation strategy which applies the reformulated transformation rules for specializing a given CLP($\mathbb{Z}$) program with respect to a given query.

There are two advantages of the verification technique we consider here. The first advantage is that, since our specialization strategy manipulates constraints

over the reals, it may exploit efficient techniques for checking satisfiability and entailment, for computing projection, and for more complex constructions, such as the widening and the convex hull operations over sets of constraints. The second advantage is that, since we use equivalence preserving transformation rules, that is, rules which preserve the perfect $\mathbb{Z}$-model, the property to be verified holds in the initial program if and only if it holds in the specialized program and, thus, we may apply to the specialized program any other verification technique we wish, including techniques based on constraints over the integers.

The rest of the paper is structured as follows. In Section 2 we introduce some basic notions concerning constraints and CLP programs. In Section 3 we present the rules for transforming CLP($\mathbb{Z}$) programs and prove that they preserve equivalence with respect to the perfect model semantics. In Section 4 we present our specialization strategy and in Section 5 we show its application to the verification of reactive systems. Finally, in Section 6 we discuss related work in the field of program specialization and verification of infinite state systems.

2 Constraint Logic Programs over Integers and Reals

We will consider CLP($\mathbb{Z}$) programs, that is, constraint logic programs with linear constraints over the set $\mathbb{Z}$ of the integer numbers. An *atomic constraint* is either of the form $r \geq 0$ or of the form $r > 0$, where r is a linear polynomial with integer coefficients. A *constraint* is a conjunction of atomic constraints. The equality $t_1 = t_2$ stands for the conjunction $t_1 \geq t_2 \wedge t_2 \geq t_1$. A clause of a CLP($\mathbb{Z}$) program is of the form $A \leftarrow c \wedge B$, where A is an atom, c is a constraint, and B is a conjunction of (positive or negative) literals. For reasons of simplicity and without loss of generality, we also assume that the arguments of all literals are variables, that is, the literals are of the form $p(X_1, \ldots, X_n)$ or $\neg p(X_1, \ldots, X_n)$, with $n \geq 0$, where p is a predicate symbol not in $\{>, \geq, =\}$ and $X_1, \ldots, X_n$ are distinct variables ranging over $\mathbb{Z}$.

Given a constraint c, by $vars(c)$ we denote the set of variables occurring in c. By $\forall(c)$ we denote the universal closure $\forall X_1 \ldots \forall X_n\ c$, where $vars(c) = \{X_1, \ldots, X_n\}$. Similarly, by $\exists(c)$ we denote the existential closure $\exists X_1 \ldots \exists X_n\ c$. Similar notation will also be used for literals, goals, and clauses.

For the constraints over the integers we assume the usual interpretation which, by abuse of language, we denote by $\mathbb{Z}$. A *$\mathbb{Z}$-model* of a CLP($\mathbb{Z}$) program P is defined to be a model of P which agrees with the interpretation $\mathbb{Z}$ for the constraints. We assume that programs are *locally stratified* [2] and, similarly to the case of logic programs without constraints, for a locally stratified CLP($\mathbb{Z}$) program P we can define its unique *perfect $\mathbb{Z}$-model* (or, simply, *perfect model*), denoted $M_{\mathbb{Z}}(P)$ (see [2] for the definition of the perfect model of a logic program).

We say that a constraint c is *$\mathbb{Z}$-satisfiable* if $\mathbb{Z} \models \exists(c)$. We also say that a constraint c *$\mathbb{Z}$-entails* a constraint d, denoted $c \sqsubseteq_{\mathbb{Z}} d$, if $\mathbb{Z} \models \forall(c \rightarrow d)$.

Let $\mathbb{R}$ be the usual interpretation of the constraints over the set of the real numbers. A constraint c is *$\mathbb{R}$-satisfiable* if $\mathbb{R} \models \exists(c)$. A constraint c *$\mathbb{R}$-entails* a

constraint d, denoted $c \sqsubseteq_{\mathbb{R}} d$, if $\mathbb{R} \models \forall(c \rightarrow d)$. The $\mathbb{R}$-*projection* of a constraint c onto the set X of variables is a constraint c_p such that: (i) $vars(c_p) \subseteq X$ and (ii) $\mathbb{R} \models \forall(c_p \leftrightarrow \exists Y_1 \ldots \exists Y_k\ c)$, where $\{Y_1, \ldots, Y_k\} = vars(c) - X$. Recall that the set of constraints over $\mathbb{Z}$ is not closed under projection.

The following lemma states some simple relationships between $\mathbb{Z}$- and $\mathbb{R}$-satisfiability, and between $\mathbb{Z}$- and $\mathbb{R}$-entailment.

Lemma 1. *Let c and d be constraints and X be a set of variables.*
(i) *If c is $\mathbb{Z}$-satisfiable, then c is $\mathbb{R}$-satisfiable.* (ii) *If $c \sqsubseteq_{\mathbb{R}} d$, then $c \sqsubseteq_{\mathbb{Z}} d$.* (iii) *If c_p is the $\mathbb{R}$-projection of c on X, then $c \sqsubseteq_{\mathbb{Z}} c_p$.*

3 Transformation Rules with Real Relaxations

In this section we present a set of transformation rules that can be used for specializing locally stratified CLP($\mathbb{Z}$) programs. The applicability conditions of the rules are given in terms of constraints interpreted over the set $\mathbb{R}$ and, as shown by Theorem 1, these rules preserve the perfect $\mathbb{Z}$-model semantics.

The rules we will consider are those needed for specializing constraint logic programs, as indicated in the Specialization Strategy of Section 4. Note, however, that the correctness result stated in Theorem 1 can be extended to a larger set of rules (including the *negative unfolding* rule [18,34]) or to more powerful rules (such as the *definition* rule with $m\,(\geq 1)$ clauses, and the *multiple positive folding* [18]).

Before presenting these rules, we would like to show through an example that, if we consider different domains for the interpretation of the constraints and, in particular, if we apply the relaxation from the integers to the reals, we may derive different programs with different intended semantics.

Let us consider, for instance, the following constraint logic program P:

1. $p \leftarrow Y > 0 \wedge Y < 1$ 2. $q \leftarrow$

If we interpret the constraints over the reals, since $\mathbb{R} \models \exists Y(Y > 0 \ \wedge \ Y < 1)$, program P can be transformed into program $P_{\mathbb{R}}$:

1′. $p \leftarrow$ 2. $q \leftarrow$

If we interpret the constraints over the integers, since $\mathbb{Z} \models \neg\exists Y(Y > 0 \wedge Y < 1)$, program P can be transformed into program $P_{\mathbb{Z}}$:

2. $q \leftarrow$

Programs $P_{\mathbb{R}}$ and $P_{\mathbb{Z}}$ are not equivalent because they have different perfect $\mathbb{Z}$-models (which in this case coincide with their least Herbrand models). Thus, when we apply a relaxation we should proceed with some care. In particular, we will admit a transformation rule only when its applicability conditions interpreted over $\mathbb{R}$ imply the corresponding applicability conditions interpreted over $\mathbb{Z}$.

The transformation rules are used to construct a *transformation sequence*, that is, a sequence $P_0, \ldots, P_n$ of programs. We assume that P_0 is locally stratified. A transformation sequence $P_0, \ldots, P_n$ is constructed as follows. Suppose

that we have constructed a transformation sequence $P_0, \ldots, P_k$, for $0 \leq k \leq n-1$. The next program P_{k+1} in the transformation sequence is derived from program P_k by the application of a transformation rule among R1–R5 defined below.

Our first rule is the *Constrained Atomic Definition* rule (or *Definition Rule*, for short), which is applied for introducing a new predicate definition.

R1. Constrained Atomic Definition. Let us consider a clause, called a *definition clause*, of the form:

δ: $newp(X_1, \ldots, X_h) \leftarrow c \wedge p(X_1, \ldots, X_h)$

where: (i) *newp* does not occur in $\{P_0, \ldots, P_k\}$, (ii) $X_1, \ldots, X_h$ are distinct variables, (iii) c is a constraint with $vars(c) \subseteq \{X_1, \ldots, X_h\}$, and (iv) p occurs in P_0. By *constrained atomic definition* from program P_k we derive the program $P_{k+1} = P_k \cup \{\delta\}$. For $k \geq 0$, $Defs_k$ denotes the set of clauses introduced by the definition rule during the transformation sequence $P_0, \ldots, P_k$. In particular, $Defs_0 = \emptyset$.

R2. (Positive) Unfolding. Let $\gamma: \ H \leftarrow c \wedge G_L \wedge A \wedge G_R$ be a clause in program P_k and let

γ_1: $K_1 \leftarrow c_1 \wedge B_1 \quad \ldots \quad \gamma_m$: $K_m \leftarrow c_m \wedge B_m \qquad (m \geq 0)$

be all clauses of (a renamed apart variant of) program P_k such that, for $i=1, \ldots, m$, the constraint $c \wedge c_i\rho_i$ is $\mathbb{R}$-satisfiable, where ρ_i is a renaming substitution such that $A = K_i\rho_i$ (recall that all atoms in a CLP($\mathbb{Z}$) program have distinct variables as arguments).

By *unfolding clause* γ *w.r.t. the atom* A we derive the clauses

$\eta_1: \ H \leftarrow c \wedge c_1\rho_1 \wedge G_L \wedge B_1\rho_1 \wedge G_R$

$\ldots$

$\eta_m: \ H \leftarrow c \wedge c_m\rho_m \wedge G_L \wedge B_m\rho_m \wedge G_R$

and from program P_k we derive the program $P_{k+1} = (P_k - \{\gamma\}) \cup \{\eta_1, \ldots, \eta_m\}$.

Note that if $m=0$ then, by unfolding, clause γ is deleted from P_k.

Example 1. Let P_k be the following CLP($\mathbb{Z}$) program:

1. $p(X) \leftarrow X > 1 \wedge q(X)$
2. $q(Y) \leftarrow Y > 2 \wedge Z = Y - 1 \wedge q(Z)$
3. $q(Y) \leftarrow Y < 2 \wedge 5\,Z = Y \wedge q(Z)$
4. $q(Y) \leftarrow Y = 0$

Let us unfold clause 1 w.r.t. the atom $q(X)$. We have the renaming substitution $\rho = \{Y/X\}$, which unifies the atoms $q(X)$ and $q(Y)$, and the following three constraints:

(a) $X > 1 \wedge X > 2 \wedge Z = X - 1$, derived from clauses 1 and 2,
(b) $X > 1 \wedge X < 2 \wedge 5\,Z = X$, derived from clauses 1 and 3,
(c) $X > 1 \wedge X = 0$, derived from clauses 1 and 4.

Only (a) and (b) are $\mathbb{R}$-satisfiable, and only (a) is $\mathbb{Z}$-satisfiable. By unfolding clause 1 w.r.t. $q(X)$ we derive the following clauses:

1.a $p(X) \leftarrow X > 1 \wedge X > 2 \wedge Z = X - 1 \wedge q(Z)$
1.b $p(X) \leftarrow X > 1 \wedge X < 2 \wedge 5\,Z = X \wedge q(Z)$

Now we introduce two versions of the folding rule: *positive folding* and *negative folding*, depending on whether folding is applied to positive or negative literals in the body of a clause.

R3. Positive Folding. Let γ: $H \leftarrow c \wedge G_L \wedge A \wedge G_R$ be a clause in P_k and let δ: $K \leftarrow d \wedge B$ be a clause in (a renamed apart variant of) $Defs_k$. Suppose that there exists a renaming substitution ρ such that: (i) $A = B\,\rho$, and (ii) $c \sqsubseteq_{\mathbb{R}} d\,\rho$. By *folding* γ *using* δ we derive the clause η: $H \leftarrow c \wedge G_L \wedge K\rho \wedge G_R$ and from program P_k we derive the program $P_{k+1} = (P_k - \{\gamma\}) \cup \{\eta\}$.

The following example illustrates an application of Rule R3.

Example 2. Suppose that the following clause belongs to P_k:

γ: $h(X) \leftarrow X \geq 1 \wedge 2\,Y = 3\,X + 2 \wedge p(X, Y)$

and suppose that the following clause is a definition clause in $Defs_k$:

δ: $new(V, Z) \leftarrow Z > 2 \wedge p(V, Z)$

We have that the substitution $\rho = \{V/X, Z/Y\}$ satisfies Conditions (i) and (ii) of the positive folding rule because $X \geq 1 \wedge 2\,Y = 3\,X + 2 \sqsubseteq_{\mathbb{R}} (Z > 2)\rho$. Thus, by folding clause γ using clause δ, we derive:

η: $h(X) \leftarrow X \geq 1 \wedge 2\,Y = 3\,X + 2 \wedge new(X, Y)$

R4. Negative Folding. Let γ: $H \leftarrow c \wedge G_L \wedge \neg A \wedge G_R$ be a clause in P_k and let $\delta : K \leftarrow d \wedge B$ be a clause in (a renamed apart variant of) $Defs_k$. Suppose that there exists a renaming substitution ρ such that: (i) $A = B\,\rho$, and (ii) $c \sqsubseteq_{\mathbb{R}} d\,\rho$. By *folding* γ *using* δ we derive the clause η: $H \leftarrow c \wedge G_L \wedge \neg K\rho \wedge G_R$ and from program P_k we derive the program $P_{k+1} = (P_k - \{\gamma\}) \cup \{\eta\}$.

The following notion will be used for introducing the *clause removal* rule. Given two clauses of the form γ: $H \leftarrow c \wedge B$ and δ: $H \leftarrow d$, respectively, we say that γ is $\mathbb{Z}$-*subsumed* by δ, if $c \sqsubseteq_{\mathbb{Z}} d$. Similarly, we say that γ is $\mathbb{R}$-*subsumed* by δ, if $c \sqsubseteq_{\mathbb{R}} d$.

By Lemma 1, if γ is $\mathbb{R}$-subsumed by δ, then γ is $\mathbb{Z}$-subsumed by δ.

R5. Clause Removal. Let γ be a clause in P_k. By *clause removal* we derive the program $P_{k+1} = P_k - \{\gamma\}$ if clause γ is $\mathbb{R}$-subsumed by a clause occurring in $P_k - \{\gamma\}$.

The following Theorem 1 states that the transformation rules R1–R5 preserve the perfect $\mathbb{Z}$-model semantics.

Theorem 1 (Correctness of the Transformation Rules). *Let P_0 be a locally stratified program and let $P_0, \ldots, P_n$ be a transformation sequence obtained by applying rules* R1–R5*. Let us assume that for every k, with $0 < k < n-1$, if P_{k+1} is derived by applying positive folding to a clause in P_k using a clause δ in $Defs_k$, then there exists j, with $0 < j < n-1$, such that:* (i) *δ belongs to P_j, and* (ii) *P_{j+1} is derived by unfolding δ w.r.t. the only atom in its body.*
Then P_n is locally stratified and for every ground atom A whose predicate occurs in P_0, we have that $A \in M_{\mathbb{Z}}(P_0)$ iff $A \in M_{\mathbb{Z}}(P_n)$.

Proof. (Sketch) Let us consider variants of Rules R1–R5 where the applicability conditions are obtained from those for R1–R5 by replacing $\mathbb{R}$ by $\mathbb{Z}$. Let us denote $\mathrm{R1}_{\mathbb{Z}}$–$\mathrm{R5}_{\mathbb{Z}}$ these variants of the rules. Rules $\mathrm{R1}_{\mathbb{Z}}$, $\mathrm{R2}_{\mathbb{Z}}$, $\mathrm{R3}_{\mathbb{Z}}$, $\mathrm{R4}_{\mathbb{Z}}$, and $\mathrm{R5}_{\mathbb{Z}}$ can be viewed as instances (for $\mathcal{D} = \mathbb{Z}$) of the rules R1, R2p, R3(P), R3(N), and R4s, respectively, for specializing CLP($\mathcal{D}$) programs presented in [15]. By Theorem 3.3.10 of [15] we have that P_n is locally stratified and for every ground atom A whose predicate occurs in P_0, we have that $A \in M_{\mathbb{Z}}(P_0)$ iff $A \in M_{\mathbb{Z}}(P_n)$. Since, by Lemma 1 we have that the applicability conditions of R1–R5 imply the applicability conditions of $\mathrm{R1}_{\mathbb{Z}}$–$\mathrm{R5}_{\mathbb{Z}}$, we get the thesis. □

4 The Specialization Strategy

Now we present a strategy for specializing a program P_0 with respect to a query of the form $c \wedge p(X_1, \ldots, X_h)$, where c is a constraint and p is a predicate occurring in P_0. Our strategy constructs a transformation sequence $P_0, \ldots, P_n$ by using the rules R1–R5 defined in Section 3. The last program P_n is the specialized version of P_0 with respect to $c \wedge p(X_1, \ldots, X_h)$. P_n is the output program P_{sp} of the specialization strategy below.

The Specialization Strategy makes use of two auxiliary operators: an *unfolding operator* and a *generalization operator* that tell us how to apply the unfolding rule R2 and the constrained atomic definition rule R1, respectively. The problem of designing suitable unfolding and generalization operators has been addressed in many papers and various solutions have been proposed in the literature (see, for instance, [16,19,31] and [28] for a survey in the case of logic programs). In this paper we will not focus on this aspect and we will simply assume that we are given: (i) an operator $\mathit{Unfold}(\delta, P)$ which, for every clause δ occurring in a program P, returns a set of clauses derived from δ by applying $n\,(\geq 1)$ times the unfolding rule R2, and (ii) an operator $\mathit{Gen}(c \wedge A, \mathit{Defs})$ which, for every constraint c, atom A with $\mathit{vars}(c) \subseteq \mathit{vars}(A)$, and set Defs of the definition clauses introduced so far by Rule R1 during the Specialization Strategy, returns a constraint g that is *more general than* c, that is: (i) $\mathit{vars}(g) \subseteq \mathit{vars}(c)$ and (ii) $c \sqsubseteq_{\mathbb{R}} g$. An example of the generalization operator Gen will be presented in Section 5.

The Specialization Strategy

Input: A program P_0 and a query $c \wedge p(X_1, \ldots, X_h)$ where: (i) c is a constraint with $\mathit{vars}(c) \subseteq \{X_1, \ldots, X_h\}$, and (ii) p occurs in P_0.

Output: A program P_{sp} such that for every tuple $\langle n_1, \ldots, n_h \rangle \in \mathbb{Z}^h$,

$$p_{sp}(n_1, \ldots, n_h) \in M_{\mathbb{Z}}(P_0 \cup \{\delta_0\}) \text{ iff } p_{sp}(n_1, \ldots, n_h) \in M_{\mathbb{Z}}(P_{sp}),$$

where: (i) δ_0 is the definition clause $p_{sp}(X_1, \ldots, X_h) \leftarrow c \wedge p(X_1, \ldots, X_h)$ and (ii) p_{sp} is a predicate not occurring in P_0.

INITIALIZATION:

$P_{sp} := P_0 \cup \{\delta_0\}$; $\mathit{Defs} := \{\delta_0\}$;

while there exists a clause δ in $P_{sp} \cap \mathit{Defs}$ *do*

UNFOLDING: $\Gamma := \mathit{Unfold}(\delta, P_{sp})$;

CLAUSE REMOVAL:
while in Γ there exist two distinct clauses γ_1 and γ_2 such that γ_1 is $\mathbb{R}$-subsumed by γ_2 *do* $\Gamma := \Gamma - \{\gamma_1\}$ *end-while*;

DEFINITION & FOLDING:
while in Γ there exists a clause γ: $H \leftarrow c \wedge G_1 \wedge L \wedge G_2$, where L is a literal whose predicate occurs in P_0 *do*

let c_p be the $\mathbb{R}$-projection of c on $\mathit{vars}(L)$ and let A be the atom such that L is either A or $\neg A$;

if in *Defs* there exists a clause $K \leftarrow d \wedge B$ and a renaming substitution ρ such that: (i) $A = B\,\rho$ and (ii) $c_p \sqsubseteq_{\mathbb{R}} d\,\rho$

then $\Gamma := (\Gamma - \{\gamma\}) \cup \{H \leftarrow c \wedge G_1 \wedge M \wedge G_2\}$
where M is $K\rho$ if L is A, and M is $\neg K\rho$ if L is $\neg A$;

else $P_{sp} := P_{sp} \cup \{K \leftarrow g \wedge A\}$; $\mathit{Defs} := \mathit{Defs} \cup \{K \leftarrow g \wedge A\}$
where: (i) $K = \mathit{newp}(Y_1, \ldots, Y_m)$, (ii) *newp* is a predicate symbol not occurring in $P_0 \cup \mathit{Defs}$, (iii) $\{Y_1, \ldots, Y_m\} = \mathit{vars}(A)$, and (iv) $g = \mathit{Gen}(c_p \wedge A, \mathit{Defs})$;

$\Gamma := (\Gamma - \{\gamma\}) \cup \{H \leftarrow c \wedge G_1 \wedge M \wedge G_2\}$
where M is K if L is A, and M is $\neg K$ if L is $\neg A$;

end-while;

$P_{sp} := (P_{sp} - \{\delta\}) \cup \Gamma$;

end-while

In the Specialization Strategy we use real relaxations at several points: (i) when we apply the *Unfold* operator (because for applying rule R2 we check $\mathbb{R}$-satisfiability of constraints); (ii) when we check $\mathbb{R}$-subsumption during clause removal; (iii) when we compute the $\mathbb{R}$-projection c_p of the constraint c occurring in a clause γ of the form $H \leftarrow c \wedge G_1 \wedge L \wedge G_2$, (iv) when we check whether or not $c_p \sqsubseteq_{\mathbb{R}} d\rho$, and (v) when we compute the constraint $g = \mathit{Gen}(c_p \wedge A, \mathit{Defs})$ such that $c_p \sqsubseteq_{\mathbb{R}} g$. (Note that the condition $c_p \sqsubseteq_{\mathbb{R}} g$ ensures that clause γ can be folded using the new clause $K \leftarrow g \wedge A$, as it can be checked by looking at Rules R3 and R4 and recalling that, by Lemma 1, $c \sqsubseteq_{\mathbb{R}} c_p$.)

The correctness of the Specialization Strategy derives from the correctness of the transformation rules (see Theorem 1). Indeed, the sequence of values assigned to P_{sp} during the strategy can be viewed as (a subsequence of) a transformation sequence satisfying the hypotheses of Theorem 1.

We assume that the unfolding and the generalization operators guarantee that the Specialization Strategy terminates. In particular, we assume that: (i) the *Unfold* operator performs a finite number of unfolding steps, and (ii) the set *Defs* stabilizes after a finite number of applications of the *Gen* operator, that is, there exist two consecutive values, say Defs_k and Defs_{k+1}, of *Defs* such that $\mathit{Defs}_k = \mathit{Defs}_{k+1}$. This stabilization property can be enforced by defining the

generalization operator similarly to the *widening* operator on polyhedra, which is often used in static analysis of programs [10].

5 Application to the Verification of Reactive Systems

In this section we show how our Specialization Strategy based on real relaxations can be used for the verification of properties of infinite state reactive systems.

Suppose that we are given an infinite state reactive system such that: (i) the set of *states* is a subset of $\mathbb{Z}^k$, and (ii) the state *transition relation* is a binary relation on $\mathbb{Z}^k$ specified as a set of constraints over $\mathbb{Z}^k \times \mathbb{Z}^k$. In this section we will take into consideration *safety* properties, but our technique can be applied to more complex properties, such as CTL temporal properties [9,19]. A reactive system is said to be *safe* if from every *initial state* it is not possible to reach, by zero or more applications of the transition relation, a state, called an *unsafe state*, satisfying an undesired property. Let *Unsafe* be the set of all unsafe states. A standard method to verify whether or not the system is safe consists in: (i) computing (backward from *Unsafe*) the set BR of the states from which it is possible to reach an unsafe state, and (ii) checking whether or not $BR \cap \mathit{Init} = \emptyset$, where *Init* denotes the set of initial states.

In order to compute the set BR of backward reachable states, we introduce a CLP($\mathbb{Z}$) program P_{BR} defining a predicate br such that $\langle n_1, \ldots, n_k \rangle \in BR$ iff $br(n_1, \ldots, n_k) \in M_{\mathbb{Z}}(P_{BR})$. Then we can show that the reactive system is safe, by showing that there is no atom $br(n_1, \ldots, n_k) \in M_{\mathbb{Z}}(P_{BR})$ such that $\mathit{init}(n_1, \ldots, n_k)$ holds, where $\mathit{init}(X_1, \ldots, X_k)$ is a constraint that represents the set *Init* of states. Unfortunately, the computation of the perfect $\mathbb{Z}$-model $M_{\mathbb{Z}}(P_{BR})$ by a bottom-up evaluation of the immediate consequence operator, may not terminate and in that case we are unable to check whether or not the system is safe.

It has been shown in [19] that the termination of the bottom-up construction of the perfect model of a program can be improved by first specializing the program with respect to the query of interest. In this paper, we use a variant of the specialization-based method presented in [19] which is tailored to the verification of safety properties.

Our specialization-based method for verification consists of two steps. In Step 1 we apply the Specialization Strategy of Section 4 and specialize program P_{BR} with respect to the initial states of the system, that is, w.r.t. the query $\mathit{init}(X_1, \ldots, X_k) \wedge br(X_1, \ldots, X_k)$. In Step 2 we compute the perfect $\mathbb{Z}$-model of the specialized program by a bottom-up evaluation of the immediate consequence operator associated with the program.

Before presenting an example of application of our verification method, let us introduce the generalization operator we will use in the Specialization Strategy. We will define our generalization operator by using the widening operator [10], but we could have made other choices by using suitable combinations of the widening operator, the *convex hull* operator, and *thin well-quasi orderings* based on the coefficients of the polynomials (see [11,19,31] for details).

First, we need to structure the set *Defs* of definition clauses as a tree, also called *Defs* (a similar approach is followed in [19]): (i) the root clause of that tree is δ_0, and (ii) the children of a definition clause δ are the new definition clauses added to *Defs* (see the *else* branch in the body of the inner while-loop of the Specialization Strategy) during the execution relative to δ (see the test 'δ in $P_{sp} \cap$ *Defs*') of the body of outer while-loop of the Specialization Strategy.

Given a constraint c_p and an atom A obtained from a clause δ as described in the Specialization Strategy, *Gen*($c_p \wedge A$, *Defs*) is the constraint g defined as follows. If in *Defs* there exists a (most recent) ancestor clause $K \leftarrow d \wedge B$ of δ (possibly δ itself) such that: (i) $A = B\,\rho$ for some renaming substitution ρ, and (ii) $d\,\rho = a_1 \wedge \ldots \wedge a_m$ then $g = \bigwedge_{i=1}^{m} \{a_i \mid c_p \sqsubseteq_{\mathbb{R}} a_i\}$. Otherwise, if no such ancestor of δ exists in *Defs*, then $g = c_p$.

Now let us present an example of application of our verification technique based on the Specialization Strategy of Section 4. The states of the infinite state reactive system we consider are pairs of integers and the transitions from states to states, denoted by $\longrightarrow$, are the following ones: for all $X, Y \in \mathbb{Z}$,

(1) $\langle X, Y\rangle \longrightarrow \langle X, Y-1\rangle$ if $X \geq 1$
(2) $\langle X, Y\rangle \longrightarrow \langle X, Y+2\rangle$ if $X \leq 2$
(3) $\langle X, Y\rangle \longrightarrow \langle X, -1\rangle$ if $\exists Z \in \mathbb{Z}\ (Y = 2\,Z+1)$

(Thus, transition (3) is applicable only if Y is a positive or negative odd number.) The initial state is $\langle 0, 0\rangle$ and, thus, *Init* is the singleton $\{\langle 0, 0\rangle\}$. We want to prove that the system is safe in the sense that from the initial state we cannot reach any state $\langle X, Y\rangle$ with $Y < 0$. As mentioned above, we define the set $BR = \{\langle m, n\rangle \in \mathbb{Z}^2 \mid \exists \langle x, y\rangle \in \mathbb{Z}^2\ (\langle m, n\rangle \longrightarrow^* \langle x, y\rangle \wedge y < 0)\}$, where $\longrightarrow^*$ is the reflexive, transitive closure of the transition relation $\longrightarrow$. Thus, BR is the set of states from which an unsafe state is reachable. We have to prove that $Init \cap BR = \emptyset$.

We proceed as follows. First, we introduce the following program P_{BR}:

1. $br(X, Y) \leftarrow X \geq 1 \wedge X' = X \wedge Y' = Y-1 \wedge br(X', Y')$
2. $br(X, Y) \leftarrow X \leq 2 \wedge X' = X \wedge Y' = Y+2 \wedge br(X', Y')$
3. $br(X, Y) \leftarrow Y = 2\,Z+1 \wedge X' = X \wedge Y' = -1 \wedge br(X', Y')$
4. $br(X, Y) \leftarrow Y < 0$

The predicate br computes the set BR of states, in the sense that: for all $\langle m, n\rangle \in \mathbb{Z}^2$, $\langle m, n\rangle \in BR$ iff $br(m, n) \in M_{\mathbb{Z}}(P_{BR})$. Thus, in order to prove the safety of the system it is enough to show that $br(0, 0) \notin M_{\mathbb{Z}}(P_{BR})$. Unfortunately, the construction of $M_{\mathbb{Z}}(P_{BR})$ performed by means of the bottom-up evaluation of the immediate consequence operator does not terminate.

Note that the use of a *tabled* logic programming system [8], augmented with a solver for constraints on the integers, would not overcome this difficulty. Indeed, a top-down evaluation of the query $br(0, 0)$ generates infinitely many calls of the form $br(0, 2n)$, for $n \geq 1$.

Now we show that our two step verification method successfully terminates. *Step* 1. We apply the Specialization Strategy which takes as input the program P_{BR} and the query $X = 0 \wedge Y = 0 \wedge br(X, Y)$. Thus, the clause δ_0 is:

δ_0. $br_{sp}(X,Y) \leftarrow X=0 \wedge Y=0 \wedge br(X,Y)$

By applying the *Unfold* operator we obtain the two clauses:

5. $br_{sp}(X,Y) \leftarrow X=0 \wedge Y=0 \wedge X'=0 \wedge Y'=2 \wedge br(X',Y')$
6. $br_{sp}(X,Y) \leftarrow X=0 \wedge Y=0 \wedge Y=2\,Z+1 \wedge X'=0 \wedge Y'=-1 \wedge$ $br(X',Y')$

Since clause δ_0 cannot be used for folding clause 5, we apply the generalization operator and we compute $Gen((X'=0 \wedge Y'=2 \wedge br(X',Y')),\ \{\delta_0\})$ as follows. We consider the definition clause δ_0 to be an ancestor clause of itself, and we generalize the constraint $d\,\rho \equiv (X' \geq 0 \wedge X' \leq 0 \wedge Y' \geq 0 \wedge Y' \leq 0)$, using $c_p \equiv (X'=0 \wedge Y'=2)$, thereby introducing the following definition (modulo variable renaming):

δ_1. $new1(X,Y) \leftarrow X=0 \wedge Y \geq 0 \wedge br(X,Y)$

Similarly, in order to fold clause 6, we introduce the following definition:

δ_2. $new2(X,Y) \leftarrow X=0 \wedge Y \leq 0 \wedge br(X,Y)$

By folding clauses 5 and 6 by using definitions δ_1 and δ_2, respectively, we derive the following clauses:

7. $br_{sp}(X,Y) \leftarrow X=0 \wedge Y=0 \wedge X'=0 \wedge Y'=2 \wedge new1(X',Y')$
8. $br_{sp}(X,Y) \leftarrow X=0 \wedge Y=0 \wedge Y=2\,Z+1 \wedge X'=0 \wedge Y'=-1 \wedge$ $new2(X',Y')$

Then, we proceed with the next iterations of the body of the outermost while-loop of the Specialization Strategy, and we process first clause δ_1 and then clause δ_2. By using clauses δ_0, δ_1, and δ_2, we cannot fold all the clauses which are obtained by unfolding δ_1 and δ_2 w.r.t. the atom $br(X,Y)$. Thus, we again apply the generalization operator and we introduce the following definition (modulo variable renaming):

δ_3. $new3(X,Y) \leftarrow X=0 \wedge br(X,Y)$

After processing also this clause δ_3 and performing the unfolding and folding steps as indicated by the Specialization Strategy, we obtain the clauses:

9. $new1(X,Y) \leftarrow X=0 \wedge Y \geq 0 \wedge X'=0 \wedge Y'=Y+2 \wedge new1(X',Y')$
10. $new1(X,Y) \leftarrow X=0 \wedge Y \geq 0 \wedge Y=2\,Z+1 \wedge X'=0 \wedge Y'=-1 \wedge$ $new2(X',Y')$
11. $new2(X,Y) \leftarrow X=0 \wedge Y \leq 0 \wedge X'=0 \wedge Y'=Y+2 \wedge new3(X',Y')$
12. $new2(X,Y) \leftarrow X=0 \wedge Y \leq 0 \wedge Y=2\,Z+1 \wedge X'=0 \wedge Y'=-1 \wedge$ $new2(X',Y')$
13. $new2(X,Y) \leftarrow X=0 \wedge Y<0$
14. $new3(X,Y) \leftarrow X=0 \wedge X'=0 \wedge Y'=Y+2 \wedge new3(X',Y')$
15. $new3(X,Y) \leftarrow X=0 \wedge Y=2\,Z+1 \wedge X'=0 \wedge Y'=-1 \wedge new3(X',Y')$
16. $new3(X,Y) \leftarrow X=0 \wedge Y<0$

The final program P_{sp} consists of clauses 7–16.

Step 2. Now we construct the perfect $\mathbb{Z}$-model of P_{sp} by computing the least fixpoint of the immediate consequence operator associated with P_{sp} (note that in our case the least fixpoint exists, because the program is definite, and is reached after a finite number of iterations) and we have that:

$$M_{\mathbb{Z}}(P_{sp}) = \{new1(X,Y) \mid X=0 \wedge Y \geq 0 \wedge Y = 2\,Z+1\} \quad \cup$$
$$\{new2(X,Y) \mid X=0 \wedge (Y<0 \vee Y = 2\,Z+1)\} \cup$$
$$\{new3(X,Y) \mid X=0 \wedge (Y<0 \vee Y = 2\,Z+1)\}.$$

By inspection, we immediately get that $br_{sp}(0,0) \notin M_{\mathbb{Z}}(P_{sp})$ and, thus, the safety property has been proved.

Our Specialization Strategy has been implemented on the MAP transformation system (available at `http://www.iasi.cnr.it/~proietti/system.html`) by suitably modifying the specialization strategy presented in [19], so as to use the transformation rules based on real relaxations we have presented in this paper. We have tested our implementation on the set of infinite state systems used for the experimental evaluation in [19] and we managed to prove the same properties. However, the technique proposed in [19] encodes the temporal properties of the reactive systems we consider as CLP($\mathbb{Q}$) programs, where $\mathbb{Q}$ is the set of rational numbers. Thus, a proof of correctness of the encoding is needed for each system, to show that the properties of interest hold in the CLP($\mathbb{Q}$) encoding iff they hold in the CLP($\mathbb{Z}$) one. In contrast, the method presented in this paper makes use of constraint solvers over the real numbers, but it preserves *equivalence* with respect to the perfect $\mathbb{Z}$-model, thereby avoiding the need for *ad hoc* proofs of the correctness of the encoding.

Finally, note that the example presented in this section cannot be worked out by first applying the relaxation from integers to reals to the initial program and then applying polyhedral approximations, such as those considered in static program analysis [10]. Indeed, we have that $br(0,0) \notin M_{\mathbb{Z}}(P_{BR})$, but if the system is interpreted over the reals, instead of the integers, we have that $br(0,0) \in M_{\mathbb{R}}(P_{BR})$ (where $M_{\mathbb{R}}$ denotes the perfect model constructed over $\mathbb{R}$). This is due to the fact that $\exists Z(0=2\,Z+1)$ holds on the reals (but it does not hold on the integers) and, hence, we derive $br(0,0)$ from clauses 3 and 4 of program P_{BR}. Thus, $br(0,0)$ is a member of every over-approximation of $M_{\mathbb{R}}(P_{BR})$ and the safety property cannot be proved.

6 Related Work and Conclusions

We have presented a technique for specializing a CLP($\mathbb{Z}$) program with respect to a query of interest. Our technique is based on the unfold/fold transformation rules and its main novelty is that it makes use of the relaxation from the integers to the reals, that is, during specialization the constraints are interpreted over the set $\mathbb{R}$ of the real numbers, instead of $\mathbb{Z}$. The most interesting feature of our specialization technique is that, despite the relaxation, the initial program and the derived, specialized program are equivalent with respect to the perfect model constructed over $\mathbb{Z}$ (restricted to the query of interest). In essence, the reason for this equivalence is that, if the unsatisfiability or entailment between constraints that are present in the applicability conditions of the transformation rules hold in $\mathbb{R}$, then they hold also in $\mathbb{Z}$.

The main practical advantage of our specialization technique is that, during transformation, we can use tools for manipulating constraints over the reals, such

as the libraries for constraint solving, usually available within CLP($\mathbb{R}$) systems and, in particular, the Parma Polyhedral Library [3]. These tools are significantly more efficient than constraint solvers over the integers and, moreover, they implement operators which are often used during program specialization and program analysis, such as, the widening and convex hull operators. The price we pay, at least in principle, for the efficiency improvement, is that the result of program specialization may be sub-optimal with respect to the one which can be achieved by manipulating integer constraints. Indeed, our specialization strategy might fail to exploit properties which hold for the integers and not for the reals, while transforming the input program. For example, it may be unable to detect that a clause could be removed because it contains constraints which are unsatisfiable on the integers. However, we have checked that, for the significant set of examples taken from [19], this sub-optimality never occurs.

The main application of our specialization technique is the verification of infinite state reactive systems by following the approach presented in [19]. Those systems are often specified by using constraints over integer variables, and their properties (for instance, reachability, safety and liveness) can be specified by using CLP($\mathbb{Z}$) programs [20,21]. It has been shown in [19] that properties of infinite state reactive systems can be verified by first (1) specializing the program that encodes the properties of the system with respect to the property of interest, and then (2) constructing the perfect model of the specialized program by the standard bottom-up procedure based on the evaluation of the immediate consequence operator. However, in [19] the reactive systems and their properties were encoded by using CLP programs over the rational numbers (or, equivalently for linear constraints, real numbers), instead of integer numbers. Thus, a proof of correctness of the encoding is needed for each system (or for classes of systems, as in [7,13]). In contrast, our specialization technique makes use of constraint solvers over the real numbers, but preserves equivalence with respect to the perfect model constructed over the integer numbers, thereby avoiding the need for *ad hoc* proofs of the correctness of the encoding.

Specialization techniques for constraint logic programs have been presented in several papers [12,16,23,31,35]. However, those techniques consider CLP($\mathcal{D}$) programs, where $\mathcal{D}$ is either a generic domain or the domain of the rational numbers or the domain of the real numbers. None of those papers proposes techniques for specializing CLP($\mathbb{Z}$) programs by manipulating constraints interpreted over the real numbers, as we do here.

Also the application of program specialization to the verification of infinite state systems is not a novel idea [17,19,29,30,31] and, indeed, the technique outlined in Section 5 is a variant of the one proposed in [19]. The partial deduction techniques presented in [29,30] do not make use of constraints. The papers [17,19,31] propose verification techniques for reactive systems which are based on the specialization of constraint logic programs, where the constraints are linear equations and inequations over the rational or real numbers. When applying these specialization techniques to reactive systems whose native specifications are given by using constraints over the integers, we need to prove the

correctness of the encoding. Indeed, as shown by our example in Section 3, if we specify a system by using constraints over the integers and then we interpret those constraints over the reals (or the rationals), we may get an incorrect result. The approach investigated in this paper avoids extra correctness proofs, and allows us to do the specialization by interpreting constraints over the reals.

The verification of program properties based on real convex polyhedral approximations (that is, linear inequations over the reals) has been first proposed in the field of static program analysis [10,11] and then applied in many contexts. In particular, [4,5,13] consider CLP($\mathbb{R}$) encodings of infinite state reactive systems. In the case where a reactive system is specified by constraints over the integers and we want to prove a property of a set of reachable states, these encodings determine an (over-)approximation of that set. Thus, by static analysis a further (over-)approximation is computed, besides the one due the interpretation over the reals, instead of the integers, and the property of interest is checked on the approximated set of reachable states. (Clearly this method can only be applied to prove that certain states are *not* reachable.)

A relevant difference between our approach and the program analysis techniques based on polyhedral approximations is that we apply equivalence preserving transformations and, therefore, the property to be verified holds in the initial CLP($\mathbb{Z}$) program *if and only if* it holds in the specialized CLP($\mathbb{Z}$) program. In some cases this equivalence preservation is an advantage of the specialization-based verification techniques over the approximation-based techniques. For instance, if we want to prove that a given state is not reachable and this property does not hold in the CLP($\mathbb{R}$) encoding (even if it holds in the CLP($\mathbb{Z}$) encoding), then we will not be able to prove the unreachability property of interest by computing any further approximation (see our example in Section 5).

Another difference between specialization-based verification techniques and static program analysis techniques is that program specialization allows *polyvariance* [24], that is, it can produce several specialized versions for the same predicate (see our example in Section 5), while static program analysis produces one approximation for each predicate. Polyvariance is a potential advantage, as it could be exploited for a more precise analysis, but, at the same time, it requires a suitable control to avoid the explosion in size of the specialized program. The issue of controlling polyvariance is left for future work.

In this paper we have considered constraints consisting of conjunctions of linear inequations. In the case of non-linear inequations the relaxation from integer to real numbers is even more advantageous, as the satisfiability of non-linear inequations in undecidable on the integers and decidable on the reals. Our techniques smoothly extend to the non-linear case which, for reasons of simplicity, we have not considered.

Finally, in this paper we have considered transformation rules and strategies for program specialization. An issue for future research is the extension of relaxation techniques to more general unfold/fold rules, including, for instance: (i) negative unfolding, and (ii) folding using multiple clauses with multiple literals in their bodies (see, for instance, [18]).

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Proving Properties of Co-logic Programs by Unfold/Fold Transformations

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Abstract. We present a framework for unfold/fold transformation of co-logic programs, where each predicate is annotated as either inductive or coinductive, and the declarative semantics of co-logic programs is defined by an alternating fixpoint model: the least fixpoints for inductive predicates and the greatest fixpoints for coinductive predicates. We show that straightforward applications of conventional program transformation rules are not adequate for co-logic programs, and propose new conditions which ensure the preservation of the intended semantics of co-logic programs through program transformation. We then examine the use of our transformation rules for proving properties of co-logic programs which specify computations over infinite structures. We show by some examples in the literature that our method based on unfold/fold transformation can be used for verifying some properties of Büchi automata and synchronous circuits.

1 Introduction

Co-logic programming (co-LP) is an extension of logic programming recently proposed by Gupta et al. [5] and Simon et al. [18, 19], where each predicate in definite programs is annotated as either *inductive* or *coinductive*, and the declarative semantics of co-logic programs is defined by an alternating fixpoint model: the least fixpoints for inductive predicates and the greatest fixpoints for coinductive predicates. Predicates in co-LP are defined over infinite structures such as infinite trees or infinite lists as well as finite ones, and co-logic programs allow us to represent and reason about properties of programs over such infinite structures. Co-LP therefore has interesting applications to reactive systems and verifying properties such as safety and liveness in model checking and so on.

In co-LP, Simon et al. also proposed the operational semantics defined by combining standard SLD-resolution for inductive predicates and *co-SLD* resolution for coinductive predicates. However, to the best of our knowledge, methodologies for reasoning about co-LP such as the familiar unfold/fold transformation rules have not been studied. In fact, as discussed in [14], very few methods which

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use logic programs over infinite structures, have been reported so far for proving properties of infinite computations. The work by Pettorossi, Proietti and Senni [14] is one of few exceptions of such proposals, and they gave a method based on their unfold/fold transformation rules for *ω-programs*, locally stratified programs on infinite lists, for verifying properties of such programs. The semantics of ω-programs is defined based on perfect model semantics [15], where the semantics is defined in terms of iterated least fixpoints only (without using greatest fixpoints).

In this paper we consider a framework for unfold/fold transformation of co-logic programs. We first show that straightforward applications of conventional transformation rules for definite programs such as those by Tamaki and Sato [20] are not adequate for co-logic programs, and then propose new conditions which ensure the preservation of the intended semantics of co-logic programs through program transformation.

One of the motivations of this paper is to further study the applicability of techniques based on program transformation not only to program development originally due to Burstall and Darlington [1], but also for proving properties of programs. We show by examples that our method based on unfold/fold transformation can be used for verifying some properties of Büchi automata and synchronous circuits.

The organization of this paper is as follows. In Section 2, we summarise some preliminary definitions on co-logic programs. In Section 3, we present our transformation rules, and give some conditions which ensure the correctness of our transformation system. In Section 4, we explain by examples how our proof method via unfold/fold transformations proves properties of co-logic programs. Finally, we discuss about the related work and give a summary of this work in Section 5. [1]

Throughout this paper, we assume that the reader is familiar with the basic concepts of logic programming, which are found in [9].

2 Preliminaries: Co-Logic Programs

In this section, we recall some basic definitions and notations concerning co-logic programs. The details and more examples are found in [5, 18, 19]. We also explain some preliminaries on constraint logic programming (CLP) (e.g., [8] for a survey).

Since co-logic programming can deal with infinite terms such as infinite lists or trees like $f(f(\dots))$ as well as finite ones, we consider the *complete* (or *infinitary*) Herbrand base [9, 7], denoted by HB_P^*, where P is a program. Therefore, an equation $X = f(X)$, for example, has a solution $X = f(f(\dots))$. The equality theory in co-logic programming is the same as that of the standard one [9], except that we have no axiom corresponding to "occur-check", i.e.,

[1] Due to space constraints, we omit most proofs and some details, which will appear in the full paper.

$\forall t \neq X$ for each term t containing X and different from X. The theory of equality in this case is studied by Colmerauer [3]. Throughout this paper, we assume that there exists at least one constant and one function symbol of arity ≥ 1, thus HB_P^* is non-empty.

It is well-known that pure logic programming (LP for short) can be seen as an instance of the CLP scheme obtained by considering the following simple translation: let $\gamma : p(\tilde{t}_0) \leftarrow p_1(\tilde{t}_1), \ldots, p_n(\tilde{t}_n)$ be a clause in LP, where $\tilde{t}_0, \ldots, \tilde{t}_n$ are tuples of terms. Then, γ is mapped into the following *pure* CLP clause:

$$p(\tilde{x}_0) \leftarrow \tilde{X}_0 = \tilde{t}_0 \wedge \tilde{X}_1 = \tilde{t}_1 \wedge \cdots \wedge \tilde{X}_n = \tilde{t}_n \,[\!]\, p_1(\tilde{X}_1), \ldots, p_n(\tilde{X}_n),$$

where $\tilde{X}_0, \ldots, \tilde{X}_n$ are tuples of new and distinct variables, and $[\!]$ means conjunction ("$\wedge$"). Therefore, in examples we will use the conventional representation of a LP clause as a shorthand for a pure CLP clause, for the sake of readability.

In the following, for a CLP clause γ of the form: $H \leftarrow c \,[\!]\, B_1, \ldots, B_n$, the head H and the body $B_1, \ldots, B_n$ are denoted by $hd(\gamma)$ and $bd(\gamma)$, respectively. We call c the *constraint* of γ. A conjunction $c \,[\!]\, B_1, \ldots, B_n$ is said to be a *goal* (or a *query*). The predicate symbol of the head of a clause is called the *head predicate* of the clause.

2.1 Syntax

In co-logic programming, predicate symbols are annotated as either inductive or coinductive.[2] We denote by $\mathcal{P}^{in}$ ($\mathcal{P}^{co}$) the set of inductive (coinductive) predicates in P, respectively. However, there is one restriction, referred to as the *stratification restriction*: Inductive and coinductive predicates are not allowed to be mutually recursive. This notion is defined formally in Def. 1. The following is an example of co-logic programs.

Example 1. [19]. Suppose that predicates *member* and *drop* are annotated as inductive, while predicate *comember* is annotated as coinductive.

$$\begin{array}{ll} member(H, [H|\_]) \leftarrow & drop(H, [H|T], T) \leftarrow \\ member(H, [\_|T]) \leftarrow member(H, T) & drop(H, [\_|T], T_1) \leftarrow drop(H, T, T_1) \end{array}$$

$$comember(X, L) \leftarrow drop(X, L, L_1), comember(X, L_1)$$

The definition of *member* is a conventional one, and, since it is an inductive predicate, its meaning is defined in terms of the least fixpoint (Sect. 2.2). Therefore, the prefix ending in the desired element H must be finite. The similar thing also holds for predicate *drop*.

On the other hand, predicate *comember* is coinductive, whose meaning is defined in terms of the greatest fixpoint (Sect. 2.2). Therefore, it is true if and only if the desired element X occurs an infinite number of times in the list L. Hence it is false when the element does not occur in the list or when the element only occurs a finite number of times in the list. □

[2] We call an atom, A, an *inductive* (a *coinductive*) atom when the predicate of A is an inductive (a coinductive) predicate, respectively.

The notion of stratification restriction is defined using *predicate dependency*, which is defined as usual: a predicate p *depends on* a predicate q in P iff either (i) $p = q$, (ii) there exists in P a clause of the form: $p(\dots) \leftarrow c \,[]\, B$ such that predicate q occurs in B or (iii) there exists a predicate r such that p depends on r in P and r depends on q in P. The *dependency graph* of program P has the set of its predicates as vertices, and the graph has an edge from p to q if and only if p depends on q.

The set of all clauses in a program P with the same predicate symbol p in the head is called the definition of p and denoted by $Def(p, P)$. The *extended definition* [12] of p in P, denoted by $Def^*(p, P)$, is the conjunction of the definition of p and the definitions of all the predicates on which p depends in P.

Definition 1. Co-logic Program

A co-logic program is a definite program such that it satisfies the stratification restriction, namely, for any strongly connected component G in the dependency graph of the program, either every predicate in G is coinductive, or every predicate in G is inductive, i.e., every predicate in G has the same annotation. □

In order to define the semantics of co-logic programs in Sect. 2.2, some notions are necessary. A *reduced graph* is derived from a dependency graph by collapsing each strongly connected component of the dependency graph into a single node. A vertex in a reduced graph of a program P is called a *stratum*, as the set $\mathcal{P}$ of predicates in P is stratified into a collection (called a *stratification*) of mutually disjoint strata $\mathcal{P}_1, \dots, \mathcal{P}_m$ $(1 \leq m)$ of predicates. It follows from the stratification restriction that all vertices in the same stratum are of the same kind, i.e., every stratum is either inductive or coinductive. A stratum v depends on a stratum v', when there is an edge from v to v' in the reduced graph. When there is a path in the reduced graph from v to v', v is said to be higher than v' and v' is said to be lower than v. Moreover, when v_1 is higher (lower) than v_2 and $v_1 \neq v_2$, v_1 is said to be "strictly" higher (lower) than v_2, respectively.

2.2 Semantics of Co-Logic Programs

The declarative semantics of a co-logic program is a stratified interleaving of the least fixpoint semantics and the greatest fixpoint semantics.

In this paper, we consider the complete Herbrand base HB_P^* as the set of elements in the domain of a *structure* $\mathcal{D}$ (i.e., a complete Herbrand interpretation [9]), and as a constraint a set of equations of the form $s = t$, where s and t are finite terms.

Given a structure $\mathcal{D}$ and a constraint c, $\mathcal{D} \models c$ denotes that c is true under the interpretation for constraints provided by $\mathcal{D}$. Moreover, if θ is a ground *substitution* (i.e., a mapping of variables on the domain $\mathcal{D}$, HB_P^* in this case) and $\mathcal{D} \models c\theta$ holds, then we say that c is *satisfiable*, and θ is called a *solution* (or ground *satisfier*) of c, where $c\theta$ denotes the application of θ to the variables in c.

Suppose that P is a program and I is an interpretation (i.e., a subset of HB_P^*). The operator $\mathcal{T}_{P,I}$ assigns to every set T of ground atoms a new set

$\mathcal{T}_{P,I}(T)$ of ground atoms. Intuitively, I represents facts currently known to be true and $\mathcal{T}_{P,I}(T)$ contains *new* facts (i.e., facts not contained in I), whose truth can be immediately derived form the program P assuming that all facts in I hold and assuming that all facts in T are true.

Definition 2. For set T of ground atoms we define:

$\mathcal{T}_{P,I}(T) = \{A : A \notin I,$ and there is a ground substitution θ and a clause in P

$H \leftarrow c \,[]\, B_1, \cdots, B_n,\ n \geq 0,$ such that

(i) $A = H\theta$, (ii) θ is a solution of c, and

(iii) for every $1 \leq i \leq n$, either $B_i\theta \in I$ or $B_i\theta \in T\}$. □

We consider $\mathcal{T}_{P,I}$ to be the operator defined on the set of all subsets of HB_P^*, ordered by standard inclusion. Next, two subsets $T_{P,I}^{\uparrow\omega}$ and $T_{P,I}^{\downarrow\omega}$ of complete Herbrand base are defined by iterating the operators $\mathcal{T}_{P,I}$.

Definition 3. Let I be an interpretation. Define:

$$T_{P,I}^{\uparrow 0} = \emptyset \text{ and } T_{P,I}^{\downarrow 0} = HB_P^* ;$$
$$T_{P,I}^{\uparrow n+1} = \mathcal{T}_{P,I}(T_{P,I}^{\uparrow n}) \text{ and } T_{P,I}^{\downarrow n+1} = \mathcal{T}_{P,I}(T_{P,I}^{\downarrow n}) ;$$
$$T_{P,I}^{\uparrow\omega} = \cup_{n<\omega} T_{P,I}^{\uparrow n} \text{ and } T_{P,I}^{\downarrow\omega} = \cap_{n<\omega} T_{P,I}^{\downarrow n}.$$

□

Finally, the model M_P of a co-logic program P is defined as follows:

Definition 4. Suppose that a co-logic program P has a stratification $\mathcal{P}_i$ $(1 \leq i \leq m)$, where $\mathcal{P}_i$ is a set of predicates with stratum i. We denote by P_i the union of the definitions of the predicates in $\mathcal{P}_i$, and let $P_{<i}$ be the union of P_j such that $\mathcal{P}_j$ is strictly lower than $\mathcal{P}_i$.

Let:

$$M(P_i) = \begin{cases} T_{P_i,M(P_{<i})}^{\uparrow\omega}, & \text{if } \mathcal{P}_i \text{ is inductive,} \\ T_{P_i,M(P_{<i})}^{\downarrow\omega}, & \text{if } \mathcal{P}_i \text{ is coinductive.} \end{cases}$$

Then, the model of P, denoted by $M(P)$, is the union of the model $M(P_i)$ $(i = 1, \ldots, m)$. □

We note that Simon et al. [18, 19] defined the semantics $M(P)$ in terms of the greatest fixpoint of $\mathcal{T}_{P,I}$. On the other hand, we use $T_{P,I}^{\downarrow\omega}$ instead. This is justified by the notable fact that $gfp(\mathcal{T}_{P,I}) = \mathcal{T}_{P,I}^{\downarrow\omega}$ in the complete Herbrand base HB_P^* [9].

3 Unfold/fold Transformation of Co-Logic Programs

We first explain our transformation rules here, and then give some conditions imposed on the transformation rules which are necessary for correctness of transformation. Our transformation rules are formulated in the framework of CLP,

following that by Etalle and Gabbrielli [4]. The set of variables in an expression E is denoted by $var(E)$. Given atoms A, H, we write $A = H$ as a shorthand for: (i) $a_1 = t_1 \wedge \cdots \wedge a_n = t_n$, if, for some predicate symbol p and $n \geq 0$, $A \equiv p(a_1, \ldots, a_n)$ and $H \equiv p(t_1, \ldots, t_n)$ (where $\equiv$ denotes syntactic equality), (ii) *false*, otherwise. This notation readily extends to conjunctions of atoms.

Let c_i be constraints, G_i be conjunctions of atoms, and $\gamma_i : A_i \leftarrow c_i \,[\!]\, G_i$ be clauses $(i = 1, 2)$. We say that a goal $c_1 \,[\!]\, G_1$ is an *instance* of the goal $c_2 \,[\!]\, G_2$ iff, for any solution θ of c_1, there exists a solution τ of c_2 such that $G_1\theta \equiv G_2\tau$. We write $\gamma_1 \simeq \gamma_2$ iff, for any $i, j \in [1, 2]$ and for any solution θ of c_i, there exists a solution τ of c_j such that $A_i\theta \equiv A_j\tau$ and $G_i\theta$ and $G_j\tau$ are equal as multisets.

3.1 Transformation Rules

Definition 5. Initial Program

An initial program P_0 is a co-logic program satisfying the following conditions:

1. P_0 is divided into two disjoint sets of clauses, P_{new} and P_{old}. The predicates defined in P_{new} are called *new predicates*, while those defined in P_{old} are called *old predicates*. The set of new (old) predicates is denoted by $\mathcal{P}_{new}$ ($\mathcal{P}_{old}$), respectively. [3]
2. The new predicates appear neither in P_{old} nor in the bodies of the clauses in P_{new}.
3. Let γ be a clause in P_0 whose head predicate h is new. Then, h is annotated as *inductive* iff there exists at least one inductive atom in each body of the definition of h, while h is annotated as *coinductive* iff every predicate symbol occurring in each body of the definition of h is annotated as *coinductive*. □

The conditions 1 and 2 are the same as those in the original framework by Tamaki and Sato [20]. An extra condition 3 is required for the case of co-logic programs, which is explained in Example 2.

Our transformation rules consist of standard rules such as unfolding, folding and replacement rule. In particular, unfolding and folding are the same as those in Etalle and Gabbrielli [4], which are CLP counterparts of those by Tamaki and Sato [20] for definite programs. The definitions of the transformation rules are given modulo reordering of the bodies of clauses, and we assume that the clauses of a program have been renamed so that they do not share variables pairwise.

R1. Unfolding Let γ be a clause in a program P of the form: $A \leftarrow c \,[\!]\, H, G$, where c is a constraint, H is an atom, and G is a (possibly empty) conjunction of atoms. Let $\gamma_1, \ldots, \gamma_k$ with $k \geq 0$, be all clauses of P such that $c \wedge c_i \wedge (H = hd(\gamma_i))$ is satisfiable for $i = 1, \ldots, k$, where c_i is the constraint of γ_i.

[3] We call an atom, A, a *new atom* (an *old atom*) when the predicate of A is a new predicate (an old predicate), respectively. We call a clause, γ, a *new clause* (an *old clause*) when γ is in P_{new} (P_{old}), respectively.

By *unfolding* γ w.r.t. H, we derive from P the new program P' by replacing γ by $\eta_1, \ldots, \eta_k$, where η_i is the clause $A \leftarrow c \wedge c_i \wedge (H = hd(\gamma_i)) \,[\!]\, bd(\gamma_i), G$, for $i = 1, \ldots, k$. We say that clauses $\eta_1, \ldots, \eta_k$ are *derived from* γ.
In particular, if $k = 0$, i.e., there exists no clause in P such that $c \wedge c_i \wedge (H = hd(\gamma_i))$ is satisfiable, then we derive from P the new program P' by deleting clause γ.
R2. Folding Let γ be a clause in P of the form: $A \leftarrow c_A \,[\!]\, K, G$, where K and G are conjunctions of atoms. Let δ be a clause in P_{new} of the form: $D \leftarrow c_D \,[\!]\, M$, where M is a non-empty conjunction of atoms, and $c_A \,[\!]\, K$ is an instance of $c_D \,[\!]\, M$.
Suppose that there exists a constraint e such that $var(e) \subseteq var(D) \cup var(\gamma)$, and the following conditions hold:
(i) $\mathcal{D} \models \exists_{-var(A,G,M)}\ c_A \wedge e \wedge c_D \leftrightarrow \exists_{-var(A,G,M)}\ c_A \wedge (M = K)$, where $\exists_{-\tilde{X}}\ \phi$ is the notation, due to [8], to denote the existential closure of the formula ϕ except for the variables $\tilde{X}$ which remain unquantified, and
(ii) there is no clause $\delta' : B \leftarrow c_B \,[\!]\, M'$ in P_{new} such that $\delta' \neq \delta$ and $c_A \wedge e \wedge (D = B) \wedge c_B$ is satisfiable.
By applying *folding* to γ w.r.t. K using clause δ, we get the clause η: $A \leftarrow c_A \wedge e \,[\!]\, D, G$, and we say that η is *derived from* γ. We derive from P the new program $P' = (P \setminus \{\gamma\}) \cup \{\eta\}$.
The clause γ is called the *folded clause* and δ the *folding clause* (or *folder clause*).
R3. Replacement Rule We consider the following two rules depending on the annotation of a predicate.
- The set of the *useless* inductive predicates[4] of a program P is the maximal set U of inductive predicates of P such that a predicate p is in U if, for the body of each clause of $Def(p, P)$, it has an inductive atom whose predicate is in U. By applying *replacement rule* to P w.r.t. the useless inductive predicates in P, we derive the new program P' from P by removing the definitions of the useless inductive predicates.
- Let $p(\tilde{t})$ be a coinductive atom, and γ be a clause (modulo $\simeq$) in P of the form: $p(\tilde{t}) \leftarrow p(\tilde{t})$. By applying *replacement rule* to P w.r.t. the coinductive atom $p(\tilde{t})$, we derive from P the new program $P' = P \setminus \{\gamma\} \cup \{p(\tilde{t}) \leftarrow\}$.

We note that we do not explicitly consider *definition introduction* as a transformation rule, which allows us to define a new predicate in terms of old (i.e., previously defined) predicates. The reason is that new predicates introduced in the course of transformation can be assumed to be present in an initial program from scratch as is done in [20].

Etalle and Gabbrielli [4] show that we can always replace any clause γ in a program P by a clause γ' without affecting the results of the transformations, provided that $\gamma \simeq \gamma'$. Since this operation is useful to *clean up* the constraints, thereby presenting a clause in a more readable form, we will use it in examples.

Let P_0 be an initial co-logic program (thus satisfying the conditions in Def. 5). A sequence of programs $P_0, \ldots, P_n$ is said to be a *transformation sequence* with

[4] This notion is originally due to Pettorossi and Proietti [12], where the rule is called *clause deletion rule*.

the input P_0, if each P_i $(1 \leq i \leq n)$ is obtained from P_{i-1} by applying to a *new* clause in P_{i-1} one of the above-mentioned transformation rules R1-R3.

We note that every old clause in P_0 remains *untransformed* at any step in a transformation sequence.

Example 2. Consider the following transformation sequence from program P_0 to P_1, which is obtained by applying unfolding to the second clause in P_0 and then applying folding to the resultant clause, assuming that a is a new atom, while p is an old atom.

$$\begin{array}{rr} P_0 : p \leftarrow p & \qquad P_1 : p \leftarrow p \\ \qquad a \leftarrow p & \qquad\quad a \leftarrow a \end{array}$$

We note that $\mathit{lfp}(P_0) = \mathit{lfp}(P_1) = \emptyset$ and $\mathit{gfp}(P_0) = \mathit{gfp}(P_1) = \{p, a\}$, thus the above transformation preserves the least fixpoint and the greatest fixpoint of the initial program. In fact, the above transformation is a legitimate transformation in the sense of Tamaki-Sato [20] as well as Seki [17].

Table 1 shows the alternating fixpoint semantics of P_0 and P_1, depending on the predicate annotations. In P_0, there exists a stratification $\sigma = \{\{p\}, \{a\}\}$. Since the definition of a in P_0 is non-recursive, the truth value of a is determined by those predicates with lower strata (i.e., p), regardless of whether a is inductive or not. After the unfold/fold transformation, however, the annotation of a does matter to its truth value in P_1, where a is recursively defined. We note that condition 3 in Def. 5 gives such a restriction on predicate annotations. □

Table 1. The Alternating Fixpoint Semantics in Example 2

annotations		$M(P_0)$	$M(P_1)$
p: inductive	a: inductive	$\emptyset$	$\emptyset$
	a: coinductive	$\emptyset$	$\{a\}$
p: coinductive	a: inductive	$\{p, a\}$	$\{p\}$
	a: coinductive	$\{p, a\}$	$\{p, a\}$

3.2 Conditions on Transformation Rules

In the following, we will explain the conditions imposed on unfolding and folding rules to preserve the alternating fixpoint semantics of a co-logic program.

Let f be a new inductive predicate. We call an inductive predicate p *primitive*, if, for some coinductive predicate q occurring in $\mathit{Def}^*(f, P_0)$, p occurs in $\mathit{Def}^*(q, P_0)$. We denote by $\mathcal{P}_{pr}$ the set of all the primitive predicates, i.e., $\mathcal{P}_{pr} = \{p \in \mathcal{P}^{in} \mid p \text{ occurs in } \mathit{Def}^*(q, P_0), q \text{ occurs in } \mathit{Def}^*(f, P_0), q \in \mathcal{P}^{co}, f \in \mathcal{P}^{in} \cap \mathcal{P}_{new}\}$. We call an inductive predicate p *non-primitive*, if it is not primitive.

We call an atom with non-primitive (primitive) predicate symbol a *non-primitive* (primitive) atom, respectively.

The following example will be helpful to understand the notion of primitive atoms.

Example 3. Consider the following transformation sequence from program P_0 to P_1, where $p, f \in \mathcal{P}^{in}$, $q \in \mathcal{P}^{co}$, and p, q are old predicates, while f is a new predicate:

$$\begin{array}{ll} P_0 : f \leftarrow p, q & P_1 : f \leftarrow f \\ \quad\quad p \leftarrow & \quad\quad p \leftarrow \\ \quad\quad q \leftarrow p, q & \quad\quad q \leftarrow p, q \end{array}$$

We note that $M(P_0) = \{p, q, f\}$, while and $M(P_1) \not\models f$, thus the above transformation does not preserves the alternating fixpoint semantics.

In P_0, p is a *primitive* inductive predicate, since p occurs in the definition of coinductive predicate q in the definition of f, which is new and inductive.

In the above transformation, unfolding is applied to $f \leftarrow p, q$ w.r.t. inductive *primitive* atom p. □

The next notion is due to [17], which is originally introduced to give a condition on folding to preserve the finite failure set.

Definition 6. Inherited Atom [17], Fair Folding

Let $P_0, \ldots, P_n$ be a transformation sequence starting from P_0, and η a clause in P_i $(0 \leq i \leq n)$ whose head is a new atom. Then, an atom in the body of η is called an atom *inherited from* P_0 if one of the following conditions is satisfied:

1. $\eta \in P_{new}$. Then, each atom in $bd(\eta)$ is *inherited from* P_0.
2. Suppose that η is derived by unfolding $\gamma \in P_{i-1}$ w.r.t. H. Thus, γ and η are of the form: $A \leftarrow c_A \,[\!]\, H, G$ and $A \leftarrow c \wedge c_i \wedge (H = hd(\gamma_i)) \,[\!]\, bd(\gamma_i), G$, respectively, where γ_i is an unfolding clause. Then, each atom B occurring in G of η is *inherited from* P_0, if B in G of γ is inherited from P_0.
3. Suppose that η is derived by folding γ in P_{i-1}. Thus, γ and η are of the form: $A \leftarrow c_A \,[\!]\, K, G$ and $A \leftarrow c_A \wedge e \,[\!]\, D, G$, respectively, for a folding clause δ with $hd(\delta) = D$. Then, each atom B in G of η is *inherited from* P_0, if B in G of γ is inherited from P_0.

Moreover, the application of folding is said to be *fair*, if, in condition 3, there is no atom in K which is inherited from P_0. □

Intuitively, an inherited atom is an atom such that it was in the body of some clause in P_{new} and no unfolding has been applied to it.

In order to give conditions of folding, we need the following notion of marking: Let $P_0, \ldots, P_n$ be a transformation sequence with input P_0. We mark each clause in $P_{new} \subseteq P_0$ "*not TS-foldable*". Let η be a clause in P_{k+1} $(0 \leq k < n)$.

(i) Suppose that η is derived from $\gamma \in P_k$ by unfolding $\gamma : A \leftarrow c \,[\!]\, H, G$ w.r.t. H. If H is a *non-primitive* inductive atom, then we mark η "*TS-foldable*". Otherwise, η inherits the mark of γ.

(ii) Suppose that η is derived from $\gamma \in P_k$ by folding. Then, η inherits the mark of γ.
(iii) Suppose that η is not involved in the derivation from P_k to P_{k+1}. Then, η inherits its mark in P_k.

Conditions on Folding Let $P_0, \ldots, P_n$ be a transformation sequence with input P_0. Suppose that P_k $(0 < k \leq n)$ is derived from P_{k-1} by folding $\gamma \in P_{k-1}$. The application of folding is said to be *admissible* if the following conditions are satisfied:
(1) P_k satisfies the stratification restriction,
(2) if $hd(\gamma)$ is an inductive atom, then γ is marked "TS-foldable" in P_{k-1}, and
(3) if $hd(\gamma)$ is a coinductive atom, then the application of folding is fair. □
We call condition (2) in the above as *TS-folding condition*.

The following shows the correctness of our transformation system.

Proposition 1. Correctness of Transformation
Let P_0 be an initial co-logic program, and $P_0, \ldots, P_n$ $(0 \leq n)$ a transformation sequence, where every application of folding is admissible. Then, the alternating fixpoint semantics $M(P_0)$ of P_0 is preserved, i.e., $M(P_n) = M(P_0)$. □

Remark 1. Table 2 summarizes the conditions imposed on the transformation rules. The results on the least fixpoint semantics $T_P^{\uparrow\omega}$ for definite programs (column $T_P^{\uparrow\omega}$ in Table 2) are due to Tamaki-Sato [20], while those on the finite failure set (FF) (column $T_P^{\downarrow\omega}$ in Table 2) are found in [17]. It is known (e. g., [9]) that $FF(P) = \overline{T_P^{\downarrow\omega}}$, the complement of $T_P^{\downarrow\omega}$ for definite program P, and that $gfp(P) = \overline{T_P^{\downarrow\omega}}$ in complete (infinitary) Herbrand base HB_P^*. Therefore, one might think that unfold/fold transformation simply using fair folding would be appropriate for co-logic programs. However, Example 2 and Example 3 show that it is not the case, since a co-logic program consists of the definitions of predicates defined either inductively or coinductively, and its semantics is defined in terms of alternating the least fixpoints and the greatest fixpoints. Proposition 1 gives some additional conditions (shown in column $M(P)$ in Table 2) which are necessary to preserve the alternating fixpoint semantics of co-logic programs. □

4 Proving Properties of Co-Logic Programs

In this section, we explain our approach based on the transformation rules given in Sect. 3 to proving properties of co-logic programs. We use two examples studied in the literature: One is the non-emptiness of the language accepted by a Büchi automaton [14]. The other is an example of proving a liveness property of a modulo 4 counter [18].

Let P be a co-inductive program and *prop* be a predicate specifying a property of interest which is defined in terms of the predicates in P. Then, in order to check whether or not $M(P) \models \exists X\, prop(X)$, our proving approach is very

Table 2. Conditions Imposed on the Transformations Rules: The application conditions in column $M(P)$ are newly given in this paper. Those in column $T_P^{\uparrow\omega}$ ($T_P^{\downarrow\omega}$) are due to [20] ([17]), respectively. When the predicate symbol of atom A is inductive (coinductive), we denote it by $A \in \mathcal{P}^{in}$ ($\mathcal{P}^{co}$), respectively.

trans. rule	$T_P^{\uparrow\omega}$	$T_P^{\downarrow\omega}$	$M(P)$
definition (init. prog. P_0) (Def. 5)	$P_0 \ni \forall\, C : H \leftarrow L_1, \ldots, L_k$, $\forall i$ L_i is old, if H is new	the same	the same & $\forall i$ $L_i \in \mathcal{P}^{co}$, if $H \in \mathcal{P}^{co}$ $\exists i$ $L_i \in \mathcal{P}^{in}$, if $H \in \mathcal{P}^{in}$
folding	TS-folding	fair folding	strat. restriction & TS-folding, if $hd(C) \in \mathcal{P}^{in}$ fair folding, if $hd(C) \in \mathcal{P}^{co}$

simple: (i) we introduce a new predicate f defined by clause C_f of the form: $f \leftarrow prop(X)$, then (ii) we apply the transformation rules for co-logic programs given in Sect. 3 to $P \cup \{C_f\}$ as (possibly a subset of) an initial program. The annotation of predicate f is defined according to Def. 5.

Example 4. Adapted from [14]. A Büchi automaton $\mathcal{A}$ is a nondeterministic finite automaton $\langle \Sigma, Q, q_0, \delta, F \rangle$, where Σ is the input alphabet, Q is the set of states, q_0 is the initial state, $\delta \subseteq Q \times \Sigma \times Q$ is the transition relation, and F is the set of final states. A *run* of the automaton $\mathcal{A}$ on an infinite input word $w = a_0 a_1 \cdots \in \Sigma^\omega$ is an infinite sequence $\rho = \rho_0 \rho_1 \cdots \in Q^\omega$ of states such that ρ_0 is the initial state q_0 and, for all $n \geq 0$, $\langle \rho_n, a_n, \rho_{n+1} \rangle \in \delta$. Let $Inf(\rho)$ denote the set of states that occur infinitely often in the infinite sequence ρ of states. An infinite word $w \in \Sigma^\omega$ is *accepted* by $\mathcal{A}$ if there exists a run ρ of $\mathcal{A}$ on w such that $Inf(\rho) \cap F \neq \emptyset$. The language accepted by $\mathcal{A}$ is the subset of Σ^ω, denoted by $\mathcal{L}(\mathcal{A})$, of the infinite words accepted by $\mathcal{A}$.

In order to check whether or not the language $\mathcal{L}(\mathcal{A})$ is empty, we consider the following co-logic program which includes the definition of a unary predicate *accepting_run* such that: $\mathcal{L}(\mathcal{A}) \neq \emptyset$ iff $\exists X\, accepting\_run(X)$.
1. $automata([X|Xs], [Q, Q'|Qs]) \leftarrow trans(Q, X, Q'), automata(Xs, [Q'|Qs])$
2. $run([Q_0|Qs]) \leftarrow initial(Q_0), automata(Xs, [Q_0|Qs])$
3. $accepting\_run(Qs) \leftarrow run(Qs), final(Q), comember(Q, Qs)$
where, for all $q, q_1, q_2 \in Q$, for all $a \in \Sigma$,

(i) $initial(q)$ iff $q = q_0$,
(ii) $trans(q_1, a, q_2)$ iff $\langle q_1, a, q_2 \rangle \in \delta$,
(iii) $final(q)$ iff $q \in F$.

We note that predicates *automata* and *comember* (defined in Example 1) are annotated as coinductive, while the other predicates are inductive. Now, let us consider a Büchi automaton $\mathcal{A}$ such that: $\Sigma = \{a, b\}, Q = \{1, 2\}, q_0 = 1, \delta = \{\langle 1, a, 1\rangle, \langle 1, b, 1\rangle, \langle 1, a, 2\rangle, \langle 2, a, 2\rangle\}, F = \{2\}$ which can be represented in Fig. 1. For this automaton $\mathcal{A}$, program $P_\mathcal{A}$ consists of clauses 1-3 and the following

clauses 4-9 that encode the initial state (clause 4), the final state (clause 5) and the transition relation (clauses 6-9):

4. $initial(1) \leftarrow$ 6. $trans(1, a, 1) \leftarrow$ 8. $trans(1, a, 2) \leftarrow$
5. $final(2) \leftarrow$ 7. $trans(1, b, 1) \leftarrow$ 9. $trans(2, a, 2) \leftarrow$

To check the non-emptiness of $\mathcal{L}(\mathcal{A})$, we introduce the following clause:
C_f : $f \leftarrow accepting\_run(X)$,
where f is a new inductive predicate. By some unfolding steps, from C_f we obtain:
10. $f \leftarrow automata(Xs, [1|Qs]), comember(2, [1|Qs])$
By some unfolding steps, from clause 10 we get as one of the derived clauses:
11. $f \leftarrow automata(Xs, [2|Qs]), comember(2, [1, 2|Qs])$
By applying unfolding to clause 11 w.r.t. $comember(2, [1, 2|Qs])$, we get:
12. $f \leftarrow automata(Xs, [2|Qs]), comember(2, Qs)$

Now, we introduce:
C_g : $g \leftarrow automata(Xs, [2|Qs]), comember(2, Qs)$
where g is a new coinductive predicate. Since clause 12 satisfies the conditions of fair folding, we apply folding to that clause with folder clause C_g and get:
13. $f \leftarrow g$

By some unfolding steps, from C_g we obtain as one of the derived clauses:
14. $g \leftarrow automata(Xs, [2|Qs]), comember(2, Qs)$

Again, we can apply fair folding to clause 14 and obtain:
15. $g \leftarrow g$

Since g is a coinductive predicate, we apply replacement rule to the above clause, and obtain:
16. $g \leftarrow$

Then, we apply unfolding to clause 13 with unfolding clause 16, obtaining:
17. $f \leftarrow$

This means that $M(P_{\mathcal{A}}) \models \exists X\, accepting\_run(X)$, and we thus have that $\mathcal{L}(\mathcal{A}) \neq \emptyset$.

It will be interesting to compare our approach with the original method by Pettorossi, Proietti and Senni [14]. In their method, (i) the given problem is encoded in an *ω-program* P, a locally stratified program on infinite lists, then (ii) their transformation rules in [14] are applied to P, deriving a *monadic* ω-program T, and finally (iii) the decision procedure in [13] is applied to T to check whether or not $PERF(T) \models \exists prop(X)$, where $PERF(T)$ is the perfect model of T.

To represent $Inf(\rho) \cap F \neq \emptyset$, their ω-program first introduces a new predicate $rejecting(Qs)$, meaning that run Qs is rejecting (not accepting). Then, the non-emptyness of the language is represented by using nested negations. This process of definition introduction will be inevitable, because their semantics is based on perfect model semantics which is defined by a least model characterization. On the other hand, co-logic programming allows us to use predicate *comember* in this case, which makes the representation succinct and easy to understand. □

Fig. 1. Examples: a Büchi automaton (left) [14] and a modulo 4 counter (right) [18]

The next example due to [18] is on proving a liveness property of a modulo 4 counter in Fig. 1 (right).

Example 5. Adapted from [18]. The following co-logic program P encodes the modulo 4 counter in Fig. 1:

1. $t_{-1}(N, [s_{-1}|T]) \leftarrow N_1 = N + 1 \bmod 4, t_0(N_1, T), N_1 \geq 0$
2. $t_0(N, [s_0|T]) \leftarrow N_1 = N + 1 \bmod 4, t_1(N_1, T), N_1 \geq 0$
3. $t_1(N, [s_1|T]) \leftarrow N_1 = N + 1 \bmod 4, t_2(N_1, T), N_1 \geq 0$
4. $t_2(N, [s_2|T]) \leftarrow N_1 = N + 1 \bmod 4, t_3(N_1, T), N_1 \geq 0$
5. $t_3(N, [s_3|T]) \leftarrow N_1 = N + 1 \bmod 4, t_0(N_1, T), N_1 \geq 0$

where each t_i $(-1 \leq i \leq 3)$ is a coinductive predicate, and s_0, s_1, s_2, s_3, and s_{-1} denote the states labelled with $0, 1, 2, 3$, and -1, respectively.

Suppose that we want to prove a property of the counter, ensuring that there is an infinite path through the system that never passes through the state labelled with -1. The counterexamples to the property can be specified as: $\exists T\ t_{-1}(-1, T), comember(s_{-1}, T)$, which means that there exists an infinite trace T along which state s_{-1} occurs infinitely often.

We first introduce the following clause:
$C_f:\ \ f \leftarrow t_{-1}(-1, T), comember(s_{-1}, T),$
where f is a new coinductive predicate. By some unfolding steps, from C_f we obtain:
6. $f \leftarrow t_1(1, T), drop(s_{-1}, T, T'), comember(s_{-1}, T')$

We then introduce:
$C_g:\ \ g(T') \leftarrow t_1(1, T), drop(s_{-1}, T, T')$
where g is a new inductive predicate. Since clause 6 satisfies the conditions of fair folding, we apply folding to that clause with folder clause C_g and get:
7. $f \leftarrow g(T'), comember(s_{-1}, T')$

By some unfolding steps, from C_g we obtain:
8. $g(T') \leftarrow t_1(1, T), drop(s_{-1}, T, T')$

Again, we can apply fair folding to clause 8 and obtain:
9. $g(T) \leftarrow g(T)$

Since g is a inductive predicate, we apply replacement rule to the above clause, thereby removing the single clause defining predicate g.

Then, we apply unfolding to clause 7 w.r.t. $g(T')$, which removes the single clause 7 defining predicate f. This means that $M(P \cup \{f\}) \not\models f$, which implies that there is no counterexample to the original property.

It will be interesting to compare our approach with the operational semantics of co-logic programs by Simon [18, 19], which is a combination of standard SLD-resolution for inductive predicates, and *co-SLD* resolution for coinductive predicates. A new inference rule called *coinductive hypothesis rule* is introduced in co-SLD resolution. Stated informally, if a current subgoal A in a derivation is a coinductive atom, and it appears as an ancestor of the derivation, A is supposed to be true.

It is easy to see that folding together with replacement rule w.r.t. coinductive predicates plays the same role as coinductive hypothesis rule in the above example. In general, however, the pair of folding and the replacement rule is more powerful than coinductive hypothesis rule, in that folding allows several atoms in a folded clause to be folded, while only a single atom is concerned in coinductive hypothesis rule.

Moreover, the pair of folding together with replacement rule for *inductive* predicates works as a loop-check mechanism for inductive predicates, while such a mechanism is not employed in the operational semantics by Simon et al. Although it is possible to incorporate such a mechanism into their operational semantics, it would inevitably make the description of the semantics more complicated. □

5 Related Work and Concluding Remarks

We have proposed a new a framework for unfold/fold transformation of co-logic programs. We have explained that straightforward applications of conventional unfold/fold rules by Tamaki-Sato [20] and Seki [17] are not adequate for co-logic programs, and proposed new conditions which ensure the preservation of the intended semantics of co-logic programs through transformation.

Simon et al. have already realized a prototypical implementation based on their operational semantics [18]. Our framework for unfold/fold transformation of co-logic programs will hopefully become a basis of developing methodologies for program optimization such as partial evaluation for co-logic programs. We have already made some comparison with their operational semantics in Example 5.

As discussed in [14], very few methods have been reported so far for proving properties of infinite computations by using logic programs over infinite structures, and as a notable exception, we have discussed the work by Pettorossi, Proietti and Senni [14] in Example 4. Although the example is taken from their paper, the proof illustrated here has shown that, as far as this particular example is concerned, our method using co-logic programs can prove the given property in a simpler and more intuitive manner.

On the other hand, the framework by Pettorossi, Proietti and Senni is very general in that arbitrary first order formulas are allowed to specify properties of a given program, while our framework is restricted in that only definite co-logic programs are allowed. One of the future work is therefore to extend the current framework to allow negation. Min and Gupta [10], for example, have already proposed such an extension, where they extend co-LP with negation. We hope

that our results reported in this paper will be a contribution to promote further cross-fertilization between program transformation and model checking.

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Simplifying Questions in Maude Declarative Debugger by Transforming Proof Trees*

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Abstract. Declarative debugging is a debugging technique that abstracts the execution details, that may be difficult to follow in general in declarative languages, to focus on results. It relies on a data structure representing the wrong computation, the *debugging tree*, which is traversed by asking questions to the user about the correction of the computation steps related to each node. Thus, the complexity of the questions is an important factor regarding the applicability of the technique. In this paper we present a transformation for debugging trees for Maude specifications that ensures that any subterm occurring in a question has been previously replaced by the most reduced form that it has taken during the computation, thus ensuring that questions become as simple as possible.

Keywords: declarative debugging, Maude, proof tree transformation

1 Introduction

Declarative debugging [14], also called *algorithmic debugging*, is a debugging technique that abstracts the execution details, that may be difficult to follow in general in declarative languages, to focus on results. This approach, that has been used in logic [16], functional [10], and multi-paradigm [7] languages, is a two-phase process [9]: first, a data structure representing the computation, the so-called *debugging tree*, is built; in the second phase this tree is traversed following a *navigation strategy* and asking to an external oracle about the correctness of the computation associated to the current node until a *buggy node*, an incorrect node with all its children correct, is found. The structure of the debugging tree must ensure that buggy nodes are associated to incorrect fragments of code, that is, finding a buggy node is equivalent to finding a bug in the program. Note that, since the oracle used to navigate the tree is usually the user, the number and complexity of the questions are the main issues when discussing the applicability of the technique.

Maude [4] is a high-level language and high-performance system supporting both equational and rewriting logic computation. Maude modules correspond to specifications in rewriting logic [8], a simple and expressive logic which allows the representation of many models of concurrent and distributed systems. This logic is an extension of equational logic, that in the Maude case corresponds to membership equational logic (MEL) [1], which, in addition to equations, allows the statement of membership axioms

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characterizing the elements of a sort. Rewriting logic extends MEL by adding rewrite rules, that represent transitions in a concurrent system.

In previous papers we have faced the problem of declarative debugging of Maude specifications both for *wrong answers* (incorrect results obtained from a valid input), and for missing answers (incomplete results obtained from a valid input); a complete description of the system can be found in [13]. Conceptually debugging trees in Maude are obtained in two steps. First a *proof tree* for the erroneous result (either a wrong or missing answer) in a suitable semantic calculus is considered. Then this tree is pruned by removing those nodes that correspond to logic inference steps that does not depend on the program and are consequently valid. The result is an *abbreviated proof tree* (APT) which has the property of requiring less questions to find the error in the program. Moreover, the terms in the APT nodes appear in their most reduced forms (for instance function calls have been replaced by their results). Although unnecessary from the theoretical point of view, this property of containing terms in their most reduced form has been required since the earlier works in declarative debugging (see Section 2) since otherwise the debugging process becomes unfeasible in practice due to the complexity of the questions performed to the user.

However, the situation changes when debugging Maude specifications with the `strat` attribute [4], that directs the evaluation order and can prevent some arguments from being reduced, that is, this attribute introduces a particular notion of laziness, making some subterms to be evaluated later than they would be in a "standard" Maude computation. For this reason we will use in this paper a slightly different notion of normal form that takes into account `strat`: a term is in normal form if neither the term nor its subterms has been further reduced in the current computation. When dealing with specifications with this attribute the APT no longer contains the terms in their most reduced forms, and thus the questions performed by the tool become too involved.

The purpose of this work is to define a program transformation that converts an arbitrary proof tree T built for a specification with the `strat` attribute into a proof tree T' whose APT contains all the subterms in their most reduced form. Since T' is also a proof tree for the same computation the soundness and completeness of the technique obtained in previous papers remain valid. Note that this improvement, described for the equational subset of Maude (where `strat` is applied) improves the questions asked in the debugging of both wrong and missing answers, including system modules, because reductions are used by all the involved calculuses. Note that, although we present here a transformation for arbitrary proof trees, our tool builds the debugging trees in such a way that some of this transformations are not needed (more specifically, we do not need the "canonical" transformation we will see later). We prefer to build the proof tree and then transform it to make the approach conservative: the user can decide whether he wants to use the transformation or not.

The rest of the paper is organized as follows: the following section introduces some related work and shows the contributions of our approach with respect to related proposals. Section 3 introduces Maude functional modules, the debugging trees used to debug this kind of modules, and the trees we want to obtain to improve the debugging process. Section 4 presents the transformations applied to obtain these trees and the

theoretical results that ensure that the transformation is safe. Finally, we present the conclusions and discuss some related ongoing work.

The source code of the debugger, examples, and much more information is available at `http://maude.sip.ucm.es/debugging/`. Detailed proofs of the results shown in this paper and extended information about the transformations can be found in [2].

2 Related Work

Since the introduction of declarative debugging [14] the main concerns with respect to this technique were the complexity of the questions performed to the user, and also that the process can become very tedious, and thus error-prone. The second point is related to the number of questions and has been addressed in different ways [13,15]: nodes whose correction only depends on the correction of their children are removed; statements and modules can be trusted, and thus the corresponding nodes can be removed from the debugging tree; a database can be used to prevent debuggers from asking the same question twice; trees can be compressed [5], which consists in removing from the debugging tree the children of nodes that are related to the same error as the father, in such a way that the father will provide all the debugging information; a different approach consists in *adding* nodes to the debugging tree to balance it and thus traverse it more efficiently [6]; finally, other techniques reduce the number of questions by allowing complex answers, that direct the debugging process in a more specific direction, e.g. [7] provides an answer to point out a specific subterm as erroneous.

This paper faces the first concern, the complexity of the questions, considering the case of Maude specifications including the `strat` attribute. This attribute can be used to alter the execution order, and thus the same subterm can be found in different forms in the tree. The unpredictability of the execution order was already considered in the first declarative debuggers proposed for lazy functional programming. In [11] the authors proposed two ways of constructing the debugging trees. The first one was based on source code transformations and the introduction of an impure primitive employed for ensuring that all the subterms take the most reduced form (or a special symbol denoting unevaluated calls). This idea was implemented in Buddha [12], a declarative debugger for Haskell, and in the declarative debugger of the functional-logic language Toy [3]. The second proposal was to change the underlying language implementation, which offers better performance. This technique was exploited in [10], where an implementation based on graph reduction was proposed for the language Haskell.

In this paper we address a similar problem from a different point of view. We are interested in proving formally the adequacy of the proposal and thus we propose a transformation at the level of the proof trees, independent of the implementation. The transformation takes an arbitrary proof tree and generates a new proof tree. We prove that the transformed tree is a valid proof tree with respect to rewriting logic calculus underlying Maude and that the subterms in questions are in their most reduced form.

3 Declarative Debugging in Maude

We present here Maude and the debugging trees used to debug Maude specifications.

3.1 Maude

For our purposes in this paper we are interested in the equational subset of Maude, which corresponds with specifications in MEL [1]. Maude functional modules [4], introduced with syntax `fmod ... endfm`, are executable MEL specifications and their semantics is given by the corresponding initial membership algebra in the class of algebras satisfying the specification. In a functional module we can declare sorts (by means of keyword `sort(s)`); subsort relations between sorts (`subsort`); operators (`op`) for building values of these sorts, giving the sorts of their arguments and result, and which may have attributes such as being associative (`assoc`) or commutative (`comm`), for example; memberships (`mb`) asserting that a term has a sort; and equations (`eq`) identifying terms. Both memberships and equations can be conditional (`cmb` and `ceq`). The executability requirements for equations and memberships are confluence, termination, and sort-decreasingness [4].

We illustrate the features described before with an example. The `LAZY-LISTS` module below specifies lists with a lazy behavior. At the beginning of the module we define the sort `NatList` for lists of natural numbers, which has `Nat` as a subsort, indicating that a natural number constitutes the singleton list:

```
(fmod LAZY-LISTS is
  pr NAT .
  sort NatList .
  subsort Nat < NatList .
```

Lists are built with the operator `nil` for empty lists and with the operator `_ _` for bigger lists, which is associative and has `nil` as identity. It also has the attribute `strat(0)` indicating that only reductions at the top (the position `0`) are allowed:

```
  op nil : -> NatList [ctor] .
  op _ _ : NatList NatList -> NatList [ctor assoc id: nil strat(0)] .
```

Next, we define a function `from` that generates a potentially infinite list starting from the number given as argument. Note that the attribute `strat(0)` in `_ _`, used in the righthand side of the equation, does not permit reductions in the subterms of `N from(s(N))`, thus preventing an infinite computation because no equations can be applied to `from(s(N))`:

```
  op from : Nat -> NatList .
  eq [f] : from(N) = N from(s(N)) .
```

where `f` is a label identifying the equation. The module also contains a function `take` that extracts the number of elements indicated by the first argument from the list given as the second argument. Since the `strat(0)` attribute in `_ _` prevents the list from evolving, we take the first element of the list and apply the function to the rest of the list in a matching condition, thus separating the terms built with `_ _` into two different terms and allowing the lazy lists to develop all the needed elements:

```
  op take : Nat NatList -> NatList .
  ceq [t1] : take(s(N), N' NL) = N' NL' if NL' := take(N, NL) .
  eq [t2] : take(N, NL) = 0 [owise] .
```

where `owise` stands for otherwise, indicating that the equation is used when no other equation can be applied. Finally, the function `head` extracts the first element of a list, where `~>` indicates that the function is partial:

(**Reflexivity**) (**Congruence**)

$$\frac{}{t \to t}\ \mathsf{Rf} \qquad \frac{t_1 \to t_1' \quad \ldots \quad t_n \to t_n'}{f(t_1,\ldots,t_n) \to f(t_1',\ldots,t_n')}\ \mathsf{Cong}$$

(**Transitivity**) (**Replacement**)

$$\frac{t_1 \to t' \quad t' \to t_2}{t_1 \to t_2}\ \mathsf{Tr} \qquad \frac{\{\theta(u_i) \downarrow \theta(u_i')\}_{i=1}^{n} \quad \{\theta(v_j) : s_j\}_{j=1}^{m}}{\theta(t) \to \theta(t')}\ \mathsf{Rep}$$
$$\text{if } t \to t' \Leftarrow \textstyle\bigwedge_{i=1}^{n} u_i = u_i' \wedge \bigwedge_{j=1}^{m} v_j : s_j$$

Fig. 1. Semantic calculus for reductions

```
  op head : NatList ~> Nat .
  eq [h] : head(N NL) = N .
endfm)
```

We can now introduce the module in Maude and reduce the following term:

```
Maude> (red take(2 * head(from(1)), from(1)) .)
result NatList : 1 2 0
```

However, instead of returning the first two elements of the list, it appends `0` to the result. The unexpected result of this computation indicates that there is some error in the program. The following sections show how to build a debugging tree for this reduction, how to improve it, and how to use this improved tree to debug the specification.

3.2 Debugging trees

Debugging trees for Maude specifications [13] are conceptually built in two steps:[1] first, a proof tree is built with the proof calculus in Figure 1, which is a modification of the calculus in [1], where we use the notation $t \downarrow t'$ to indicate that t and t' are reduced to the same term and we assume that the equations are terminating and confluent and hence they can be oriented from left to right, and that replacement inferences keep the label of the applied statement in order to point it out as wrong when a buggy node is found. In the second step a pruning function, called *APT*, is applied to the proof tree in order to remove those nodes whose correctness only depends on the correctness of their children (and thus they are useless for the debugging process) and to improve the questions asked to the user. This transformation can be found in [13].

Figure 1 describes the part of MEL we will use throughout this paper, the extension to full MEL is straightforward and can be found in [2]. The figure shows that the proof trees can infer *judgments* of the form $t \to t'$, indicating that t is reduced to t' by using equations. The inference rules in this calculus are reflexivity, that proves that a term can be reduced to itself; congruence, that allows to reduce the subterms; transitivity, used to compose reductions; and replacement, that applies a equation to a term if a substitution θ making the term match the lefthand side of the equation and fulfilling the conditions

[1] The implementation applies these two steps at once.

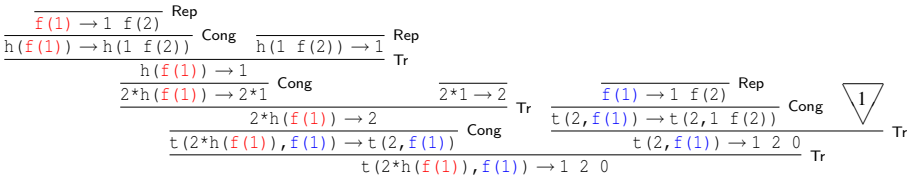

Fig. 2. Proof tree for the reduction on Section 3.1

is found. It is easy to see that the only inference rule whose correctness depends on the specification is replacement; intuitively, nodes inferred with this rule will be the only ones kept by *APT*. Thus, *APT* removes some nodes from the tree and can attach the debugging information to some others in order to ease the questions asked to the user, but cannot modify the judgments in the nodes, since it would require to modify the whole structure of the tree, as we will see later.

We show in Figures 2 and 3 the proof tree associated to the reduction presented in the previous section, obtained following Maude execution strategies,[2] where `t` stands for `take`, `h` for `head`, and `f` for `from`. The left child of the root of the tree in Figure 2 obtains the number of elements that must be extracted from the list, while the right child unfolds the list one step further and takes the element thus obtained, repeating this operation until all the required elements have been taken. Note that Maude cannot reduce `f(1)` to its normal form (with respect to the tree) `1 2 3 f(4)` with three consecutive replacement steps because the attribute `strat(0)` prevents it.

From the point of view of declarative debugging, this tree is not very satisfactory, because it contains nodes like `t(2,1 f(2))` $\longrightarrow$ `1 2 0`, the root of the tree in Figure 3, where the subterm `f(2)` is not fully reduced, which forces the user to obtain its expected result and then (mentally) substitute it in the node in order to answer the question about the correction of the node. We show the APT corresponding to this tree in Figure 4; note that a transformation like *APT* cannot improve this kind of questions because there is no node with the information we want to use, and thus the node (†) described above is kept and will be used in the debugging process. Intuitively, we would like to gather all the replacements related to the same term so we can always ask about terms with the subterms in normal form, like `t(2,1 2` $\bot$`)`, where $\bot$ is a special symbol indicating that a term could be further reduced but its value is not necessary. The next section explains how to transform proof trees in order to obtain questions with this form.

When examining a proof tree we are interested in distinguishing whether two syntactically identical terms are copies of the same term or not. The reason is that it is more natural for the user to have each copy in its more reduced form, without considering the reductions of other copies of the same term (as happens with the term `f(1)` in the example above; one of these terms is reduced to `1 f(2)` while the second one is reduced to `1 2 3 f(4)`). We achieve this goal by "painting" related terms in a proof tree with

[2] Actually, the value `3` in Figure 3 has been computed to mimic Maude's behavior. Once it has obtained `take(0, f(3))` it tries to reduce its subterms, obtaining `3` although it will be never used. All the transformations in this paper also work if this term is not computed.

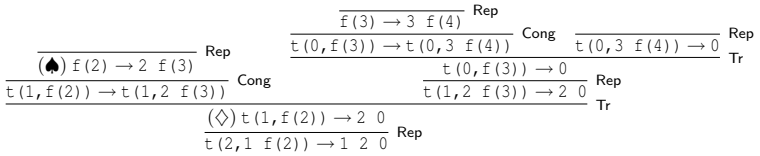

Fig. 3. Proof tree for the subtree $\overset{1}{\triangledown}$ on Figure 2

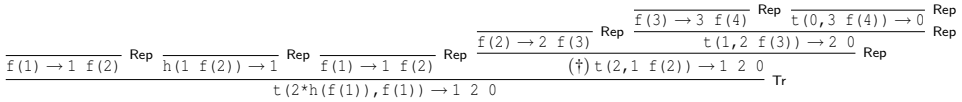

Fig. 4. Abbreviated proof tree for the proof tree in Figure 2

the same color. Hence the same term can be repeated in several places in a proof tree, but only those copies coming from the same original term will have the same color. We refer to colored terms as *c-terms* and to trees with colored terms in their nodes as *c-trees*. When talking about colored trees, $t_1 = t_2$ means that t_1 and t_2 are equally colored. Therefore talking about two occurrences of a c-term t implicitly means that there are two copies of the same term equally colored. Intuitively, all the terms in the lefthand side of the root have different colors; the replacement inference rule introduces new colors, while the reflexivity, transitivity, and congruence rules propagate them. More details can be found in [2].

3.3 The Lists Example Revisited

As explained in the previous section, the debugging tree in Figure 4 presents the drawback of containing nodes of the form `t(2,1 f(2)) → 1 2 0`, whose correction is difficult to state because the subterms must be mentally reduced by the user in order to compute the final result. We give in this section the intuitions motivating the transformations in the next section, transforming the trees and in Figures 2 and 3, that give rise to the proof trees in Figures 5 and 6. The tree $\overset{2}{\triangledown}$ in Figure 5 has the same left premise as the one in Figure 2, which shows the importance of coloring the terms in the proof trees, because the algorithm distinguishes between the two `f(1)` thanks to their different colors. The part of the tree depicted in Figure 5 shows how the reduction of the subterms is "anticipated" by the algorithm in the previous section and thus the node (♡) performs the reduction of `f(1)` to its normal form (with respect to the tree), and all the replacement steps that where needed to reach it are contained in this subtree. The tree $\overset{3}{\triangledown}$ in Figure 6 shows the other part of the transformations: we get rid of the relocated replacement inferences by using reflexivity steps.

The APT of our transformed proof tree is depicted in Figure 7. It has removed all the useless information like reflexivity and congruence inferences, and has associated the replacement inferences, that contain debugging information, to the transitivity inferences below them, returning a debugging tree where the lefthand side of all the

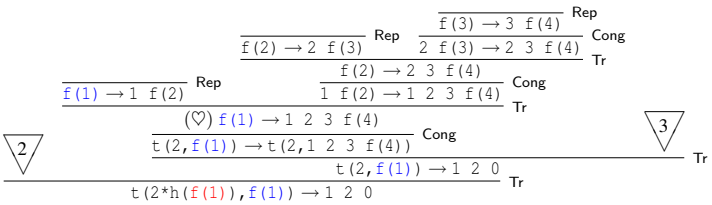

Fig. 5. Proof tree for the reduction on Section 3.1

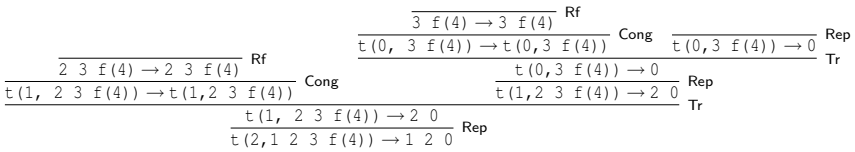

Fig. 6. Proof tree for the subtree $\overset{3}{\bigtriangledown}$ on Figure 5

reductions have their subterms in normal form, as expected because the transformation works driven by the *APT* transformation.

Since this transformation has been implemented in our declarative debugger, we can start a debugging session to find the error in the specification described in Section 3.1. The debugging process starts with the command:

```
Maude> (debug take(2 * head(from(1)), from(1)) -> 1 2 0 .)
```

This command builds the tree shown in Figure 7,[3] which is traversed following the navigation strategy divide and query [15], that selects in each case a node rooting a subtree with approximately half the size of the whole tree, and the first question, associated with the node (‡) in Figure 7, is:

```
Is this reduction (associated with the equation t1) correct?
take(2,1 2 3 ?:NatList) -> 1 2 0
Maude> (no .)
```

where we must interpret `?:NatList` as a term that has not reached a normal form (in the sense it is not built with operators with the `ctor` attribute) but whose value is irrelevant to compute the final result. The answer is `(no .)` because we expected to take only `1 2`. Note that this node is the transformed version of the node (†) in Figure 4, that would perform the question:

```
Is this reduction (associated with the equation t1) correct?
take(2,1 from(2)) -> 1 2 0
```

which is more difficult to answer because we have to think first about the reduction of `from(2)` and then use the result to reason about the complete reduction. With the answer given above the subtree rooted by (‡) in Figure 7 is considered as the current one and the next questions are:

[3] Actually, it builds the tree in Figure 4 and then transforms it into the tree in Figure 7.

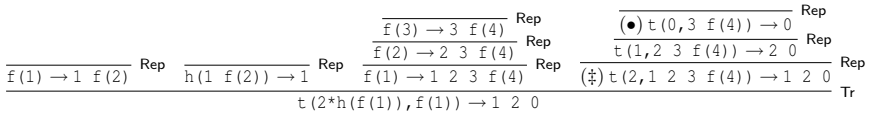

Fig. 7. Abbreviated proof tree for the transformed tree

```
Is this reduction (associated with the equation t1) correct?
take(1,2 3 ?:NatList) -> 2 0
Maude> (no .)
Is this reduction (associated with the equation t2) correct?
take(0,3 ?:NatList) -> 0
Maude> (no .)
```

We answer `(no .)` in both cases for the same reason as in the previous case. With these answers we have discovered that the node (•) is wrong. Hence, since it has no children, it is the buggy node and is associated with a wrong statement:

```
The buggy node is: take(0,3 ?:NatList) -> 0
with the associated equation: t2
```

In fact, the equation `t2` returns `0` but it should return `nil`.

4 Transforming Debugging Trees

In this section we present the transformation that ensures that the abbreviated proof tree contains every term reduced as much as possible. This transformation is a two-step process. First, a sequence of three tree transformations prepares the proof tree for the second phase. We call the trees obtained by this transformation *canonical trees*. The second phase takes a canonical tree as input and applies the algorithm that replaces terms by its most reduced forms. The result is a proof tree for the same computation whose APT verifies that every term is reduced as much as possible.

4.1 Reductions

We need to formally define the concepts of reduction and number of steps, which will be necessary to ensure that a tree is in its most reduced form.

Definition 1. *Let T be an APT, and t, t' two c-terms. We say that $t \to t'$ is a reduction w.r.t. T if there is a node $N \in T$ of the form $t_1 \to t_2$ verifying:*

- *$pos(t, t_1) \neq \emptyset$, where $pos(t, t_1)$ is the set of positions of t containing t_1.*
- *$t' = t[t_1 \mapsto t_2]$, where $t[t_1 \mapsto t_2]$ represents the replacement of every occurrence of the c-term t_1 by t_2 in t.*

In this case we also say that t is reducible (w.r.t. T). A reduction chain *for t will be a sequence of reductions $t_0 = t \to t_1 \to t_2 \to \cdots \to t_n$ s.t. each $t_i \to t_{i+1}$ is a reduction and that t_n cannot be further reduced w.r.t. T.*

Definition 2. *Let T be an APT. Then:*

- *The number of reductions of a term t w.r.t. T, denoted as $reduc(t,T)$ is the sum of the length of all the possible different reduction chains of t w.r.t. T.*
- *The number of reductions of a node of the form $N = f(t_1,\ldots,t_n) \rightarrow t$ w.r.t. T, denoted as $reduc(N,T)$ is defined as $(\sum_{i=1}^{n} reduc(t_i,T)) + reduc(t,T)$.*

In this definition the length of a reduction chain $t_0 \rightarrow \cdots \rightarrow t_n$ is defined as n. Remember that the aim of this paper is to present a technique to put together these reductions chains, transforming appropriately the proof tree, and using colors to distinguish terms; when dealing with commutative or associativity, we will assume flatten terms with the subterms ordered in an alphabetical fashion. Moreover, our technique assumes that there is only one normal form for each c-term in the tree.

Definition 3. *We say that an occurrence of a c-term t occurring in an APT T is in* normal form w.r.t. *T if there is no reduction for any c-subterm of t in T.*

Definition 4. *Let T be an APT. We say that T is* confluent *if every c-term t occurring in T has a unique normal form with respect to T.*

Note that this notion of confluence is different from the usual notion of confluence required in Maude functional modules: it requires all the copies of a (colored) term, that can be influenced by the `strat` attribute, to be reduced to the same term. In the rest of the paper we assume that, unless stated otherwise, all the APTs are colored and confluent. With these definitions we are ready to define the concept of *norm*:

Definition 5. *Let T be a proof tree, and $T' = APT(T)$. The* norm *of T, represented by $\| T \|$, is the sum of the lengths of all the reduction chains that can be applied to terms in T'. More formally, given the reduc function in Definition 2:*

$$\| T \| = \sum_{\substack{N \in T' \\ N \neq root(T')}} reduc(N,T')$$

Thus, the norm is the number of reductions that can be performed in the corresponding APT. Our goal is to obtain proof trees with associated norm 0, ensuring that the questions performed to the user contain terms as reduced as possible. This is the purpose of the proof tree transformations in the following section, which start with some initial proof tree and produces an equivalent proof tree with norm 0.

4.2 Canonical trees

Canonical trees are obtained from proof trees as explained in the following definition.

Definition 6. *We define the canonical form of a proof tree T, which will be denoted from now on as $Can(T)$, as*

$$Can(T) = RemInf(NTr(InsCong(T)))$$

where InsCong (insert congruences), NTr (normalize transitivities), and RemInf (remove superfluous inferences) are defined in Figures 8, 9, and 10, respectively.

($\mathbf{InsCong_1}$)

$$InsCong\left(\frac{T_1 \ldots T_m}{f(t_1,\ldots,t_n) \to t}\mathsf{Rep}\right) =$$

$$\frac{\dfrac{\dfrac{}{t_1 \to t_1}\mathsf{Rf} \;\ldots\; \dfrac{}{t_n \to t_n}\mathsf{Rf}}{f(t_1,\ldots,t_n) \to f(t_1,\ldots,t_n)}\mathsf{Cong} \quad \dfrac{InsCong(T_1)\ldots InsCong(T_m)}{f(t_1,\ldots,t_n) \to t}\mathsf{Rep}}{f(t_1,\ldots,t_n) \to t}\mathsf{Tr}$$

($\mathbf{InsCong_2}$)

$$InsCong\left(\frac{T_1 \ldots T_m}{aj}\mathsf{R}\right) = \frac{InsCong(T_1)\ldots InsCong(T_m)}{aj}\mathsf{R}$$

aj any judgment, R any inference rule, $n > 0$

Fig. 8. Insert Congruences (*InsCong*)

($\mathbf{NTr_1}$)

$$NTr\left(\frac{\dfrac{T_{t_1\to t_2} \quad T_{t_2\to t_3}}{t_1 \to t_3}\mathsf{Tr} \quad T_{t_3\to t_4}}{t_1 \to t_4}\mathsf{Tr}\right) = NTr\left(\frac{NTr(T_{t_1\to t_2}) \quad NTr\left(\dfrac{T_{t_2\to t_3} \quad T_{t_3\to t_4}}{t_2 \to t_4}\mathsf{Tr}\right)}{t_1 \to t_4}\mathsf{Tr}\right)$$

($\mathbf{NTr_2}$)

$$NTr\left(\frac{T_1 \ldots T_n}{aj}\mathsf{R}\right) = \frac{NTr(T_1)\ldots NTr(T_n)}{aj}\mathsf{R} \qquad aj \text{ any judgment, R any inference rule}$$

Fig. 9. Normalize Transitivities (*NTr*)

It is assumed that the rules of each transformation are applied top-down. The first transformation, *InsCong*, prepares the proof tree for allowing reductions on the arguments t_i of judgments of the form $f(t_1,\ldots,t_n) \to t$ by introducing congruence inferences before these judgments take place. Initially no reduction is applied, and each argument is simply reduced to itself using a reflexivity inference. Replacing these reflexivities by non-trivial reductions for the arguments is the role of the algorithm introduced in the next section. The next transformation, *NTr*, takes care of righthand sides. The idea is that transitivity inferences occurring as left premises of other transitivity are associated to intermediate, not fully-reduced computations. Thus, *NTr* ensures that righthand sides can be completely reduced by the algorithm in the next section. Finally, *RemInf* eliminates some superfluous steps involving reflexivities, and combines consecutive congruences in a "bigger step" single congruence, which avoids the production of unnecessary intermediate results in the proof tree. This last process is done with the help of an auxiliary transformation *merge* (Figure 11), that combines two trees by using a transitivity.

A proof tree in canonical form is also a proof tree proving the same judgment.

Proposition 1. *Let T be a proof tree. Then $Can(T)$ is a proof tree with the same root.*

Moreover, applying these transformations cannot produce an increase of the norm:

$$(\mathbf{RemInf_1}) \qquad \mathit{RemInf}\left(\dfrac{\dfrac{T_{t_1\to t'_1}\dots T_{t_n\to t'_n}}{f(t_1,\dots,t_n)\to f(t'_1,\dots,t'_n)}\mathsf{Cong} \qquad \dfrac{T_{t'_1\to t''_1}\dots T_{t'_n\to t''_n}}{f(t'_1,\dots,t'_n)\to f(t''_1,\dots,t''_n)}\mathsf{Cong}}{f(t_1,\dots,t_n)\to f(t''_1,\dots,t''_n)}\mathsf{Tr}\right) =$$

$$\dfrac{\mathit{RemInf}\left(\mathit{merge}\left(T_{t_1\to t'_1},\ T_{t'_1\to t''_1}\right)\right)\dots\mathit{RemInf}\left(\mathit{merge}\left(T_{t_n\to t'_n},\ T_{t'_n\to t''_n}\right)\right)}{f(t_1,\dots,t_n)\to f(t''_1,\dots,t''_n)}\mathsf{Cong}$$

$$(\mathbf{RemInf_2}) \qquad \mathit{RemInf}\left(\dfrac{\dfrac{T_{t_1\to t'_1}\dots T_{t_n\to t'_n}}{f(t_1,\dots,t_n)\to f(t'_1,\dots,t'_n)}\mathsf{Cong} \qquad \dfrac{\dfrac{T_{t'_1\to t''_1}\dots T_{t'_n\to t''_n}}{f(t'_1,\dots,t'_n)\to f(t''_1,\dots,t''_n)}\mathsf{Cong}\ T_{f(t''_1,\dots,t''_n)\to e}}{f(t'_1,\dots,t'_n)\to e}\mathsf{Tr}}{f(t_1,\dots,t_n)\to e}\mathsf{Tr}\right) =$$

$$\mathit{RemInf}\left(\dfrac{\dfrac{\mathit{merge}\left(T_{t_1\to t'_1},\ T_{t'_1\to t''_1}\right)\dots\mathit{merge}\left(T_{t_n\to t'_n},\ T_{t'_n\to t''_n}\right)}{f(t_1,\dots,t_n)\to f(t''_1,\dots,t''_n)}\mathsf{Cong} \qquad \mathit{RemInf}(T_{f(t''_1,\dots,t''_n)\to e})}{f(t_1,\dots,t_n)\to e}\mathsf{Tr}\right)$$

$$(\mathbf{RemInf_3}) \qquad \mathit{RemInf}\left(\dfrac{\dfrac{F}{t\to t_1}\mathsf{Cong} \qquad \dfrac{\dfrac{}{t_1\to t_1}\mathsf{Rf}\ T_{t_1\to t'}}{t_1\to t'}\mathsf{Tr}}{t\to t'}\mathsf{Tr}\right) = \mathit{RemInf}\left(\dfrac{\dfrac{F}{t\to t_1}\mathsf{Cong} \qquad T_{t_1\to t'}}{t\to t'}\mathsf{Tr}\right)$$

$$(\mathbf{RemInf_4}) \qquad \mathit{RemInf}\left(\dfrac{T\ \mathsf{Rf}\quad T'}{aj}\mathsf{Tr}\right) = \mathit{RemInf}\left(\dfrac{T'\quad T\ \mathsf{Rf}}{aj}\mathsf{Tr}\right) = \mathit{RemInf}(T'),\ aj \text{ any judgment}$$

$$(\mathbf{RemInf_5}) \qquad \mathit{RemInf}\left(\dfrac{T_1\dots T_n}{aj}\mathsf{R}\right) = \dfrac{\mathit{RemInf}(T_1)\dots\mathit{RemInf}(T_n)}{aj}\mathsf{R},\ aj \text{ any judgment, } \mathsf{R} \text{ any inference rule}$$

Fig. 10. Remove superfluous inferences (*RemInf*)

$$(\mathbf{Merge_1})$$
$$merge\left(\frac{T_{t\to t_1}\ \ T_{t_1\to t'}}{t\to t'}\mathsf{Tr}, T_{t'\to t''}\right) = \frac{T_{t\to t_1}\ \ merge\,(T_{t_1\to t'}, T_{t'\to t''})}{t\to t''}\mathsf{Tr}$$
$$(\mathbf{Merge_2})$$
$$merge\,(T_{t\to t'}, T_{t'\to t''}) = \frac{T_{t\to t'}\ \ T_{t'\to t''}}{t\to t''}\mathsf{Tr}$$

Fig. 11. Merge Trees

Proposition 2. *Let T be proof tree and $T' = Can(T)$. Then $\| T \| \geq \| T' \|$.*

4.3 Reducing the norm of canonical trees

We describe in this section the main transformation applied to the proof trees. This transformation relies on the following proposition, that declares that in any proof tree in canonical form there exist (1) a node with a reduction $t_1 \to t_1'$ such that t_1' is in normal form, that will be used to further reduce the terms, (2) a node that contains a reduction $t_2 \to t_2'$, with $t_1 \in t_2'$ (t_1 is a subterm of t_2'), which means that t_2' can be further reduced by the previous reduction, and (3) a node such that it is not affected by the transformations in the previous nodes. We will use node (1) to improve the reductions in node (2); this transformation will only affect the nodes in the subtree that has (3) as root:

Proposition 3. *Let T be a confluent c-proof tree in canonical form such that $\| T \| > 0$. Then T contains:*

1. *A node related to a judgment $t_1 \to t_1'$ such that:*
   - *It is either the consequence of a transitivity inference with a replacement as left premise, or the consequence of a replacement inference which is not the left premise of a transitivity.*
   - *t_1' is in normal form w.r.t. T.*
2. *A node related to a judgment $t_2 \to t_2'$ with $t_1 \in t_2'$.*
3. *A node related to a judgment $t_3 \to t_3'$ consequence of a transitivity step, with $t_1 \notin t_3'$.*

Algorithm 1 presents the transformation in charge of reducing the norm of the proof trees until it reaches 0. It first selects a node N_{ible} (from *reducible node*), that contains a term that has been further reduced during the computation,[4] a node N_{er} (from *reducer node*) that contains the reduction needed by the terms in N_{ible}, and a node p_0 limiting the range of the transformation. Note that we can distinguish two parts in the subtree rooted by the node in p_0, the left premise, where N_{ible} is located, and the right premise, where N_{er} is located. Then, we create some copies of these nodes in order to use them after the transformations. For example, the first step of the loop for the proof tree in Figures 2 and 3 would set N_{ible} to `f(2)` $\to$ `2 f(3)` and N_{er} to `f(3)` $\to$ `3 f(4)`; they are located in the subtree rooted by p_0, the node ($\diamondsuit$).

[4] We select the first one in post-order to ensure that this node is the one that generated the term.

Step 6 replaces the proof of the reduction $t_1 \rightarrow t_1'$ by reflexivity steps $t_1' \rightarrow t_1'$. Since the algorithm is trying to use this reduction before its current position, a natural consequence will be to transform all the appearances of t_1 in the path between the old and the new position by t_1', what means that in this particular place we would obtain the reduction $t_1' \rightarrow t_1'$ inferred, by Proposition 3, by either a transitivity or a replacement rule, and with the appropriate proof trees as children. Since this would be clearly incorrect, the whole tree is replaced by a reflexivity. In our example, the replacement `f(3)` $\rightarrow$ `3 f(4)` (N_{er}) would be transformed into the reflexivity step `3 f(4)` $\rightarrow$ `3 f(4)`.

Step 7 replaces all the occurrences of t_1 by t_1' in the right premise of p_0, as explained in the previous step. In this way, the right premise of p_0 is a new subtree where t_1 has been replaced by t_1' and all the proofs related to $t_1 \rightarrow t_1'$ have been replaced by reflexivity steps $t_1' \rightarrow t_1'$. Note that intuitively these steps are correct because t_1' is required to be in normal form, the tree is confluent, and the norm of this tree is 0, that is, all the possible reductions of terms with the same color have been previously modified by the algorithm to create a $t_1 \rightarrow t_1'$ proof. In our example, the appearances of `f(3)` in the right premise of the node ($\diamondsuit$) are replaced by `3 f(4)`; this subtree is already a proof tree.

Step 8 replaces the occurrences of t_1 by t_1' in the left premise of p_0. We apply this transformation only in the righthand sides because they are in charge of transmitting the information, and in this way we prevent the algorithm from changing correct values (inherited perhaps from the root). This substitution can be used thanks to the position p_0, which ensures that only the righthand sides are affected. In our example, we substitute the term `f(3)` by `3 f(4)` in the left child of ($\diamondsuit$).

Step 9 combines the reduction in N_{ible} with the reduction in N_{er} (actually, it merges their copies, since the previous transformations have modified them). If the term t_1 we are further reducing corresponds to the term t_2' in the lefthand side of the judgment in N_{ible}, then it is enough to use a transitivity to "join" the two subtrees. In other case, the term we are reducing is a subterm of t_2' and thus we must use a congruence inference rule to reduce it, using again a transitivity step to infer the new judgment. This last step would generate, in our example, a node combining the replacement ($\spadesuit$) and the one in N_{er} in a transitivity step, giving rise to the node `f(2)` $\rightarrow$ `2 3 f(4)`; in this way the left child of ($\diamondsuit$), and consequently the tree, becomes a proof tree again.

Finally, these transformations make the trees to lose their canonical form, and hence the canonical form of the tree is computed again in step 10.

Algorithm 1 *Let T be a proof tree in canonical form.*

1. *Let $T_r = T$*
2. *Loop while $\| T_r \| > 0$*
3. *Let $N_{er} = t_1 \rightarrow t_1'$ be a node satisfying the conditions of item 1 in Proposition 3, $N_{ible} = t_2 \rightarrow t_2'$ the first node in T's post-order verifying the conditions of item 2 in Proposition 3, and p_0 the position of the subtree of T rooted by the first (furthest from the root) ancestor of N_{ible} satisfying item 3 in Proposition 3, such that the right premise of the node in p_0, T_{rp}, has $\| T_{rp} \| = 0$.*
4. *Let C_{er} be a copy of the tree rooted by N_{er}.*
5. *Let C_{ible} be a copy of the tree rooted by N_{ible} and p_{ible} the position of N_{ible}.*
6. *Let T_1 be the result of replacing in T all the subtrees rooted by N_{er} by a reflexivity inference step with conclusion $t_1' \rightarrow t_1'$.*

7. *Let T_2 be the result of substituting all the occurrences of the c-term t_1 by t_1' in the right premise of the subtree at position p_0 in T_1.*
8. *Let T_3 be the result of substituting all the occurrences of the c-term t_1 with t_1' in the righthand sides of the left premise of the subtree at position p_0 in T_2.*
9. *Let T_4 be the result of replacing the subtree at position p_{ible} in T_3 by the following subtree:*
   (a) if $t_2' = t_1$.

$$\frac{C_{ible} \quad C_{er}}{t_2 \rightarrow t_1'}\ \mathsf{Tr}$$

   (b) if $t_2' \neq t_1$.

$$\frac{C_{ible} \quad \dfrac{C_{er}}{t_2' \rightarrow t_2'[t_1 \mapsto t_1']}\ \mathsf{Cong}}{t_2 \rightarrow t_2'[t_1 \mapsto t_1']}\ \mathsf{Tr}$$

10. *Let T_r be the result of normalizing T_4.*
11. *End Loop*

The next theorem is the main result of this paper. It states that after applying the algorithm we obtain a proof tree for the same computation whose nodes are as reduced as possible. Thus, the declarative debugging tool that uses this tree as debugging tree will ask questions in its most simplified form.

Theorem 1. *Let T be a proof tree in canonical form. Then the result of applying Algorithm 1 to T is a proof tree T_r such that $root(T_r) = root(T)$ and $\| T_r \| = 0$.*

Observe that we have improved the "quality" of the information in the nodes without increasing the number of questions, since the transformations do not introduce new replacement inferences in the APT.

5 Concluding Remarks and Ongoing Work

One of the main criticisms to declarative debugging is the high complexity of the questions performed to the user. Thus, if the same computation can be represented by different debugging trees, we must choose the tree containing the simplest questions. In Maude, an improvement in this direction is to ensure that the judgments involving reductions are presented to the user with the terms reduced as much as possible. We have presented a transformation that allows us to produce debugging trees fulfilling this property starting with any valid proof tree for a wrong computation. The result is a debugging tree with questions as simple as possible without increasing the number of questions, which is specially useful when dealing with the `strat` attribute. Moreover, the theoretical results supporting the debugging technique presented in previous papers remain valid since we have proved that our transformation transforms proof trees into proof trees for the same computation.

Although for the sake of simplicity we have focused in this paper on the equational part of Maude, this transformation has been applied to all the judgments $t \rightarrow t'$ appearing in the debugging of both wrong (including system modules) and missing answers.

However, our calculus for missing answers also considers judgments $t \rightarrow_{norm} t'$, indicating that t' is the normal form of t; when facing the `strat` attribute, the inferences for these judgments have the same problem shown here; we are currently working to define a transformation for this kind of judgment.

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Automatic Synthesis of Specifications for Curry Programs*
– Extended Abstract –

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Abstract This extended abstract presents a technique to automatically infer specifications from Curry programs. Program specifications (in particular, automatically derived specifications) have been used for program verification, understanding, documentation, service discovering or testing. Our technique, statically infers from the source code of a Curry program a specification which consists of a set of semantic properties that the program operations satisfy. These properties are given by means of equations relating (nested) operation calls that have the same behavior. Our method relies on the semantics of [1] for achieving, to some extent, the correctness of the inferred specification, as opposed to other similar tools based on testing.
In this paper, we present the main ideas of the approach emphasizing the difficulties addressed for the case of the Curry language.

1 Introduction

Specifications have been widely used for several purposes: they can be used to aid (formal) verification, as summaries in program understanding, as documentation of programs, to discover services in a network context, or to guide the testing process [2,3,4,5,6,7,8]. It is possible to define specifications before or during the program coding. We are interested in the (automatic) inference of high-level specifications from an executable or the source code of a system, which has been shown very helpful in the literature [2,4,5,9]. More specifically, by high-level specification we mean a *property-based* specification in contrast to a *functional* specification. In other words, our specification does not represent the functionality of the program (the output of the system), but the relation among the operations that can be invoked in the program (i.e., the pairs of calls that have the same behaviour when executed).

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We can identify two main approaches for the inference of specifications. The glass-box approach [2,4] assumes that the source code of the program, or at least some kind of low-level specification, is available. In this context, the goal of inferring a specification is mainly applied to document the code, or to understand it [4]. Therefore, the specification must be more succinct and comprehensible than the source code itself. The inferred specification can also be used to automatize the testing process of the program [4] or to verify that a given property holds [2]. The black-box approach [5,9] can only work with the executable. This means that the only information used during the inference process is the input-output behavior of the program. In this setting, the inferred specification is often used to discover the functionality of the system (or services in a network) [9].

The task of automatically inferring program specifications has shown to be very complex. There exists a large number of different proposals and, due to the complexity of the problem, it becomes natural to impose some restrictions on the general case. Many aspects vary from one solution to another: the restriction of the considered programming language (for glass-box approaches), the kind of specifications that are computed (functional specifications vs. property-based specifications), the kind of programs considered, etc. Although black-box approaches work without any restriction on the considered language—which is rarely the case in a glass-box approach—in general they cannot *guarantee* the correctness of the results (which indeed glass-box can).

For this work, we took inspiration from QuickSpec [4], a black-box approach defined to infer specifications from Haskell programs. However there are significant differences between our approach and QuickSpec. First we propose a glass-box semantic-based approach, since our aim is to infer *correct* algebraic specifications. Moreover, we consider the language Curry, which introduces some extra difficulties w.r.t. Haskell. Curry is a multi-paradigm programming language that combines functional and logic programming. Because of all this very high-level features, the problem of inferring specifications for this kind of languages poses several additional problems w.r.t. other paradigms. We discuss these issues in Section 2.

In the rest of the paper, we present some basic notions that we have used in order to get, hopefully, interesting and useful specifications for the functional-logic setting. The core of our inference method is based on the use of a compact bottom-up semantics for the first order fragment of Curry proposed by [1].

2 Specifications for Functional-logic Languages

A language is said to be referentially transparent if for all of its expressions and contexts, if the semantics of a pair of expressions e and e' coincides, then it also coincides when used within any context $C[\cdot]$ (written $[\![C[e]]\!] = [\![C[e']]\!]$). In a pure functional setting, this property holds by language definition. The language Curry is not referentially transparent w.r.t. its operational behavior: a term can produce different computed values when it is embedded in a context that binds its free variables (see Example 2). However, the semantics introduced in [1] fulfills

referential transparency for Curry, and our approach exploits this feature. Let us show the main issues when considering a functional-logic language by means of an illustrative example.

Example 1 (The Queue example). Assume we have an implementation of a two-sided queue where it is possible to insert or delete elements on both left and right sides[3]:

```
data Queue a = Q [a] [a]
new = Q [] []
null (Q [] []) = True
null (Q (_:_) _) = False
null (Q [] (_:_)) = False
inl x (Q xs ys) = Q (x:xs) ys
inr x (Q xs ys) = Q xs (x:ys)
outl (Q [] ys) = Q (tail (reverse ys)) []
outl (Q (_:xs) ys) = Q xs ys
outr (Q xs []) = Q [] (tail (reverse xs))
outr (Q xs (_:ys)) = Q xs ys
```

Intuitively, for this program one expects a specification with properties like

```
null new = True
inl y (inr x q) = inr x (inl y q)
outr (inr q) = outl (inl q)
null (inl x q) = False
outl (inl x q) = q
```

These equations can be read as *all possible outcomes for the term on the left hand side of the equation are also outcomes for the term on the right hand side*, and vice versa. All previous equations are valid in this sense.

One could *additionally* ask that the outcomes should be equal also when the two terms are embedded within any context. However, only the first three equation holds in this sense for the program above. In fact, the rest of equations are not valid since the computed answers over `q` do not coincide. This is different from the pure functional case where equations are interpreted as properties that hold for any *ground* instance of the variables occurring in the equation.

This notion of equivalence poses a very restrictive condition. Therefore, we also use another notion of equivalence that allows to compute equations that hold for any non variable instantiation of the variables. In this way, the following equations, variants of the previous ones, now hold.[4]

```
null (inl x q:nonvar) = False
outl (inl x q:nonvar) = q:nonvar
```

[3] `tail` and `reverse` are language predefined functions.
[4] The label `:nonvar` states that the the associated variable is not a free variable.

3 What is a specification?

In this section, we present the kinds of term equivalence notions that are used to compute equations of the specification. We first introduce some basic notions that are used throughout the paper. For a complete description of the Curry language, the interested reader can consult [10].

We say that a program is composed by a signature Σ and a set of rules $\mathcal{R}$. $\mathcal{V}$ denotes a (fixed) countably infinite set of variables and $\mathcal{T}(\Sigma, \mathcal{V})$ denotes the terms built over signature Σ and variables $\mathcal{V}$. $t_1, \ldots, t_n$ are terms in $\mathcal{T}(\Sigma, \mathcal{V})$. A *fresh* variable is a variable that appears nowhere else. We evaluate Curry programs on the collecting, goal-independent semantics recently defined in [1,11] for functional logic programs. Given a term $t \in \mathcal{T}(\Sigma, \mathcal{V})$ and an interpretation $\mathcal{I}$, the evaluation of t w.r.t. $\mathcal{I}$ is denoted by $\mathcal{E}[\![t]\!]_{\mathcal{I}}$. Given a program $\mathcal{R}$, the semantics $\mathcal{F}[\![\mathcal{R}]\!]$ for $\mathcal{R}$ is the least fixed-point of the immediate consequences operator $\mathcal{P}[\![\mathcal{R}]\!]$. Intuitively, the evaluation $\mathcal{E}[\![t]\!]_{\mathcal{F}[\![\mathcal{R}]\!]}$ of a term t computes a tree-like structure which collects the "relevant history" of the computation of all computed solutions of t, abstracting from function calls and focusing only on the way in which the solution evolves. Thus, every leaf of the tree represents a normal form of the initial term.

In our setting, the computed (algebraic) specification (called $\mathcal{S}$) consists of a set of equations that state properties among operations of the program. Equations are of the form $t_1 =_K t_2$ with $K \in \{C, CA, CBI, G\}$ and $t_1, t_2 \in \mathcal{T}(\Sigma, \mathcal{V})$. K distinguish the kinds of equations that we handle. We denote the domain of equations as $\mathcal{Q}$, thus $\mathcal{S} \in \wp(\mathcal{Q})$. Moreover, variables appearing in a term t_i can be *normal* variables (in the set $\mathcal{V}_n$), or variables representing instantiated values (in the set $\mathcal{V}_{nv}$), thus $\mathcal{V} = \mathcal{V}_n \cup \mathcal{V}_{nv}$.

Now we are ready to present the four equivalence relations among terms:

Congruence Equivalence $=_C$. States that two terms t_1 and t_2 are equivalent if they have the same behavior and for any context $C[\cdot]$, $C[t_1] =_C C[t_2]$ still holds. It is the most difficult equivalence to be established by looking at the operational semantics. However, by using the semantics recently defined in [1,11] for functional logic programs (which is correct and fully abstract w.r.t. the program behavior) it becomes easy to establish congruence equivalence. Two terms t_1 and t_2 are related by the congruence relation $=_C$ if their semantics coincide, formally $t_1 =_C t_2$ iff $\mathcal{E}[\![t_1]\!]_{\mathcal{F}[\![\mathcal{R}]\!]} = \mathcal{E}[\![t_2]\!]_{\mathcal{F}[\![\mathcal{R}]\!]}$[5].
Intuitively, this means that all the way in which these two terms reach their normal forms coincide. This is the key point in order to state the closedness under contexts.

Computed-solution equivalence $=_{CS}$. This equivalence states that two terms are equivalent when the outcomes of their evaluation are the same.
The $=_{CS}$ equivalence is coarser than $=_C$ ($=_C \subseteq =_{CS}$) as shown by the following example.

[5] Note that $=_C$ does not capture termination properties, which is out of our scope.

Example 2. Given a program `f (C x) B = B`, `g' A = C A`, `g x = C (h x)`, and `h A = A`, it is easy to note that the computed solutions for `g x` and `g' x` are the same. Consider now the context $C[\cdot] := f[\cdot]\ x$. We see that `f (g' x) x` has no solutions while `f (g x) x` has one, namely $\{x/B\} \cdot B$.

Constructor Based Instances Equivalence $=_{CBI}$. It states that two terms are equivalent if for all possible instances of the terms with constructor terms $\mathcal{T}(\mathcal{C}, \mathcal{V})$ the same values are computed (with empty substitution). This equivalence is coarser than the former.

Ground Equivalence $=_{G}$. This equivalence states that two terms are equivalent if for all possible ground instances we have the same values. Also this equivalence is coarser than the former.

The last equivalence is the easier equivalence to be established. It is the only possible notion in the pure functional paradigm. This fact allows one to have an intuition of the reason why the problem of specification synthesis is more complex in the functional logic paradigm. To summarize, we have $=_{C} \subseteq =_{CS} \subseteq =_{CBI} \subseteq =_{G}$.

4 Deriving Specifications from Programs

In this section, we describe the process of inferring specifications. The pseudocode in Algorithm 1 shows the main steps of the process. The input of the process consists of the Curry program to be analyzed and two additional parameters: a *relevant* API and a maximum term size. The *relevant* API, called Σ^r, allows the user to choose the operations in the program that will be present in the inferred specification, whereas the maximum term size limits the depth (hence the complexity) of the terms in the specification. As a consequence, these two parameters tune the granularity of the specification, allowing the user to keep the specification concise and easy to understand. The output consists of a set of equations represented by equivalence classes of terms belonging to $\mathcal{T}(\Sigma^r, \mathcal{V})$. Note that inferred equations may differ for the same program depending on the considered API and on the maximum term size.

The process consists of two main steps. First, a partition of terms of size less or equal to the provided maximum size is computed. The equivalence classes of the partition contain equivalent terms w.r.t. the congruence equivalence defined in Section 3. Once the partition is created, the set of equations is generated.

The first step of the algorithm is to compute the (abstract) semantics of the program. The semantics of a program is in general infinite, therefore something has to be done in order to have a terminating method. Following the approximation of [11,1], we use abstract interpretation [12] in order to achieve finiteness by giving up precision of the results. We discuss this issue at the end of the section. Let us now explain more in detail how terms are generated, and how equivalence classes are defined. We first explain the generation of the first partition, based

[6] $|ec|$ denotes the number of terms in the equivalence class.

Algorithm 1 Inference of an algebraic specification

Require: Program : $\mathcal{R}$, Program *relevant* API : Σ^r, Maximum term size : *maxSize*
  Compute $\mathcal{F}[\![\mathcal{R}]\!]$: the (abstract) semantics of $\mathcal{R}$
  $size = 0$; $part = initial\_part()$;
  while $size \leq maxSize$ **do**
    $part' = part$
    for all $f/n \in \Sigma^r$ **do**
      for all $t_1, \ldots t_n \in part$ **do**
        $t = f(t_1, \ldots, t_n)$
        Compute $\mathcal{E}[\![t]\!]_{\mathcal{F}[\![\mathcal{R}]\!]}$: the (abstract) semantics of term t
        $add\_to\_partition(t, \mathcal{E}[\![t]\!]_{\mathcal{F}[\![\mathcal{R}]\!]}, part')$
      end for
    end for
    $size = size + 1$; $part = part'$
  end while
  $specification = \emptyset$
  for all $kind \in \{C, CS, CBI, G\}$ **do**
    for all $ec \in part$ s.t. $|ec| > 1$[6] **do**
      Compute equations of ec and add them to *specification*; $part = part \setminus \{ec\}$
    end for
    $part = transform\_semantics(kind, part)$
  end for
  return *specification*

on the congruence relation. This is the basis for the generation of terms, and also for the definition of the other kinds of equivalence classes. A partition P consists of a set of equivalence classes EC, and each equivalence class is formed by

- the semantics of the terms in that class,
- the *representative term* of the class, which is defined as the smallest term in the class (by using the function *size*), and
- the set of terms belonging to that equivalence class.

Generation of congruence classes. The first step is to generate the initial partition which contains one equivalence class for a (logical) variable. Then we iteratively select all symbols f, of arity n, of the relevant API and n representative terms $t_1, \ldots, t_n$ from the current partition. We build term $t = f(t_1, \ldots, t_n)$, compute the semantics $s = \mathcal{E}[\![t]\!]_{\mathcal{F}[\![\mathcal{R}]\!]}$ and update the current partition P with $add\_to\_partition(t, s, P)$. The $add\_to\_partition(t, s, P)$ function looks for an equivalence class ec in P whose semantics coincides with s. Then, the term t is added to the set of terms in ec. If no equivalence class is found with that semantics s, then a new one is created.

Generation of congruence equations. Once the partition has been computed, we define the equations between terms of a partition. We can just take each con-

gruence class with more than one element, and define equations for all possible pairs of terms in the class. [7]

Generation of computed solution equations. From the semantics of a term (which models its congruence behavior) it is possible to construct (by losing some internal structure) a semantics modeling its computed solution behavior: we transform all the semantics of the congruence classes to its "computed solutions version". Some of the congruence classes which had a different semantics may now collapse into the same class. The reclassification w.r.t. this semantics creates the (coarser) partition which is used to produce computed solution equations. This is performed by the *transform_semantics* function.

To make the specification concise, before the transformation of the semantics, we replace all sets of terms of all congruence class with its representative term. Thanks to this we do not include in the specification the less precise versions of an equation if a more restrictive one holds. For example, if $t_1 =_C t_2$ holds, then $t_1 =_{\{CA,CBI,G\}} t_2$ are not present in the specification.

From the coarser partition we generate new equations analogously to the previous case.

Generation of other equivalence equations. The same strategy is used to generate the other two kinds of equations. Intuitively, the semantics are transformed by removing further internal structure to compute the constructor-based and ground versions. Since these relations are less precise than the previous ones, again classes may collapse and new equations (w.r.t. a different equivalence notion) are generated.

Effectivity/Efficiency considerations. In a semantic-based approach, one of the main problems to be tackled is effectiveness. The semantics of a program is in general infinite and thus we use abstract interpretation [12] in order to have a terminating method, similarly to [11,1].

Due to the loss of precision given by the abstraction, our method may compute a specification that include both, correct (concrete) equations, and approximated equations. We call these approximated equations *maybe equations*, following the idea of the interpretation of equations in the testing-based approach. In other words, these equations are not *correct* equations, but equations that *have not been falsified up to that point.*

It is important to reach a compromise between efficiency of the computation and accuracy of the specifications. A "fast" domain typical of program analysis may produce very inaccurate specifications. Thus, as our first effort, we are using the (much concrete) $depth(k)$ abstraction defined in [11].

[7] Note that this is the strategy implemented in the current version. However, this may introduce some redundancy between equations coming from different equivalence classes. As future work, we plan to use a more elaborated method to generate the equations in order to avoid that redundancy. We recall that much redundancy is nevertheless avoided when computing the partition thanks to the use of the congruence relation.

The main advantage of this choice w.r.t. the testing-based approaches is the fact that we are able to distinguish when an equation *certainly* holds, and when a *maybe equation* just *can* hold. In the case of the *depth*(k) abstraction, the presence of cut variables in the semantics of an equivalence class means that any equation generated from it will be a maybe equation.

5 The prototype in practice

We have implemented the basic functionality of this approach in a prototype written in Haskell. For the example shown in Section 2, an extract of the computed specification is the following one:

```
null new =C True
new =C outl (inl x new)
new =C outr (inr x new)
q : nonvar =CS outl (inl x q : nonvar)
q : nonvar =CS outr (inr x q : nonvar)
inl y (inr x new) =C inr x (inl y new)
inl y (inr x q) =CS inr x (inl y q)
null (inl x new) =C null (inr x new)
null (inr x q : nonvar) =C null (inl x q : nonvar)
```

We see that `new` always computes a queue which, when applied to the operator `null` is true. One can also see (fourth line) that if we do `outl` after an `inl`, nothing changes (in the sense that the same queue `q` is obtained). In the sixth line, we see that, the order in which `inl` and `inr` are called does not affect the result, etc.

6 Related Work

Regarding related work, QuickSpec [4] computes an algebraic specification by means of (almost black-box) testing. Its inferred specifications are complete up to a certain depth of the analyzed terms because of its exhaustiveness. However, the specification may be incorrect due to the use of testing for the equation generation. Instead, we follow a (glass-box) semantic-based approach that allows us to compute specifications as complete as those of QuickSpec, but with correctness guarantees (depending on the abstraction). In the functional-logic setting, EasyCheck [13] is a testing tool in which specifications are used as the input for the testing process. It is not a tool to automatically deduce specifications. Properties are given as input, and EasyCheck executes ground tests in order to check whether the property holds.

7 Ongoing and Future Work

This extended abstract presents a method to automatically infer high-level, property-based (algebraic) specifications in a functional-logic setting. A concise

specification is obtained from the source code of the program. The specification represents relations that hold between operations in the program. Our main goal is to get a concise and clear specification of program properties that is useful for the programmer in order to detect possible errors, or to check that the program corresponds to the intended behavior.

The approach relies on the computation of the semantics. Therefore, to achieve effectiveness and good performance results, we use a suitable abstract semantics instead of the concrete one. This means that we may lose correctness of the equations in the specification, but we can also have correct equations thanks to a good compromise between abstraction and efficiency. We can use the computed specification for testing or verification purposes. For verification, correct equations can be the basis for the check, whereas maybe equations can be used in combination with some formal verification technique.

We have developed a prototype that implements the basic functionality of the approach. We are working on the inclusion of all the functionality described in this extended abstract, in particular to use the abstract semantics instead of the concrete one. As future (ongoing) work, we will improve the implementation in order to evaluate the quality of the generated specifications by means of several examples (mainly using the abstract semantics). The current results are promising, but we need to extensively analyze the tool for other cases. We also plan to add another notion of equivalence class. More specifically, when dealing with a user-defined data type, the user may have defined a specific notion of equivalence by means of an "equality" function. In this context, some interesting equations could show up. For instance, in the Queue example, a possible equality may identify queues which contain the same elements. Then, we would have the equation `inl x new = inr x new`. Note that, although the internal structure of the queue differs, the content coincides.

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A Declarative Embedding of XQuery in a Functional-Logic Language *

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Abstract. This paper addresses the problem of integrating a fragment of XQuery, a language for querying XML documents, into the functional-logic language $\mathcal{TOY}$. The queries are evaluated by an interpreter, and the declarative nature of the proposal allows us to prove correctness and completeness with respect to the semantics of the subset of XQuery considered. The different fragments of XML that can be produced by XQuery expressions are obtained using the non-deterministic features of functional-logic languages. As an application of this proposal we show how the typical *generate and test* techniques of logic languages can be used for generating test-cases for XQuery expressions.

1 Introduction

XQuery has been defined as a query language for finding and extracting information from XML [15] documents. Originally designed to meet the challenges of large-scale electronic publishing, XML also plays an important role in the exchange of a wide variety of data on the Web and elsewhere. For this reason many modern languages include libraries or encodings of XQuery, including logic programming [1] and functional programming [6]. In this paper we consider the introduction of a simple subset of XQuery [18, 20] into the functional-logic language $\mathcal{TOY}$ [11].

One of the key aspects of declarative languages is the emphasis they pose on the logic semantics underpinning declarative computations. This is important for reasoning about computations, proving properties of the programs or applying declarative techniques such as abstract interpretation, partial evaluation or algorithmic debugging [14]. There are two different declarative alternatives that can be chosen for incorporating XML into a (declarative) language:

1. Use a domain-specific language and take advantage of the specific features of the host language. This is the approach taken in [9], where a rule-based

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language for processing semi-structured data that is implemented and embedded into the functional-logic language Curry, and also in [13] for the case of logic programming.
2. Consider an existing query language such as XQuery, and embed a fragment of the language in the host language, in this case $\mathcal{TOY}$. This is the approach considered in this paper.

Thus, our goal is to include XQuery using the purely declarative features of the host languages. This allows us to prove that the semantics of the fragment of XQuery has been correctly included in $\mathcal{TOY}$. To the best of our knowledge, it is the first time a fragment of XQuery has been encoded in a functional-logic language. A first step in this direction was proposed in [5], where XPath [16] expressions were introduced in $\mathcal{TOY}$. XPath is a subset of XQuery that allows navigating and returning fragments of documents in a similar way as the path expressions used in the *chdir* command of many operating systems. The contributions of this paper with respect to [5] are:
- The setting has been extended to deal with a simple fragment of XQuery, including *for* statements for traversing XML sequences, *if/where* conditions, and the possibility of returning XML elements as results. Some basic XQuery constructions such as *let* statements are not considered, but we think that the proposal is powerful enough for representing many interesting queries.
- The soundness of the approach is formally proved, checking that the semantics of the fragment of XQuery is correctly represented in $\mathcal{TOY}$.

Next section introduces the fragment of XQuery considered and a suitable operational semantics for evaluating queries. The language $\mathcal{TOY}$ and its semantics are presented in Section 3. Section 4 includes the interpreter that performs the evaluation of simple XQuery expressions in $\mathcal{TOY}$. The theoretical results establishing the soundness of the approach with respect to the operational semantics of Section 2 are presented in Section 4.1. Section 5 explains the automatic generation of test cases for simple XQuery expressions. Finally, Section 6 concludes summarizing the results and proposing future work.

An extended version of the paper including proofs of the theoretical results can be found at [2].

2 XQuery and its Operational Semantics

XQuery allows the user to query several documents, applying join conditions, generating new XML fragments, and using many other features [18, 20]. The syntax and semantics of the language are quite complex [19], and thus only a small subset of the language is usually considered. The next subsection introduces the fragment of XQuery considered in this paper.

2.1 The subset SXQ

In [4] a declarative subset of XQuery, called XQ, is presented. This subset is a core language for XQuery expressions consisting of *for*, *let* and *where/if* statements.

$$
\begin{aligned}
query ::= {} & ( ) \mid query\ query \mid tag \\
& \mid doc(File) \mid doc(File)/axis :: \nu \mid var \mid var/axis :: \nu \\
& \mid \texttt{for}\ var\ \texttt{in}\ query\ \texttt{return}\ query \\
& \mid \texttt{if}\ cond\ \texttt{then}\ query \\
cond ::= {} & var{=}var \mid query \\
tag ::= {} & \langle a \rangle\ var \ldots var\ \langle /a \rangle \mid \langle a \rangle\ tag\ \langle /a \rangle
\end{aligned}
$$

Fig. 1. Syntax of SXQ, a simplified version of XQ

In this paper we consider a simplified version of XQ which we call SXQ and whose syntax can be found in Figure 1. where *axis* can be one of *child*, *self*, *descendant* or *dos* (i.e. descendant or self), and ν is a node test. The differences of SXQ with respect to XQ are:

1. XQ includes the possibility of using variables as tag names using a constructor *lab(\$x)*.
2. XQ permits enclosing any query Q between tag labels $\langle a \rangle Q \langle /a \rangle$. SXQ only admits either variables or other tags inside a tag.

Our setting can be easily extended to support the *lab(\$x)* feature, but we omit this case for the sake of simplicity in this presentation. The second restriction is more severe: although *let*s are not part of XQ, they could be simulated using *for* statements inside tags. In our case, forbidding other queries different from variables inside tag structures imply that our core language cannot represent *let* expressions. This limitation is due to the non-deterministic essence of our embedding, since a *let* expression means collecting all the results of a query instead of producing them separately using non-determinism. In spite of these limitations, the language SXQ is still useful for solving many common queries as the following example shows.

Example 1. Consider an XML file *"bib.xml"* containing data about books, and another file *"reviews.xml"* containing reviews for some of these books (see [17], sample data 1.1.2 and 1.1.4 to check the structure of these documents and an example). Then we can list the reviews corresponding to books in *"bib.xml"* as follows:

```
for $b in doc("bib.xml")/bib/book,
    $r in doc("reviews.xml")/reviews/entry
where $b/title = $r/title
for $booktitle in $r/title,
    $revtext in $r/review
return <rev> $booktitle  $revtext </rev>
```

The variable $\$b$ takes the value of the different books, and $\$r$ the different reviews. The *where* condition ensures that only reviews corresponding to the book are considered. Finally, the last two variables are only employed to obtain

the book title and the text of the review, the two values that are returned as output of the query by the *return* statement.

It can be argued that the code of this example does not follow the syntax of Figure 1. While this is true, it is very easy to define an algorithm that converts a query formed by *for*, *where* and *return* statements into a SXQ query (as long as it only includes variables inside tags, as stated above). The idea is simply to convert the *where* into *if*s, following each *for* by a *return*, and decomposing XPath expressions including several steps into several *for* expressions by introducing a new auxiliary variable and each one consisting of a single step.

Example 2. The query of Example 1 using SXQ syntax:

```
for $x1 in doc("bib.xml")/child::bib return
for $x2 in $x1/child::book  return
for $x3 in doc("reviews.xml")/child::reviews return
for $x4 in $x3/entry  return
if ($x2/title = $x4/title) then
    for $x5 in $x4/title return
     for $x6 in $x4/review return  <rev> $x5  $x6 </rev>
```

We end this subsection with a few definitions that are useful for the rest of the paper. The set of variables in a query Q is represented as $Var(Q)$. Given a query Q, we use the notation $Q_{|p}$ for representing the subquery Q' that can be found in Q at position p. Positions are defined as usual in syntax trees:

Definition 1. *Given a query Q and a position p, $Q_{|p}$ is defined as follows:*

$$\begin{array}{ll} Q_{|\varepsilon} & = Q \\ (Q_1\ Q_2)_{|(i\cdot p)} & = (Q_i)_{|p}\ i \in \{1,2\} \\ (\texttt{for}\ \text{var}\ \texttt{in}\ Q_1\ \texttt{return}\ Q_2)_{|(i\cdot p)} & = (Q_i)_{|p}\ i \in \{1,2\} \\ (\texttt{if}\ Q_1\ \texttt{then}\ Q_2)_{|(i\cdot p)} & = (Q_i)_{|p}\ i \in \{1,2\} \\ (\texttt{if}\ \text{var}{=}\text{var}\ \texttt{then}\ Q_1)_{|(1\cdot p)} & = (Q_1)_{|p} \end{array}$$

Hence the position of a subquery is the path in the syntax tree represented as the concatenation of children positions $p_1 \cdot p_2 \ldots \cdot p_n$. For every position p, $\varepsilon \cdot p = p \cdot \varepsilon = p$. In general $Q_{|p}$ is not a proper SXQ query, since it can contain *free variables*, which are variables defined previously in *for* statements in Q. The set of variables of Q that are *relevant* for $Q_{|p}$ is the subset of $Var(Q)$ that can appear free in any subquery at position p. This set, denoted as $Rel(Q,p)$ is defined recursively as follows:

Definition 2. *Given a query Q, and a position p, $Rel(Q,p)$ is defined as:*

1. $\emptyset$, *if* $p = \varepsilon$.
2. $Rel(Q_1,p')$, *if* $Q \equiv Q_1\ Q_2$, $p = 1 \cdot p'$.
3. $Rel(Q_2,p')$, *if* $Q \equiv Q_1\ Q_2$, $p = 2 \cdot p'$.
4. $Rel(Q_1,p')$, *if* $Q \equiv \texttt{for}\ \text{var}\ \texttt{in}\ Q_1\ \texttt{return}\ Q_2$, $p = 1 \cdot p'$.
5. $\{\text{var}\} \cup Rel(Q_2,p')$, *if* $Q \equiv \texttt{for}\ \text{var}\ \texttt{in}\ Q_1\ \texttt{return}\ Q_2$, $p = 2 \cdot p'$.
6. $Rel(Q_1,p')$, *if* $Q \equiv \texttt{if}\ Q_1\ \texttt{then}\ Q_2$, $p = 1 \cdot p'$.

7. $Rel(Q_2, p')$, *if* $Q \equiv$ `if` Q_1 `then` Q_2, $p = 2 \cdot p'$.

Observe that cases $Q \equiv ()$, $Q \equiv tag$, $Q \equiv \mathrm{var}$, $Q \equiv \mathrm{var}/\chi :: \nu$, *and* $\mathrm{var} = \mathrm{var}$ *correspond to* $p \equiv \varepsilon$.

Without loss of generality we assume that all the relevant variables for a given position are indexed starting from 1 at the outer level. We also assume that every `for` statement introduces a new variable. A query like `for X in ((for Y in ...) (for Y in ...)) ...` is then renamed to an equivalent query of the form `for` X_1 `in ((for` X_2 `in ...) (for` X_3 `in ...)) ...` (notice that the two Y variables occurred in different scopes).

2.2 XQ Operational Semantics

Figure 2 introduces the operational semantics of XQ that can be found in [4]. The only difference with respect to the semantics of this paper is that there is no rule for the constructor *lab*, for the sake of simplicity.

$$
\begin{aligned}
[\![(\,)]\!]_k(\mathcal{F}, \overline{e}) &= (\mathcal{F}, [\,]) \\
[\![Q_1\ Q_2]\!]_k(\mathcal{F}, \overline{e}) &= [\![Q_1]\!]_k(\mathcal{F}, \overline{e}) \uplus [\![Q_2]\!]_k(\mathcal{F}, \overline{e}) \\
[\![\texttt{for}\ \$x_{k+1}\ \texttt{in}\ Q_1\ \texttt{return}\ Q_2]\!]_k(\mathcal{F}, \overline{e}) &= \text{let } (\mathcal{F}', \bar{l}) = [\![Q_1]\!]_k(\mathcal{F}, \overline{e}) \text{ in} \\
&\qquad \biguplus_{1 \le i \le |\bar{l}|} [\![Q_2]\!]_{k+1}(\mathcal{F}', \overline{e} \cdot l_i) \\
[\![\$x_i]\!]_k(\mathcal{F}, [e_1, \ldots, e_k]) &= (\mathcal{F}, [e_i]) \\
[\![\$x_i/\chi :: \nu]\!]_k(\mathcal{F}, [e_1, \ldots, e_k]) &= (\mathcal{F}, \text{list of nodes } v \text{ such that } \chi^{\mathcal{F}}(e_i, v) \text{ and} \\
&\qquad \text{label name of } v = \nu \text{ in order } <_{doc}^{tree(e_i)}) \\
[\![\texttt{if}\ C\ \texttt{then}\ Q_1]\!]_k(\mathcal{F}, \overline{e}) &= \text{if } \pi_2([\![C]\!]_k(\mathcal{F}, \overline{e})) \neq [\,] \text{ then } [\![Q_1]\!]_k(\mathcal{F}, \overline{e}) \\
&\qquad \text{else } (\mathcal{F}, [\,]) \\
[\![\$x_i = \$x_j]\!]_k(\mathcal{F}, [e_1, \ldots, e_k]) &= \text{if } e_i = e_j \text{ then } \mathit{construct}(\mathit{yes}, (\mathcal{F}, [\,])) \\
&\qquad \text{else } (\mathcal{F}, [\,])
\end{aligned}
$$

Fig. 2. Semantics of Core XQuery

As explained in [4], the previous semantics defines the denotation of an XQ expression Q with k relevant variables, under a graph-like representation of a data forest $\mathcal{F}$, and a list of indexes $\overline{e}$ in $\mathcal{F}$, denoted by $[\![Q]\!]_k(\mathcal{F}, \overline{e})$. In particular, each relevant variable $\$x_i$ of Q has as value the tree of $\mathcal{F}$ indexed at position e_i. $\chi^{\mathcal{F}}(e_i, v)$ is a boolean function that returns *true* whenever v is the subtree of $\mathcal{F}$ indexed at position e_i. The operator $\mathit{construct}(a, (\mathcal{F}, [w_1 ... w_n]))$, denotes the construction of a new tree, where a is a label, $\mathcal{F}$ is a data forest, and $[w_1 \ldots w_n]$ is a list of nodes in $\mathcal{F}$. When applied, *construct* returns an indexed forest $(\mathcal{F} \cup T', [\mathit{root}(T')])$, where T' is a tree with domain a new set of nodes, whose root is labeled with a, and with the subtree rooted at the i-th (in sibling order) child of root(T') being an isomorphic copy of the subtree rooted by w_i in $\mathcal{F}$. The symbol $\biguplus$ used in the rules takes two indexed forests $(\mathcal{F}_1, l_1), (\mathcal{F}_2, l_2)$ and returns

an indexed forest $(\mathcal{F}_1 \cup \mathcal{F}_2, l)$, where $l = l_1 \cdot l_2$. Finally, $tree(e_i)$ denotes the maximal tree within the input forest that contains the node e_i, hence $<_{doc}^{tree(e_i)}$ is the document order on the tree containing e_i.

Without loss of generality this semantics assumes that all the variables relevant for a subquery are numbered consecutively starting by 1 as in Example 2. It also assumes that the documents appear explicitly in the query. That is, in Example 2 we must suppose that instead of *doc("bib.xml")* we have the XML corresponding to this document. Of course this is not feasible in practice, but simplifies the theoretical setting and it is assumed in the rest of the paper.

These semantic rules constitute a term rewriting system (TRS in short, see [3]), with each rule defining a single reduction step. The symbol $:=^*$ represents the reflexive and transitive closure of $:=$ as usual. The TRS is terminating and confluent (the rules are not overlapping). Normal forms have the shape $(\mathcal{F}, e_1, \ldots, e_n)$ where $\mathcal{F}$ is a forest of XML fragments, and e_i are nodes in $\mathcal{F}$, meaning that the query returns the XML fragments (**indexed by**) $e_1, \ldots, e_n$. The semantics evaluates a query starting with the expression $[\![Q]\!]_0(\emptyset, ())$. Along intermediate steps, expressions of the form $[\![Q']\!]_k(\mathcal{F}, \overline{e}_k)$ are obtained. The idea is that Q' is a subquery of Q with k relevant variables (which can occur free in Q'), that must take the values $\overline{e}_k$. The next result formalizes these ideas.

Proposition 1. *Let Q be a SXQ query. Suppose that*

$$[\![Q]\!]_0(\emptyset, ()) :=^* [\![Q']\!]_n(\mathcal{F}, \overline{e}_n)$$

Then:

- *Q' is a subquery of Q, that is, $Q' = Q_p$ for some p.*
- *$Rel(Q, p) = \{X_1, \ldots, X_n\}$.*
- *Let S be the set of free variables in Q'. Then $S \subset Rel(Q, p)$.*
- *$[\![Q']\!]_n(\mathcal{F}, \overline{e}_n) = [\![Q'\theta]\!]_0(\emptyset, ())$, with $\theta = \{X_1 \mapsto e_1, \ldots, X_n \mapsto e_n\}$*

Proof. Straightforward from Definition 2, and from the XQ semantic rules of Figure 2.

A more detailed discussion about this semantics and its properties can be found in [4].

3 $\mathcal{TOY}$ and Its Semantics

A $\mathcal{TOY}$ [11] program is composed of data type declarations, type alias, infix operators, function type declarations and defining rules for functions symbols. The syntax of *partial expressions* in $\mathcal{TOY}$ $e \in Exp_\perp$ is $e ::= \perp \mid X \mid h \mid (e\ e')$ where X is a variable and h either a function symbol or a data constructor. Expressions of the form $(e\ e')$ stand for the application of expression e (acting as a function) to expression e' (acting as an argument). Similarly, the syntax of *partial patterns* $t \in Pat_\perp \subset Exp_\perp$ can be defined as $t ::= \perp \mid X \mid c\ t_1 \ldots t_m \mid f\ t_1 \ldots t_m$ where X represents a variable, c a data constructor of arity greater or equal to

m, and f a function symbol of arity greater than m, being t_i partial patterns for all $1 \leq i \leq m$. Each rule for a function f in $\mathcal{TOY}$ has the form:

$$\underbrace{f\ t_1 \ldots t_n}_{\text{left-hand side}} \rightarrow \underbrace{r}_{\text{right-hand side}} \Leftarrow \underbrace{C_1, \ldots, C_k}_{\text{condition}} \text{ where } \underbrace{s_1 = u_1, \ldots, s_m = u_m}_{\text{local definitions}}$$

where u_i and r are expressions (that can contain new extra variables), C_j are strict equalities, and t_i, s_i are patterns. In $\mathcal{TOY}$, variable names must start with either an uppercase letter or an underscore (for anonymous variables), whereas other identifiers start with lowercase.

Data type declarations and type alias are useful for representing XML documents in $\mathcal{TOY}$:

```
data node      = txt    string
               | comment string
               | tag     string [attribute] [node]
data attribute = att     string string
type xml       = node
```

The data type `node` represents nodes in a simple XML document. It distinguishes three types of nodes: texts, tags (element nodes), and comments, each one represented by a suitable data constructor and with arguments representing the information about the node. For instance, constructor `tag` includes the tag name (an argument of type `string`) followed by a list of attributes, and finally a list of child nodes. The data type `attribute` contains the name of the attribute and its value (both of type `string`). The last type alias, `xml`, renames the data type `node`. Of course, this list is not exhaustive, since it misses several types of XML nodes, but it is enough for this presentation.

$\mathcal{TOY}$ includes two primitives for loading and saving XML documents, called `load_xml_file` and `write_xml_file` respectively. For convenience all the documents are started with a dummy node `root`. This is useful for grouping several XML fragments. If the file contains only one node `N` at the outer level, the `root` node is unnecessary, and can be removed using this simple function:

```
load_doc F = N <== load_xml_file F == xmlTag "root" [] [N]
```

where `F` is the name of the file containing the document. Observe that the strict equality `==` in the condition forces the evaluation of `load_xml_file F` and succeeds if the result has the form `xmlTag "root" [] [N]` for some `N`. If this is the case, `N` is returned.

The constructor-based ReWriting Logic (CRWL) [7] has been proposed as a suitable declarative semantics for functional-logic programming with lazy nondeterministic functions. The calculus is defined by five inference rules (see Figure 3): (BT) that indicates that any expression can be approximated by bottom, (RR) that establishes the reflexivity over variables, the decomposition rule (DC), the (JN) (join) rule that indicates how to prove strict equalities, and the function application rule (FA). In every inference rule, $r, e_i, a_j \in Exp_\perp$ are partial expres-

BT $\quad e \to \bot$

RR $\quad X \to X \qquad$ with $X \in Var$

DC $\quad \dfrac{e_1 \to t_1 \ \ldots \ e_m \to t_m}{h\ \overline{e}_m \to h\ \overline{t}_m} \qquad h\ \overline{t}_m \in Pat_\bot$

JN $\quad \dfrac{e \to t \quad e' \to t}{e \ == \ e'} \qquad t \in Pat$ (total pattern)

FA $\quad \dfrac{e_1 \to t_1 \ \ldots \ e_n \to t_n \quad C \quad r\ \overline{a}_k \to t}{f\ \overline{e}_n\ \overline{a}_k \ \to t}$
if $(f\ \overline{t}_n \to r \Leftarrow C) \in [P]_\bot, t \neq \bot$

Fig. 3. CRWL Semantic Calculus

sions and $t, t_k \in Pat_\bot$ are partial patterns. The notation $[P]_\bot$ of the inference rule *FA* represents the set $\{(l \to r \Leftarrow C)\theta \mid (l \to r \Leftarrow C) \in P,\ \theta \in Subst_\bot\}$ of partial instances of the rules in program P ($Subst_\bot$ represents the set of partial substitutions that replace variables by partial terms). The most complex inference rule is FA (Function Application), which formalizes the steps for computing a *partial pattern* t as approximation of a function call $f\ \overline{e}_n$:

1. Obtain partial patterns t_i as suitable approximations of the arguments e_i.
2. Apply a program rule $(f\ \overline{t}_n \to r \Leftarrow C) \in [P]_\bot$, verify the condition C, and check that t approximates the right-hand side r.

In this semantic notation, local declarations $a = b$ introduced in $\mathcal{TOY}$ syntax by the reserved word `where` are part of the condition C as approximation statements of the form $b \to a$.
The semantics in $\mathcal{TOY}$ allows introducing non-deterministic functions, such as the following function `member` that returns all the elements in a list:

```
member:: [A]  -> A
member  [X | Xs] =  X
member  [X | Xs] =  member Xs
```

Another example of $\mathcal{TOY}$ function is the definition of the infix operator `.:::.` for XPath expressions (the operator `::` in XPath syntax):

```
(.:::.) :: (A -> B) -> (B -> C) -> (A -> C)
(F .:::. G) X = G (F X)
```

As the examples show, $\mathcal{TOY}$ is a typed language. However the type declaration is optional and in the rest of the paper they are omitted for the sake of simplicity. *Goals* in $\mathcal{TOY}$ are sequences of strict equalities. A strict equality $e_1 == e_2$ holds (inference JN) if both e_1 and e_2 can be reduced to the same total pattern t. For instance, the goal `member [1,2,3,4] == R` yields four answers, the four values for `R` that make the equality true: $\{$`R` $\mapsto$ `1`$\}$, ..., $\{$`R` $\mapsto$ `4`$\}$.

4 Transforming SXQ into $\mathcal{TOY}$

In order to represent SXQ queries in $\mathcal{TOY}$ we use some auxiliary datatypes:

```
type xPath = xml-> xml

data sxq  = xfor xml sxq sxq | xif cond sxq | xmlExp xml |
                     xp path | comp sxq sxq
data cond = xml := xml | cond sxq
data path = var xml | xml :/ xPath | doc string xPath
```

The structure of the datatype `sxq` allows representing any SXQ query (see SXQ syntax in Figure 1). It is worth noticing that a variable introduced by a *for* statement has type `xml`, indicating that the variable always contains a value of this type. $\mathcal{TOY}$ includes a primitive `parse_xquery` that translates any SXQ expression into its corresponding representation as a term of this datatype, as the next example shows:

Example 3. The translation of the SXQ query of Example 2 into the datatype `sxq` produces the following $\mathcal{TOY}$ data term:

```
Toy> parse_xquery  "for $x1 in doc(\"bib.xml\")/child::bib return
           for $x2 in .....  <rev> $x5  $x6 </rev>" == R
yes
{R --> xfor X1 (xp (doc "bib.xml" (child .::. (nameT "bib"))))
    (xfor X2 (xp ( X1 :/ (child .::.(nameT "book"))))
    (xfor X3 (xp (doc "reviews.xml" (child  .::. (nameT "reviews"))))
    (xfor X4 (xp ( X3 :/ (child .::.(nameT "entry"))))
    (xif  ((xp(X2 :/ (child .::.(nameT "title")))) :=
             (xp(X4 :/ (child .::.(nameT "title")))))
    (xfor X5 (xp ( X4 :/ (child .::.(nameT "title"))))
    (xfor X6 (xp ( X4 :/ (child .::.(nameT "review"))))
       (xmlExp (xmlTag "rev" [] [X5,X6])))))))))
 }
```

The interpreter assumes the existence of the infix operator `.::.` that connects axes and tests to build steps, defined as the sequence of applications in Section 3.

The rules of the $\mathcal{TOY}$ interpreter that processes SXQ queries can be found in Figure 4. The main function is `sxq`, which distinguishes cases depending of the form of the query. If it is an XPath expression then the auxiliary function `sxqPath` is used. If the query is an XML expression, the expression is just returned (this is safe thanks to our constraint of allowing only variables inside XML expressions). If we have two queries (`comp` construct), the result of evaluating any of them is returned using non-determinism. The `for` statement (`xfor` construct) forces the evaluation of the query `Q1` and binds the variable `X` to the result. Then the result query `Q2` is evaluated. The case of the `if` statement is analogous. The XPath subset considered includes tests for attributes (`attr`), label names (`nameT`), general elements (`nodeT`) and text nodes (`textT`). It also

```
sxq (xp E)              = sxqPath E
sxq (xmlExp X)          = X
sxq (comp Q1 Q2)        = sxq Q1
sxq (comp Q1 Q2)        = sxq Q2
sxq (xfor X Q1 Q2)      = sxq Q2 <== X== sxq Q1
sxq (xif (Q1:=Q2) Q3)   = sxq Q3 <== sxq Q1  == sxq Q2
sxq (xif (cond Q1) Q2) = sxq Q2 <== sxq Q1  == _

sxqPath (var X)  = X
sxqPath (X :/ S) = S X
sxqPath (doc F S) = S (load_xml_file F)

%%%% XPATH %%%%%%
attr A (xmlTag S Attr L ) = xmlText T <== member Attr == xmlAtt A T
nameT S (xmlTag S Attr L ) = xmlTag S Attr L
nodeT X = X
textT (xmlText S) = xmlText S
commentT S (xmlComment S) = xmlComment S

self X = X
child (xmlTag _Name _Attr L) = member L
descendant X = child X
descendant X = descendant Y <== child X == Y
dos = self
dos = descendant
```

Fig. 4. $\mathcal{TOY}$ transformation rules for SXQ

includes the axes `self`, `child`, `descendant` and `dos`. Observe that we do not include reverse axes like `ancestor` because they can be replaced by expressions including forward axes, as shown in [12]. Other constructions such as filters can be easily included (see [5]). The next example uses the interpreter to obtain the answers for the query of our running example.

Example 4. The goal `sxq (parse_xquery "for....")) == R` applies the interpreter of Figure 4 to the code of Example 2 (assuming that the string after `parse_xquery` is the query in Example 2), and returns the $\mathcal{TOY}$ representation of the expected results:

```
<rev>
 <title>TCP/IP Illustrated</title>
 <review>  One of the best books on TCP/IP.  </review>
</rev>
...
```

4.1 Soundness of the Transformation

One of the goals of this paper is to ensure that the embedding is semantically correct and complete. This section introduces the theoretical results establishing

these properties. If V is a set of indexed variables of the form $\{X_1, \ldots, X_n\}$ we use the notation $\theta(V)$ to indicate the sequence $\theta(X_1), \ldots, \theta(X_n)$. In these results it is implicitly assumed that there is a bijective mapping f from XML format to the datatype `xml` in $\mathcal{TOY}$. Also, variables in XQuery $\$x_i$ are assumed to be represented in $\mathcal{TOY}$ as X_i and conversely. However, in order to simplify the presentation, we omit the explicit mention to f and to f^{-1}.

Lemma 1. *Let P be a $\mathcal{TOY}$ program, Q' an SXQ query, and Q, p such that $Q \equiv Q'_{|p}$. Define $V = Rel(Q', p)$ (see Definition 2), and $k = |V|$. Let θ be a substitution such that $\mathcal{P} \vdash (\texttt{sxq}\ Q\theta == t)$ for some pattern t.*
Then $[\![Q]\!]_k(\mathcal{F}, [\theta(V)]) :=^* (\mathcal{F}', L)$, for some forests $\mathcal{F}, \mathcal{F}'$ and with L verifying $t \in L$.

The theorem that establishes the correctness of the approach is an easy consequence of the Lemma.

Theorem 1. *Let P be the $\mathcal{TOY}$ program of Figure 4, Q an SXQ query, t a $\mathcal{TOY}$ pattern, and θ a substitution such that $\mathcal{P} \vdash (\texttt{sxq}\ Q\theta == t)$ for some θ. Then $[\![Q]\!]_0(\emptyset, []) :=^* (\mathcal{F}, L)$, for some forest $\mathcal{F}$, and L verifying $t \in L$.*

Proof. In Lemma 1 consider the position $p \equiv \varepsilon$. Then $Q' \equiv Q$, $V = \emptyset$ and $k = 0$. Without loss of generality we can restrict in the conclusion to $\mathcal{F} = \emptyset$, because $\theta(V) = \emptyset$ and therefore $\mathcal{F}$ is not used during the rewriting process. Then the conclusion of the theorem is the conclusion of the lemma.

Thus, our approach is correct. The next Lemma allows us to prove that it is also complete, in the sense that the $\mathcal{TOY}$ program can produce every answer obtained by the XQ operational semantics.

Lemma 2. *Let $\mathcal{P}$ be the $\mathcal{TOY}$ program of Figure 4. Let Q' be a SXQ query and Q, p such that $Q \equiv Q'_{|p}$. Define $V = Rel(Q', p)$ (see Definition 2) and $k = |V|$. Suppose that $[\![Q]\!]_k(\mathcal{F}, \overline{e}_k) :=^* (\mathcal{F}', \overline{a}_n)$ for some $\mathcal{F}$, $\mathcal{F}'$, $\overline{e}_k$, $\overline{a}_n$.*
Then, for every a_j, $1 \leq j \leq n$, there is a substitution θ such that $\theta(X_i) = e_i$ for $X_i \in V$ and a CRWL-proof proving $\mathcal{P} \vdash \texttt{sxq}\ Q\theta == a_j$.

As in the case of correctness, the completeness theorem is just a particular case of the Lemma:

Theorem 2. *Let $\mathcal{P}$ be the $\mathcal{TOY}$ program of Figure 4. Let Q be a SXQ query and suppose that $[\![Q]\!]_k(\emptyset, []) :=^* (\mathcal{F}, \overline{a}_n)$ for some $\mathcal{F}, \overline{a}_n$. Then for every a_j, $1 \leq j \leq n$, there is $\mathcal{P} \vdash (\texttt{sxq}\ Q)\theta == a_j$ for some substitution θ.*

Proof. As in Theorem 1, suppose $p \equiv \varepsilon$ and thus $Q' \equiv Q$. Then $V = \emptyset$ and $k = 0$. Then, if $[\![Q]\!]_0(\emptyset, \emptyset) :=^* (\mathcal{F}, \overline{a}_n)$ it is easy to check that $[\![Q]\!]_0(\mathcal{F}', \emptyset) :=^* (\mathcal{F}, \overline{a}_n)$ for any $\mathcal{F}'$. Then the conclusion of the lemma is the same as the conclusion of the Theorem.

The proofs of Lemmata 1 and 2 can be found in [2].

5 Application: Test Case Generation

In this section we show how an embedding of SXQ into $\mathcal{TOY}$ can be used for obtaining test-cases for the queries. For instance, consider the erroneous query of the next example.

Example 5. Suppose that the user also wants to include the publisher of the book among the data obtained in Example 1. The following query tries to obtain this information:

```
Q = for $b in doc("bib.xml")/bib/book,
        $r in doc("reviews.xml")/reviews/entry,
        where $b/title = $r/title
        for $booktitle in $r/title,
            $revtext in $r/review,
            $publisher in $r/publisher
        return  <rev> $booktitle $publisher $revtext </rev>
```

However, there is an error in this query, because in `$r/publisher` the variable `$r` should be `$b`, since the publisher is in the document *"bib.xml"*, not in *"reviews.xml"*. The user does not notice that there is an error, tries the query (in $\mathcal{TOY}$ or in any XQuery interpreter) and receives an empty answer.

In order to check whether a query is erroneous, or even to help finding the error, it is sometimes useful to have test-cases, i.e., XML files which can produce some answer for the query. Then the test-cases and the original XML documents can be compared, and this can help finding the error. In our setting, such test-cases are obtained for free, thanks to the generate and test capabilities of logic programming. The general process can be described as follows:

1. Let `Q'` be the translation `parse_xquery Q` of query `Q` into $\mathcal{TOY}$.
2. Let $F_1, \ldots, F_k$ be the names of the XML documents occurring in `Q'`. That is, for each F_i, $1 \leq i \leq k$, there is an occurrence of an expression of the form `load_xml_file(`F_i`)` in `Q'` (which corresponds to expressions `doc(`F_i`)` in `Q`). Let `Q''` be the result of replacing each `doc(`F_i`)` expression by a new variable D_i, for $i = 1 \ldots k$.
3. Let ``expected.xml'' be a document containing an expected answer for the query `Q`.
4. Let `E` the expression `Q''==load_doc ``expected.xml''`.
5. Try the goal
   `G` $\equiv$ `E, write_xml_file` D_1 F'_1`, ..., write_xml_file` D_k F'_k

The idea is that the goal `G` looks for values of the logic variables D_i fulfilling the strict equality. The result is that after solving this goal, the D_i variables contain XML documents that can produce the expected answer for this query. Then each document is saved into a new file with name F'_i. For instance F'_i can consist of the original name F_i preceded by some suitable prefix *tc*. The process can be automatized, and the result is the code of Figure 5.

```
prepareTC (xp E)            = (xp E',L)
                              where (E',L) = prepareTCPath E
prepareTC (xmlExp X)        = (xmlExp X, [])
prepareTC (comp Q1 Q2)      = (comp Q1' Q2', L1++L2)
                               where (Q1',L1) = prepareTC Q1
                                     (Q2',L2) = prepareTC Q2
prepareTC (xfor X Q1 Q2)    = (xfor X Q1' Q2', L1++L2)
                              where (Q1',L1) = prepareTC Q1
                                    (Q2',L2) = prepareTC Q2
prepareTC (xif (Q1:=Q2) Q3) = (xif (Q1':=Q2') Q3',L1++(L2++L3))
                               where (Q1',L1) = prepareTC Q1
                                     (Q2',L2) = prepareTC Q2
                                     (Q3',L3) = prepareTC Q3
prepareTC (xif (cond Q1) Q2) = (xif (cond Q1) Q2, L1++L2)
                               where (Q1',L1) = prepareTC Q1
                                    (Q2',L2) = prepareTC Q2

prepareTCPath (var X)   = (var X, [])
prepareTCPath (X :/ S)  = (X :/ S, [])
prepareTCPath (doc F S) = (A :/ S, [write_xml_file A ("tc"++F)])

generateTC Q F = true <==  sxq Qtc == load_doc F, L==_
                where (Qtc,L) = prepareTC Q
```

Fig. 5. $\mathcal{TOY}$ transformation rules for SXQ

The code uses the list concatenation operator ++ which is defined in $\mathcal{TOY}$ as usual in functional languages such as Haskell. It is worth observing that if there are no test-case documents that can produce the expected result for the query, the call to `generateTC` will loop. The next example shows the generation of test-cases for the wrong query of Example 5.

Example 6. Consider the query of Example 5 , and suppose the user writes the following document "`expected.xml`":

```
<rev>
 <title>Some title</title>
 <review>The review</review>
 <publisher>Publisher</publisher>
</rev>
```

This is a possible expected answer for the query. Now we can try the goal:

```
Toy> Q == parse_xquery "for....", R == generateTC Q "expected.xml"
```

The first strict equality parses the query, and the second one generates the XML documents which constitute the test cases. In this example the test-cases obtained are:

```
% bibtc.xml
<bib>
 <book>
  <title>Some title</title>
 </book>
</bib>
```

```
% revtc.xml
<reviews>
 <entry>
  <title>Some title</title>
  <review>The review </review>
  <publisher>Publisher</publisher>
 </entry>
</reviews>
```

By comparing the test-case ‘‘`revtc.xml`’’ with the file ‘‘`reviews.xml`’’ we observe that the publisher is not in the reviews. Then it is easy to check that in the query the publisher is obtained from the reviews instead of from the *bib* document, and that this constitutes the error.

6 Conclusions

The paper shows the embedding of a fragment of the XQuery language for querying XML documents into the functional-logic language $\mathcal{TOY}$. Although only a small subset of XQuery consisting of *for*, *where/if* and *return* statements has been considered, the users of $\mathcal{TOY}$ can now perform simple queries such as *join* operations. The formal definition of the embedding allows us to prove the soundness of the approach with respect to the operational semantics of XQuery. The proposal respects the declarative nature of $\mathcal{TOY}$, exploiting its non-deterministic nature for obtaining the different results produced by XQuery expressions. An advantage of this approach with respect to the use of lists usually employed in functional languages is that our embedding allows the user to generate test-cases automatically when possible, which is useful for testing the query, or even for helping to find the error in the query. An extended version of this paper, including the proofs of the theoretical results and more detailed explanations about how to install $\mathcal{TOY}$ and run the prototype can be found in [2].

The most obvious future work would be introducing the *let* statement, which presents two novelties. The first is that they are *lazy*, that is, they are not evaluated if they are not required by the result. This part is easy to fulfill since we are in a lazy language. In particular, they could be introduced as local definitions (*where* statements in $\mathcal{TOY}$). The second novelty is more difficult to capture, and it is that the variables introduced by *let* represent an XML sequence. The natural representation in $\mathcal{TOY}$ would be a list, but the non-deterministic nature of our proposal does not allow us to collect all the results provided by an expression in a declarative way. A possible idea would be to use the functional-logic language Curry [8] and its encapsulated-search [10], or even the non-declarative *collect* primitive included in $\mathcal{TOY}$. In any case, this will imply a different theoretical framework and new proofs for the results. A different line for future work is the use of test cases for finding the error in the query using some variation of declarative debugging [14] that could be applied to this setting.

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Marker-directed Optimization of UnCAL Graph Transformations

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Abstract. Buneman et al. proposed a graph algebra called UnCAL (Unstructured CALculus) for compositional graph transformations based on structural recursion, and we have recently applied to model transformations. The compositional nature of the algebra greatly enhances the modularity of transformations. However, intermediate results generated between composed transformations cause overhead. Buneman et al. proposed fusion rules that eliminate the intermediate results, but auxiliary rewriting rules that enable the actual application of the fusion rules are not apparent so far. UnCAL graph model includes the concept of markers, which correspond to recursive function call in the structural recursion. We have found that there are many optimization opportunities at rewriting level based on static analysis, especially focusing on markers. The analysis can safely eliminate redundant function calls. Performance evaluation shows its practical effectiveness for non-trivial examples in model transformations.
Keywords: program transformations, graph transformations, UnCAL

1 Introduction

Graph transformation has been an active research topic [9] and plays an important role in model-driven engineering [5, 11]; models such as UML diagrams are represented as graphs, and model transformation is essentially graph transformation. We have recently proposed a bidirectional graph transformation framework [6] based on providing bidirectional semantics to an existing graph transformation language UnCAL [4], and applied it to bidirectional model transformation by translating from existing model transformation language to UnCAL [10]. Our success in providing well-behaved bidirectional transformation framework was due to structural recursion in UnCAL, which is a powerful mechanism of visiting and transforming graphs. Transformation based on structural recursion

is inherently compositional, thus facilitates modular model transformation programming.

However, compositional programming may lead to many unnecessary intermediate results, which would make a graph transformation program terribly inefficient. As actively studied in programming language community, optimization like fusion transformation [12] is desired to make it practically useful. Despite a lot of work being devoted to fusion transformation of programs manipulating lists and trees, little work has been done on fusion on programs manipulating graphs. Although the original UnCAL has provided some fusion rules and rewriting rules to optimize graph transformations [4], we believe that further work and enhancement on fusion and rewriting are required.

The key idea presented in this paper is to analyze input/output markers, which are sort of labels on specific set of nodes in the UnCAL graph model and are used to compose graphs by connecting nodes with matching input and output markers. By statically analyzing connectivity of UnCAL by our marker analysis, we can simplify existing fusion rule. Consider, for instance, the following existing generic fusion rule of the structural recursion in UnCAL:

$$\begin{aligned}&\mathbf{rec}(\lambda(\$l_2, \$t_2).e_2)(\mathbf{rec}(\lambda(\$l_1, \$t_1).e_1)(e_0))\\ &\quad = \mathbf{rec}(\lambda(\$l_1, \$t_1).\, \mathbf{rec}(\lambda(\$l_2, \$t_2).e_2)(e_1 \mathbin{@} \mathbf{rec}(\lambda(\$l_1, \$t_1).e_1)(\$t_1)))(e_0)\end{aligned}$$

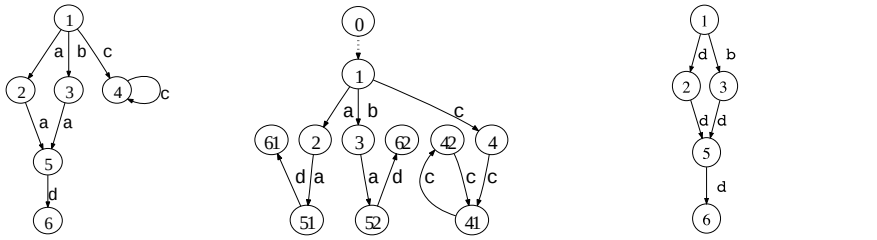
where $\mathbf{rec}(\lambda(\$l, \$t).e)$ encodes a structural recursive function which is an important computation pattern and will be explained later. The graph constructor @ connects two graphs by matching markers on nodes, and in this case, result of transformation e_1 is combined to another structural recursion $\mathbf{rec}(\lambda(\$l_1, \$t_1).e_1)$. If we know by static analysis that e_1 creates no output markers, or equivalently, $\mathbf{rec}(\lambda(\$l_1, \$t_1).e_1)$ makes no recursive function call, then we can eliminate $@\,\mathbf{rec}(\lambda(\$l_1, \$t_1).e_1)(\$t_1)$ and further simplify the fusion rule. Our preliminary performance analysis reports relatively good evidence of usefulness of this optimization.

The main technical contributions of this paper are two folds: a sound and refined static inference of markers and a set of powerful rewriting rules for optimization using inferred markers. All have been implemented and tested with graph transformations widely recognized in software engineering research. The source code of the implementation can be downloaded via our project web site at `www.biglab.org`.

The rest of this paper is organized as follows. Section 2 reviews UnCAL graph model, graph transformation language and existing optimizations. Section 3 proposes enhanced static analysis of markers. In Section 4, we build enhanced rewriting optimization algorithm based on the static analysis. Section 5 reports preliminary performance results. Section 6 reviews related work, and Section 7 concludes this paper.

2 UnCAL Graph Algebra and Prior Optimizations

In this section, we review the UnCAL graph algebra [3, 4], in which our graph transformation is specified.



(a) A Simple Graph (b) An Equivalent Graph (c) Result of $a2d\_xc$ on Fig. 1(a)

Fig. 1. Graph Equivalence Based on Bisimulation

2.1 Graph Data Model

We deal with rooted, directed, and edge-labeled graphs with no order on outgoing edges. UnCAL graph data model has two prominent features, *markers* and ε-*edges*. Nodes may be marked with *input* and *output markers*, which are used as an interface to connect them to other graphs. An ε-edge represents a shortcut of two nodes, working like the ε-transition in an automaton. We use *Label* to denote the set of labels and $\mathcal{M}$ to denote the set of markers.

Formally, a graph G, is a quadruple (V, E, I, O), where V is a set of nodes, $E \subseteq V \times (\mathit{Label} \cup \{\varepsilon\}) \times V$ is a set of edges, $I \subseteq \mathcal{M} \times V$ is a set of pairs of an input marker and the corresponding node, and $O \subseteq V \times \mathcal{M}$ is a set of pairs of nodes and associated output markers. For each marker $\&x \in \mathcal{M}$, there is at most one node v such that $(\&x, v) \in I$. The node v is called an *input node* with marker $\&x$ and is denoted by $I(\&x)$. Unlike input markers, more than one node can be marked with an identical output marker. They are called *output nodes*. Intuitively, input nodes are root nodes of the graph (we allow a graph to have multiple root nodes, and for singly rooted graphs, we often use default marker $\&$ to indicate the root), while an output node can be seen as a "context-hole" of graphs where an input node with the same marker will be plugged later. We write $\mathsf{inMarker}(G)$ to denote the set of input markers and $\mathsf{outMarker}(G)$ to denote the set of output markers in a graph G.

Note that multiple-marker graphs are meant to be an internal data structure for graph composition. In fact, the initial source graphs of our transformation have one input marker (single-rooted) and no output markers (no holes). For instance, the graph in Fig. 1(a) is denoted by (V, E, I, O) where $V = \{1, 2, 3, 4, 5, 6\}$, $E = \{(1, \mathsf{a}, 2), (1, \mathsf{b}, 3), (1, \mathsf{c}, 4), (2, \mathsf{a}, 5), (3, \mathsf{a}, 5), (4, \mathsf{c}, 4), (5, \mathsf{d}, 6)\}$, $I = \{(\&, 1)\}$, and $O = \{\}$. $DB^{\mathcal{X}}_{\mathcal{Y}}$ denotes graphs with sets of input markers $\mathcal{X}$ and output markers $\mathcal{Y}$. $DB^{\{\&\}}_{\mathcal{Y}}$ is abbreviated to $DB_{\mathcal{Y}}$.

2.2 Notion of Graph Equivalence

Two graphs are value equivalent if they are bisimilar. Please refer to [4] for the complete definition. For instance, the graph in Fig. 1(b) is value equivalent to

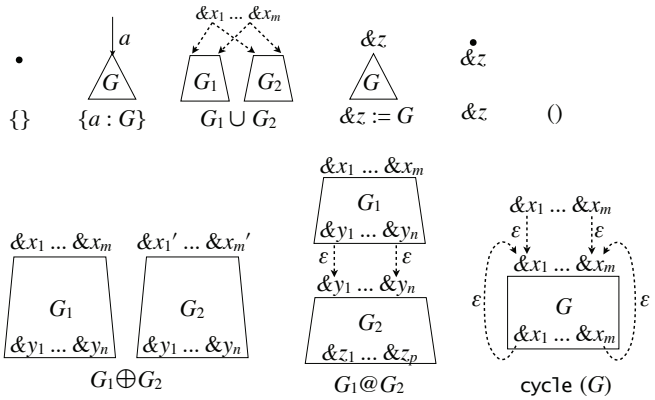


Fig. 2. Graph Constructors

the graph in Fig. 1(a); the new graph has an additional ε-edge (denoted by the dotted line), duplicates the graph rooted at node 5, and unfolds and splits the cycle at node 4. Unreachable parts are also disregarded, i.e., two bisimilar graphs are still bisimilar if one adds subgraphs unreachable from input nodes.

This value equivalence provides optimization opportunities because we can rewrite transformation so that transformation before and after rewriting produce results that are bisimilar to each other [4]. For example, optimizer can freely cut off expressions that is statically determined to produce unreachable parts.

2.3 Graph Constructors

Figure 2 summarizes the nine graph constructors that are powerful enough to describe arbitrary (directed, edge-labeled, and rooted) graphs [4]. Here, $\{\}$ constructs a root-only graph, $\{a : G\}$ constructs a graph by adding an edge with label $a \in \mathit{Label} \cup \{\varepsilon\}$ pointing to the root of graph G, and $G_1 \cup G_2$ adds two ε-edges from the new root to the roots of G_1 and G_2. Also, $\&x := G$ associates an input marker, $\&x$, to the root node of G, $\&y$ constructs a graph with a single node marked with one output marker $\&y$, and $()$ constructs an empty graph that has neither a node nor an edge. Further, $G_1 \oplus G_2$ constructs a graph by using a componentwise (V, E, I and O) union. $\cup$ differs from $\oplus$ in that $\cup$ unifies input nodes while $\oplus$ does not. $\oplus$ requires input markers of operands to be disjoint, while $\cup$ requires them to be identical. $G_1 \mathbin{@} G_2$ composes two graphs vertically by connecting the output nodes of G_1 with the corresponding input nodes of G_2 with ε-edges, and $\mathbf{cycle}(G)$ connects the output nodes with the input nodes of G to form cycles. Newly created nodes have unique identifiers. They are, together with other operators, bisimulation generic [4], i.e., bisimilar result is obtained for bisimilar operands.

$$
\begin{array}{rcll}
e & ::= & \{\} \mid \{l : e\} \mid e \cup e \mid \&x := e \mid \&y \mid () & \\
& \mid & e \oplus e \mid e \mathbin{@} e \mid \mathbf{cycle}(e) & \{ \text{ constructor } \} \\
& \mid & \$g & \{ \text{ graph variable } \} \\
& \mid & \mathbf{let}\, \$g = e\, \mathbf{in}\, e & \{ \text{ variable binding } \} \\
& \mid & \mathbf{if}\, l = l\, \mathbf{then}\, e\, \mathbf{else}\, e & \{ \text{ conditional } \} \\
& \mid & \mathbf{rec}(\lambda(\$l, \$g).e)(e) & \{ \text{ structural recursion application } \} \\
l & ::= & a \mid \$l & \{ \text{ label } (a \in \mathit{Label}) \text{ and label variable } \}
\end{array}
$$

Fig. 3. Core UnCAL Language

Example 1. The graph equivalent to that in Fig. 1(a) can be constructed as follows (though not uniquely).

$$
\begin{array}{l}
\&z \mathbin{@} \mathbf{cycle}((\&z := \{\mathtt{a} : \{\mathtt{a} : \&z_1\}\} \cup \{\mathtt{b} : \{\mathtt{a} : \&z_1\}\} \cup \{\mathtt{c} : \&z_2\}) \\
\qquad\qquad \oplus (\&z_1 := \{\mathtt{d} : \{\}\}) \\
\qquad\qquad \oplus (\&z_2 := \{\mathtt{c} : \&z_2\}))
\end{array}
$$

□

For simplicity, we often write $\{a_1 : G_1, \ldots, a_n : G_n\}$ to denote $\{a_1 : G_1\} \cup \cdots \cup \{a_n : G_n\}$, and $(G_1, \ldots, G_n)$ to denote $(G_1 \oplus \cdots \oplus G_n)$.

2.4 UnCAL Syntax

UnCAL (Unstructured Calculus) is an internal graph algebra for the graph query language UnQL, and its core syntax is depicted in Fig. 3. It consists of the graph constructors, variables, variable bindings, conditionals, and structural recursion. We have already detailed the data constructors, while variables, variable bindings and conditionals are self explanatory. Therefore, we will focus on *structural recursion*, which is a powerful mechanism in UnCAL to describe graph transformations.

A function f on graphs is called a structural recursion if it is defined by the following equations

$$
\begin{array}{ll}
f(\{\}) & = \{\} \\
f(\{\$l : \$g\}) & = e \mathbin{@} f(\$g) \\
f(\$g_1 \cup \$g_2) & = f(\$g_1) \cup f(\$g_2),
\end{array}
$$

and f can be encoded by $\mathbf{rec}(\lambda(\$l, \$g).e)$. Despite its simplicity, the core UnCAL is powerful enough to describe interesting graph transformation including all graph queries (in UnQL) [4], and nontrivial model transformations [8].

Example 2. The following structural recursion *a2d_xc* replaces all labels `a` with `d` and removes edges labeled `c`.

$$
\begin{array}{rll}
\mathit{a2d\_xc}(\$db) = \mathbf{rec}(\lambda(\$l, \$g).\, & \mathbf{if}\, \$l = \mathtt{a}\, \mathbf{then} & \{\mathtt{d} : \&\} \\
& \mathbf{else\ if}\, \$l = \mathtt{c}\, \mathbf{then} & \{\varepsilon : \&\} \\
& \mathbf{else} & \{\$l : \&\})\ (\$db)
\end{array}
$$

The nested **if**s correspond to e in the above equations. Applying the function *a2d_xc* to the graph in Fig. 1(a) yields the graph in Fig. 1(c). □

2.5 Revisiting Original Marker Analysis

There were actually previous work on marker analysis by original authors of UnCAL. The original typing rules appeared in the technical report version of [2]. Note that we call type to denote sets of input and output markers. Compared to our analysis, these rules were provided declaratively. For example, the rule for **if** says that if sets of output markers in both branches are equal, then the result have that set of output markers. It is not apparent how we obtain the output marker of **if** if the branches have different sets of output markers.

Buneman et al. [4] did mention optimization based on marker analysis, to avoid evaluating unnecessary subexpressions. But it was mainly based on *run-time* analysis. As we propose in the following sections, we can *statically* compute the set of markers and further simplify the transformation itself.

2.6 Fusion Rules and Output Marker Analysis

Buneman et al. [3, 4] proposed the following fusion rules that aim to remove intermediate results in successive applications of structural recursion **rec**.

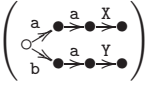
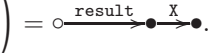
$$\begin{aligned}&\mathbf{rec}(\lambda(\$l_2, \$t_2).e_2)(\mathbf{rec}(\lambda(\$l_1, \$t_1).e_1)(e_0))\\ &= \begin{cases} \mathbf{rec}(\lambda(\$l_1, \$t_1).\, \mathbf{rec}(\lambda(\$l_2, \$t_2).e_2)(e_1))(e_0) & \text{if } t_2 \text{ appears free in } e_2 \\ \mathbf{rec}(\lambda(\$l_1, \$t_1).\, \mathbf{rec}(\lambda(\$l_2, \$t_2).e_2) \\ \quad (e_1 \mathbin{@} \mathbf{rec}(\lambda(\$l_1, \$t_1).e_1)(\$t_1)))(e_0) & \text{for arbitrary } e_2 \end{cases}\end{aligned} \tag{1}$$

If you can statically guarantee that e_1 does not produce any output marker, then the second rule is promoted to the first rule, opening another optimization opportunities.

Non-recursive Query. Now questions that might be asked would be how often do such kind of "non-recursive" queries appear. Actually it frequently appears as *extraction* or *join*. Extraction transformation is a transformation in which some subgraph is simply extracted. It is achieved by direct reference of the bound graph variable in the body of **rec**. Join is achieved by nesting of these extraction transformations. Finite steps of edge traversals are expressed by this nesting.

Example 3. The following structural recursion *consecutive* extracts subgraphs that can be accessible by traversing two connected edges of the same label.

$$\begin{aligned}\mathit{consecutive}(\$db) = \mathbf{rec}(\lambda(\$l, \$g).\, &\mathbf{rec}(\lambda(\$l', \$g'). \\ &\mathbf{if}\ \$l = \$l'\ \mathbf{then}\ \{\texttt{result} : \$g'\} \\ &\mathbf{else}\qquad\quad \{\}\qquad\quad)(\$g))(\$db)\end{aligned}$$

For example, we have $\mathit{consecutive}\left(\right.$  $\left.\right) =$  .

If this transformation is followed by $\mathbf{rec}(\lambda(\$l_2, \$t_2).e_2)$ where e_2 refers to $\$t_2$, the second condition of fusion rule applies, but it will be promoted to the first, since the body of **rec** in *consecutive*, which corresponds to e_1 in the fusion rule, does not have output markers. We revisit this case in Example 4 in Section 4.

$$\&x := (\&z := e) \longrightarrow \&x.\&z := e \quad \&x := (e_1 \oplus e_2) \longrightarrow (\&x := e_1) \oplus (\&x := e_2)$$
$$e \cup \{\} \longrightarrow e \quad \{\} \cup e \longrightarrow e \quad e \oplus () \longrightarrow e \quad () \oplus e \longrightarrow e$$
$$() \mathbin{@} e \longrightarrow () \quad \frac{e :: DB^{\mathcal{X}}_{\mathcal{Y}} \quad \mathcal{X} \cap \mathcal{Y} = \phi}{\mathbf{cycle}(e) \longrightarrow e}$$

Fig. 4. Auxiliary Rewriting Rules

2.7 Other Prior Rewriting Rules

Apart from fusion rules, the following rewriting rules for **rec** are proposed in [4] for optimizations. Type of e is assumed to be $DB^{\mathcal{Z}}_{\mathcal{Z}}$. They simplify the argument of **rec** and increases chances of fusions. Some of them are recapped below.

$$\begin{aligned}\mathbf{rec}(\lambda(\$l, \$t).e)(\{\}) &= {}^{1}\textstyle\bigoplus_{\&z \in \mathcal{Z}} \&z := \{\} \\ \mathbf{rec}(\lambda(\$l, \$t).e)(\{l : d\}) &= e[l/\$l][d/\$t] \mathbin{@} \mathbf{rec}(\lambda(\$l, \$t).e)(d)\end{aligned}$$

The first rule eliminates **rec**, while the second rule eliminates an edge from the argument.

Additional rules proposed by (full version of) Hidaka et al. [8] to further simplify the body of **rec** are given in Fig. 4. The rules in the last line in Fig. 4 can be generalized by static analysis of the marker in the following section. And given the static analysis, we can optimize further as described in Section 4.

3 Enhanced Static Analysis

This section proposes our enhanced marker analysis. Figure 5 shows the proposed marker *inference* rules for UnCAL. Static environment Γ denotes mapping from variables to their types. We assume that the types of free variables are given. Since we focus on graph values, we omit rules for labels. Roughly speaking, $DB^{\mathcal{X}}_{\mathcal{Y}}$ is a type for graphs that have $\mathcal{X}$ input markers exactly and have at most $\mathcal{Y}$ output markers, which will be shown formally by Lemma 1.

The original typing rules were provided based on the subtyping rule

$$\frac{\Gamma \vdash e :: DB^{\mathcal{X}}_{\mathcal{Y}} \quad \mathcal{Y} \subseteq \mathcal{Y}'}{\Gamma \vdash e :: DB^{\mathcal{X}}_{\mathcal{Y}'}}$$

and required the arguments of $\cup$, $\oplus$, **if** to have identical sets of output markers. Unlike the original rules, the proposed type system does not use the subtyping rule directly for inference. Combined with the forward evaluation semantics $\mathcal{F}[\![]\!]$ that is summarized in [6], we have the following type safety property.

[1] Original right hand side was {} in [4], but we corrected here.

[5] Original rule (let's say $@_o$) which requires $\mathcal{Y}_1 = \mathcal{X}_2$ is relaxed here. Our @ can be defined by $g_1 \mathbin{@} g_2 = (g_1 \mathbin{@_o} \mathsf{Id}^{\mathcal{X}_2 \setminus \mathcal{Y}_1}_{\mathcal{X}_2 \setminus \mathcal{Y}_1}) \mathbin{@_o} (\mathsf{Bot}^{\mathcal{Y}_1 \setminus \mathcal{X}_2}_{\emptyset} \oplus g_2)$. This particular definition in which markers $\mathcal{Y}_1 \setminus \mathcal{X}_2$ are peeled off is close to the original semantics because final output markers coincide. Extension in which these excess output markers remain would be possible, allowing the markers to be used later to connect to other graphs.

$$\mathcal{X} \cdot \mathcal{Y} \stackrel{\text{def}}{=} \{\&x \cdot \&y \mid \&x \in \mathcal{X}, \&y \in \mathcal{Y}\} \quad \& \cdot \&x = \&x \cdot \& = \&x \quad (\&x \cdot \&y) \cdot \&z = \&x \cdot (\&y \cdot \&z)$$

$$\frac{}{\Gamma \vdash \{\} :: DB_{\emptyset}} \quad \frac{\Gamma \vdash l :: \mathit{Label} \quad \Gamma \vdash e :: DB_{\mathcal{Y}}}{\Gamma \vdash \{l : e\} :: DB_{\mathcal{Y}}} \quad \frac{\Gamma \vdash e_1 :: DB^{\mathcal{X}}_{\mathcal{Y}_1} \quad \Gamma \vdash e_2 :: DB^{\mathcal{X}}_{\mathcal{Y}_2}}{\Gamma \vdash e_1 \cup e_2 :: DB^{\mathcal{X}}_{\mathcal{Y}_1 \cup \mathcal{Y}_2}}$$

$$\frac{}{\Gamma \vdash () :: DB^{\emptyset}_{\emptyset}} \quad \frac{\Gamma \vdash e :: DB^{\mathcal{Z}}_{\mathcal{Y}}}{\Gamma \vdash \&x := e :: DB^{\{\&x\} \cdot \mathcal{Z}}_{\mathcal{Y}}} \quad \frac{}{\Gamma \vdash \&y :: DB_{\{\&y\}}}$$

$$\frac{\Gamma \vdash e_1 :: DB^{\mathcal{X}_1}_{\mathcal{Y}_1} \quad \Gamma \vdash e_2 :: DB^{\mathcal{X}_2}_{\mathcal{Y}_2} \quad \mathcal{X}_1 \cap \mathcal{X}_2 = \emptyset}{\Gamma \vdash e_1 \oplus e_2 :: DB^{\mathcal{X}_1 \cup \mathcal{X}_2}_{\mathcal{Y}_1 \cup \mathcal{Y}_2}} \quad \frac{\Gamma \vdash e_1 :: DB^{\mathcal{X}_1}_{\mathcal{Y}_1} \quad \Gamma \vdash e_2 :: DB^{\mathcal{X}_2}_{\mathcal{Y}_2}}{\Gamma \vdash e_1 \mathbin{@} e_2 :: DB^{\mathcal{X}_1}_{\mathcal{Y}_2}}{}^{5} \quad \frac{\Gamma \vdash e :: DB^{\mathcal{X}}_{\mathcal{Y}}}{\Gamma \vdash \mathbf{cycle}(e) :: DB^{\mathcal{X}}_{\mathcal{Y} \setminus \mathcal{X}}}$$

$$\frac{\Gamma(\$g) = DB^{\mathcal{X}}_{\mathcal{Y}}}{\Gamma \vdash \$g :: DB^{\mathcal{X}}_{\mathcal{Y}}} \quad \frac{\Gamma \vdash e_{\mathrm{a}} :: DB^{\mathcal{X}}_{\mathcal{Y}} \quad \Gamma\{\$l \mapsto \mathit{Label}, \$g \mapsto DB_{\mathcal{Y}}\} \vdash e_b :: DB^{\mathcal{Z}_i}_{\mathcal{Z}_o} \quad \mathcal{Z} = \mathcal{Z}_i \cup \mathcal{Z}_o}{\Gamma \vdash \mathbf{rec}(\lambda(\$l, \$g).e_{\mathrm{b}})(e_{\mathrm{a}}) :: DB^{\mathcal{X} \cdot \mathcal{Z}}_{\mathcal{Y} \cdot \mathcal{Z}}}$$

$$\frac{\Gamma \vdash l_1 :: \mathit{Label} \quad \Gamma \vdash l_2 :: \mathit{Label} \quad \Gamma \vdash e_{\mathrm{t}} :: DB^{\mathcal{X}}_{\mathcal{Y}_{\mathrm{t}}} \quad \Gamma \vdash e_{\mathrm{f}} :: DB^{\mathcal{X}}_{\mathcal{Y}_{\mathrm{f}}}}{\Gamma \vdash \mathbf{if}\, l_1 = l_2\, \mathbf{then}\, e_{\mathrm{t}}\, \mathbf{else}\, e_{\mathrm{f}} :: DB^{\mathcal{X}}_{\mathcal{Y}_{\mathrm{t}} \cup \mathcal{Y}_{\mathrm{f}}}} \quad \frac{\Gamma \vdash e_1 :: DB^{\mathcal{X}_1}_{\mathcal{Y}_1} \quad \Gamma\{\$g \mapsto DB^{\mathcal{X}_1}_{\mathcal{Y}_1}\} \vdash e_2 :: DB^{\mathcal{X}_2}_{\mathcal{Y}_2}}{\Gamma \vdash \mathbf{let}\, \$g = e_1\, \mathbf{in}\, e_2 :: DB^{\mathcal{X}_2}_{\mathcal{Y}_2}}$$

Fig. 5. UnCAL Static Typing (Marker Inference) Rules: Rules for *Label* are Omitted

Lemma 1 (Type Safety). *Assume that g is the graph obtained by $g = \mathcal{F}[\![e]\!]$ for an expression e. Then, $\vdash e :: DB^{\mathcal{X}}_{\mathcal{Y}}$ implies both* $\mathsf{inMarker}(g) = \mathcal{X}$ *and* $\mathsf{outMarker}(g) \subseteq \mathcal{Y}$.

Lemma 1 guarantees that the set of input markers estimated by the type inference is exact in the sense that the set of input markers generated by evaluation exactly coincides with that of the inferred type. For the output markers, the type system provides an over-approximation in the sense that the set of output markers generated by evaluation is a subset of the inferred set of output markers. Since the statement on the input marker is a direct consequence of the rules in [4], we focus that on the output markers and prove it. The proof, which is based on induction on the structure of UnCAL expression, is in the full version [7] of this paper.

4 Enhanced Rewiring Optimization

This section proposes enhanced rewriting optimization rules based on the static analysis shown in the previous section.

4.1 Rule for @ and Revised Fusion Rule

Statically-inferred markers enables us to optimize expressions much more. We can generalize the rewriting rules in the last row of Fig. 4 by not just referring to the pattern of subexpressions but its estimated markers, such as

$$() \mathbin{@} e \longrightarrow () \qquad \Rightarrow \qquad \frac{e_1 :: DB^{\mathcal{X}}_{\emptyset}}{e_1 \mathbin{@} e_2 \longrightarrow e_1} \qquad (2)$$

As we have seen in Sect. 2, we have two fusion rules for **rec**. Although the first rule can be used to gain performance, the second rule is more complex so less performance gain is expected. Using (2), we can relax the condition of the first condition of the fusion rule (1) to increase chances to apply the first rule as follows.

$$\begin{aligned}&\mathbf{rec}(\lambda(\$l_2, \$t_2).e_2)(\mathbf{rec}(\lambda(\$l_1, \$t_1).e_1)(e_0))\\ &\quad = \mathbf{rec}(\lambda(\$l_1, \$t_1).\, \mathbf{rec}(\lambda(\$l_2, \$t_2).e_2)(e_1))(e_0)\\ &\qquad \text{if } \$t_2 \text{ does not appear free in } e_2, \underline{\text{ or } e_1 :: DB^{\mathcal{X}}_{\emptyset}}\end{aligned}$$

Here, the underlined part is changed.

4.2 Further Optimization with Static Marker Information

In this section, general rules for $e_1 \mathbin{@} e_2$ is investigated. First to eliminate $@\ e_2$, and then to statically compute @ by plugging e_2 into e_1.

4.2.1 Static Output-Marker Removal Algorithm and Soundness

For more general cases of @ where connections by ε do not happen, we have the following rule.

$$\frac{e_1 :: DB^{\mathcal{X}}_{\mathcal{Y}_1} \quad e_2 :: DB^{\mathcal{Y}_2}_{\mathcal{Z}} \quad \mathcal{Y}_1 \cap \mathcal{Y}_2 = \emptyset \quad \mathsf{Rm}_{\mathcal{Y}_1}\langle\!\langle e_1 \rangle\!\rangle = e}{e_1 \mathbin{@} e_2 \longrightarrow e}$$

$\mathsf{Rm}_{\mathcal{Y}}\langle\!\langle e \rangle\!\rangle$ denotes static removal of the set of output markers. Without this, rewriting result in spurious output markers from e_1 remained in the final result. The formal definition of $\mathsf{Rm}_{\mathcal{Y}}\langle\!\langle e \rangle\!\rangle$ is shown below.

$$\begin{aligned}\mathsf{Rm}_{\emptyset}\langle\!\langle e \rangle\!\rangle = e \quad \mathsf{Rm}_{\mathcal{X}\cup\mathcal{Y}}\langle\!\langle e \rangle\!\rangle &= \mathsf{Rm}_{\mathcal{Y}}\langle\!\langle \mathsf{Rm}_{\mathcal{X}}\langle\!\langle e \rangle\!\rangle \rangle\!\rangle \quad \mathsf{Rm}_{\{\&y\}}\langle\!\langle \{\} \rangle\!\rangle = \{\}\\ \mathsf{Rm}_{\{\&y\}}\langle\!\langle () \rangle\!\rangle = () \quad \mathsf{Rm}_{\{\&y\}}\langle\!\langle \&y \rangle\!\rangle &= \{\} \quad \mathsf{Rm}_{\{\&y\}}\langle\!\langle \&x \rangle\!\rangle = \&x\\ \mathsf{Rm}_{\{\&y\}}\langle\!\langle e_1 \odot e_2 \rangle\!\rangle &= \mathsf{Rm}_{\{\&y\}}\langle\!\langle e_1 \rangle\!\rangle \odot \mathsf{Rm}_{\{\&y\}}\langle\!\langle e_2 \rangle\!\rangle \quad (\odot \in \{\cup, \oplus\})\\ \mathsf{Rm}_{\{\&y\}}\langle\!\langle \&x := e \rangle\!\rangle &= (\&x := \mathsf{Rm}_{\{\&y\}}\langle\!\langle e \rangle\!\rangle)\\ \mathsf{Rm}_{\{\&y\}}\langle\!\langle \{l : e\} \rangle\!\rangle &= \{l : \mathsf{Rm}_{\{\&y\}}\langle\!\langle e \rangle\!\rangle\}\\ \mathsf{Rm}_{\{\&y\}}\langle\!\langle e_1 \mathbin{@} e_2 \rangle\!\rangle &= e_1 \mathbin{@} \mathsf{Rm}_{\{\&y\}}\langle\!\langle e_2 \rangle\!\rangle\\ \mathsf{Rm}_{\{\&y\}}\langle\!\langle \mathbf{if}\ b\ \mathbf{then}\ e_1\ \mathbf{else}\ e_2 \rangle\!\rangle &= \mathbf{if}\ b\ \mathbf{then}\ \mathsf{Rm}_{\{\&y\}}\langle\!\langle e_1 \rangle\!\rangle\ \mathbf{else}\ \mathsf{Rm}_{\{\&y\}}\langle\!\langle e_2 \rangle\!\rangle\end{aligned}$$

Since the output markers of the result of @ are not affected by that of e_1, e_1 is not visited in the rule of @. In the following, $\mathsf{Id}^{\mathcal{Y}}_{\mathcal{Y}}$ and $\mathsf{Bot}^{\mathcal{Y}}_{\emptyset}$ are respectively defined as $\bigoplus_{\&z\in\mathcal{Y}} \&z := \&z$ and $\bigoplus_{\&z\in\mathcal{Y}} \&z := \{\}$.

$$\frac{e :: DB^{\mathcal{X}}_{\mathcal{Y}} \quad \&y \in (\mathcal{Y} \setminus \mathcal{X}) \quad \mathsf{Rm}_{\{\&y\}}\langle\!\langle e \rangle\!\rangle = e'}{\mathsf{Rm}_{\{\&y\}}\langle\!\langle \mathbf{cycle}(e) \rangle\!\rangle = \mathbf{cycle}(e')} \qquad \frac{e :: DB^{\mathcal{X}}_{\mathcal{Y}} \quad \&y \notin (\mathcal{Y} \setminus \mathcal{X})}{\mathsf{Rm}_{\{\&y\}}\langle\!\langle \mathbf{cycle}(e) \rangle\!\rangle = \mathbf{cycle}(e)}$$

$$\frac{\$v :: DB^{\mathcal{X}}_{\mathcal{Y}} \quad \&y \notin \mathcal{Y}}{\mathsf{Rm}_{\{\&y\}}\langle\!\langle \$v \rangle\!\rangle = \$v} \qquad \frac{\$v :: DB^{\mathcal{X}}_{\mathcal{Y}} \quad \&y \in \mathcal{Y}}{\mathsf{Rm}_{\{\&y\}}\langle\!\langle \$v \rangle\!\rangle = \$v \mathbin{@} (\mathsf{Bot}^{\{\&y\}}_{\emptyset} \oplus \mathsf{Id}^{\mathcal{Y}\setminus\{\&y\}}_{\mathcal{Y}\setminus\{\&y\}})}$$

The first rule of $\$v$ says that according to the safety of type inference, $\&y$ is guaranteed not to result at run-time, so the expression $\$v$ remains unchanged. The second rule actually removes the output marker $\&y_j$, but static removal is impossible. So the removal is deferred till run-time. The output node marked $\&y_j$ is connected to node produced by $\&y := \{\}$. Since the latter node has no output marker, the original output marker disappears from the graph produced by the evaluation. The rest of the $\&y_k := \&y_k$ does no operation on the marker. Since estimation $\mathcal{Y}$ is the upper bound, the output maker may not be produced at run-time. If it is the case, connection with ε-edge by @ does not occur, and the nodes produced by the := expressions are left unreachable, so the transformation is still valid. As another side effect, @ may connect identically marked output nodes to single node. However, the graph before and after this "funneling" connection are bisimilar, since every leaf node with identical output markers are bisimilar by definition. Should the output nodes are to be further connected to other input nodes, the target node is always single, because more than one node with identical input marker is disallowed by the data model. So this connection does no harm. Note that the second rule increases the size of the expression, so it may increase the cost of evaluation.

$$\frac{\mathbf{rec}(\lambda(\$l, \$t).e_{\mathrm{b}})(e_{\mathrm{a}}) :: DB^{\mathcal{X}\cdot\mathcal{Z}}_{\mathcal{Y}\cdot\mathcal{Z}} \quad \&y \in \mathcal{Y} \quad \mathsf{Rm}_{\{\&y\}}\langle\!\langle e_{\mathrm{a}} \rangle\!\rangle = e'_{\mathrm{a}}}{\mathsf{Rm}_{\{\&y.\&z \mid \&z \in \mathcal{Z}\}}\langle\!\langle \mathbf{rec}(\lambda(\$l, \$t).e_{\mathrm{b}})(e_{\mathrm{a}}) \rangle\!\rangle = \mathbf{rec}(\lambda(\$l, \$t).e_{\mathrm{b}})(e'_{\mathrm{a}})}$$

For **rec**, one output marker $\&y$ in e_{a} corresponds to $\{\&y\} \cdot \mathcal{Z} = \{\&y.\&z \mid \&z \in \mathcal{Z}\}$ in the result. So removal of $\&y$ from e_{a} results in removal of all of the $\{\&y\} \cdot \mathcal{Z}$. So only removal of all of $\{\&y.\&z \mid \&z \in \mathcal{Z}\}$ at a time is allowed.

Lemma 2 (Soundness of Static Output-Marker Removal Algorithm). *Assume that $G = (V, E, I, O)$ is a graph obtained by $G = \mathcal{F}[\![e]\!]$ for an expression e, and e' is the expression obtained by $\mathsf{Rm}_{\mathcal{Y}}\langle\!\langle e \rangle\!\rangle$. Then, we have $\mathcal{F}[\![e']\!] = (V, E, I, \{(v, \&y) \in O \mid \&y \notin \mathcal{Y}\})$.*

Lemma 2 guarantees that no output marker in $\mathcal{Y}$ appears at run-time if $\mathsf{Rm}_{\mathcal{Y}}\langle\!\langle e \rangle\!\rangle$ is evaluated.

4.2.2 Plugging Expression to Output Marker Expression

The following rewriting rule is to plug an expression into another through correspondingly marked node.

$$\{l : \&y\} \mathbin{@} (\&y := e) \longrightarrow \{l : e\}$$

This kind of rewriting was actually implicitly used in the exemplification of optimization in [4], but was not generalized. We can generalize this rewriting as

$$e \mathbin{@} (\&y := e') \longrightarrow \begin{cases} \mathsf{Rm}_{\mathcal{Y}\setminus\&y}\langle\!\langle e \rangle\!\rangle[e'/\&y] & \text{if } \&y \in \mathcal{Y} \text{ where } e :: DB^{\mathcal{X}}_{\mathcal{Y}} \\ \mathsf{Rm}_{\mathcal{Y}}\langle\!\langle e \rangle\!\rangle & \text{otherwise.} \end{cases}$$

where $e[^{e'}/_{\&y}]$ denotes substitution of $\&y$ by e' in e. Since nullrary constructors $\{\}$, $()$, and $\&x \neq \&y$ do not produce output marker $\&y$, the substitution takes no effect and the rule in the latter case apply. So we focus on the former case in the sequel. For most of the constructors the substitution rules are rather straightforward:

$$\begin{aligned}
\&y[^{e}/_{\&y}] &= e \\
(e_1 \odot e_2)[^{e}/_{\&y}] &= (e_1[^{e}/_{\&y}]) \odot (e_2[^{e}/_{\&y}]) \quad (\odot \in \{\cup, \oplus\}) \\
(\&x := e)[^{e'}/_{\&y}] &= (\&x := (e[^{e'}/_{\&y}])) \\
\{l : e\}[^{e'}/_{\&y}] &= \{l : (e[^{e'}/_{\&y}])\} \\
(e_1 \mathbin{@} e_2)[^{e}/_{\&y}] &= e_1 \mathbin{@} (e_2[^{e}/_{\&y}]) \\
(\textbf{if } b \textbf{ then } e_1 \textbf{ else } e_2)[^{e}/_{\&y}] &= \textbf{if } b \textbf{ then } (e_1[^{e}/_{\&y}]) \textbf{ else } (e_2[^{e}/_{\&y}])
\end{aligned}$$

Since the final output marker for @ is not affected by that of e_1, e_1 is not visited in the rule of @. For **cycle**, we should be careful to avoid capturing of marker.

$$\textbf{cycle}(e)[^{e'}/_{\&y}] = \begin{cases} \textbf{cycle}(e[^{e'}/_{\&y}]) & \text{if } (\mathcal{Y}' \cap \mathcal{X}) = \emptyset \text{ where } e :: DB^{\mathcal{X}}_{\mathcal{Y}} \quad e' :: DB_{\mathcal{Y}'} \\ \overline{\textbf{cycle}}(e)[^{e'}/_{\&y}] & \text{otherwise.} \end{cases}$$

The above rule says that if $\&y$ will be a "free" marker in e, that is, the output markers in e', namely $\mathcal{Y}'$ will not be captured by **cycle**, then we can plug e' into output marker expression in e. If some of the output markers in $\mathcal{Y}'$ are included in $\mathcal{X}$, then the renaming is necessary. As suggested in the full version of [3], markers in $\mathcal{X}$ instead of those in $\mathcal{Y}'$ should be renamed. And that renaming can be compensated outside of **cycle** as follows:

$$\overline{\textbf{cycle}}(e) \stackrel{\text{def}}{=} (\bigoplus_{\&x \in \mathcal{X}} \&x := \&tmp_x) \mathbin{@} \textbf{cycle}(e[\&tmp_{x_1}/_{\&x_1}] \ldots [\&tmp_{x_M}/_{\&x_M}])$$

where $\&x_1, \ldots, \&x_M = \mathcal{X}$ are the markers to be renamed, and $\mathcal{X}$ of $e :: DB^{\mathcal{X}}_{\mathcal{Y}}$ is used. Note that in the renaming, not only output markers, but also input markers are renamed. $\&tmp_{x_1}, \ldots, \&tmp_{x_M}$ are corresponding fresh (temporary) markers. The left hand side of @ recovers the original name of the markers. After renaming by $\overline{\textbf{cycle}}$, no marker is captured anymore, so substitution is guaranteed to succeed. For variable reference and **rec**, static substitution is impossible. So we resort to the following generic "fall back" rule.

$$\frac{e \in \{\$v, \textbf{rec}(\_)(\_)\} \quad e :: DB^{\mathcal{X}}_{\mathcal{Y}} \quad \mathcal{Y} = \{\&y_1, \ldots, \&y_j, \ldots, \&y_n\}}{e[^{e'}/_{\&y_j}] = e \mathbin{@} \begin{pmatrix} \&y_1 := \&y_1, \ldots, \&y_{j-1} := \&y_{j-1}, \&y_j := e', \\ \&y_{j-1} := \&y_{j-1}, \ldots, \&y_n := \&y_n \end{pmatrix}}$$

The "fall back" rule is used for **rec** because unlike output marker removal algorithm, we can not just plug e into e_{a} since that will not plug e but $\textbf{rec}(\lambda(\$l, \$t).e_{\mathrm{b}})(e)$ in the result. We could have used the inverse $\textbf{rec}(\lambda(\$l, \$t).e_{\mathrm{b}})^{-1}$ to plug $\textbf{rec}(\lambda(\$l, \$t).e_{\mathrm{b}})^{-1}(e')$ instead, but the inverse does not always exist in general.

The overall rewriting is conducted by two mutually recursive functions as follows: driver function P first apply itself to subexpressions recursively, and then apply function F that implements $\longrightarrow$ and other rewriting rules recursively such as fusions described in this paper, on the result of P.

With respect to proposed rewriting rules in this section, the following theorem hold.

Theorem 1 (Soundness of Rewriting). *If $e \longrightarrow e'$, then $\mathcal{F}[\![e]\!]$ is bisimilar to $\mathcal{F}[\![e']\!]$.*

It can be proved by simple induction on the structure of UnCAL expressions, and omitted here.

Example 4. The following transformation that apply selection after *consecutive* in Example 3

$\mathbf{rec}(\lambda(\$l_1, \$g_1).\, \mathbf{if}\ \$l_1 = \mathtt{a}\ \mathbf{then}\ \{\$l_1 : \$g_1\}\ \mathbf{else}\ \{\})(\mathit{consecutive}(\$db))$

is rewritten as follows:

$$
\begin{aligned}
& \{ \text{ expand definition of } \textit{consecutive} \text{ and apply 2nd fusion rule } \} \\
= \ & \mathbf{rec}(\lambda(\$l, \$g).\, \mathbf{rec}(\lambda(\$l_1, \$g_1).\, \mathbf{if}\ \$l_1 = \mathtt{a}\ \mathbf{then}\ \{\$l_1 : \$g_1\}\ \mathbf{else}\ \{\}) \\
& \qquad (\mathbf{rec}(\lambda(\$l', \$g').\, \mathbf{if}\ \$l = \$l'\ \mathbf{then}\ \{\mathtt{result} : \$g'\}\ \mathbf{else}\ \{\})(\$g) \\
& \qquad\quad @\, \mathbf{rec}(\lambda(\$l, \$g).\, \mathbf{rec}(\lambda(\$l', \$g'). \\
& \qquad\qquad \mathbf{if}\ \$l = \$l'\ \mathbf{then}\ \{\mathtt{result} : \$g'\}\ \mathbf{else}\ \{\})(\$g))(\$g)))(\$db) \\
& \{ \ (2) \ \} \\
= \ & \mathbf{rec}(\lambda(\$l, \$g).\, \mathbf{rec}(\lambda(\$l_1, \$g_1).\, \mathbf{if}\ \$l_1 = \mathtt{a}\ \mathbf{then}\ \{\$l_1 : \$g_1\}\ \mathbf{else}\ \{\}) \\
& \qquad (\mathbf{rec}(\lambda(\$l', \$g').\, \mathbf{if}\ \$l = \$l'\ \mathbf{then}\ \{\mathtt{result} : \$g'\}\ \mathbf{else}\ \{\})(\$g)))(\$db) \\
& \{ \text{ 2nd fusion rule, (2), } \mathbf{rec} \text{ rule for } \mathbf{if} \text{ and } \{l : d\}, \text{ static label comparison } \} \\
= \ & \mathbf{rec}(\lambda(\$l, \$g).\, \mathbf{rec}(\lambda(\$l', \$g').\{\})(\$g))(\$db)
\end{aligned}
$$

This example demonstrates the second fusion rule promotes to the first. The top level edges of the result of *consecutive* are always labeled `result` while the selection selects subgraphs under edges labeled `a`. So the result will always be empty, and correspondingly the body of **rec** in the final result is {}.

More examples can be found in the full version [7] of this paper.

5 Implementation and Performance Evaluation

This section reports preliminary performance evaluations.

5.1 Implementation in GRoundTram

All of the transformation in the paper are implemented in GRoundTram, or Graph Roundtrip Transformation for Models, which is a system to build a bidirectional transformation between two models (graphs). All the source codes are available online at `www.biglab.org`. The following experimental results are obtained by the system.

Table 1. Summary of Experiments (running time is in CPU seconds)

	direction	no rewriting	previous [4, 8]	ours
Class2RDB	forward	1.18	0.68	0.68
	backward	14.5	7.99	7.89
PIM2PSM	forward	0.08	0.77 (2*3)	0.07 (2*13)
	backward	1.62	3.64	0.75
C2Osel	forward	0.04	0.04 (2*1)	0.05 (2*11)
	backward	2.26	0.26	0.27
C2Osel'	forward	0.05	0.06 (2*1)	0.04 (2*11)
	backward	2.53	2.58	1.26
UnQL	forward	0.022	0.016 (1*1)	0.010 (1*1)
	backward	0.85	0.30	0.15

5.2 Performance Results

Performance evaluation was conducted on GRoundTram, running on MacOSX over MacBookPro 17 inch, with 3.06 GHz Intel Core 2 Duo CPU. Time complexity is PTIME for the size of input graph[4], and exponential in the size (number of compositions or nesting of **rec**s) of the transformation. In the experiments, the size of input data (graph) is not very large (up to a hundred of nodes).

Table 1 shows the experimental results. Each running time includes time for forward and backward transformations [6], and for backward transformations, algorithm for edge-renaming is used, and no modification on the target is actually given. However, we suppose presence of modification would not make much difference in the running time. Running time of forward transformation in which rewriting is applied (last two columns) includes time for rewriting. Rewriting took 0.006 CPU seconds at the worst case (*PIM2PSM*, ours). *Class2RDB* stands for class diagram to table diagram transformation, *PIM2PSM* for platform independent model to platform specific model transformation, C2Osel is for transformation of customer oriented database into order oriented database, followed by a simple selection, and *UnQL* is the example that is extracted from our previous paper [8], which was borrowed from [4]. It is a composition of two **rec**s.

The numbers in parentheses show how often the fusion transformation happened. For example, *PIM2PSM* led to 3 fusions based on the second rule, and further enhanced rewriting led to 10 more fusion rule applications, all of which promoted to the first rule via proposed rewriting rule (2). Same promotions happened to *C2Osel*. Except for *C2Osel'*, a run-time optimization in which unreachable parts are removed after every application of **rec** is applied. Enhanced rewriting led to performance improvements in both forward and backward evaluations, except *C2Osel*. Comparing "previous" with "no rewriting", *PIM2PSM* and *C2Osel'* led to slowdown. These slowdown are explained as follows. The fusion turns composition of **rec**s to their nesting. In the presence of the run-

time optimization, composition is advantageous than nesting when only small part of the result is passed to the subsequent **rec**s, which will run faster than when passed entire results (including unreachable parts). Once nested, intermediate result is not produced, but the run-time optimization is suppressed because every execution of the inner rec traverses the input graph. *C2Osel'* in which run-time optimization is turned off, shows that the enhanced rewriting itself lead to performance improvements.

6 Related Work

Some optimization rules were mentioned in [8], but relationship with static marker analysis was not covered in depth. By enhanced marker analysis and rewriting rules in present paper, all the rules in [8] can be generalized uniformly.

An implementation of rewriting optimizations was reported in [6] but concrete strategies were not included in the paper.

Full (technical report) version of [3] dealt with plugging constructor-only expressions into output marker expressions. It was motivated by authors need to express semantics of @ at the constructor expression level and not graph data level as in [4]. It also mentioned renaming of markers to avoid capture of the output markers in the cycle expressions. We do attempt the same thing at the expression level but we argue here more formally.

The technical report also mentioned the semantics of **rec** on the cycle constructor expressions, even when the body expressions refer to graph variables, although marker environment that maps markers to connected subgraphs introduced there makes the semantics complex. The journal version [4] did not include this semantics on the cycle constructor expressions. But we could use the semantics to enhance rewriting rules for **rec** with **cycle** arguments.

The journal version mentioned run-time evaluation strategy in which only necessary components of structural recursion is executed. For example, only $\&z_1$ component of **rec** in $\&z_1 \mathbin{@} \mathbf{rec}(\_)(\_)$ is evaluated.

A static analysis of UnCAL was described in [1], but the main motivation was to analyze structure of graphs using graph schema.

7 Conclusion

In this paper, under the context of graph transformation using UnCAL graph algebra, enhanced static marker inference is first formalized. Fusion rule becomes more powerful thanks to the static marker analysis. Further rewriting rules based on this inference are also explored. Marker renaming for capture avoidance is formalized to support the rewriting rules.

Preliminary performance evaluation shows the usefulness of the optimization for various non-trivial transformations in the field of software engineering research.

Under the context of bidirectional graph transformations [6], one of the advantage of static analysis is that we can keep implementation of bidirectional

interpreter intact. Future work under this context includes reasoning about effects on the backward updatability. Although rewriting is sound with respect to well-behavedness of bidirectional transformations, backward transformation before and after rewriting may accept different update operations. Our conjecture is that simplified transformation accepts more updates, but this argument requires further discussions.

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Towards Resource-driven CLP-based Test Case Generation

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Abstract. Test Data Generation (TDG) aims at automatically obtaining *test inputs* which can then be used by a software testing tool to validate the functional behaviour of the program. In this paper, we propose *resource-aware* TDG, whose purpose is to generate test cases (from which the test inputs are obtained) with associated *resource consumption*s. The framework is parametric w.r.t. the notion of resource (it can measure memory, steps, etc.) and allows using software testing to detect bugs related to non-functional aspects of the program. As a further step, we introduce *resource-driven* TDG whose purpose is to guide the TDG process by taking resource consumption into account. Interestingly, given a *resource policy*, TDG is guided to generate test cases that adhere to the policy and avoid the generation of test cases which violate it.

1 Introduction

Test data generation (TDG) is the process of automatically generating *test inputs* for interesting test *coverage criteria*. Examples of coverage criteria are: *statement coverage* which requires that each line of the code is executed; *loop-k* which limits to a threshold k the number of times we iterate on loops. The standard approach to generating test cases statically is to perform a *symbolic execution* of the program [6,7,11,13,16,17,19], where the contents of variables are expressions rather than concrete values. Symbolic execution produces a system of constraints over the input variables consisting of the conditions to execute the different paths. The conjunction of these constraints represents the equivalence class of inputs that would take this path. In what follows, we use the term *test cases* to refer to such constraints. Concrete instantiations of the test cases that satisfy the constraints are generated to obtain test inputs for the program. Testing tools can later test the *functionality* of an application by executing such test inputs and checking that the output is as expected. The CLP-based approach to TDG of *imperative*[3] programs [4,10] consists of two phases: (1) first, an imperative program is translated into an equivalent CLP program and (2) symbolic execution is performed on the CLP program by relying on the standard CLP's evaluation mechanisms (extended with a special treatment for heap-allocated data [10]) which provide symbolic execution for free.

[3] The application of this approach to TDG of logic programs must consider failure [19] and, to functional programs, should consider laziness, higher-order, etc. [8].

Non-functional aspects of an application, like its resource consumption, are often more difficult to understand than functional properties. Profiling tools execute a program for concrete inputs to assess the associated resource consumption, a non-functional aspect of the program. Profilers can be parametric w.r.t. the notion of resource which often includes cost models like time, number of instructions, memory consumed, number of invocations to methods, etc. Usually, the purpose of profiling is to find out which parts of a device or software contribute most to its poor performance and find bugs related to the resource consumption.

In this paper, we propose *resource-aware TDG* which strives to build performance into test cases by additionally generating their resource consumption, thus enriching standard TDG with non-functional properties. The main idea is that, during the TDG process, we keep track of the exercised instructions to obtain the test case. Then, in a simple post-process we map each instruction into a corresponding cost, we obtain for each class of inputs a detailed information of its resource consumption (including the cost models above). Our approach is not reproducible by first applying TDG, then instantiating the test cases to obtain concrete inputs and, finally, performing profiling on the concrete data. This is because, for some cost criteria, resource-aware TDG is able to generate symbolic (i.e., non-constant) costs. E.g., when measuring memory usage, the amount of memory to create might depend on an input parameter (e.g., the length of an array to be created is an input argument). The resource consumption of the test case will be a symbolic expression that profilers cannot compute.

A well-known problem of TDG is that it produces a large number of test cases even for medium size programs. This introduces scalability problems as well as complicates human reasoning on them. An interesting aspect of resource-aware TDG is that resources can be taken into account in order to filter out test cases which do not consume more (or less) than a given amount of resources, i.e, one can consider a *resource policy*. This leads to the idea of resource-*driven* TDG, i.e., a new heuristics which aims at guiding the TDG process to generate test cases that adhere to the resource policy. The potential interest is that we can prune the symbolic execution tree and produce, more efficiently, test cases for inputs which otherwise would be very expensive (and even impossible) to obtain.

Our approach to resource-driven CLP-based TDG consists of two phases. First, in a pre-process, we obtain (an over-approximation of) the set of *traces* in the program which lead to test cases that adhere to the resource policy. We sketch several ways of automatically inferring such traces, starting from the simplest one that relies on the call graph of the program to more sophisticated ones that enrich the abstraction to reduce the number of unfeasible paths. An advantage of formalizing our approach in a CLP-based setting is that traces can be partially defined and the TDG engine then completes them. Second, executing standard CLP-based TDG with a (partially) instantiated trace generates a test case that satisfies the resource policy (or it fails if the trace is unfeasible). An interesting aspect is that, if the trace is fully instantiated, TDG becomes deterministic and solutions can be found very efficiently. Also, since there is no need to backtrack, test cases for the different traces can be computed in parallel.

2 CLP-based Test Case Generation

This section summarizes the CLP-based approach to TDG of [10] and extends it to incorporate *traces* in the CLP programs that will be instrumental later to define the resource-aware framework. CLP-based TDG consists of two main steps: (1) imperative programs are translated into an extended form of equivalent CLP-programs which incorporate built-in operations to handle dynamic data, and, (2) symbolic execution is performed on the CLP-translated programs by relying on the standard evaluation mechanisms of CLP with special operations to treat such built-ins. The next two sections overview these steps.

2.1 CLP-Translation with Traces

The translation of imperative (object-oriented) programs into equivalent CLP program has been subject of previous work (see, e.g., [1, 9]). Therefore, we will not go into details of how the transformation is done, but rather simply recap the features of the translated programs in the next definition.

Definition 1 (CLP-translated program with trace). *Given a method* `m` *with input arguments* $\bar{x}$ *and output arguments* $\bar{y}$*. Its CLP-translation consists of a set of predicates* $m, m_1, \ldots, m_n$ *such that each of them is defined by a set of rules of the form "*m_i`(I,O,`$\mathtt{H_{in}}$`,`$\mathtt{H_{out}}$`,`$\mathtt{T_m}$`):-` $g, b_1, \ldots, b_n$*." where:*

1. *m is the entry predicate (named as the method) and its arguments* `I` *and* `O` *are lists of variables that correspond to* $\bar{x}$ *and* $\bar{y}$*.*
2. *For the remaining predicates* $m_1, \ldots, m_n$*,* `I` *and* `O` *are, resp., the list of input and output arguments of this predicate.*
3. $\mathtt{H_{in}}$ *and* $\mathtt{H_{out}}$ *are, resp., the input and output heaps to each predicate.*
4. *If a predicate* m_i *is defined by multiple rules, the guards in each rule contain mutually exclusive conditions. We denote by* m_i^j *the* $j-th$ *rule defining* m_i*.*
5. $g, b_1, \ldots, b_n$ *are CLP-representations of equivalent instructions in the imperative language (as usual, a SSA transformation is performed on the variables), method invocations are replaced by calls to corresponding predicates, and operations that handle data in the heap are translated into built-in predicates (e.g.,* `new_object(H,Class,Ref,H')`*, *`get_field(H,Ref,Fld,Val)`*, etc.).*
6. *Let us denote by* $c_1, \ldots, c_k$ *the sequence of calls within instructions* $b_1, \ldots, b_n$*, the* trace term `T` *for* m_i^j *is* $\mathsf{m_i}(\mathsf{j}, \mathsf{P}, [\mathsf{T_{c_1}}, \ldots, \mathsf{T_{c_k}}])$*, where* $\mathsf{T_{c_g}}$ *is a variable that represents the trace term of the call* c_g *for* $g = 1, \ldots, k$*, and* `P` *is the list of trace parameters, i.e., the subset of the variables in rule* m_i^j *on which the resource consumption depends.*

Given a rule m_i^j*, we denote by* $instr(m_i^j)$ *the sequence of instructions in the original program that have been translated inside rule* m_i^j*.*

As the imperative program is deterministic, the CLP translation is deterministic as well (point 4 in Def. 1). Observe that the global memory (or heap) is explicitly handled in the CLP program by means of logic variables that represent the heap. When a rule is invoked, the input heap $\mathtt{H_{in}}$ is received and, after executing its

```
class Foo {
  Vector[] classify(int[] ns,
                    int div1,
                    int div2,
                    int icap){
    Vector[] r = new Vector[2];
    r[0] = new Vector(icap);
    r[1] = new Vector(icap);
    for (int i=0; i<ns.length; i++){
      if (ns[i]%div1 == 0)
        r[0].add(ns[i]);
      if (ns[i]%div2 == 0)
        r[1].add(ns[i]);
    }
    return r;}}
```

```
class Vector {
  private int[] elems;
  private int size = 0, cap;
  Vector(int iCap) throws Exception{
    if (iCap > 0){
      cap = iCap;
      elems = new int[cap];
    }else{throw Exception;}
  void add(int x){
    if (size == cap){reallocate();}
    elems[size++] = x;
  }
  void reallocate(){
    int nCap = cap*2;
    int[] nElems = new int[nCap];
    for (int i=0; i<cap; i++)
      nElems[i] = elems[i];
    cap = nCap; elems = nElems;}}
```

Fig. 1: Running example - Java source code

body, the heap might be modified, resulting in H_{out}. The operations that modify the heap will be shown in the example. A new aspect of the above transformation is that we add as additional argument to each rule a *trace term* which allows keeping track of the sequence of rules that are executed.

Example 1. Our running example in Fig. 1 is made up of two classes. Class Foo implements method classify that receives an array of integers and returns an array of two objects of type Vector with initial capacity icap and containing, each of them, those elements of ns that are multiples of, resp., div1 and div2. The interesting aspect of class Vector is that, when adding an element using method add, the size of the array is duplicated (in method reallocate) if the size reaches the maximum capacity determined by field cap. Fig. 2 shows an excerpt of the (simplified and pretty-printed) CLP translations obtained by the PET system [4] from the bytecode associated to methods classify, the constructor of Vector (named init), add and reallocate. For brevity, we have omitted the predicates that model the exceptional behavior and some intermediate predicates (where ellipsis appear). Observe that the method classify is transformed into the set of predicates classify, loop1, cond1, if0 (omitted), if1, some of them defined by several (guarded) rules. The operations that handle the heap remain as built-in predicates. Function *instr* in Def. 1 keeps the mapping between rules and bytecode instructions. For instance, *instr*(init)=⟨`iload icap, ifgt, aload this, iload icap, putfield cap, aload this, aload this, getfield cap, newarray int, putfield elems, aload this, iconst 0, putfield size, return`⟩ is the sequence of bytecode instructions that have been translated into rule init.

2.2 Symbolic Execution

When the imperative language does not use dynamic memory, CLP-translated programs can be executed by using the standard CLP's execution mechanism with all arguments being free variables. However, in order to generate heap-allocated data structures, it is required to define heap-related operations which

```
classify([Ns,Div1,Div2,ICap],Out,H,H0,classify(1,[],[T1,T2,T3]) :-
   new_array(H,'Vector',2,V,H1), new_object(H1,'Vector',V0,H2),
   init([r(V0),ICap],[],H2,H3,T1), set_array(H3,V,0,r(V0),H4),
   new_object(H4,'Vector',V1,H5), init([r(V1),ICap],[],H5,H6,T2),
   set_array(H6,V,1,r(V1),H7), loop1([r(Ns),Div1,Div2,r(V),0],Out,H7,H0,T3).
loop1([r(Ns),Div1,Div2,r(V),I],Out,H,H0,loop1(1,[],[T])) :-
   length(H,Ns,L), cond1([L,I,r(Ns),Div1,Div2,r(V)],Out,H,H0,T).
cond1^1([L,I,_,_,_,r(V)],[r(V)],H,H,cond1(1,[],[]) :- I #>= L.
cond1^2([L,I,r(Ns),Div1,Div2,r(V)],Out,H,H0,cond1(2,[],[T]) :- I #< L,
   get_array(H,Ns,I,Nsi), M1 #= Nsi mod Div1,
   if0([M1,r(Ns),Div1,Div2,r(V),I],Out,H,H0,T).
                  ....
if1^1([M,r(Ns),Div1,Div2,r(V),I],Out,H,H0,if1(1,[],[T]) :- M #\= 0,
   Ip #= I+1, loop1([r(Ns),Div1,Div2,r(V),Ip],Out,H,H0,T).
if1^2([0,r(Ns),Div1,Div2,r(V),I],Out,H,H0,if1(2,[],[T1,T2]) :-
   get_array(H,V,1,r(V1)), get_array(H,Ns,I,Nsi),
   add([r(V1),Nsi],[],H,H1,T1), Ip #= I+1,
   loop1([r(Ns),Div1,Div2,r(V),Ip],Out,H1,H0,T2).
```

```
init([r(V),ICap],[],H,H0,init(1,[ICap],[])) :- ICap #> 0,
   set_field(H,V,cap,ICap,H1), get_field(H1,V,cap,Cap),
   new_array(H1,int,Cap,E,H2),set_field(H2,V,elems,r(E),H3),
   set_field(H3,V,size,0,H0).
```

```
add([r(V),X],[],H,H0,add(1,[],[T]) :- get_field(H,V,size,S),
     get_field(H,V,cap,C), if2([C,S,r(V),X],[],H,H0,T).
if2^1([C,S,r(V),X],[],H,H0,if2(1,[],[T]) :- S #\= C, addc([r(V),X],[],H,H0,T).
if2^2([C,S,r(V),X],[],H,H0,if2(2,[],[T1,T2]) :- S #= C,
    reallocate([r(V)],[],H,H1,T1), addc([r(V),X],[],H1,H0,T2).
addc([r(V),X],[],H,H0,addc(1,[],[]) :-
    get_field(H,V,elems,r(Es)), get_field(H,V,size,S),
    set_array(H,Es,S,X,H1), NS #= S+1, set_field(H1,V,size,NS,H0).
```

```
reallocate([r(V)],[],H,H0,reallocate(1,[NC],[T]) :- get_field(H,V,cap,Cap),
    NC #= Cap*2, new_array(H,int,NC,NEs,H1),
    loop2([r(V),NC,r(NEs),0],[],H1,H0,T).
loop2([r(V),NCap,r(NEs),I],[],H,H0,loop2(1,[],[T]) :-
    get_field(H,V,cap,Cap), cond2([Cap,I,r(V),NCap,r(NEs)],[],H,H0,T).
                  ....
```

Fig. 2: (Excerpt of) CLP translation of running example

build the heap associated with a given path by using only the constraints induced by the visited code. We rely in the CLP-implementation presented in [10], where operations to create, read and modify heap-allocated data structures are presented in detail. For instance, a new object is created through a call to predicate new_object(H_{In},Class,Ref,H_{Out}), where H_{In} is the current heap, Class is the new object's type, Ref is a unique reference in the heap for accessing the new object and H_{Out} is the new heap after allocating the object. Read-only operations do not produce any output heap (e.g. get_field(H,Ref,Field,Value)). The remaining operations are implemented likewise.

It is well-known that the execution tree to be traversed in symbolic execution is in general infinite. This is because iterative constructs such as loops and recur-

sion whose number of iterations depends on the input values usually induce an infinite number of execution paths when executed with unknown input values. It is therefore essential to establish a *termination criterion*. In the context of TDG, termination is usually ensured by the *coverage criterion* which guarantees that the set of paths generated produces test cases which meet certain degree of code coverage and the process terminates. In what follows, we denote by $\mathcal{T}_m^C$ the finite symbolic execution tree of method m obtained using coverage criterion C.

Definition 2 (test case with trace and TDG). *Given a method m, a coverage criterion C and a successful branch b in $\mathcal{T}_m^C$ with root $m(Args_{in}, Args_{out}, H_{in}, H_{out}, T)$, a* test case with trace *for m w.r.t. C is a 6-tuple of the form: $\langle \sigma(Args_{in}), \sigma(Args_{out}), \sigma(H_{in}), \sigma(H_{out}), \sigma(T), \theta \rangle$, where σ and θ are the set of bindings and constraint store, resp., associated to b. TDG is the set of test cases with traces obtained for all successful branches in $\mathcal{T}_m^C$.*

Intuitively, each test case represents a class of inputs that will follow the same execution path, and its trace the sequence of rules applied along such path.

Example 2. Let us consider loop-1 as coverage criterion. In this example this forces the input array to be at most of length 1. The symbolic execution tree of `classify(`$\mathtt{Args}_{\mathsf{in}}$`,`$\mathtt{Args}_{\mathsf{out}}$`,`$\mathtt{H}_{\mathsf{in}}$`,`$\mathtt{H}_{\mathsf{out}}$`,T)` will contain the following five successful derivations (ignoring exceptions):

1. If the input array has length 0, the output vectors are empty.

If the input array is of length 1, four test cases are generated:

2. If ns[0] is not a multiple of div1 nor div2, the output vectors are empty.
3. If ns[0] is a multiple of div1 but not of div2, it is added only to vector r[0].
4. If ns[0] is a multiple of div2 but not of div1, it is added only to vector r[1].
5. If ns[0] is a multiple of both div1 and div2, it is added to both vectors.

Fig. 3 shows in detail the test case for point 3. Heaps are graphically represented by using rounded boxes for arrays (the array length appears to the left and the array itself to the right) and square boxes for Vector objects (field elems appears at the top, fields size and cap to the left and right bottom of the square). The trace-term `T` contains the rules that were executed along the derivation. At the bottom of the figure, an (executable) instantiation of this test case is shown.

3 Resource-aware Test Case Generation

In this section, we present the extension of the TDG framework of Sec. 2 to build resource consumption into the test cases. First, in Sec. 3.1 we describe the cost models that we will consider in the present work. Then, Sec. 3.2 presents our approach to resource-aware TDG.

3.1 Cost Models

A cost model defines how much the execution of an instruction costs. Hence, the resource consumption of a test case can be measured by applying the selected cost model to each of the instructions exercised to obtain it.

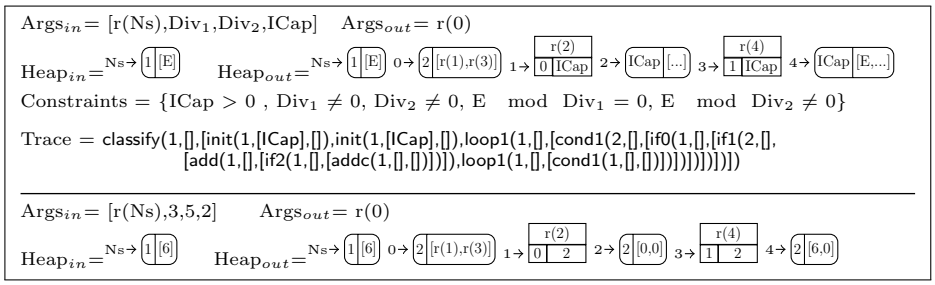


Fig. 3: Example of test case (up) and test input (down) for classify with loop-1

Number of Instructions. The most traditional model, denoted $\mathcal{M}_{ins}$, is used to estimate the number of instructions executed. In our examples, since the input to our system is the bytecode of the Java program, we count the number of bytecode instructions. All instructions are assigned cost 1.

Memory Consumption. Memory consumption can be estimated by counting the actual size of all objects and arrays created along an execution [3].

$$\mathcal{M}_{mem}(b) = \begin{cases} size(Class) & if\ b \equiv \mathsf{new}\ Class \\ S_{ref} * Length & if\ b \equiv \mathsf{anewarray}\ Class\ Length \\ S_{prim} * Length & if\ b \equiv \mathsf{newarray}\ PrimType\ Length \\ 0 & otherwise \end{cases}$$

We denote by S_{prim} and S_{ref}, resp., the size of primitive types and references. In the examples, by assuming a standard JVM implementation, we set both values to 4 bytes. The size of a class is the sum of the sizes of the fields it defines.

Number of calls. This cost model, $\mathcal{M}_{call}$, counts the number of invocations to methods. It can be specialized to $\mathcal{M}^m_{call}$ to count calls to a specific method m which, for instance, can be one that triggers a billable event.

Example 3. The application of the cost models $\mathcal{M}_{ins}$, $\mathcal{M}_{mem}$ and $\mathcal{M}_{call}$ to the sequence of instructions in rule init (i.e., $instr(\mathsf{init})$ of Ex. 1) results in, resp., 14 bytecode instructions, $4 * ICap$ bytes and 0 calls.

3.2 Resource-aware TDG

Given the test cases with trace obtained in Def. 2, the associated cost can be obtained as a simple post-process in which we apply the selected cost models to all instructions associated to the rules in its trace.

Definition 3 (test case with cost). *Consider a test case with trace Test obtained in Def. 2 for method m w.r.t. C of the form: Test* $\equiv \langle \_, \_, \_, \_, \mathrm{Trace}, \_ \rangle$. *For a a cost model* $\mathcal{M}$*, the cost of Test w.r.t.* $\mathcal{M}$*, denoted* $C(Test, \mathcal{M})$ *is defined as* $\mathtt{cost}(\mathrm{Trace}, \mathcal{M})$ *where function* cost *is recursively defined as:*

$$\mathtt{cost}(\mathtt{m}(\mathtt{k}, \mathtt{P}, \mathtt{L}), \mathcal{M}) = \textstyle\sum_{\forall i \in instr(m^k)} \mathcal{M}(i) + \sum_{\forall l \in \mathtt{L}} \mathtt{cost}(\mathtt{l}, \mathcal{M})$$

$Args_{in}$=[r(Ns),Div_1,Div_2,1] $Heap_{out}$= Ns→ (4 | [E_1,E_2,E_3,E_4]) 0→ (2 | [r(1),r(3)]) 1→ (r(7) | 4 | 4) 2→ (1 | [E_1]) 3→ (r(8) | 4 | 4) 4→ (1 | [E_1]) 5→ (2 | [E_1,E_2]) 6→ (2 | [E_1,E_2]) 7→ (4 | [E_1,E_2,E_3,E_4]) 8→ (4 | [E_1,E_2,E_3,E_4])

$Args_{out}$=r(0)

$Heap_{in}$= Ns→ (4 | [E_1,E_2,E_3,E_4])

Constraints = {$Div_1 \neq 0$, $Div_2 \neq 0$, E_1 mod Div_1=0, E_1 mod Div_2=0, E_2 mod Div_1=0, E_2 mod Div_2=0, E_3 mod Div_1=0, E_3 mod Div_2=0, E_4 mod Div_1=0, E_4 mod Div_2=0}

$\mathcal{M}_{mem}$=2*S_{Ref}+2*(2*$S_{PrimType}$+S_{Ref}+$S_{PrimType}$*1+$S_{PrimType}$*2+$S_{PrimType}$*4)=88 bytes

$\mathcal{M}_{ins}$ = 497 bytecode instructions $\mathcal{M}_{call}^{\text{reallocate}}$ = 4

$Args_{in}$=[r(Ns),Div_1,Div_2,ICap] $Heap_{out}$= Ns→ (4 | [E_1,E_2,E_3,E_4]) 0→ (2 | [r(1), r(3)]) 1→ (r(2) | 4 | ICap) 2→ (3 | [E_1,E_2,E_3,,E_4,...]) 3→ (r(4) | 4 | ICap) 4→ (1 | [E_1,E_2,E_3,E_4,...])

$Args_{out}$=r(0) $Heap_{in}$= Ns→ (4 | [E_1,E_2,E_3,E_4])

Constraints = {ICap≥4, $Div_1 \neq 0$, $Div_2 \neq 0$, E_1 mod Div_1=0, E_1 mod Div_2=0, E_2 mod Div_1=0, E_2 mod Div_2=0, E_3 mod Div_1=0, E_3 mod Div_2=0, E_4 mod Div_1=0, E_4 mod Div_2=0}

Trace = classify(1,[],[init(1,[ICap],[]),init(1,[ICap],[]),loop1(1,[],[cond1(2,[],[if0(2,[],[add(1,[],[if2(1,[], [addc(1,[],[])])]),if1(2,[],[add(1,[],[if2(1,[],[addc(1,[],[])])])]),loop1(1,[],[cond1(2,[],[if0(2,[], [add(1,[],[if2(1,[],[addc(1,[],[])])])]),if1(2,[],[add(1,[],[if2(1,[],[addc(1,[],[])])])]),loop1(1,[], [cond1(2,[],[if0(2,[],[add(1,[],[if2(1,[],[addc(1,[],[])])])]),if1(2,[],[add(1,[],[if2(1,[],[addc(1,[],[])])])]), loop1(1,[],[cond1(2,[],[if0(2,[],[add(1,[],[if2(1,[],[addc(1,[],[])])])]),if1(2,[],[add(1,[],[if2(1,[], [addc(1,[],[])])])]),loop1(1,[],[cond1(1,[],[])])])])])])])])])])])])])])])])])])

$\mathcal{M}_{mem}$ = 2*S_{Ref}+2*(2*$S_{PrimType}$+S_{Ref}+$S_{PrimType}$*ICap) = 32+8*ICap

$\mathcal{M}_{ins}$ = 327 bytecode instructions $\mathcal{M}_{call}^{\text{reallocate}}$ = 0

$Args_{in}$=[r(Ns),Div_1,Div_2,3] $Args_{out}$=r(0)

$Heap_{in}$= Ns→ (4 | [E_1,E_2,E_3,E_4]) $Heap_{out}$= Ns→ (4 | [E_1,E_2,E_3,E_4]) 0→ (2 | [r(1), r(3)]) 1→ (r(5) | 4 | 6) 2→ (3 | [E_1,E_2,E_3]) 3→ (r(6) | 4 | 6) 4→ (1 | [E_1,E_2,E_3]) 5→ (6 | [E_1,E_2,E_3,E_4,0,0]) 6→ (6 | [E_1,E_2,E_3,E_4,0,0])

Constraints = {$Div_1 \neq 0$, $Div_2 \neq 0$, E_1 mod Div_1=0, E_1 mod Div_2=0, E_2 mod Div_1=0, E_2 mod Div_2=0, E_3 mod Div_1=0, E_3 mod Div_2=0, E_4 mod Div_1=0, E_4 mod Div_2=0}

$\mathcal{M}_{mem}$ = 2*S_{Ref}+2*(2*$S_{PrimType}$+S_{Ref}+$S_{PrimType}$*3+$S_{PrimType}$*6) = 104 bytes

$\mathcal{M}_{ins}$ = 451 bytecode instructions $\mathcal{M}_{call}^{\text{reallocate}}$ = 2

Fig. 4: Selected test cases with cost for method classify with loop-4

For the cost models in Sec. 3.1, we define the test case with cost *as a tuple of the form* $\langle Test, C(Test, \mathcal{M}_{ins}), C(Test, \mathcal{M}_{mem}), C(Test, \mathcal{M}_{call})\rangle$.

Observe that this could also be done by profiling the resource consumption of the execution of the test-case. However this demands developing a profiler for the language (which would require a non trivial implementation effort). Besides, our approach goes beyond the capabilities of TDG + profiling, as it can also obtain *symbolic* (non-constant) resource usage estimations while profilers cannot.

Example 4. Let us consider the TDG of method classify with loop-4 as coverage criterion. We get 808 test cases, which correspond to all possible executions for input arrays of length not greater than 4, i.e., at most 4 iterations of the *for* loop. Fig. 4 shows three test cases. The upper one corresponds to the test case that executes the highest number of instructions, in which method reallocate is executed 4 times (worst case for $\mathcal{M}_{call}^{\text{reallocate}}$ as well). The one in the middle corresponds to that with the highest parametric memory consumption (for brevity,

only the trace for this case is shown), and the one at the bottom to that with the highest constant memory consumption. In the middle one, the input array Ns is of length 4, all elements in the array are multiple of both Div1 and Div2, and the initial capacity is constrained by ICap ≥ 4. With such input configuration, the array is fully traversed and all its elements are inserted in both vectors. By applying the cost model $\mathcal{M}_{mem}$ to the trace in the figure, we obtain a symbolic heap consumption which is parametric on ICap (observe that ICap is a parameter of the second and third calls in the trace). Importantly, this parameter remains as a variable because method reallocate is not executed. Symbolic execution of reallocate would give a concrete value to ICap when determining the number of iterations of its loop. The test case at the bottom in contrast executes reallocate twice, as both vectors run out of capacity at the fourth iteration of the loop. Hence, their capacities are duplicated.

Resource-aware TDG has interesting applications. It can clearly be useful to detect, early within the software development process, bugs related to an excessive consumption of resources. Additionally, one of the well-known problems of TDG is that, even for small programs, it produces a large set of test cases which complicate the software testing process which, among other things, requires reasoning on the correctness of the program by verifying that the obtained test cases lead to the expected result. Resource-aware TDG can be used in combination with a *resource policy* in order to filter out test cases which do not adhere to the policy. For instance, the resource policy can state that the resource consumption of the test cases must be larger (or smaller) than a given threshold so that one can focus on the (potentially problematic) test cases which consume a certain amount of resources. For instance, in Ex. 4, we had obtained 808 test cases and by focusing on those that consume more than 104 bytes, we filter out 467 test cases. Also, one can yield to the user the test cases ordered according to the amount of resources they consume. For instance, for the cost model $\mathcal{M}_{mem}$ the test cases in Ex. 4 would be shown first. It is easy to infer the condition ICap ≥ 9, which determines when the parametric test case is the most expensive one. Besides, one can implement a *worst-case* resource policy which shows to the user only the test case that consumes more resources among those obtained by the TDG process (e.g., the one at the top together with the previous condition for $\mathcal{M}_{mem}$), or display the k test cases with highest resource consumption (e.g., the two cases in Fig. 4 for $k = 2$).

4 Resource-driven TDG

This section introduces *resource-driven TDG*, a novel heuristics to guide the symbolic execution process which improves, in terms of scalability, over the resource-aware approach, especially in those cases where restrictive resource policies are supplied. The main idea is to try to avoid, as much as possible, the generation of paths during symbolic execution that do not satisfy the policy. If the resource policy imposes a maximum threshold, then symbolic execution can stop an execution path as soon as the resource consumption exceeds it. However, it is often more useful to establish resource policies that impose a minimum threshold. In

such case, it cannot be decided if a test case adheres to the policy until it is completely generated. Our heuristics to avoid the unnecessary generation of test cases that violate the resource policy is based on this idea: 1) in a pre-process, we look for traces corresponding to potential paths (or sub-paths) that adhere to the policy, and 2) we use such traces to guide the symbolic execution.

An advantage of relying on a CLP-based TDG approach is that the trace argument of our CLP-transformed programs can be used, not only as an output, but also as an input argument. Let us observe also that, we could either supply fully or partially instantiated traces, the latter ones represented by including free logic variables within the trace terms. This allows guiding, completely or partially, the symbolic execution towards specific paths.

Definition 4 (guided TDG). *Given a method m, a coverage criterion C, and a (possibly partial) trace π, guided TDG, denoted $gTDG(m, C, \pi)$, is the set of test cases with traces obtained for all successful branches in $\mathcal{T}_m^C$.*

Observe that the symbolic execution guided by one trace (a) generates exactly one test case if the trace is complete and corresponds to a feasible path, (b) none if it is unfeasible, or (c) can also generate several test cases in case it is partial. In this case the traces of all test cases are instantiations of the partial trace.

Example 5. Let us consider the following partial trace `classify(1,[],[init(1,[ICap],[]),init(1,[ICap],[]),loop1(1,[],[cond1(2,[],[if0(2,[],[V1,if1(2,[],[V1,loop1(1,[],[cond1(2,[],[if0(2,[],[V2,if1(2,[],[V3,...)` which represents the paths that iterate four times in the loop and enter in both *if's* of the *for* loop of method classify. The trace is partial since it does not specify where the execution goes after each *if* is entered. This is expressed by the corresponding variables (`V1,V2 and V3`) in the trace-term arguments. The symbolic execution guided by such trace produces four test cases differentiated by their constraint on $ICap$, which is resp. $ICap = 1$, $ICap = 2$, $ICap = 3$ and $ICap \geq 4$. The first and the third test cases are the ones shown at the top and the bottom resp. of Fig 4.

By relying on an oracle O that provides the traces, we now define resource-driven TDG as follows.

Definition 5 (resource-driven TDG). *Given a method m, a coverage criterion C and a resource-policy R, resource-driven TDG is defined as*

$$\bigcup_{i=1}^{n} gTDG(m, C, \pi_i)$$

where $\{\pi_1, \ldots, \pi_n\}$ is the set of traces computed by an oracle O w.r.t R and C. The result is thus a set of test cases with traces.

An interesting observation is that the symbolic executions of the different traces computed by the oracle are independent of each other and therefore can be performed in parallel. This also saves symbolic execution from the overhead

of maintaining the constraint stores for performing the backtrackings which is usually the main cause of its lack of scalability.

This definition relies on a generic oracle. We will now sketch different techniques for defining specific oracles. Ideally, an oracle should be *sound*, *complete* and *effective*. An oracle is sound if every trace it generates satisfies the resource policy. It is complete if it generates all traces that satisfy the policy. Effectiveness is related to the number of unfeasible traces it generates. The larger the number, the less effective the oracle and the less efficient the TDG process. For instance, assuming a worst-case resource policy, one can think of an oracle that relies on the results of a static cost analyzer [1] to detect the methods with highest cost. It can then generate partial traces that force the execution go through such costly methods (combined with a terminating criterion). Such oracle can produce a trace as the one in Ex. 5 with the aim of trying to maximize the number of times method `add` (the potentially most costly one) is called. This kind of oracle can be quite effective though it will be in general unsound and incomplete.

4.1 On Soundness and Completeness of Oracles

In the following we develop a concrete scheme of an oracle which is sound, complete, and parametric w.r.t. both the cost model and the resource policy. Intuitively, an oracle is complete if, given a resource policy and a coverage criterion, it produces an over-approximation of the set of traces (obtained as in Def. 2) satisfying the resource policy and coverage criterion. We first propose a naive way of generating such an over-approximation which is later improved.

Definition 6 (trace-abstraction program). *Given a CLP-translated program with traces P, its trace-abstraction is obtained as follows: for every rule of P, (1) remove all atoms in the body of the rule except those corresponding to rule calls, and (2) remove all arguments from the head and from the surviving atoms of (1) except the last one (i.e., the trace term).*

The trace-abstraction of a program corresponds to its control-flow graph, and can be directly used as a trace-generator that produces a superset of the (usually infinite) set of traces of the program. The coverage criterion is applied in order to obtain a concrete and finite set of traces. Note that this is possible as long as the coverage criterion is structural, i.e., it only depends in the program structure (like loop-k). The resource policy can then be applied over the finite set: (1) in a post-processing where the traces that do not satisfy the policy are filtered out or (2) depending on the policy, by employing a specialized search method.

As regards soundness, the intuition is that an oracle is sound if the resource consumption for the selected cost model is *observable* from the traces, i.e, it can be computed and it is equal to the one computed after the guided TDG.

Definition 7 (resource observability). *Given a method m, a coverage criterion C and a cost-model $\mathcal{M}$, we say that $\mathcal{M}$ is* observable *in the trace-abstraction for m, if for every feasible trace π generated from the trace-abstraction using C, we have that $\texttt{cost}(\pi, \mathcal{M}) = \texttt{cost}(\pi', \mathcal{M})$, where π' is a corresponding trace obtained for $gTDG(m, C, \pi)$.*

Observe that π can only have variables in trace parameters (second argument of a trace-term). This means that the only difference between π and π' can be made by means of instantiations (or associated constraints) performed during the symbolic execution on those variables. Trivially, $\mathcal{M}_{ins}$ and $\mathcal{M}_{call}$ are observable since they do not depend on such trace parameters. Instead, $\mathcal{M}_{mem}$ can depend on trace parameters and is therefore non-observable in principle on this trace-abstraction, as we will discuss later in more detail.

Enhancing trace-abstractions. Unfortunately the oracle proposed so far is in general very far from being effective since trace-abstractions can produce a huge amount of unfeasible traces. To solve this problem, we propose to enhance the trace-abstraction with information (constraints and arguments) taken from the original program. This can be done at many degrees of precision, from the empty enhancement (the one we have seen) to the full one, where we have the original program (hence the original resource-aware TDG). The more information we include, the less unfeasible traces we get, but the more costly the process is. The goal is thus to find heuristics that enrich sufficiently the abstraction so that many unfeasible traces are avoided and with the minimum possible information.

A quite effective heuristic is based on the idea of adding to the abstraction those program variables (input arguments, local variables or object fields) which get instantiated during symbolic execution (e.g., field `size` in our example). The idea is to enhance the trace-abstraction as follows. Let us start with a set of variables V initialized with those variables (this can be soundly approximated by means of static analysis). For every $v \in V$, we add to the program all occurrences of v and the guards and arithmetic operations in which v is involved. The remaining variables involved in those guards are added to V and the process is repeated until reaching a fixpoint. The trace-abstraction with the proposed enhancement for our working example is shown in Fig. 5.

Resource Observability for $\mathcal{M}_{mem}$. As already mentioned, $\mathcal{M}_{mem}$ is in general non-observable in trace-abstractions. The problem is that the memory consumed by the creation of arrays depends on dynamic values which might be not present in the trace-abstraction. Again, this problem can be solved by enhancing the trace-abstraction with the appropriate information. In particular, the enhancement must ensure that the variables involved in the creation of new arrays (and those on which they depend) are added to the abstraction. This information can be statically approximated [2, 14, 15].

Instances of Resource-driven TDG. The resource-driven scheme has been deliberately defined as generic as possible and hence it could be instantiated in different ways for particular resource policies and cost-models producing more effective versions of it. For instance, for a worst-case resource policy, the oracle must generate all traces in order to know which is the one with maximal cost. Instead of launching a guided symbolic execution for all of them, we can try them one by one (or k by k in parallel) ordered from higher to lower cost, so that as soon as a trace is feasible the process stops. By correctness of the oracle, the trace will necessarily correspond to the feasible path with highest cost.

```
classify(ICap,classify(1,[],[T1,T2,T3]) :- init(ICap,S1,C1,T1),
   init(ICap,S2,C2,T2), loop1(S1,C1,S2,C2,T3).
init(ICap,0,ICap,init(1,[ICap],[])).
loop1(S1,C1,S2,C2,loop1(1,[],[T])) :- cond1(S1,C1,S2,C2,T).
cond1^1(_,_,_,_,cond1(1,[],[])).
cond1^2(S1,C1,S2,C2,cond1(2,[],[T])) :- if0(S1,C1,S2,C2,T).
if0^1(S1,C1,S2,C2,if0(1,[],[T])) :- if1(S1,C1,S2,C2,T).
if0^2(S1,C1,S2,C2,if0(2,[],[T1,T2])) :- add(S1,C1,S1p,C1p,T1),
   if1(S1p,C1p,S2,C2,T2).
if1^1(S1,C1,S2,C2,if1(1,[],[T])) :- loop1(S1,C1,S2,C2,T).
if1^2(S1,C1,S2,C2,if1(2,[],[T1,T2])) :- add(S2,C2,S2p,C2p,T1),
   loop1(S1,C1,S2p,C2p,T2).
add(S,C,Sp,Cp,add(1,[],[T])) :- if2(S,C,Sp,Cp,T).
if2^1(S,C,Sp,C,if2(1,[],[T])) :- S #\= C, addc(S,Sp,T).
if2^2(S,C,Sp,Cp,if2(2,[],[T1,T2])) :- S #= C, reallocate(C,Cp,T1),
    addc(S,Sp,T2).
addc(S,NS,addc(1,[],[])) :- NS #= S+1.
reallocate(C,NC,reallocate(1,[NC],[T])) :- NC #= C*2, loop2(C,0,T).
loop2(C,I,loop2(1,[],[T])) :- cond2(C,I,T).
cond2^1(C,I,cond2(1,[],[])) :- I #>= C.
cond2^2(C,I,cond2(2,[],[T])) :- I #< C, Ip #= I+1, loop2(C,Ip,T).
```

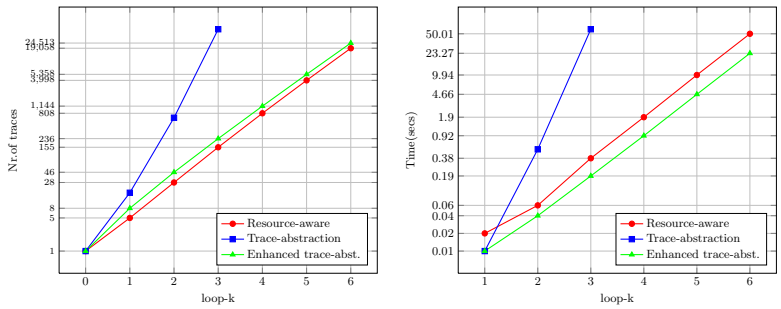
Fig. 5: Running example - Enhanced trace-abstraction program

Theorem 1 (correctness of trace-driven TDG). *Given a cost model $\mathcal{M}$, a method m, a coverage criterion C and a sound oracle O on which $\mathcal{M}$ is observable, resource-driven TDG for m w.r.t. C using O generates the same test cases as resource-aware TDG w.r.t. C for the cost model $\mathcal{M}$.*

Soundness is trivially entailed by the features of the oracle.

4.2 Performance of Trace-driven TDG

We have performed some preliminary experiments on our running example using different values for k for the loop-k coverage criterion (X axis) and using a worst-case resource policy for the $\mathcal{M}_{ins}$ cost model. Our aim is to compare resource-aware TDG with the two instances of resource-driven TDG, the one that uses the naive trace-abstraction and the enhanced one. Fig. 6a depicts the number of traces which will be explored in each case. It can be observed that the naive trace-abstraction generates a huge number of unfeasible traces and the growth is larger as k increases. Indeed, from $k = 4$ on, the system runs out of memory when computing them. The enhanced trace-abstraction reduces drastically the number of unfeasible traces and besides the difference w.r.t. this number in resource-aware is a (small) constant. Fig. 6b shows the time to obtain the worst-case test case in each case. The important point to note is that resource-driven TDG outperforms resource-aware TDG in all cases, taking in average half the



(a) Number of traces. (b) Time.

Fig. 6: Preliminary experimental results.

time w.r.t. the latter. We believe our results are promising and suggest that the larger the symbolic execution tree is (i.e., the more exhaustive TDG aims to be), the larger the efficiency gains of resource-driven TDG are. Furthermore, in a real system, the different test cases for resource-driven TDG could be computed in parallel and hence the benefits would be potentially larger.

5 Conclusions and Related work

In this paper, we have proposed resource-aware TDG, an extension of standard TDG with resources, whose purpose is to build resource consumption into the test cases. Resource-aware TDG can be considered a subset of performance engineering, an emerging software engineering practice that strives to build performance into the design and architecture of systems. Resource-aware TDG can serve different purposes. It can be used to test that a program meets performance criteria up to a certain degree of code coverage. It can compare two systems to find which one performs better in each test case. It could even help finding out what parts of the program consume more resources and can cause the system to perform badly. In general, the later a defect is detected, the higher the cost of remediation. Our approach allows thus that performance test efforts begin at the inception of the development project and extend through to deployment.

Previous work also considers extensions of standard TDG to generate resource consumption estimations for several purposes (see [5, 12, 20] and their references). However, none of those approaches can generate symbolic resource estimations, as our approach does, neither take advantage of a resource policy to guide the TDG process. The most related work to our resource-driven approach is [18], which proposes to use an abstraction of the program in order to guide symbolic execution and prune the execution tree as a way to scale up. An important difference is that our trace-based abstraction is an over-approximation of the actual paths which allows us to select the most expensive paths. However, their abstraction is an under-approximation which tries reduce the number of test cases that are generated in the context of concurrent programming, where the state explosion can be problematic, and thus could omit the most expensive paths. Besides, our extension to infer the resources from the trace-abstraction and the idea to use it as a heuristics to guide the symbolic execution is new.

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Probabilistic Termination of CHRiSM Programs

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Abstract. Termination analysis has received considerable attention in Logic Programming for several decades. In recent years, probabilistic extensions of Logic Programming languages have become increasingly important. Languages like PRISM, CP-Logic, ProbLog and CHRiSM have been introduced and proved very useful for addressing problems in which a combination of logical and probabilistic reasoning is required. As far as we know, the termination of probabilistic logical programs has not received any attention in the community so far.
Termination of a probabilistic program is not a crisp notion. Given a query, such a program does not simply either terminate or not terminate, but it terminates with a certain probability.
In this paper, we explore this problem in the context of CHRiSM, a probabilistic extension of CHR. We formally introduce the notion of probabilistic termination. We study this concept on the basis of a number of case studies. We provide some initial sufficient conditions to characterize probabilistically terminating programs and queries. We also discuss some challenging examples that reveal the complexity and interest of more general settings. The paper is intended as a first step in a challenging and important new area in the analysis of Logic Programs.

Keywords: Termination Analysis, Probabilistic LP, Constraint Handling Rules.

1 Introduction

Termination analysis has received considerable attention from the Logic Programming research community. Over several decades, many key concepts have been defined and formally studied (e.g. acceptability [3] and various variants of it), several powerful techniques for automatic verification of termination have been designed (e.g. the query-mapping pairs [15], constraint-based termination [7], the dependency-pairs framework [20]) and systems, implementing these techniques, currently provide very refined analysis tools for the termination property (e.g. cTI [17], Aprove [12], Polytool [21]). The main goals have been to support the study of total correctness of programs, to facilitate debugging tasks and to provide termination information for program optimization techniques such as partial evaluation and other transformation systems [16, 14, 29].

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Several Logic Programming related languages have been considered in all this work. Most research has addressed pure Prolog, but other languages, such as full Prolog [25, 28], CLP [18] and CHR [8, 30, 22] have also been considered.

In the past decade, probabilistic extensions of Logic Programming have become increasingly more important. Languages like PRISM [24] and ProbLog [6] extend Logic Programming with probabilistic reasoning and allow to tackle applications that require combinations of logical and probabilistic inference. Probabilistic termination analysis for imperative languages [19, 13] and for rewrite systems [5, 4] has already been studied in the past. However, as far as we know, termination analysis in the context of probabilistic logic programming has not yet received any attention, with the exception of some comments on probabilistic termination in [10]. It is the aim of the current paper to provide an initial investigation of the problem, mostly based on case studies.

Our study will be performed in the context of the probabilistic-logical language CHRiSM [26], a language based on CHR [9, 27, 11] and PRISM [24].

CHR – Constraint Handling Rules – is a high-level language extension based on multi-headed rules. Originally, CHR was designed as a special-purpose language to implement constraint solvers (see e.g. [2]), but in recent years it has matured into a general purpose programming language. Being a language *extension*, CHR is implemented on top of an existing programming language, which is called the *host language*. An implementation of CHR in host language X is called CHR(X). For instance, several CHR(Prolog) systems are available [27].

PRISM – PRogramming In Statistical Modeling – is a probabilistic extension of Prolog. It supports several probabilistic inference tasks, including sampling, probability computation, and expectation-maximization (EM) learning.

In [26], a new formalism was introduced, called CHRiSM, short for CHance Rules Induce Statistical Models. It is based on CHR(PRISM) and it combines the advantages of CHR and those of PRISM.

By way of motivation, let us consider a simple example of a CHRiSM program and briefly look at its termination properties.

Example 1 (Repeated Coin Flipping) *Suppose we flip a fair coin, and if the result is* `tail`*, we stop, but if it is* `head`*, we flip the coin again. We can model this process in* CHRiSM *as follows:*

```
flip <=> head:0.5 ; tail:0.5.
head <=> flip.
```

In Section 2 we formally introduce the syntax and semantics of CHRiSM*, but intuitively, the first rule states that the outcome of a* `flip` *event has an equal probability of 0.5 to result in* `head` *or in* `tail`*. The second rule is not probabilistic (or has probability 1): if there is* `head`*, we always* `flip` *again.*

The program would typically be activated by the query `flip`*. In a computation for the query* `flip`*, the first rule will either select* `head` *or* `tail`*, with equal probability. The choice is not backtrackable.*

It is unclear whether we should consider this program as terminating or non-terminating. The program has an infinite derivation in which the coin always lands on `head`. *However, out of all the possible derivations, there is only one infinite one and its probability of being executed is* $\lim_{n\to\infty}(0.5)^n = 0$. *So, if we execute this program, the probability of it terminating is equal to 1. Therefore, it is debatable whether we should call the program non-terminating and we will need the more refined notion of probabilistic termination.* □

In this paper we will study the notion of probabilistic termination. Most of this study is based on a number of case studies, where we compute the probabilities of termination for specific programs. We also compute the expected number of rule applications for some of these programs. For some classes of programs, we are able to generalize the results of our examples and formulate and prove probabilistic termination theorems. However, for the more complex programs, our study reveals that the mathematical equations modelling the probability of termination sometimes become too complex to solve.

The paper is organized as follows. In Section 2 we recall the syntax and semantics of CHRiSM. In Section 3 we define probabilistic termination of a CHRiSM program. We relate it to universal termination and we study some simple examples. Section 4 introduces a class of programs that behave like Markov chains, for which we provide a termination criterion. In Section 5 we discuss more complex examples and show that solving such examples provides a challenge for currently available mathematical techniques. We conclude in Section 6.

2 CHRiSM

In this section we briefly recall the CHRiSM programming language, in order to make this paper as self-contained as possible given the limited space. However we encourage the reader to refer to [26] for a more detailed description.

A CHRiSM program $\mathcal{P}$ consists of a sequence of *chance rules*. Chance rules rewrite a multiset $\mathbb{S}$ of data elements, which are called (CHRiSM) *constraints* (mostly for historical reasons). Syntactically, a constraint $\texttt{c(t}_1\texttt{,..,t}_n\texttt{)}$ looks like a Prolog predicate: it has a functor `c` of some arity n and arguments $\texttt{t}_1\texttt{,..,t}_n$ which are Prolog terms. The multiset $\mathbb{S}$ of constraints is called the *constraint store* or just *store*. The initial store is called the *query* or *goal*, the final store (obtained by exhaustive rule application) is called the *answer* or *result*.

We use $\{\!|\ |\!\}$ to denote multisets, $\uplus$ for multiset union, $\Subset$ for multiset subset, and $\bar{\exists}_A B$ to denote $\exists x_1, \ldots, x_n : B$, with $\{x_1, \ldots, x_n\} = vars(B) \setminus vars(A)$, where $vars(A)$ are the (free) variables in A; if A is omitted it is empty.

Chance rules. A chance rule has the following form: `P ?? Hk \ Hr <=> G | B.` where `P` is a probability expression (as defined below), `Hk` is a conjunction of (kept head) constraints, `Hr` is a conjunction of (removed head) constraints, `G` is a guard condition, and `B` is the body of the rule. If `Hk` is empty, the rule is called a *simplification* rule and the backslash is omitted; if `Hr` is empty, the rule

is called a *propagation* rule, written as "`P ?? Hk ==> G | B`". If both `Hk` and `Hr` are non-empty, the rule is called a *simpagation* rule. The guard `G` is optional; if it is omitted, the "`|`" is also omitted. The body `B` is a conjunction of CHRiSM constraints, Prolog goals, and probabilistic disjunctions (as defined below).

Intuitively, the meaning of a chance rule is as follows: If the constraint store $\mathbb{S}$ contains elements that match the head of the rule (i.e. if there is a (satisfiable) matching substitution θ such that $(\theta(\texttt{Hk}) \uplus \theta(\texttt{Hr})) \trianglelefteq \mathbb{S}$), and furthermore, the guard $\theta(\texttt{G})$ is satisfied, then we can consider rule application. The subset of $\mathbb{S}$ that corresponds to the head of the rule is called a rule *instance*. Depending on the probability expression `P`, the rule instance is either ignored or it actually leads to a rule application. Every rule instance may only be considered once.

Rule application has the following effects: the constraints matching `Hr` are removed from the constraint store and then the body `B` is executed, that is, Prolog goals are called and CHRiSM constraints are added into the store.

Probability expressions. In this paper, we assume probabilities to be fixed numbers. The CHRiSM system also supports learnable probabilities and other types of probability expressions. We refer to [26] for an overview.

Probabilistic disjunction. The body `B` of a CHRiSM rule may contain probabilistic disjunctions: "`D1:P1 ; ... ; Dn:Pn`" indicates that a disjunct `D`i is chosen with probability `P`i. The probabilities should sum to 1 (otherwise a compile-time error occurs). Unlike CHR$^\vee$ disjunctions [1], which create a choice point, probabilistic disjunctions are *committed-choice*: once a disjunct is chosen, the choice is not undone later. However, when later on in a derivation, the same disjunction is reached again, the choice can of course be different.

Operational Semantics. The operational semantics of a CHRiSM program $\mathcal{P}$ is given by a state-transition system that resembles the abstract operational semantics ω_t of CHR [27]. The execution states are defined analogously, except that we additionally define a unique failed execution state, which is denoted by *"fail"* (because we don't want to distinguish between different failed states). We use the symbol $\omega_t^{??}$ to refer to the (abstract) operational semantics of CHRiSM.

Definition 1 (identifiers). *An* identified *constraint $c\#i$ is a* CHRiSM *constraint c associated with some unique integer i. This number serves to differentiate between copies of the same constraint. We introduce the functions $chr(c\#i) = c$ and $id(c\#i) = i$, and extend them to sequences and sets, e.g.:*

$$chr(S) = \{\!|\, c | c\#i \in S \,|\!\}$$

Definition 2 (execution state). *An* execution state *σ is a tuple $\langle \mathbb{G}, \mathbb{S}, \mathbb{B}, \mathbb{T} \rangle_n$. The* goal *$\mathbb{G}$ is a multiset of constraints to be rewritten to solved form. The* store *$\mathbb{S}$ is a set of* identified *constraints that can be matched with rules in the program $\mathcal{P}$. Note that $chr(\mathbb{S})$ is a multiset although $\mathbb{S}$ is a set. The* built-in store *$\mathbb{B}$ is the conjunction of all Prolog goals that have been called so far. The* history *$\mathbb{T}$ is a*

1. Fail. $\langle \{\!|\, b \,|\!\} \uplus \mathbb{G}, \mathbb{S}, \mathbb{B}, \mathbb{T} \rangle_n \overset{1}{\underset{\mathcal{P}}{\rightarrowtail}} \mathit{fail}$
where b is a built-in (Prolog) constraint and $\mathcal{D}_\mathcal{H} \models \neg\bar{\exists}(\mathbb{B} \wedge b)$.

2. Solve. $\langle \{\!|\, b \,|\!\} \uplus \mathbb{G}, \mathbb{S}, \mathbb{B}, \mathbb{T} \rangle_n \overset{1}{\underset{\mathcal{P}}{\rightarrowtail}} \langle \mathbb{G}, \mathbb{S}, b \wedge \mathbb{B}, \mathbb{T} \rangle_n$
where b is a built-in (Prolog) constraint and $\mathcal{D}_\mathcal{H} \models \bar{\exists}(\mathbb{B} \wedge b)$.

3. Introduce. $\langle \{\!|\, c \,|\!\} \uplus \mathbb{G}, \mathbb{S}, \mathbb{B}, \mathbb{T} \rangle_n \overset{1}{\underset{\mathcal{P}}{\rightarrowtail}} \langle \mathbb{G}, \{c\#n\} \cup \mathbb{S}, \mathbb{B}, \mathbb{T} \rangle_{n+1}$
where c is a CHRiSM constraint.

4. Probabilistic-Choice. $\langle \{\!|\, d \,|\!\} \uplus \mathbb{G}, \mathbb{S}, \mathbb{B}, \mathbb{T} \rangle_n \overset{p_i}{\underset{\mathcal{P}}{\rightarrowtail}} \langle \{\!|\, d_i \,|\!\} \uplus \mathbb{G}, \mathbb{S}, \mathbb{B}, \mathbb{T} \rangle_n$
where d is a probabilistic disjunction of the form $d_1 \texttt{:} p_1 \ \texttt{;} \ \ldots \ \texttt{;} \ d_k \texttt{:} p_k$ or of the form `P ??` $d_1 \ \texttt{;} \ \ldots \ \texttt{;} \ d_k$, where the probability distribution given by `P` assigns the probability p_i to the disjunct d_i.

5. Maybe-Apply. $\langle \mathbb{G}, H_1 \uplus H_2 \uplus \mathbb{S}, \mathbb{B}, \mathbb{T} \rangle_n \overset{1-p}{\underset{\mathcal{P}}{\rightarrowtail}} \langle \mathbb{G}, H_1 \uplus H_2 \uplus \mathbb{S}, \mathbb{B}, \mathbb{T} \cup \{h\} \rangle_n$
$\langle \mathbb{G}, H_1 \uplus H_2 \uplus \mathbb{S}, \mathbb{B}, \mathbb{T} \rangle_n \overset{p}{\underset{\mathcal{P}}{\rightarrowtail}} \langle B \uplus \mathbb{G}, H_1 \uplus \mathbb{S}, \theta \wedge \mathbb{B}, \mathbb{T} \cup \{h\} \rangle_n$
where the r-th rule of $\mathcal{P}$ is of the form `P ??` $H_1' \setminus H_2'$ `<=> G | B`,
θ is a matching substitution such that $chr(H_1) = \theta(H_1')$ and $chr(H_2) = \theta(H_2')$, $h = (r, id(H_1), id(H_2)) \notin \mathbb{T}$, and $\mathcal{D}_\mathcal{H} \models \mathbb{B} \rightarrow \bar{\exists}_{\mathbb{B}}(\theta \wedge G)$. If `P` is a number, then $p =$ `P`. Otherwise p is the probability assigned to the success branch of `P`.

Fig. 1. Transition relation $\overset{}{\underset{\mathcal{P}}{\rightarrowtail}}$ of the abstract operational semantics $\omega_t^{??}$ of CHRiSM.

set of tuples, each recording the identifiers of the CHRiSM *constraints that fired a rule and the rule number. The history is used to prevent trivial non-termination: a rule instance is allowed to be considered only once. Finally, the counter $n \in \mathbb{N}$ represents the next free identifier.*

We use $\sigma, \sigma_0, \sigma_1, \ldots$ to denote execution states and Σ to denote the set of all execution states. We use $\mathcal{D}_\mathcal{H}$ to denote the theory defining the host language (Prolog) built-ins and predicates used in the CHRiSM program. For a given program $\mathcal{P}$, the transitions are defined by the binary relation $\overset{}{\underset{\mathcal{P}}{\rightarrowtail}} \subset \Sigma \times \Sigma$ shown in Figure 1. Every transition is annotated with a probability.

Execution of a query Q proceeds by exhaustively applying the transition rules, starting from an initial state (root) of the form $\sigma_Q = \langle Q, \emptyset, \mathit{true}, \emptyset \rangle_0$ and performing a random walk in the directed acyclic graph defined by the transition relation $\overset{}{\underset{\mathcal{P}}{\rightarrowtail}}$, until a leaf node is reached, which is called a final state. We use Σ_f to denote the set of final states. The probability of a path from an initial state to the state σ is simply the product of the probabilities along the path.

We assume a given execution strategy ξ that fixes the non-probabilistic choices in case multiple transitions are applicable (see section 4.1 of [26]).

We use $\sigma_0 \overset{p}{\underset{\mathcal{P}}{\rightarrowtail}}{}^* \sigma_f$ to denote all k different derivations from σ_0 to σ_f:

$$\sigma_0 \overset{p_{1,1}}{\underset{\mathcal{P}}{\rightarrowtail}} \sigma_{1,1} \overset{p_{1,2}}{\underset{\mathcal{P}}{\rightarrowtail}} \sigma_{1,2} \overset{p_{1,3}}{\underset{\mathcal{P}}{\rightarrowtail}} \ \ldots \ \overset{p_{1,l_1}}{\underset{\mathcal{P}}{\rightarrowtail}} \sigma_f$$

$$\vdots$$

$$\sigma_0 \overset{p_{k,1}}{\underset{\mathcal{P}}{\rightarrowtail}} \sigma_{k,1} \overset{p_{k,2}}{\underset{\mathcal{P}}{\rightarrowtail}} \sigma_{k,2} \overset{p_{k,3}}{\underset{\mathcal{P}}{\rightarrowtail}} \ \ldots \ \overset{p_{k,l_k}}{\underset{\mathcal{P}}{\rightarrowtail}} \sigma_f$$

where

$$p = \sum_{i=1}^{k} \prod_{j=1}^{l_i} p_{i,j}.$$

If σ_0 is an initial state and σ_k is a final state, then we call these derivations an *explanation set* with total probability p for the query σ_0 and the result σ_k. Note that if $k = 0$, i.e. there is no derivation from σ_0 to σ_f, then $p = 0$. We define a function *prob* to give the probability of an explanation set: $prob(\sigma_0 \overset{p}{\underset{\mathcal{P}}{\rightarrowtail}}{}^{*} \sigma_k) = p$.

If σ_0 is an initial state and there exist infinite sequences s_i of transitions

$$\sigma_0 \overset{p_{i,1}}{\underset{\mathcal{P}}{\rightarrowtail}} \sigma_{i,1} \overset{p_{i,2}}{\underset{\mathcal{P}}{\rightarrowtail}} \sigma_{i,2} \overset{p_{i,3}}{\underset{\mathcal{P}}{\rightarrowtail}} \ldots$$

then we call these sequences infinite derivations from σ_0. We use $\sigma_0 \overset{p}{\underset{\mathcal{P}}{\rightarrowtail}}{}^{*} \infty$ to denote the (possibly infinite) set D of infinite derivations from σ_0, where

$$p = \lim_{l \to \infty} \sum_{i=1}^{|D|} \prod_{j=1}^{l} p_{i,j}.$$

Note that if all rule probabilities are 1 and the program contains no probabilistic disjunctions — i.e. if the CHRiSM program is actually just a regular CHR program — then the $\omega_t^{??}$ semantics boils down to the ω_t semantics of CHR.

3 Probabilistic Termination

In the contexts of Prolog and CHR, the usual notion of termination is *universal termination*: a program $\mathcal{P}$ terminates for a query Q if Q does not have an infinite derivation for $\mathcal{P}$.

For some CHRiSM programs, universal termination is too strong. In order to be able to execute (sample) a program, *probabilistic* termination is sufficient.

Definition 3 (Probabilistic termination). *A program $\mathcal{P}$ probabilistically terminates for a query Q with probability p if the probability of the event that the computation for Q in $\mathcal{P}$ halts is equal to p, i.e.*

$$p = \sum_{\sigma \in \Sigma_f} prob(\sigma_Q \overset{}{\underset{\mathcal{P}}{\rightarrowtail}}{}^{*} \sigma) = 1 - prob(\sigma_Q \overset{}{\underset{\mathcal{P}}{\rightarrowtail}}{}^{*} \infty).$$

A program $\mathcal{P}$ probabilistically terminates for a query Q if the program probabilistically terminates for Q with probability 1. A program $\mathcal{P}$ probabilistically terminates if it probabilistically terminates for all finite queries.

Note that the above definition does not give a general practical method to compute the termination probability for a given query, and like universal termination, probabilistic termination is undecidable. Note also that in general the number of finite derivations may be infinite.

Although many CHRiSM programs do not universally terminate (so they have infinite derivations) universal termination is of course sufficient for probabilistic

termination. This already provides us with a practical way of proving probabilistic termination of one class of CHRiSM programs. In general, we can associate to any CHRiSM program $\mathcal{P}$ a corresponding CHR$^\vee$ program [1], CHR$^\vee(\mathcal{P})$, by removing all the probability information from $\mathcal{P}$. As already mentioned, apart from removing the probability factors, this transformation changes committed choice disjunctions into backtrackable disjunctions. However, from a perspective of proving universal termination, this is not a problem, because we need to prove that all derivations are finite anyway.

Proposition 1. *For any* CHRiSM *program* $\mathcal{P}$ *and query* Q, $\mathcal{P}$ *is probabilistically terminating for* Q *if CHR*$^\vee(\mathcal{P})$ *is universally terminating for* Q.

Proof. If CHR$^\vee(\mathcal{P})$ has no infinite derivation for Q, then $\mathcal{P}$ has no infinite derivation for Q. Thus the probability of halting is one.

Proving that CHR$^\vee(\mathcal{P})$ universally terminates for Q can be done using the techniques presented in [8], [30] or [22]. The latter technique has been automated and implemented [23]. Of course, these techniques were developed for CHR, rather than for CHR$^\vee$, but again, a CHR$^\vee$ program can easily transformed into a CHR program with the same universal termination behavior.

Example 2 (Low-power Countdown) *Consider the* CHRiSM *program:*

```
0.9 ?? countdown(N) <=> N > 1 | countdown(N-1).
0.9 ?? countdown(0) <=> writeln('Happy New Year!').
```

representing a New Year countdown device with low battery power, which may or may not display its New Year wishes starting from a query `countdown(10)`. *At every tick, there is a 10% chance that the battery dies and the countdown stops.*

Consider the CHR program obtained by omitting the probabilities. The ranking techniques of all three of the approaches presented in [8, 30, 22], prove universal termination for that program and the same query. Thus, Low-power New Years Countdown will terminate (universally and probabilistically) as well. □

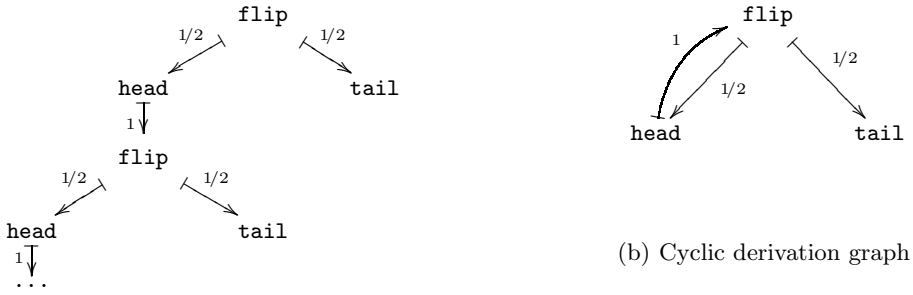
However, the main attention in this paper will be addressed to the case in which the CHRiSM program does not universally terminate.

Example 3 (Repeated Coin Flipping cont'd) *Consider again Example 1.*

```
flip <=> head:0.5 ; tail:0.5.
head <=> flip.
```

Recall that the only infinite derivation has probability $\lim_{n\to\infty}(0.5)^n = 0$, *so that we can conclude that the program probabilistically terminates.*

Figure 2 shows the derivation tree for this program, assuming the query `flip`. *This derivation tree corresponds to a finite cyclic derivation graph. There is only one cycle in this graph and its probability is less than one.* □



(a) Infinite derivation tree

(b) Cyclic derivation graph

Fig. 2. Repeated coin flipping example.

Example 4 (Basic a-to-a) *In terms of termination behavior, the coin flipping program is equivalent to the following program, given the query* `a`*:*

```
0.5 ?? a <=> a.
```

To analyze the probabilistic termination of programs we have to compute the termination probability as the sum of the probabilities of all terminating derivations. It is not difficult to see that for the above program, just as in the original coin flipping program, the termination probability is $\sum_{i=1}^{\infty}(0.5)^i = 1$. □

The above example can be generalized to the case where the probability is some `p` between 0 and 1, instead of 0.5. Consider the rule "`p ?? a <=> a.`" where `p` is a fixed probability. All terminating derivations consist of n rule applications followed by one non-applied rule instance. Thus, the probability of such a derivation is $p^n(1-p)$. Hence, the total termination probability s for the above program is $s = \sum_{n=0}^{\infty} p^n(1-p)$. To solve this infinite sum it suffices to note that $s - ps = 1 - p$, so if $p < 1$ we have $s = (1-p)/(1-p) = 1$. If $p = 1$ we get $s = 0$ since every term is zero.

We can compute the expected number of rule applications (i.e., the average run time) as follows, assuming $p < 1$ so the probability of non-termination is zero: $\sum_{n=0}^{\infty} p^n(1-p)n = p/(1-p)$. So e.g. if $p = 3/4$, then the expected number of rule applications is 3.

4 Markov Chains and MC-type computations

Example 5 (Bull-bear) *Consider the following* CHRiSM *program, which implements a Markov chain modeling the evolution of some market economy:*

```
s(T,bull) ==> (s(T+1,bull):0.9 ; s(T+1,bear):0.1).
s(T,bear) ==> (s(T+1,bear):0.7 ; s(T+1,bull):0.2 ; s(T+1,recession):0.1).
s(T,recession) ==> (s(T+1,recession):0.7 ; s(T+1,bear):0.2 ; stop:0.1).
```

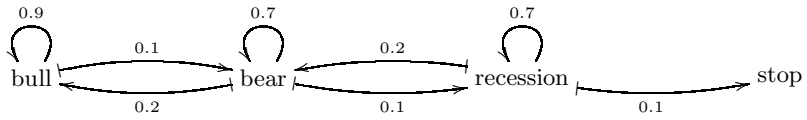


Fig. 3. Markov chain representing the economy.

Figure 3 illustrates the transitions. In every state the most likely option is to stay in that state. Also, a bull market can become a bear market, a bear market can recover to a bull market or worsen into a recession, and in a recession we can recover to a bear market or the market economy transition system may come to an end (e.g. a socialist revolution happened).

In this case, the program terminates probabilistically. This can be shown as follows. From every execution state, the probability of termination has a nonzero lower bound, as can be verified from Fig.3. Indeed, it is easy to see that in every state, the probability of terminating "immediately" (i.e. by taking the shortest path to the final state "stop") is at least 0.001*. Now, every infinite derivation has to visit one of the states in Fig.3 infinitely often. Let p_x be the total probability of all derivations that visit state x infinitely often, then the probablity of non-termination is at most $p_{bull}+p_{bear}+p_{recession}$. We now show that $p_x = 0$. Consider all subderivations of the form $x \rightarrowtail y_1 \rightarrowtail y_2 \rightarrowtail \ldots \rightarrowtail x$ where all intermediate $y_i \neq x$. The total probability for all such subderivations has to be less than* 0.999*, since there is a subderivation $x \overset{p}{\rightarrowtail}{}^* stop$ with $p \geq 0.001$ (where all intermediate steps are different from x). This means that the probability p_x is bounded from above by*

$$\lim_{n\to\infty} (0.999)^n = 0$$

so the probability of termination is one. □

In the previous two examples, the transition graph is essentially finite, in the following sense: there exists a finite set of abstractions of states and probabilistic transitions between these abstract states and an abstraction function from execution states to abstract states, such that for all reachable executions states, concrete transitions between these states are mapped to transitions between abstract states, with the same probability, and conversely.

More formally, we introduce MC-graphs and MC-type computations.

Definition 4 (MC-graph). *An MC-graph is an annotated, directed graph, (V, A, L), consisting of a finite set of vertices $V = \{v_1, \ldots, v_n\}$, a set of arcs, $A \subseteq V \times V$, and a function $L : A \rightarrow]0, 1]$. We refer to L as the probability labeling for A.*

It should be clear that an MC-graph represents a Markov Chain.

Definition 5 (MC-type computation). *Let $\mathcal{P}$ be a* CHRiSM *program and Q a query to $\mathcal{P}$. The computation for $\mathcal{P}$ and Q consists of all possible transitions $\sigma \overset{p}{\underset{\mathcal{P}}{\rightarrowtail}} \sigma'$, reachable from the initial state $\langle Q, \emptyset, true, \emptyset\rangle_0$.*

The computation for $\mathcal{P}$ and Q is an MC-type computation, if there exists an MC-graph (V, A, L) and a function $\alpha : \Sigma \to V$, such that:

- *If there is a transition $\sigma \overset{p}{\underset{\mathcal{P}}{\rightarrowtail}} \sigma'$ of type* **Probabilistic-Choice** *or* **Maybe-Apply** *(see Fig. 1) in the computation for $\mathcal{P}$ and Q, where $p > 0$ (we omit impossible transitions), then $(\alpha(\sigma), \alpha(\sigma')) \in A$ and $L((\alpha(\sigma), \alpha(\sigma'))) = p$.*
- *If $\alpha(\sigma) \in V$, $(\alpha(\sigma), v) \in A$ and $L((\alpha(\sigma), v)) = p$, then there exists a reachable execution state $\sigma' \in \Sigma$, such that $\alpha(\sigma') = v$ and $\sigma \overset{p}{\underset{\mathcal{P}}{\rightarrowtail}} \sigma'$ is in the computation for $\mathcal{P}$ and Q.*

Example 6 (a-to-a, bull-bear cont'd) *In the a-to-a example, $V = \{a, stop\}$, $A = \{(a, a), (a, stop)\}$, $L((a, a)) = p$, and $L((a, stop)) = 1 - p$. All reachable non-final execution states are mapped to a, all final states are mapped to stop.*

In the bull-bear example, the MC-graph is essentially as represented in Figure 3, with the addition of the loop-arcs on the vertices bull, bear and recession. The mapping α maps an execution state of the form $\langle \mathbb{G}, \mathbb{S}, \mathbb{B}, \mathbb{T} \rangle_n$ to the node `x` *iff* `s(_,x)` $\in \mathbb{G}$ *or* `s(_,x)#k` $\in \mathbb{S}$ *and* `(_,k)` $\notin \mathbb{T}$. □

Note that a leaf node (a node without outgoing edges) in the MC-graph corresponds to final states. We have the following criterion for probabilistic termination of MC-type computations.

Theorem 1. *Let $\mathcal{P}$ be a* CHRiSM *program and Q a query, such that the computation for $\mathcal{P}$ and Q is MC-type and let (V, A, L) be the associated MC-graph. The program $\mathcal{P}$ probabilistically terminates for Q if for every node $v_i \in V$, there is a path in A from v_i to a leaf node.*

Proof. The argument is identical to the one for the bull-bear example above.

It is tempting (but wrong) to think that a CHRiSM program $\mathcal{P}$ is probabilistically terminating if every cycle in its derivation graph has a probability $p < 1$. This is a tempting idea, because, for such programs, every infinite derivation has probability zero. However, even for MC-type computations, this is wrong.

Example 7 (Infinite Coin Flipping) *The following program terminates with probability zero, although every infinite derivation has probability zero:*

```
flip <=> head:0.5 ; tail:0.5.
head <=> flip.
tail <=> flip.
```
□

5 The Drunk Guy on a Cliff and More

Now let us analyze a more challenging toy example in which the transition graph is essentially infinite. Consider the following rule:

```
0.5 ?? a <=> a, a.
```

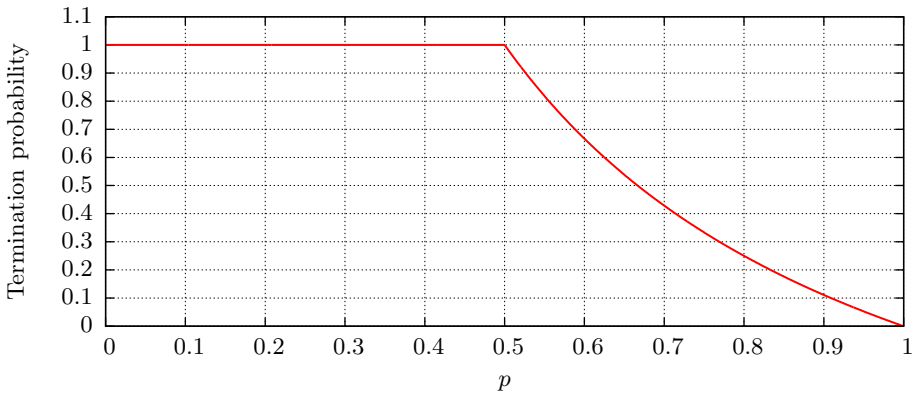


Fig. 4. Termination probability for the rule "`p ?? a <=> a,a`".

We are trying to find the termination probability s for the query `a`. With probability 0.5, the program terminates immediately (the rule instance is not applied), and with probability 0.5, it terminates if and only if it (independently) terminates two times in a row for the query `a`. If terminating once has probability s, then terminating twice has probability s^2, so we get the following equation:

$$s = 0.5 + 0.5s^2$$

The only solution to this equation is $s = 1$. Somewhat counter-intuitively, the above program does terminate probabilistically.

In general, consider the above rule with an arbitrary fixed probability p:

```
p ?? a <=> a, a.
```

We can compute the termination probability as follows. Again, either the program terminates immediately or it has to terminate twice from the query `a`, so $s = (1-p) + ps^2$. Solving for s, we get $s = 1$ or $s = \frac{1-p}{p}$, so taking into account that $0 \leq s \leq 1$ (since s is a probability), we have $s = 1$ if $p \leq 1/2$ and $s = (1-p)/p$ if $p \geq 1/2$ (see Fig. 4).

The "drunk guy on a cliff" puzzle is defined as follows. There is a sheer cliff, and a drunk guy is facing the cliff. He is staggering drunkenly back and forth. One single step forward from his current location will send him hurtling into the abyss, a step backward will bring him closer to safety. The chance of him staggering backwards (at any time) is p, the chance of him staggering forwards is $1-p$. What is the chance that he will eventually fall into the abyss?

We can model the drunk guy on a cliff as follows:

```
dist(0) <=> true.
dist(N) <=> N > 0 |  dist(N+1):p ; dist(N-1):(1-p).
```

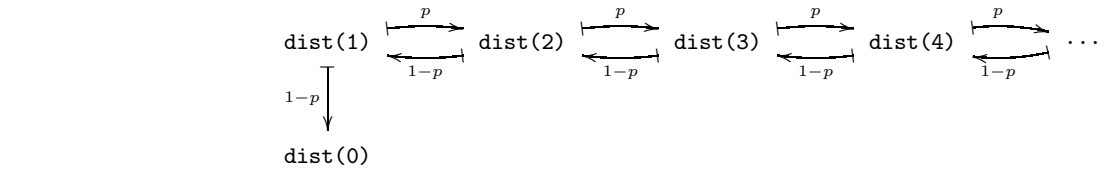


Fig. 5. Derivation graph for the drunk guy on a cliff program.

with the initial query `dist(1)`. The only way to terminate is by reaching `dist(0)`, i.e. by falling into the abyss. So the drunk guy on a cliff puzzle boils down to computing the termination probability of the above program.

For example, consider the case $p = {}^1/_2$ and the query `dist(1)`. The probability of termination $s = s(\texttt{dist(1)})$ can be computed as follows:

$$s(\texttt{dist(i)}) = \frac{1}{2}s(\texttt{dist(i - 1)}) + \frac{1}{2}s(\texttt{dist(i + 1)})$$

Given that $s(\texttt{dist(0)}) = 1$, it is easy to verify that

$$s(\texttt{dist(1)}) = \frac{1}{2} + \frac{1}{2}s(\texttt{dist(2)}) = \frac{2}{3} + \frac{1}{3}s(\texttt{dist(3)}) = \frac{3}{4} + \frac{1}{4}s(\texttt{dist(4)}) = \ldots = 1$$

It turns out that we have already solved this problem. Consider again the program consisting of the single rule "`p ?? a <=> a,a`", and consider an $\omega_t^{??}$ execution state $\sigma = \langle \mathbb{G}, \mathbb{S}, \mathbb{B}, \mathbb{T} \rangle_n$ in a derivation starting from the query "`a`". The probability of termination from state σ only depends on the number of `a`/0 constraints for which the rule could still be applied, which is the following number: $\left|\mathbb{G} \uplus \{\!\{ \texttt{a}\#n \in \mathbb{S} \mid (1,n) \notin \mathbb{T} \}\!\}\right|$. Let us call this number the *distance to termination* and denote it with $d(\sigma)$. When considering a rule instance, there are two options: with probability p, the distance increases by one (the rule is applied), and with probability $1 - p$, the distance decreases by one (the rule is not applied). The program terminates as soon as $d(\sigma) = 0$.

An alternative way to compute the termination probability of the above programs is as follows. All terminating derivations consist of n rule instances that are applied (or distances that are increased) and $n+1$ rule instances that are not applied (or distances that are decreased), for some number n. For example, for $n = 3$ we have the following five derivations: $+++----$, $++-+--$, $++--+-$, $+-++--$, and $+-+-+-$ where "+" means "applied" (or incremented) and "−" means "not applied" (or decremented). For a given number n of applied rule instances, the number of possible derivations is given by the n-th Catalan number[1] $C_n = (2n)!/(n!(n+1)!)$. This gives us the following

[1] The Catalan numbers are named after the Belgian mathematician Eugène Charles Catalan (1814-1894). They are sequence A000108 in The On-Line Encyclopedia of Integer Sequences (`http://oeis.org/A000108`).

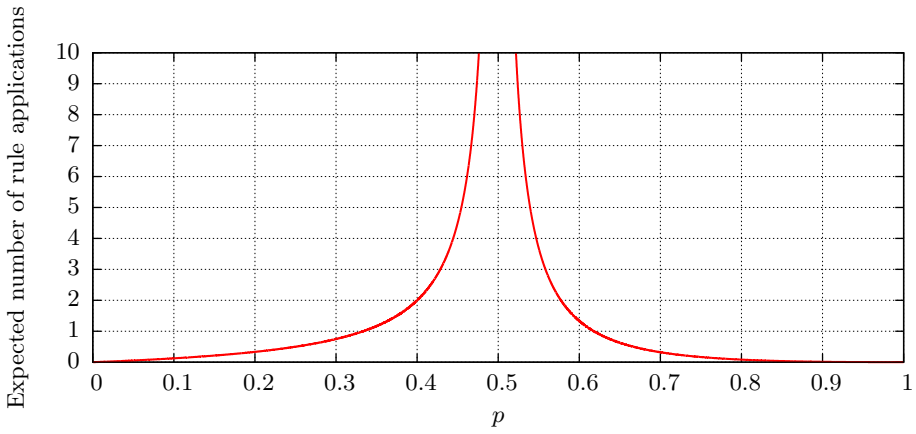


Fig. 6. Expected number of rule applications (if terminating) for "`p ?? a <=> a,a`".

formula to compute the termination probability s:

$$s = \sum_{n=0}^{\infty} p^n (1-p)^{n+1} \frac{(2n)!}{n!(n+1)!}$$

The above infinite sum converges to the same values for s we already calculated above. However, this alternative formulation allows us to compute the expected number of rule applications (of the rule "`p ?? a <=> a,a`"). The expected number of rule applications is given by:

$$E_p = \sum_{n=0}^{\infty} p^n (1-p)^{n+1} \frac{(2n)!}{n!(n+1)!} n$$

Figure 6 shows the expected number of rule applications E_p as a function of p. As p gets closer to $1/2$, the value for E_p grows quickly: for $p = \frac{2^k-1}{2^{k+1}}$, we have $E_p = \frac{2^k-1}{2}$. The border case $p = 1/2$ is interesting: the termination probability is 1 but the expected number of rule applications is $+\infty$. As p gets larger than $1/2$, the termination probability drops and so does the expected number of rule applications of the (increasingly rare) terminating derivations.

Multi-headed rules. So far, we have only considered single-headed rules. One of the simplest "interesting" cases is the following rule: (with less than three `a`'s in the body, the program terminates universally)

```
p ?? a, a <=> a, a, a.
```

Given the query "`a,a`", there are two rule instances to be considered: (`a`#1, `a`#2) and (`a`#2, `a`#1). If both instances are not applied (probability $(1-p)^2$), the program terminates; otherwise we are further away from termination.

We define the termination distance $d(\sigma)$ of an execution state $\sigma = \langle \mathbb{G}, \mathbb{S}, \mathbb{B}, \mathbb{T} \rangle_n$ as a pair $d(\sigma) = (n, m)$ where $n = \left|\mathbb{G}\right|$ is the number of "not yet considered" $\mathtt{a}$'s and $m = \left|\mathbb{S}\right|$ is the number of "considered" $\mathtt{a}$'s. Given the query "$\mathtt{a,a}$", the initial state has distance $(2, 0)$.

The termination probability $s(n, m)$ of a state with distance (n, m) can be computed as follows. If $n = 0$, the rule can no longer be applied so we have termination. If $n > 0$, we can take one $\mathtt{a}/0$ and consider all matching rule instances. Since there are m possible partner constraints and two (symmetric) occurrences of the active constraint, there are $2m$ rule instances to consider. If none of these rule instances are applied, we just add the $\mathtt{a}/0$ constraint to the store, so the new distance will be $(n - 1, m + 1)$. However, if one of the rule instances is applied, we get a new distance $(n + 2, m - 1)$. So the termination probability $s(n, m)$ is given by the following equations:

$$\begin{cases} s(0, m) = 1 \\ s(n, m) = (1 - p)^{2m} s(n - 1, m + 1) + (1 - (1 - p)^{2m}) s(n + 2, m - 1) \end{cases}$$

Note that if $m = 0$, there are no partner constraints so there are no rule instances to consider, i.e. $s(n, 0) = s(n - 1, 1)$.

Unfortunately, we have not found a closed-form solution for the above equations. The example shows that, while the complexity of the programs increases, the mathematical models representing the probability of termination become too complex to be solved by standard techniques.

6 Conclusion and Future Work

In this paper we presented the results of an initial investigation of the concept of probabilistic termination of CHRiSM programs. This research has mostly taken the form of a number of small case studies, in which we attempt to reveal the intuitions concerning the concept of probabilistic termination and present some ways of (manually) proving probabilistic termination. In the process, for some of the cases, we also study the expected number of rule applications.

For some classes of programs, we have generalised the observations in our case studies and we formulated and proved termination conditions. In particular, for universally termination programs we obviously also get probabilistic termination. Therefore, techniques developed to prove universal termination of CHR are sufficient to prove probabilistic termination of corresponding CHRiSM programs. We also identified the class of MC-type programs and formulated and proved a sufficient probabilistic termination condition for it.

For more general classes of programs, termination proofs may become quite complex. We elaborated on a few more complex (but still toy) cases, where sometimes we are able to solve the problem, but in other cases, we observe that the equations expressing probabilistic termination are too complex to be solved with standard techniques. In this exploratory paper we have focused on

intuition and examples. It would be interesting to investigate to what extent the theoretical work of [5, 4] can be transferred to our setting.

Finally, note that although this work has been in the context of CHRiSM, most of the ideas are also applicable to other probabilistic logic programming languages like PRISM and ProbLog. In most of the probabilistic inference algorithms used in the implementations of these languages (e.g. probability computation, learning), it is assumed that the program universally terminates. An interesting direction for future work is to generalize these algorithms such that they can handle (certain classes of) probabilistically terminating programs.

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Improved termination analysis of CHR using self-sustainability analysis

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Abstract. In the past few years, several successful approaches to termination analysis of Constraint Handling Rules (CHR) have been proposed. In parallel to these developments, for termination analysis of Logic Programs (LP), recent work has shown that a stronger focus on the analysis of the cycles in the strongly connected components (SCC) of the program is very beneficial, both for precision and efficiency of the analysis.
In this paper we investigate the benefit of using the cycles of the SCCs of CHR programs for termination analysis. It is a non-trivial task to define the notion of a cycle for a CHR program. We introduce the notion of a self-sustaining set of CHR rules and show that it provides a natural counterpart for the notion of a cycle in LP. We prove that non-self-sustainability of an SCC in a CHR program entails termination for all queries to that SCC. Then, we provide an efficient way to prove that an SCC of a CHR program is non-self-sustainable, providing an additional, new way of proving termination of (part of) the program.
We integrate these ideas into the CHR termination analyser CHRisTA and demonstrate by means of experiments that this extension significantly improves both the efficiency and the performance of the analyser.

1 Introduction

Termination analysis techniques for Logic Programs often make use of dependency analysis. In some approaches (e.g. [5]), this is done in order to detect (mutually) recursive predicates. For non-recursive predicates, no termination proof is needed, so that termination conditions are only expressed and verified for the recursive ones. In other approaches (e.g. [11], [17]) the termination conditions are explicitly expressed in terms of cycles in the strongly connected components (SCCs) of the dependency graph. It was shown in [17] that such an approach is both efficient and precise. On the benchmark of the termination analysis competition (see [22]) it outperformed competing systems.

Recently, in [23] and [12], we adapted termination analysis techniques from Logic Programming (LP) to Constraint Handling Rules (CHR) [1, 8] and developed the CHR termination analyser CHRisTA [13]. These techniques and system are based on recursion, rather than on cycles in SCCs.

The main motivation that led to the current work is that we wanted to adapt the approach based on SCCs to CHR, with the hope of improving efficiency and precision. It turned out that there were considerable complications to achieve this, caused by the fact that for CHR a useful notion of "cycle" is hard to define.

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Consider for example the CHR program, P, consisting of the CHR rule,

$$R \ @ \ a, b \Leftrightarrow a.$$

For each application of R, two constraints, a and b, are removed, while a new constraint, a, is added. Since R adds constraints that are required to fire R, the application of R depends on itself. An SCC analysis on the dependency graph of P would therefore consider R to be cyclic, while in fact, for every application of R, a constraint b is removed and never added again. Therefore, at some point in a computation of P, the b constraints will be depleted and thus P will terminate.

A more accurate analysis of cycles in CHR could therefore still rely on an SCC analysis, but could also verify for each SCC whether there exists a dependency for each head of the rules of a component, provided for by the component itself.

Unfortunately, such an approach is still not very accurate. Consider for example the CHR program, P, consisting of the rule,

$$R \ @ \ a, a \Leftrightarrow a.$$

For R, which is part of an SCC, both heads are provided for from within the component itself. However, for every application of R, two constraints a are removed, while only one constraint a is added. Repeated application of R will therefore result in depletion of these a constraints, and thus P will terminate.

Therefore, in order for an SCC in CHR to be cyclic, we must guarantee that the component is *self-sustainable*. That is, when the rules of an SCC are applied, they must provide the constraints to fire the same rules again.

In fact, in definite LP, an SCC of the dependency graph of a definite LP program is self-sustainable by default. The reason for this is that definite LP is a single-headed language. Therefore, each cycle in the dependency graph of a definite LP program —as described by the SCCs of the program— corresponds to rule applications that have the potential to be repeated.

In CHR, to characterise the notion of a self-sustainable SCC, we need to identify the multisets of rule applications of an SCC that can be repeated. Consider for example the CHR program, P:

$$R_1 \ @ \ a, a \Leftrightarrow b, b. \qquad R_2 \ @ \ b \Leftrightarrow a.$$

As can be verified, it is non-terminating. That is, when R_1 is applied once, it adds two b constraints, allowing R_2 to be applied twice. By applying R_2 twice, the input required for application of R_1 is provided for, thus resulting in a loop.

In this paper, we introduce the notion of *self-sustainability* for a set of CHR rules. It provides a rather precise approximation of cyclic behaviour in CHR. We characterise self-sustainability for a set of rules by means of a system of linear inequalities. Each solution to this system identifies a multiset based on the given rules, such that, if it is *traversed* —all rules in the multiset are applied once— it provides all required constraints to potentially traverse the multiset again.

Unfortunately, we cannot use this concept directly as a basis for termination analysis, similar to [11] for LP. The reason is that for any cyclic SCC in a CHR program, the system has infinitely many solutions. In [15], we describe a rather inefficient approach to cope with this problem, resulting in little gain in precision.

Alternatively, we can use the concept of self-sustainability in a "negative" way. If we can show that an SCC in a CHR program is *not* self-sustainable —the system has no solution— then this proves that the rules involved in that SCC cannot be part of an infinite computation. Therefore, we can ignore these rules in the termination analysis. By integrating this idea in the CHRisTA analyser, it turns out that precision and efficiency of the analysis is improved.

Our approach will be restricted to the abstract CHR semantics. It is however widely applicable as most other CHR semantics [18] are instances of the abstract CHR semantics. That is, if an SCC of a CHR program is not self-sustainable for the abstract semantics, it cannot be self-sustainable for any more refined semantics. Note that, under the abstract semantics, the two different kinds of rules —*simpagation* and *propagation* rules— of a CHR program behave as *simplification* rules. Hence, we discuss our approach in terms of simplification only.

Finally, note that a CHR program may contain propagation rules and that these rules do not remove the constraints on which they fire. Under the abstract CHR semantics, propagation rules are infinitely applicable on the same combination of constraints. Represented as a simplification rule, they explicitly replace the constraints on which they fire and thus are considered self-sustainable by default. Our approach can therefore only prove non-self-sustainability of an SCC without propagation. In Section 6, we provide intuitions regarding self-sustainability under the theoretical CHR semantics [8]. This refinement of the abstract CHR semantics additionally considers a *fire-once policy* on propagation rules to overcome the infinite applicability of propagation rules.

Overview of the paper. In Section 2, we discuss the syntax and semantics of abstract CHR. Section 3 defines CHR dependency graphs for an SCC analysis and CHR nets —a more accurate description of the dependencies of a CHR program— for a self-sustainability analysis. In Section 4, we formalise the notion of self-sustainability of an SCC (Section 4.1). Then, we present a test for verifying that an SCC is not self-sustainable (Section 4.2). In Section 5, we evaluate our approach and discuss CHR programs that we can only prove terminating using the test for non-self-sustainability. Finally, in Section 6, we conclude the paper.

2 Preliminaries

We assume familiarity with LP and its main results [2, 9]. By L, we denote the first order language underlying a CHR program P. By $Term_P$ and $Atom_P$, we denote, respectively, the sets of terms and atoms constructible from L.

2.1 The syntax of abstract CHR

The rules of a CHR program act on first-order atoms, called *constraints*.

Definition 1 (constraint). Constraints, $c(t_1, \ldots, t_n)$ $(n \geq 0)$, *are first-order predicates applied to terms,* t_i $(1 \leq i \leq n)$. *We distinguish between two kinds of constraints:* CHR constraints *are user-defined and are solved by the* CHR rules *of a* CHR program*;* built-in constraints *are pre-defined and are solved by a* constraint theory *(*CT*) defined in the* host language. □

Constraints are kept in a *constraint store*, of which the behaviour corresponds to a *multiset* (or bag) of constraints. Therefore, to formalise the syntax and semantics of CHR, we first recall multiset theory [4, 6].

A *multiset* is a tuple, $M_S = \langle S, m_S \rangle$, where S is a set, called the *underlying set*, and m_S a *multiplicity function*, mapping the elements, e, of S to natural numbers, $m_S(e) \in \mathbb{N}_0$, representing the number of occurrences of e in M_S. Like any function, m_S may be represented as a set, $\{(s, m_S(s)) : s \in S\}$. An example of a multiset is $\langle \{a, b\}, \{(a, 2), (b, 1)\} \rangle$. We introduce the alternative notation to represent this multiset as $[\![a, a, b]\!]$.

If a *universe* U in which the elements of S must live is specified, the definition of a multiset can be simplified to a *multiset indicator function*. Let U be a universe for a multiset $M_S = \langle S, m_S \rangle$. Then, we define the *multiset indicator function*, $\mu_S : U \to \mathbb{N}$, of M_S w.r.t. U as: $\mu_S(u) = m_S(u)$ if $u \in S$ and $\mu_S(u) = 0$ if $u \notin S$. Since it is often more favourable to discuss multisets in terms of some universe, we can —as an abuse of notation— denote a multiset $M_S = \langle S, m_S \rangle$ also by $\langle U, \mu_S \rangle$, or μ_S if its universe is clear from context.

Furthermore, we will need the notion of a *multisubset* in the constraint store since the rules of a CHR program will be applied on multisubsets of constraints. Let U be a universe for the multisets M_{S_1} and M_{S_2}. Then, multiset M_{S_1} is a *multisubset* of multiset M_{S_2}, denoted $M_{S_1} \sqsubseteq M_{S_2}$, iff the multiset indicator functions, μ_{S_1} and μ_{S_2}, w.r.t. U, of M_{S_1} and M_{S_2} respectively, are such that $\mu_{S_1}(u) \leq \mu_{S_2}(u)$, for all u in U. Associated to $\sqsubseteq$, we define *strict multisubsets*: $M_{S_1} \sqsubset M_{S_2} \leftrightarrow M_{S_1} \sqsubseteq M_{S_2} \wedge M_{S_2} \not\sqsubseteq M_{S_1}$.

We are now ready to recall the syntax of *simplification rules*.

Definition 2 (abstract CHR program). *An* abstract CHR program *is a finite set of* simplification rules*, R_i.*

A simplification rule*,*

$$R_i \ @ \ H_1^i, \ldots, H_{n_i}^i \Leftrightarrow G_1^i, \ldots, G_{k_i}^i \mid B_1^i, \ldots, B_{l_i}^i, C_1^i, \ldots, C_{m_i}^i.$$

is applicable on a multiset of CHR constraints, matching with the head*, $[\![H_1^i, \ldots, H_{n_i}^i]\!]$, of the rule, such that the* guard*, $[\![G_1^i, \ldots, G_{k_i}^i]\!]$, is satisfiable. Upon application, the multiset of constraints matching with the head is replaced by an appropriate instance of the multiset of built-in and CHR constraints, $[\![B_1^i, \ldots, B_{l_i}^i, C_1^i, \ldots, C_{m_i}^i]\!]$, from the* body *of the rule.*

Note that the guard, $[\![G_1^i, \ldots, G_{k_i}^i]\!]$, of a CHR rule may only consist of built-in constraints. Also note that naming a rule by "rulename @" is optional. □

The next example program is an introductory example to CHR(Prolog).

Example 1 (Primes). The program below implements the Sieve of Eratosthenes for finding the prime numbers up to a given number. User-defined *prime*/1 constraints are used to hold the values of the positive integers for which we derive whether they are prime. User-defined *primes*/1 constraints are used to query the program and to generate the *prime*/1 constraints for prime evaluation.

R_1 @ $primes(2) \Leftrightarrow prime(2)$.
R_2 @ $primes(N) \Leftrightarrow N > 2 \mid Np \text{ is } N-1, prime(N), primes(Np)$.
R_3 @ $prime(M), prime(N) \Leftrightarrow div(M,N) \mid prime(M)$.

R_2 generates the numbers for prime evaluation top-down. It replaces a $primes(n)$ constraint, matching with the head $primes(N)$, by the constraints Np *is* $n-1$, $prime(n)$ and $primes(Np)$, if $CT \models n > 2$. R_1 removes a $primes(2)$ constraint, replacing it with the final number for prime evaluation, $prime(2)$. R_3 implements the sieve. For any two matching constraints, $prime(m)$ and $prime(n)$, such that m divides n, we replace both $prime/1$ constraints by $prime(m)$. □

2.2 The semantics of abstract CHR

The abstract CHR semantics is defined as a state transition system.

Definition 3 (abstract CHR state). *An* abstract CHR state *is a multiset, Q, of constraints (with universe $Atom_P$), called a* constraint store. □

To define the transitions on CHR states, as given by the CHR rules of the program, we introduce the multiset operator *join*, adding multisets together. Let M_A and M_B be multisets with universe U, and let u be an element of U. Then, the multiset indicator function of the *join* $M_C = M_A \uplus M_B$ is given by the sum, $\mu_C(u) = \mu_A(u) + \mu_B(u)$, of the multiset indicator functions of M_A and M_B.

The CHR transition relation represents the consecutive CHR states for a CHR program P and constraint theory CT.

Definition 4 (abstract CHR transition relation). *Let P be a CHR program and CT a constraint theory for the built-in constraints. Let θ represent the substitutions corresponding to the bindings generated when resolving built-in constraints by CT, and let σ represent substitutions for the variables in the head of the rule as a result of matching. Then, the* transition relation, *$\rightarrow_P$, for P, where Q is a CHR state, is defined by:*

1. ***A solve transition:***
   if $Q = [\![b]\!] \uplus Q'$, *with b a built-in constraint, and* $CT \models b\theta$,
   then, $Q \rightarrow_P Q'\theta$.
2. ***Simplification:***
   if $(R_i \text{ @ } H_1^i, \ldots, H_{n_i}^i \Leftrightarrow G_1^i, \ldots, G_{k_i}^i \mid B_1^i, \ldots, B_{l_i}^i, C_1^i, \ldots, C_{m_i}^i.) \in P$,
   and if $Q = [\![h_1, \ldots, h_{n_i}]\!] \uplus Q'$ *and*
   $\exists \sigma\theta : CT \models (h_1 = H_1^i\sigma) \wedge \ldots \wedge (h_{n_i} = H_{n_i}^i\sigma) \wedge (G_1^i, \ldots, G_{k_i}^i)\sigma\theta$,
   then, $Q \rightarrow_P ([\![B_1^i, \ldots, B_{l_i}^i, C_1^i, \ldots, C_{m_i}^i]\!] \uplus Q')\sigma\theta$.

Rules in CHR are non-deterministically applied until exhaustion, thus until no more transitions are possible. Rule application is a committed choice. Built-in constraints are assumed to return an answer in finite time and cannot introduce new CHR constraints. If built-ins cannot be solved by CT, the program fails. □

By an *initial CHR state* or *query state* for a CHR program P, we mean any abstract CHR state for P. By a *final CHR state* or *answer state* for P, we mean a CHR state Q, such that no CHR state Q' exists for which $(Q, Q') \in \rightarrow_P$.

Example 2 (Primes continued). Executing the program from Example 1 on an initial CHR state $Q_0 = [\![primes(7)]\!]$, we obtain by application of R_2 the next state $Q_1 = [\![Np\ is\ 7-1, prime(7), primes(Np)]\!]$. Solving the built-in constraint, $Np\ is\ 7-1$, binds 6 to Np, yielding the state, $Q_2 = [\![prime(7), primes(6)]\!]$. Proceeding in this way, we obtain the state $Q_{10} = [\![prime(3), primes(2), prime(4), prime(5), prime(6), prime(7)]\!]$, on which R_2 is no longer applicable. Then, by application of R_1, we obtain $Q_{11} = [\![prime(2), prime(3), prime(4), prime(5), prime(6), prime(7)]\!]$.

Now only R_3 is applicable, replacing two $prime/1$ constraints by the constraint dividing the other. For example, we can remove $prime(4)$ since $prime(2)$ divides it. A next state could therefore be $Q_{12} = [\![prime(2), prime(3), prime(5), prime(6), prime(7)]\!]$. For $prime(6)$ there are two prime numbers that divide it. One possibility is that $prime(3)$ is used, and obtain $Q_{13} = [\![prime(3), prime(2), prime(5), prime(7)]\!]$.

Since on Q_{13} no more rules are applicable, we reach an answer state. This state holds all prime numbers up to 7. □

3 The CHR dependency graph and CHR net

In CHR, the head constraints of a rule represent the constraints *required* for rule application. The body CHR constraints represent the constraints *newly available* after rule application. To represent these sets, we introduce *abstract CHR constraints.*

Definition 5 (abstract CHR constraint). *An* abstract CHR constraint *is a pair $\mathcal{C} = (C, B)$, where C is a CHR constraint, and B a conjunction of built-in constraints. The denotation of an abstract CHR constraint is given by a mapping $\wp : (C, B) \mapsto \{C\sigma \mid \exists\theta : CT \models B\sigma\theta\}$.*

In a CHR program P, we distinguish between two types of abstract CHR constraints. An abstract input constraint*, $in^i_j = (H^i_j, G^i)$, represents the CHR constraints that can be used to match the head H^i_j of a CHR rule R_i, without invalidating the guards $G^i = G^i_1 \wedge \cdots \wedge G^i_{k_i}$ of R_i. An* abstract output constraint*, $out^i_j = (C^i_j, G^i)$, represents the CHR constraints that become newly available after rule application, and are related to the body CHR constraints C^i_j of R_i.* □

By $\mathcal{I}n_{R_i}$ and $\mathcal{O}ut_{R_i}$, we represent the sets of abstract input and output constraints of a rule R_i. By $\mathcal{I}n_P$ and $\mathcal{O}ut_P$, we represent the abstract input and output constraints of a CHR program P.

Example 3 (abstract CHR constraints of Primes). We revisit the Primes program from Example 1, and derive:

- $\mathcal{I}n_P = \mathcal{I}n_{R_1} \cup \mathcal{I}n_{R_2} \cup \mathcal{I}n_{R_3} = \{in^1_1, in^2_1, in^3_1, in^3_2\}$, where
  $in^1_1 = (primes(2), true)$ $in^2_1 = (primes(N), N > 2)$
  $in^3_1 = (prime(M), div(M, N))$ $in^3_2 = (prime(N), div(M, N))$
- $\mathcal{O}ut_P = \mathcal{O}ut_{R_1} \cup \mathcal{O}ut_{R_2} \cup \mathcal{O}ut_{R_3} = \{out^1_1, out^2_1, out^2_2, out^3_1\}$, where
  $out^1_1 = (prime(2), true)$ $out^2_1 = (prime(N), N > 2)$
  $out^2_2 = (primes(Np), N > 2)$ $out^3_1 = (prime(M), div(M, N))$

□

The rules of a CHR program P relate abstract inputs to abstract outputs. We call this relation the *rule transition relation* of P.

Definition 6 (rule transition relation). *A rule transition of an abstract CHR program, P, is an ordered pair $T_i = (\mathcal{I}n_{R_i}, \mathcal{O}ut_{R_i})$, relating the set of abstract input constraints $\mathcal{I}n_{R_i} = \{in_1^i, \ldots, in_{n_i}^i\}$ of $R_i \in P$ to the set of abstract output constraints $\mathcal{O}ut_{R_i} = \{out_1^i, \ldots, out_{m_i}^i\}$ of R_i. The rule transition relation $\mathcal{T}_P = \{T_i \mid R_i \in P\}$ of P is the set of rule transitions of P.* □

Example 4 (rule transition relation of Primes). The Primes program P from Example 1 defines three rule transitions:

- $\mathcal{T} = \{T_1, T_2, T_3\}$, where
  $T_1 = (\{in_1^1\}, \{out_1^1\})$ $\quad T_2 = (\{in_1^2\}, \{out_1^2, out_2^2\})$
  $T_3 = (\{in_1^3, in_2^3\}, \{out_1^3\})$

□

Abstract output constraints relate to abstract input constraints by a *match transition relation*. This second kind of relation is the result of a dependency analysis between abstract constraints, relating the constraints newly available after rule application to constraints required for rule application.

Definition 7 (match transition relation). *A match transition of an abstract CHR program P is an ordered pair $M_{(i,j,k,l)} = (out_j^i, in_l^k)$, relating an output $out_j^i = (C_j^i, G^i)$ of $\mathcal{O}ut_P$ to an input $in_l^k = (C_l^k, G^k)$ of $\mathcal{I}n_P$ such that $\exists\theta$: $CT \models (C_j^i = C_l^k \wedge G^i \wedge G^k)\theta$. The match transition relation $\mathcal{M}_P$ is the set of all match transitions $M_{(i,j,k,l)}$ in P.* □

Note that a match transition exists for an abstract output and input if the intersection of their denotation is non-empty, i.e. $\wp(out_j^i) \cap \wp(in_l^k) \neq \emptyset$.

Example 5 (match transition relation of Primes). The Primes program, P, from Example 1 defines the match transition relation,

$$\mathcal{M}_P = \{M_{(1,1,3,1)}, M_{(1,1,3,2)}, M_{(2,1,3,1)}, M_{(2,1,3,2)} \\ M_{(2,2,1,1)}, M_{(2,2,2,1)}, M_{(3,1,3,1)}, M_{(3,1,3,2)}\}.$$

□

As in LP, the dependency graph of a CHR program is a directed graph where the nodes represent rules, and the directed arcs dependencies between these rules.

Definition 8 (CHR dependency graph). *A* CHR dependency graph, *$\mathcal{D}_P$, of an abstract CHR program P is an ordered tuple $\langle T, D\rangle$ of nodes T, one for each transition in the rule transition relation, $\mathcal{T}_P$, of P, and directed arcs D, one for each ordered pair of transitions between which a match transition exists in the match transition relation, $\mathcal{M}_P$, of P.* □

For an SCC analysis, a CHR dependency graph is sufficient, however, for self-sustainability we rely in the next sections on a CHR net instead.

Definition 9 (CHR net). *A* CHR net, *$\mathcal{N}_P$, of an abstract CHR program, P, is a quadruple $\langle \mathcal{I}n_P, \mathcal{O}ut_P, \mathcal{T}_P, \mathcal{M}_P\rangle$. Here, respectively, $\mathcal{I}n_P$ and $\mathcal{O}ut_P$ are the abstract input and output constraints of P, and $\mathcal{T}_P$ and $\mathcal{M}_P$ the rule and match transition relations of P.* □

Note that a CHR net corresponds to a bipartite hypergraph. We illustrate both notions in Figure 1 for the Primes program of Example 1.

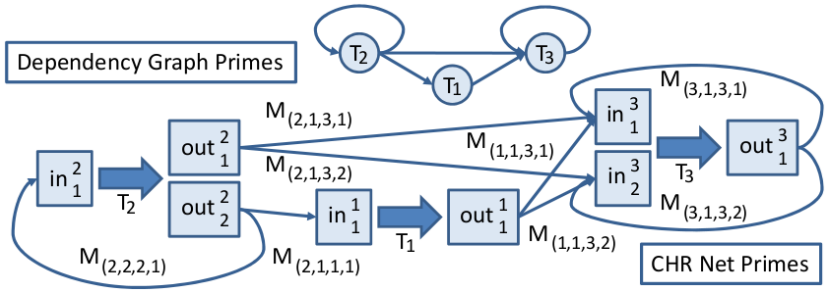

Fig. 1. Dependency graph and CHR net for Primes

4 Self-sustainable SCCs of a CHR program

To derive the SCCs of a CHR program, we perform an SCC analysis on the dependency graph of the CHR program. This is similar to such an analysis in LP and can be done efficiently using Tarjan's algorithm [21].

Example 6 (SCCs of Primes). Based on $\mathcal{D}_P = (\{T_1, T_2, T_3\}, \{(T_1, T_3), (T_2, T_1), (T_2, T_2), (T_2, T_3), (T_3, T_3)\})$, the dependency graph of Primes of Figure 1, we derive two SCCs, $\{T_2\}$ and $\{T_3\}$. □

4.1 Self-sustainable SCCs

Consider again the non-terminating example program from the Introduction:

$$R_1 \ @ \ a, a \Leftrightarrow b, b. \qquad R_2 \ @ \ b \Leftrightarrow a.$$

Its dependency graph and CHR net are shown in Figure 2. As can be verified, in Figure 2, $in_1^1 = in_2^1 = out_1^2 = (a, true)$ and $out_1^1 = out_2^1 = in_1^2 = (b, true)$. For the example, there is only one SCC: $\{T_1, T_2\}$.

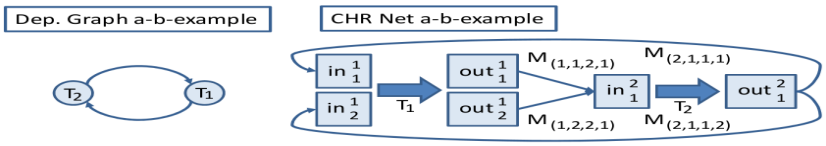

Fig. 2. Dependency graph and CHR net for the *a*-*b*-example

What we want to characterise —in the notion of self-sustainability for such an SCC— is whether we can duplicate some of the transitions of this SCC, such that for the resulting multiset of transitions and its *extended CHR net*, it is so that a multisubset of all $M_{(i,j,k,l)}$ match transitions exists, that maps a multisubset of all the out_q^p nodes *onto all of* the in_s^r nodes. Returning to our example, consider

the multiset $[\![T_1, T_2, T_2]\!]$ based on $\{T_1, T_2\}$. In Figure 3, we expand the CHR net of Figure 2 to represent all match transitions for this multiset.

It is clear that from the multiset of 8 match transitions in Figure 3, we can select 4 transitions, for example $[\![M_{(1,1,2,1)}, M_{(1,2,2,1)}, M_{(2,1,1,1)}, M_{(2,1,1,2)}]\!]$, such that these transitions define a function from a multisubset of all out_q^p nodes *onto* all in_s^r nodes. This function is represented in Figure 3 in the thick arrows.

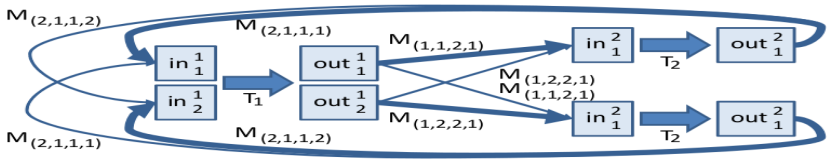

Fig. 3. Expanded CHR net for $[\![T_1, T_2, T_2]\!]$

Note that in this example, the multisubsets of out_q^p nodes on which the function is defined is equal to the entire multiset, $[\![out_1^1, out_2^1, out_1^2, out_1^2]\!]$, of out_q^p nodes. In general, this is not necessary: out_q^p nodes are allowed to be "unused" by in_s^r nodes. It suffices that a CHR constraint is produced for each in_s^r node.

We generalise the construction in the example above in the following definition. In this definition, we start off from a set of CHR rules, C, and its CHR net, $\mathcal{N}_C = \langle \mathcal{I}n_C, \mathcal{O}ut_C, \mathcal{T}_C, \mathcal{M}_C \rangle$. In the definition we will consider a multiset with universe the rule transitions $\mathcal{T}_C$, and will denote it by $\mu_{\mathcal{T}}$. Note that, given such a multiset $\mu_{\mathcal{T}}$, there are associated multisets $\mu_{\mathcal{I}n}$ and $\mu_{\mathcal{O}ut}$, with universes $\mathcal{I}n_C$ and $\mathcal{O}ut_C$, respectively. If a transition $T_i \in \mathcal{T}_C$ occurs n_i times in $\mu_{\mathcal{T}}$, then all its in_j^i and out_l^i abstract constraints occur n_i times in $\mu_{\mathcal{I}n}$ and $\mu_{\mathcal{O}ut}$, respectively.

Given $\mu_{\mathcal{T}}$, there is also an associated multiset $\mu_{\mathcal{M}}$, with universe $\mathcal{M}_C$. If transitions T_i and T_k occur respectively n_i and n_k times in $\mu_{\mathcal{T}}$, then all $M(i, j, k, l) \in \mathcal{M}_C$ occur $n_i \times n_k$ times in $\mu_{\mathcal{M}}$.

Definition 10 (self-sustainability of a set of CHR rules). *Let C be a set of simplification rules and $\mathcal{N}_C = \langle \mathcal{I}n_C, \mathcal{O}ut_C, \mathcal{T}_C, \mathcal{M}_C \rangle$ the CHR net of C. The set C is self-sustainable iff there exist*

- *a non-empty multiset $\mu_{\mathcal{T}}$, with the associated multisets $\mu_{\mathcal{I}n}$, $\mu_{\mathcal{O}ut}$ and $\mu_{\mathcal{M}}$,*
- *a multiset $\mu'_{\mathcal{O}ut} \sqsubseteq \mu_{\mathcal{O}ut}$, and*
- *a multiset $\mu'_{\mathcal{M}} \sqsubseteq \mu_{\mathcal{M}}$,*

such that $\mu'_{\mathcal{M}}$ defines a function from $\mu'_{\mathcal{O}ut}$ onto *$\mu_{\mathcal{I}n}$.* □

Before we illustrate this concept on our running example, Primes, we provide an alternative, numeric characterisation.

Proposition 1 (numeric characterisation self-sustainability). *Let C be a set of simplification rules and $\mathcal{N}_C = \langle \mathcal{I}n_C, \mathcal{O}ut_C, \mathcal{T}_C, \mathcal{M}_C \rangle$ its CHR net. The set C is self-sustainable iff there exist multisets $\mu_{\mathcal{T}}$, with associated multisets $\mu_{\mathcal{I}n}$,*

$\mu_{\mathcal{O}ut}$, $\mu_{\mathcal{M}}$, $\mu'_{\mathcal{O}ut} \sqsubseteq \mu_{\mathcal{O}ut}$ *and* $\mu'_{\mathcal{M}} \sqsubseteq \mu_{\mathcal{M}}$, *such that* $\sum_{i:T_i \in \mathcal{T}_C} \mu_{\mathcal{T}}(T_i) \geq 1$ *and such that*

$$\forall out^i_j \in \mathcal{O}ut_C : \sum_{k,l:M_{(i,j,k,l)} \in \mathcal{M}_C} \mu'_{\mathcal{M}}(M_{(i,j,k,l)}) \leq \mu_{\mathcal{T}}(T_i), \text{ and}$$

$$\forall in^i_j \in \mathcal{I}n_C : \sum_{k,l:M_{(k,l,i,j)} \in \mathcal{M}_C} \mu'_{\mathcal{M}}(M_{(k,l,i,j)}) = \mu_{\mathcal{T}}(T_i). \qquad \square$$

Proof. The first inequality expresses that $\mu_{\mathcal{T}}$ is non-empty. The second kind of inequalities —one for each out^i_j in $\mathcal{O}ut_C$— state that for an abstract output out^i_j, the number of match transitions $M_{(i,j,k,l)}$ in $\mu'_{\mathcal{M}}$ that have (i,j) as their first two arguments does not exceed the number of occurrences of T_i in $\mu_{\mathcal{T}}$. This corresponds to stating that $\mu'_{\mathcal{M}}$ can be regarded as a function defined on a multisubset $\mu'_{\mathcal{O}ut}$ of $\mu_{\mathcal{O}ut}$.

The third kind of inequalities —one for each in^i_j in $\mathcal{I}n_C$— state that for an abstract input constraint in^i_j, the number of match transitions $M_{(k,l,i,j)}$ in $\mu'_{\mathcal{M}}$ that have (i,j) as their last two arguments is exactly the number of occurrences of T_i in $\mu_{\mathcal{T}}$. This means that the function defined by $\mu'_{\mathcal{M}}$ is onto $\mu_{\mathcal{I}n}$. $\square$

Example 7 (self-sustainable SCCs for Primes). Consider the SCCs, $C_1 = \{T_2\}$ and $C_2 = \{T_3\}$, (see Example 6) of the Primes program, P, of Example 1. While the first component of the program is self-sustainable, the second is not. That is, at some point in a computation of C_2, the *prime*/1 constraints to fire the rule will be depleted. Consider their CHR nets,

$$\mathcal{N}_{C_1} = \langle \{in^2_1\}, \{out^2_1, out^2_2\}, \{T_2\}, \{M_{(2,2,2,1)}\}\rangle \quad \textit{and}$$
$$\mathcal{N}_{C_2} = \langle \{in^3_1, in^3_2\}, \{out^3_1\}, \{T_3\}, \{M_{(3,1,3,1)}, M_{(3,1,3,2)}\}\rangle.$$

Let us denote $\mu'_{\mathcal{M}}(M_{(i,j,k,l)})$ as $m_{(i,j,k,l)}$ and $\mu_{\mathcal{T}}(T_i)$ as t_i, where all $m_{(i,j,k,l)}$ and t_i are natural numbers. Then, we can characterise self-sustainability of C_1 and C_2, respectively, by the systems of linear inequalities,

$$t_2 \geq 1 \qquad m_{(2,2,2,1)} \leq t_2 \qquad m_{(2,2,2,1)} = t_2 \qquad \textit{and}$$
$$t_3 \geq 1 \qquad m_{(3,1,3,1)} + m_{(3,1,3,2)} \leq t_3 \qquad m_{(3,1,3,1)} = t_3 \qquad m_{(3,1,3,2)} = t_3.$$

If a solution to these systems exists, the underlying component is self-sustainable. C_1 is clearly self-sustainable, while C_2 is not. $\square$

Several comments with respect to Definition 10 and Proposition 1 are in order. First, the statement that $\mu'_{\mathcal{M}}$ defines a function from $\mu'_{\mathcal{O}ut}$ onto $\mu_{\mathcal{I}n}$ is imprecise. In fact, $\mu'_{\mathcal{M}}$ defines a set of functions from $\mu'_{\mathcal{O}ut}$ onto $\mu_{\mathcal{I}n}$. This is because $\mu'_{\mathcal{O}ut}$ and $\mu_{\mathcal{I}n}$ are multisets, that may contain elements more than once.

Therefore, if in^i_j or out^k_l occur multiple times in $\mu_{\mathcal{I}n}$, respectively $\mu'_{\mathcal{O}ut}$, it is unclear which mapping is defined by an element $M_{(k,l,i,j)}$ of $\mu'_{\mathcal{M}}$. Looking back at the *a*-*b*-example of Figure 3, there are four different functions in this graph, all corresponding to the multiset $\mu'_{\mathcal{M}} = [\![M_{(1,1,2,1)}, M_{(1,2,2,1)}, M_{(2,1,1,1)}, M_{(2,1,1,2)}]\!]$. The thick lines in the figure represent one of these, but selecting other arcs, with the same labels, produces the other three.

Apart from this, for a fixed multiset $\mu_{\mathcal{T}}$, there can be several mappings $\mu'_{\mathcal{M}}$ that map a multiset $\mu'_{\mathcal{O}ut}$ *onto* $\mu_{\mathcal{I}n}$. This is because there can be different abstract constraints out_l^k in $\mu_{\mathcal{O}ut}$ that all have a match transition to some abstract constraint in_j^i. This may give a number of alternative candidates for $\mu'_{\mathcal{M}}$.

Finally, by considering different multisets $\mu_{\mathcal{T}}$ based on $\mathcal{T}_C$, we may obtain a very large number of solutions for $\mu'_{\mathcal{M}}$ in Definition 10. In the context of the *a*-*b*-example, consider a multiset $\mu_{\mathcal{T}} = [\![T_1, T_1, T_2, T_2, T_2, T_2]\!]$. From the fact that there are twice as many T_2 rules than T_1 rules, it should be intuitively clear that it again allows to find multisets $\mu'_{\mathcal{O}ut}$ and $\mu'_{\mathcal{M}}$: $\mu'_{\mathcal{O}ut} \rightarrow \mu_{\mathcal{I}n}$, with the latter being *onto*. Because of the increased multiplicity of the rule transitions, the number of different functions that $\mu'_{\mathcal{M}}$ represents in this context is much higher than for the previous $\mu_{\mathcal{T}}$. Moreover, it turns out that by increasing the multiplicity of the rule transitions, we can construct concrete functions associated to $\mu'_{\mathcal{M}}$ that cannot be obtained as the union of multiple concrete functions associated to a solution for a $\mu_{\mathcal{T}}$ with lower multiplicity of rule transitions (see [14]).

This observation implies that we are unable to use the notion of a self-sustainable set of rules as a direct basis for a termination analysis. Such an approach would have to identify a finite set of minimal self-sustainable cycles and then prove that all these are terminating. But since in CHR, there are in general an infinite set of minimal cycles, such an approach is not feasible.

In [15], to tackle the problem of an infinite number of minimal cycles, a new concept of minimality is introduced, based on a finite constructive set of solutions —the Hilbert basis— for the inequalities representing self-sustainability. This approach is however slow, with little gain in precision.

Fortunately, there is another way for using the notion of a self-sustaining set of rules. After determining the SCCs of a CHR program, we can verify which SCCs are not self-sustainable, and disregard such SCCs. This observation is based on the following theorems.

Theorem 1. *If a CHR program, P, is not self-sustainable, then P terminates for every query.* □

Theorem 2. *Let P be a CHR program and let C be an SCC of P. If C is not self-sustainable and if $P \setminus C$ terminates for every query, then P terminates for every query.* □

4.2 Non-self-sustainable SCCs of a CHR program

From here on, we refer to self-sustainable as '*selfs*' and use the matrix form: $A \times X \leq B$; to represent systems of linear inequalities.

Example 8 (system in matrix form for Primes). We revisit Example 7 and represent for C_1 and C_2, respectively, their systems of inequalities in matrix form:

$$\begin{bmatrix} -1 & 1 \\ 1 & -1 \\ -1 & 1 \\ -1 & 0 \end{bmatrix} \times \begin{bmatrix} t_2 \\ m_{(2,2,2,1)} \end{bmatrix} \leq \begin{bmatrix} 0 \\ 0 \\ 0 \\ -1 \end{bmatrix} \quad \textit{and} \quad \begin{bmatrix} -1 & 1 & 0 \\ 1 & -1 & 0 \\ -1 & 0 & 1 \\ 1 & 0 & -1 \\ -1 & 1 & 1 \\ -1 & 0 & 0 \end{bmatrix} \times \begin{bmatrix} t_3 \\ m_{(3,1,3,1)} \\ m_{(3,1,3,2)} \end{bmatrix} \leq \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ -1 \end{bmatrix}.$$

Note that the equalities of the original system are replaced by two inequalities. E.g. $m_{(2,2,2,1)} = t_2$ is replaced by $m_{(2,2,2,1)} \geq t_2$ and $m_{(2,2,2,1)} \leq t_2$. □

In order to prove that a component is not *selfs*, we need to prove that no positive integer solution exists for the variables of the linear inequalities representing that it is *selfs*. Thus, we need to prove that such a system is *infeasible*.

Definition 11 (feasible). *A system, $S = A \times X \leq B$, is* (in)feasible *iff S has (not) a solution in $\mathbb{R}^+$.* □

The following lemma is due to Farkas [7].

Lemma 1 (Farkas' lemma). *Let $S = A \times X \leq B$ be a system of linear inequalities. Then, S is feasible iff $\forall P \geq 0 : A^T \times P \geq 0 \rightarrow B^T \times P \geq 0$. Alternatively, S is infeasible iff $\exists P \geq 0 : A^T \times P \geq 0 \wedge B^T \times P < 0$.* □

Note that Farkas' lemma is only applicable to the real case: if a real matrix P exists, such that $P \geq 0 \wedge A^T \times P \geq 0 \wedge B^T \times P < 0$, then, the original system, S, is infeasible. Therefore, it has no solution in $\mathbb{N} \subset \mathbb{R}^+$ and must be *non-selfs*.

Infeasibility has received much attention in linear programming (see e.g. [3]) and several approaches exist to tackle the problem. It is not in our intention to improve on these approaches. To evaluate our approach, we do however formulate a simple test, where we first represent infeasibility as a constraint problem on symbolic coefficients. That is, we introduce a symbolic matrix P', for each infeasibility problem, of the same dimensions as P, with symbolic coefficients p_i, one for each position in the matrix. Then, we derive constraints on the symbolic coefficients, based on $P' \geq 0 \wedge A^T \times P' \geq 0 \wedge B^T \times P' < 0$.

Example 9 (infeasibility for Primes). We revisit Example 8, and formulate infeasibility of the systems of linear inequalities. That is, let P_1 for C_1 be a (4×1)-matrix of (integer) symbolic coefficients $p_0^1, p_1^1, \ldots, p_3^1$, all greater or equal to 0. Then, to prove *non-selfs* for C_1, we need to satisfy:

$$\begin{bmatrix} -1 & 1 & -1 & -1 \\ 1 & -1 & 1 & 0 \end{bmatrix} \times P_1 \geq 0 \quad \textit{and} \quad \begin{bmatrix} 0 & 0 & 0 & -1 \end{bmatrix} \times P_1 < 0.$$

We derive the following problem, where $\forall i \in \{0, 1, \ldots, 3\} : p_i^1 \geq 0$:

$$-p_0^1 + p_1^1 - p_2^1 - p_3^1 \geq 0 \qquad p_0^1 - p_1^1 + p_2^1 \geq 0 \qquad -p_3^1 < 0$$

There is no solution to this problem, thus C_1 is *selfs*. For C_2, we have

$$\begin{bmatrix} -1 & 1 & -1 & 1 & -1 & -1 \\ 1 & -1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & -1 & 1 & 0 \end{bmatrix} \times P_2 \geq 0 \quad \textit{and} \quad \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -1 \end{bmatrix} \times P_2 < 0.$$

We derive the following problem, where $\forall i \in \{0, 1, \ldots, 5\} : p_i^2 \geq 0$:

$$\begin{array}{ll} -p_0^2 + p_1^2 - p_2^2 + p_3^2 - p_4^2 - p_5^2 \geq 0 & p_0^2 - p_1^2 + p_4^2 \geq 0 \\ p_2^2 - p_3^2 + p_4^2 \geq 0 & -p_5^2 < 0 \end{array}$$

One solution is: $p_0^2 = 0$, $p_1^2 = 1$, $p_2^2 = 0$, $p_3^2 = 1$, $p_4^2 = 1$, and $p_5^2 = 1$. Therefore, C_2 is *non-selfs* and thus must be terminating. □

To find a solution to these constraint problems, we can transform them to SAT problems, representing that a component is *non-selfs*, by using a transformation based on signed integer arithmetic. Thus, in this approach, we can only represent integers and not reals. This is still sufficient to represent the infeasibility problem, however, yields an incomplete approach (see Lemma 1): it is not guaranteed that a solution in the integers can be found if the original system is infeasible. Nevertheless, as it turns out, the approach works well in practice.

5 Evaluation

We have implemented the *non-selfs* test using SWI-Prolog [19] and integrated it with CHRisTA, a termination analyser for CHR(Prolog) [13]. This resulted in a new termination analyser, T-CoP [20] (Termination of CHR on top of Prolog).

CHRisTA uses CHR nets as a representation of CHR programs and implements an SCC analysis based on Tarjan's algorithm. To solve the satisfiability problems that CHRisTA is confronted with, we represent the Diophantine constraints as a sufficient SAT problem based on signed integer arithmetic and solve it with MiniSAT2 [10]. Of course, by doing so, we place limits on the domains of variables and integers of the original problem. That is, we limit on the bit-sizes used for representing the variables and the integers of the problem. We reuse this system to prove infeasibility of the linear inequalities that we obtain for *selfs*.

Therefore, integrating the *non-selfs* test into CHRisTA involved the following steps: deriving a system of linear inequalities for *selfs* from the CHR net of an SCC, formulating infeasibility of that system, and transforming the resulting infeasibility problem to a SAT problem. Afterwards, a proof of termination of the remaining SCCs, that are possibly *selfs*, is attempted by the termination proof procedure of CHRisTA.

CHR program	3bit	sec	4bit	sec	CHRisTA (sec)	T-CoP (sec)
factorial	-	0.10	-	0.14	1.50	1.64
mean	+	0.35	+	0.58	1.26	0.58
mergesortscc1	-	0.12	-	0.20	1.44	1.64
mergesortscc2	+	0.19	+	0.34	1.51	0.34
newcase1	+	0.41	+	0.74	timeout	0.74
newcase2	-	1.09	+	2.03	timeout	2.03
primesscc1	-	0.11	-	0.19	1.67	1.86
primesscc2	+	0.18	+	0.33	1.11	0.33

Table 1. Results of *non-selfs* test on terminating SCCs.

Table 1 contains a representative set of the results that we obtained. T-CoP, as well as the full benchmark, is available online for reference [20]. Note that the considered programs of Table 1 contain only a single SCC of a size and complexity similar to the SCCs expected in real-sized CHR programs.

In Table 1, there are SCCs that are *non-selfs*, which are proven terminating (+) using at most a 4 bit representation for the variables and integers of the SAT problems. The SCCs, only proven terminating by CHRisTA, are *selfs*.

Among these programs, there are two programs on which the proof procedure of CHRisTA fails (see [12]). An example, representative for such programs, is

$\{(R_1 \ @ \ a, a \Leftrightarrow b.), (R_2 \ @ \ b \Leftrightarrow a.)\}$. To prove termination, for R_1, the size of a must be greater or equal to b. For R_2, a has to be strictly smaller than b.

Our new approach can handle such programs, and integrated with CHRisTA, improves the precision of the termination analysis as shown in Table 1 under "T-CoP". From these results we may also conclude that the *non-selfs* test improves the efficiency of the analysis: If an SCC cannot be proven *non-selfs*, the overhead is acceptable; if it can be proven *non-selfs*, the gain in speed is relatively high.

Finally, note that the transformational approach of [16], combined with the technique of [17], can be used to handle programs such as newcase 1 and 2. Unfortunately, in the presence of propagation, the transformational approach of [16] cannot be applied.

6 Conclusion and future work

In this paper, we developed an approach to detect non-self-sustainability of the SCCs of a CHR program by means of a satisfiability problem. Integrating the approach with CHRisTA [13], resulted in a more efficient analyser, T-CoP. For one, the approach improves the precision of the termination analysis, being able to prove termination of a new class of CHR programs automatically. Furthermore, we improve the efficiency of the termination analyser CHRisTA (cfr. T-CoP).

Future work will consider propagation rules. For self-sustainability of propagation, we will need to assume presence of a fire-once policy. Intuitively, under such a policy, if no new combinations of constraints are ever introduced as a consequence of applying a propagation rule, such that the propagation rule can be applied again on the newly introduced combinations of constraints, then the propagation rule is non-selfs. Informally, this corresponds to verifying whether there does not exist a cycle in the CHR net of a CHR program across an abstract input constraint of the propagation rule and across some abstract output constraint *added* by a rule of the program. If so, the propagation rule can be ignored. Therefore, if we obtain by this approach an SCC that ultimately does not contain propagation, then, we can verify whether the SCC is non-selfs by the approach of this paper. Otherwise, the remaining SCC is still selfs by default.

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Automata-based Computation of Temporal Equilibrium Models*

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Abstract. Temporal Equilibrium Logic (TEL) is a formalism for temporal logic programming that generalizes the paradigm of Answer Set Programming (ASP) introducing modal temporal operators from standard Linear-time Temporal Logic (LTL). In this paper we solve some open problems that remained open for TEL like decidability, bounds for computational complexity as well as computation of temporal equilibrium models for arbitrary theories. We propose a method for the latter that consists in building a Büchi automaton that accepts exactly the temporal equilibrium models of a given theory, providing an automata-based decision procedure and illustrating the ω-regularity of such sets. We are able to show that TEL satisfiability can be solved in exponential space and it is hard for polynomial space. Finally, given two theories, we provide a decision procedure to check whether they have the same temporal equilibrium models.

1 Introduction

Stable models. Stable models have their roots in Logic Programming and in the search for a semantical interpretation of default negation [9] (or *answer set* semantics). They have given rise to a successful declarative paradigm, known as *Answer Set Programming* (ASP) [18,15], for practical knowledge representation. ASP has been applied to a wide spectrum of domains for solving several types of reasoning tasks: making diagnosis for the Space Shuttle [19], information integration of different data sources [14], distributing seaport employees in work teams [10] or automated music composition [3] to cite some examples. Some of these application scenarios frequently involve representing transition-based systems under linear time, so that discrete instants are identified with natural numbers. ASP offers interesting features for a formal treatment of temporal scenarios. For instance, it provides a high degree of *elaboration tolerance* [16], allowing a simple and natural solution to typical representational issues such as

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the *frame* problem and the *ramification* problem, see respectively [17] and [12]. Another interesting feature is that it allows a uniform treatment of different kinds of reasoning problems such as prediction, postdiction, planning, diagnosis or verification. However, since ASP is not a temporal formalism, it also involves some difficulties for dealing with temporal problems. In particular, since most ASP tools must deal with finite domains, this additionally requires fixing a finite path length with an obvious impossibility for solving problems such as proving the non-existence of a plan for a given planning scenario, or checking whether two temporal representations are *strongly equivalent* (i.e., they are interchangeable inside any context and for any path length).

Temporal Equilibrium Logic. To overcome these difficulties, in [1] a temporal extension of ASP, called *Temporal Equilibrium Logic* (TEL), was considered. This extension is an orthogonal combination of *linear-time temporal logic* (LTL) (see e.g. [22]) with the nonmonotonic formalism of *Equilibrium Logic* [20], probably the most general and best studied logical characterisation of ASP. TEL extends the stable model semantics to arbitrary LTL theories, that is, sets of formulae that combine atoms, the standard Boolean connectives, and the temporal operators X (read "next"), G (read "always"), F (read "eventually"), U (read "until") and R (read "release").

Towards arbitrary TEL theories. The definition of TEL has allowed studying problems like the aforementioned strong equivalence [1] of two temporal theories, but it had mostly remained as a theoretical tool, since there was no method for computing the temporal stable models of a temporal theory, at least until quite recently. In a first step in this direction, the paper [2] started from the normal form for TEL called *temporal logic programs* (TLPs) from [5] and showed that, when a syntactic subclass is considered (the so-called *splitable* TLPs), its temporal stable models can be obtained by a translation into LTL. This method has been implemented in a tool called `STeLP` [6] that uses an LTL model checker as a backend and provides the temporal stable models of a splitable TLP in terms of a Büchi automaton.

Although the splitable TLPs are expressive enough to capture most temporal scenarios treated in the ASP literature, a general method to compute the temporal equilibrium models for *arbitrary* TEL theories was not available until now. The interest for obtaining such a method is not only to cover the full expressiveness of this logic, but also to show its decidability and assess the complexity associated to its main reasoning tasks. In this sense, it is not convenient to use TLPs as a starting point since, despite of being a normal form for TEL, they are obtained by introducing new auxiliary atoms not present in the original propositional signature.

Our contributions. In this paper we cover this gap and introduce an automata-based method to compute the temporal equilibrium models of an arbitrary temporal theory. We will pay a special attention to recall standard relationships between LTL and Büchi automata in order to facilitate the connection between

ASP concepts and those from model-checking with temporal logics. More precisely, we propose automata-based decision procedures as follows:

1. We show that the satisfiability problem for the monotonic basis of TEL – the so-called logic of *Temporal Here-and-There* (THT) – can be solved in PSPACE by translation into the satisfiability problem for LTL. Whence, any decision procedure for LTL (automata-based, tableaux-based, resolution-based, etc.) can be used for THT. We are also able to demonstrate the PSPACE-hardness of the problem.
2. For any temporal formula, we effectively build a Büchi automaton that accepts exactly its temporal equilibrium models which allows to provide an automata-based decision procedure. We are able to show that TEL satisfiability can be solved in EXPSPACE and it is PSPACE-hard. Filling the gap is part of future work. Hence, we provide a symbolic representation for sets of temporal equilibrium models raising from temporal formulae.
3. Consequently, given two theories, we provide a decision procedure to check whether they have the same temporal equilibrium models (that is, *regular* equivalence, as opposed to *strong* equivalence).
4. Our proof technique can indeed be adapted to any extension of LTL provided that formulae can be translated into Büchi automata (as happens with LTL with past or LTL with fixed-points operators).

The rest of the paper is organised as follows. In the next section we recall the basic definitions and properties of Temporal Equilibrium Logic. Section 3 contains a brief overview of the use of automata for temporal model checking (in particular, Büchi automata for the case of LTL). Next, we explain our method for constructing a Büchi automaton that captures the temporal equilibrium models of any arbitrary temporal theory. Section 5 concludes the paper.

2 Temporal Equilibrium Logic

Let $\mathrm{AT} = \{p, q, \ldots\}$ be a countably infinite set of *atoms*. A *temporal formula* is defined with the formal grammar below:

$$\varphi ::= p \mid \bot \mid \varphi_1 \wedge \varphi_2 \mid \varphi_1 \vee \varphi_2 \mid \varphi_1 \rightarrow \varphi_2 \mid \mathsf{X}\varphi \mid \varphi_1 \mathsf{U} \varphi_2 \mid \varphi_1 \mathsf{R} \varphi_2$$

where $p \in \mathrm{AT}$. We will use the standard abbreviations:

$$\neg\varphi \stackrel{\text{def}}{=} \varphi \rightarrow \bot \qquad \mathsf{G}\varphi \stackrel{\text{def}}{=} \bot \,\mathsf{R}\, \varphi$$
$$\top \stackrel{\text{def}}{=} \neg\bot \qquad \mathsf{F}\varphi \stackrel{\text{def}}{=} \top \,\mathsf{U}\, \varphi$$
$$\varphi \leftrightarrow \varphi' \stackrel{\text{def}}{=} (\varphi \rightarrow \varphi') \wedge (\varphi' \rightarrow \varphi)$$

The temporal connectives X, G, F, U and R have their standard meaning from LTL. A *theory* Γ is defined as a finite set of temporal formulae.

In the non-temporal case, Equilibrium Logic is defined by introducing a criterion for selecting models based on a non-classical monotonic formalism called

the logic of *Here-and-There* (HT) [11], an intermediate logic between intuitionistic and classical propositional calculus. Similarly, TEL will be defined by first introducing a monotonic, intermediate version of LTL, we call the logic of *Temporal Here-and-There* (THT), and then defining a criterion for selecting models in order to obtain nonmonotonicity.

In this way, we will deal with two classes of models. An *LTL model* $\mathbf{H}$ is a map $\mathbf{H} : \mathbb{N} \to \mathcal{P}(\mathrm{AT})$, viewed as an ω-sequence of propositional valuations. By contrast, the semantics of THT is defined in terms of sequences of pairs of propositional valuations, which can be also viewed as a pair of LTL models. A *THT model* is a pair $\mathbf{M} = (\mathbf{H}, \mathbf{T})$ where $\mathbf{H}$ and $\mathbf{T}$ are LTL models and for $i \geq 0$, we impose that $\mathbf{H}(i) \subseteq \mathbf{T}(i)$. $\mathbf{H}(i)$ and $\mathbf{T}(i)$ are sets of atoms standing for *here* and *there* respectively. A THT model $\mathbf{M} = (\mathbf{H}, \mathbf{T})$ is said to be *total* when $\mathbf{H} = \mathbf{T}$.

The satisfaction relation $\models$ is interpreted as follows on THT models ($\mathbf{M}$ is a THT model and $k \in \mathbb{N}$):

1. $\mathbf{M}, k \models p \overset{\text{def}}{\Leftrightarrow} p \in \mathbf{H}(k)$.
2. $\mathbf{M}, k \models \varphi \wedge \varphi' \overset{\text{def}}{\Leftrightarrow} \mathbf{M}, k \models \varphi$ and $\mathbf{M}, k \models \varphi'$.
3. $\mathbf{M}, k \models \varphi \vee \varphi' \overset{\text{def}}{\Leftrightarrow} \mathbf{M}, k \models \varphi$ or $\mathbf{M}, k \models \varphi'$.
4. $\mathbf{M}, k \models \varphi \to \varphi' \overset{\text{def}}{\Leftrightarrow}$ for all $\mathbf{H}' \in \{\mathbf{H}, \mathbf{T}\}$, $(\mathbf{H}', \mathbf{T}), k \not\models \varphi$ or $(\mathbf{H}', \mathbf{T}), k \models \varphi'$.
5. $\mathbf{M}, k \models \mathsf{X}\varphi \overset{\text{def}}{\Leftrightarrow} \mathbf{M}, k+1 \models \varphi$.
6. $\mathbf{M}, k \models \varphi \mathsf{U} \varphi' \overset{\text{def}}{\Leftrightarrow}$ there is $j \geq k$ such that $\mathbf{M}, j \models \varphi'$ and for all $j' \in [k, j-1]$, $\mathbf{M}, j' \models \varphi$.
7. $\mathbf{M}, k \models \varphi \mathsf{R} \varphi' \overset{\text{def}}{\Leftrightarrow}$ for all $j \geq k$ such that $\mathbf{M}, j \not\models \varphi'$, there exists $j' \in [k, j-1]$, $\mathbf{M}, j' \models \varphi$.
8. never $\mathbf{M}, k \models \bot$.

A *model* for a theory Γ is a THT model $\mathbf{M}$ such that for every formula $\varphi \in \Gamma$, we have $\mathbf{M}, 0 \models \varphi$. A formula φ is *THT valid* $\overset{\text{def}}{\Leftrightarrow}$ $\mathbf{M}, 0 \models \varphi$ for every THT model $\mathbf{M}$. Similarly, a formula φ is *THT satisfiable* $\overset{\text{def}}{\Leftrightarrow}$ there is a THT model $\mathbf{M}$ such that $\mathbf{M}, 0 \models \varphi$.

As we can see, the main difference with respect to LTL is the interpretation of implication (item 4), that must be checked in both components, $\mathbf{H}$ and $\mathbf{T}$, of $\mathbf{M}$. In fact, it is easy to see that when we take total models $\mathbf{M} = (\mathbf{T}, \mathbf{T})$, THT satisfaction $(\mathbf{T}, \mathbf{T}), k \models \varphi$ collapses to standard LTL satisfaction $\mathbf{T}, k \models \varphi$ so that we will sometimes write the latter when convenient. For instance, item 4 in the above definition can be rewritten as:

4′. $\mathbf{M}, k \models \varphi \to \varphi' \overset{\text{def}}{\Leftrightarrow}$ ($\mathbf{M}, k \models \varphi$ implies $\mathbf{M}, k \models \varphi'$) and $\mathbf{T}, k \models \varphi \to \varphi'$ (LTL satisfaction)

Note that $\mathbf{M}, k \models \neg p$ iff $\mathbf{M}, k \models p \to \bot$ iff ($\mathbf{M}, k \models p$ implies $\mathbf{M}, k \models \bot$ and $\mathbf{T}, k \models p$ implies $\mathbf{T}, k \models \bot$) iff ($p \notin \mathbf{H}(k)$ and $p \notin \mathbf{T}(k)$).

Similarly, a formula φ is *LTL valid* $\overset{\text{def}}{\Leftrightarrow}$ $\mathbf{M}, 0 \models \varphi$ for every total THT model $\mathbf{M}$ whereas a formula φ is *LTL satisfiable* $\overset{\text{def}}{\Leftrightarrow}$ there is a total THT model $\mathbf{M}$

such that $\mathbf{M}, 0 \models \varphi$. We write $\mathrm{Mod}(\varphi)$ to denote the set of LTL models for φ (restricted to the set of atoms occurring φ denoted by $\mathrm{AT}(\varphi)$).

Obviously, any THT valid formula is also LTL valid, but not the other way around. For instance, the following are THT valid equivalences:

$$\begin{array}{ll} \neg(\varphi \wedge \psi) \leftrightarrow \neg\varphi \vee \neg\psi & \mathsf{X}(\varphi \oplus \psi) \leftrightarrow \mathsf{X}\varphi \oplus \mathsf{X}\psi \\ \neg(\varphi \vee \psi) \leftrightarrow \neg\varphi \wedge \neg\psi & \mathsf{X} \otimes \varphi \leftrightarrow \otimes \mathsf{X}\varphi \end{array}$$

for any binary connective $\oplus$ and any unary connective $\otimes$. This means that De Morgan laws are valid, and that we can always shift the X operator to all the operands of any connective. On the contrary, the LTL valid formula $\varphi \vee \neg\varphi$ (known as *excluded middle* axiom) is not THT valid. This is inherited from the intermediate/intuitionistic nature of THT: in fact, the addition of this axiom makes THT collapse into LTL. By adding a copy of this axiom for any atom at any position of the models, we can force that THT models of any formula are total, as stated next.

Proposition 1. *Given a temporal formula φ built over the propositional atoms in $\mathrm{AT}(\varphi)$, for every THT model $(\mathbf{H}, \mathbf{T})$, the propositions below are equivalent:*

(I) $(\mathbf{H}, \mathbf{T}), 0 \models \varphi \wedge \bigwedge_{p \in \mathrm{AT}(\varphi)} \mathsf{G}(p \vee \neg p)$,
(II) $\mathbf{T}, 0 \models \varphi$ *in LTL, and for* $i \geq 0$ *and* $p \in \mathrm{AT}(\varphi)$, *we have* $p \in \mathbf{H}(i)$ *iff* $p \in \mathbf{T}(i)$.

As a consequence, we can easily encode LTL in THT, since LTL models of φ coincide with its total THT models. Let us state another property whose proof can be obtained by structural induction.

Proposition 2 (Persistence). *For any formula φ, any THT model $\mathbf{M} = (\mathbf{H}, \mathbf{T})$ and any $i \geq 0$, if $\mathbf{M}, i \models \varphi$, then $\mathbf{T}, i \models \varphi$.*

Corollary 1. $(\mathbf{H}, \mathbf{T}), i \models \neg\varphi$ *iff* $\mathbf{T}, i \not\models \varphi$ *in LTL.*

We proceed now to define an ordering relation among THT models, so that only the minimal ones will be *selected* for a temporal theory. Given two LTL models $\mathbf{H}$ and $\mathbf{H}'$, we say that $\mathbf{H}$ is *less than or equal to* $\mathbf{H}'$ (in symbols $\mathbf{H} \leq \mathbf{H}'$) $\stackrel{\text{def}}{\Leftrightarrow}$ for $k \geq 0$, we have $\mathbf{H}(k) \subseteq \mathbf{H}'(k)$. We write $\mathbf{H} < \mathbf{H}'$ if $\mathbf{H} \leq \mathbf{H}'$ and $\mathbf{H} \neq \mathbf{H}'$. The relations $\leq$ and $<$ can be lifted at the level of THT models. Given two THT models $\mathbf{M} = (\mathbf{H}, \mathbf{T})$ and $\mathbf{M}' = (\mathbf{H}', \mathbf{T}')$, $\mathbf{M} \leq \mathbf{M}' \stackrel{\text{def}}{\Leftrightarrow} \mathbf{H} \leq \mathbf{H}'$ and $\mathbf{T} = \mathbf{T}'$. Similarly, we write $\mathbf{M} < \mathbf{M}'$ if $\mathbf{M} \leq \mathbf{M}'$ and $\mathbf{M} \neq \mathbf{M}'$.

Definition 1 (Temporal Equilibrium Model). *A THT model $\mathbf{M}$ is a* temporal equilibrium model *(or* TEL model*, for short) of a theory Γ if $\mathbf{M}$ is a total model of Γ and there is no $\mathbf{M}' < \mathbf{M}$ such that $\mathbf{M}', 0 \models \Gamma$.*

Temporal Equilibrium Logic (TEL) is the logic induced by temporal equilibrium models and it is worth noting that any temporal equilibrium model of Γ is a *total* THT model of the form $(\mathbf{T}, \mathbf{T})$ (by definition). The corresponding LTL model $\mathbf{T}$ of Γ is said to be a *temporal stable model* of Γ.

When we restrict the syntax to non-modal theories and semantics to HT interpretations $\langle \mathbf{H}(0), \mathbf{T}(0) \rangle$ we talk about (non-temporal) equilibrium models, which coincide with stable models in their most general definition [8].

The TEL satisfiability problem consists in determining whether a temporal formula has a TEL model. As an example, consider the formula

$$\mathsf{G}(\neg p \rightarrow \mathsf{X}p) \tag{1}$$

Its intuitive meaning corresponds to the logic program consisting of rules of the form: $p(s(X)) \leftarrow \mathit{not}\ p(X)$ where time has been reified as an extra parameter $X = 0, s(0), s(s(0)), \ldots$. Notice that the interpretation of $\neg$ is that of default negation *not* in logic programming. In this way, (1) is saying that, at any situation $i \geq 0$, if there is no evidence on p, then p will become true in the next state $i + 1$. In the initial state, we have no evidence on p, so this will imply $\mathsf{X}p$. As a result $\mathsf{XX}p$ will have no applicable rule and thus will be false by default, and so on. It is easy to see that the unique temporal stable model of (1) is defined by the formula $\neg p \wedge \mathsf{G}(\neg p \leftrightarrow \mathsf{X}p)$.

It is worth noting that an LTL satisfiable formula may have no temporal stable model. As a simple example (well-known from non-temporal ASP) the logic program rule $\neg p \rightarrow p$, whose only (classical) model is $\{p\}$, has no stable models. This is because if we take a model $\mathbf{M} = (\mathbf{H}, \mathbf{T})$ where p holds in $\mathbf{T}$, then (Corollary 1) $\mathbf{M} \not\models \neg p$ and so $\mathbf{M} \models \neg p \rightarrow p$ true regardless $\mathbf{H}$, so we can take a strictly smaller $\mathbf{H} < \mathbf{T}$ whose only difference with respect to $\mathbf{T}$ is that p does not hold. On the other hand, if we take any $\mathbf{T}$ in which p does not hold, then $\mathbf{M} \models \neg p$ and so $\neg p \rightarrow p$ would make p true both in $\mathbf{H}$ and $\mathbf{T}$ reaching a contradiction. When dealing with logic programs, it is well-known that non-existence of stable models is always due to a kind of cyclic dependence on default negation like this.

In the temporal case, however, non-existence of temporal stable models may also be due to a lack of a finite justification for satisfying the criterion of minimal knowledge. As an example, take the formula $\mathsf{GF}p$, typically used in LTL to assert that property p occurs infinitely often. This formula has no temporal stable models: all models must contain infinite occurrences of p and there is no way to establish a minimal $\mathbf{H}$ among them. Thus, formula $\mathsf{GF}p$ is LTL satisfiable but it has no temporal stable model. By contrast, forthcoming Proposition 4 states that for a large class of temporal formulae, LTL satisfiability is equivalent to THT satisfiability and TEL satisfiability.

3 Automata-Based Approach for LTL in a Nutshell

Before presenting our decision procedures, let us briefly recall what are the main ingredients of the automata-based approach. It consists in reducing logical problems into automata-based decision problems in order to take advantage of known results from automata theory. The most standard target problems on automata used in this approach are the nonemptiness problem (checking whether an automaton admits at least one accepting computation) and the inclusion problem

(checking whether the language accepted by the automaton $\mathcal{A}$ is included in the language accepted by the automaton $\mathcal{B}$). In a pioneering work [4] Büchi introduced a class of automata showing that they are equivalent to formulae in monadic second-order logic (MSO) over $(\mathbb{N}, <)$.

In full generality, here are a few desirable properties of the approach. The reduction should be conceptually simple, see the translation from LTL formulae into alternating automata [27]. Formula structure is reflected directly in the transition formulae of alternating automata. The computational complexity of the automata-based target problem should be well-characterized – see, for instance, the translation from PDL formulae into nondeterministic Büchi tree automata [28]. It is also highly desirable that not only the reduction is conceptually simple but also that it is semantically faithful so that the automata involve in the target instance are closely related to the instance of the original logical problem. Last but not least, preferrably, the reduction might allow to obtain the optimal complexity for the source logical problem. For instance, CTL model-checking can be shown in PolyTime by reduction into hesitant alternating automata (HAA) [13] and we know this is the optimal upper bound.

3.1 Basics on Büchi automata

We recall that a *Büchi automaton* $\mathcal{A}$ is a tuple $\mathcal{A} = (\Sigma, Q, Q_0, \delta, F)$ such that Σ is a finite *alphabet*, Q is a finite set of *states*, $Q_0 \subseteq Q$ is the set of *initial* states, the *transition relation* δ is a subset of $Q \times \Sigma \times Q$ and $F \subseteq Q$ is a set of *final* states. Given $q \in Q$ and $a \in \Sigma$, we also write $\delta(q, a)$ to denote the set of states q' such that $(q, a, q') \in \delta$.

A *run* ρ of $\mathcal{A}$ is a sequence $q_0 \xrightarrow{a_0} q_1 \xrightarrow{a_1} q_2 \dots$ such that for every $i \geq 0$, $(q_i, a_i, q_{i+1}) \in \delta$ (also written $q_i \xrightarrow{a_i} q_{i+1}$). The run ρ is *accepting* if $q_0 \in Q_0$ is initial and some state of F is repeated infinitely often in ρ: $\inf(\rho) \cap F \neq \emptyset$ where we let $\inf(\rho) = \{q \in Q : \forall\, i,\ \exists\, j > i,\ q = q_j\}$. The *label* of ρ is the word $\sigma = a_0 a_1 \cdots \in \Sigma^\omega$. The automaton $\mathcal{A}$ *accepts* the language $\mathrm{L}(\mathcal{A})$ of ω-words $\sigma \in \Sigma^\omega$ such that there exists an accepting run of $\mathcal{A}$ on the word σ, i.e., with label σ.

Now, we introduce a standard generalization of the Büchi acceptance condition by considering conjunctions of classical Büchi conditions. A *generalized Büchi automaton* (GBA) is a structure $\mathcal{A} = (\Sigma, Q, Q_0, \delta, \{F_1, \dots, F_k\})$ such that $F_1, \dots, F_k \subseteq Q$ and Σ, Q, Q_0 and δ are defined as for Büchi automata. A run is defined as for Büchi automata and a run ρ of $\mathcal{A}$ is *accepting* iff the first state is initial and for $i \in [1, n]$, we have $\inf(\rho) \cap F_i \neq \emptyset$. It is known that every GBA $\mathcal{A}$ can be easily translated in logarithmic space into a Büchi automaton, preserving the language of accepted ω-words (see e.g. [21]). Moreover, the nonemptiness problem for GBA or BA is known to be NLogSpace-complete.

3.2 From LTL formulae to Büchi automata

We recall below how to define a Büchi automaton that accepts the linear models of an LTL formula. Given an LTL formula φ, we define its *closure* $cl(\varphi)$ to denote

a finite set of formulae that are relevant to check the satisfiability of φ. For each LTL formula φ, we define its *main components* (if any) according to the table below:

formula φ	main components
p or $\neg p$	none
$\neg\neg\psi$ or $\mathsf{X}\psi$	ψ
$\neg\mathsf{X}\psi$	$\neg\psi$
$\psi_1 \mathsf{U} \psi_2$ or $\psi_1 \wedge \psi_2$ or $\psi_1 \mathsf{R} \psi_2$	ψ_1, ψ_2
$\neg(\psi_1 \mathsf{U} \psi_2)$ or $\neg(\psi_1 \wedge \psi_2)$ or $\neg(\psi_1 \mathsf{R} \psi_2)$	$\neg\psi_1$, $\neg\psi_2$

We write $cl(\varphi)$ to denote the least set of formulae such that $\varphi \in cl(\varphi)$ and $cl(\varphi)$ is closed under main components. It is routine to check that $\mathrm{card}(cl(\varphi)) \leq |\varphi|$ (the size of φ). Moreover, one can observe that if $\psi \in cl(\varphi)$, then for each immediate subformula (if any), either it belongs to $cl(\varphi)$ or its negation belongs to $cl(\varphi)$. A subset $\Gamma \subseteq cl(\varphi)$ is *consistent and fully expanded* whenever

- $\psi_1 \wedge \psi_2 \in \Gamma$ implies $\psi_1, \psi_2 \in \Gamma$,
- $\neg(\psi_1 \wedge \psi_2) \in \Gamma$ implies $\neg\psi_1 \in \Gamma$ or $\neg\psi_2 \in \Gamma$,
- $\neg\neg\psi \in \Gamma$ implies $\psi \in \Gamma$,
- Γ does not contain a contradictory pair ψ and $\neg\psi$.

The pair of consistent and fully expanded sets (Γ_1, Γ_2) is *one-step consistent* $\stackrel{\text{def}}{\Leftrightarrow}$

1. $\mathsf{X}\psi \in \Gamma_1$ implies $\psi \in \Gamma_2$ and $\neg\mathsf{X}\psi \in \Gamma_1$ implies $\neg\psi \in \Gamma_2$.
2. $\psi_1 \mathsf{U} \psi_2 \in \Gamma_1$ implies $\psi_2 \in \Gamma_1$ or ($\psi_1 \in \Gamma_1$ and $\psi_1 \mathsf{U} \psi_2 \in \Gamma_2$),
3. $\neg(\psi_1 \mathsf{U} \psi_2) \in \Gamma_1$ implies $\neg\psi_2 \in \Gamma_1$ and ($\neg\psi_1 \in \Gamma_1$ or $\neg(\psi_1 \mathsf{U} \psi_2) \in \Gamma_2$).
4. $\psi_1 \mathsf{R} \psi_2 \in \Gamma_1$ implies $\psi_2 \in \Gamma_1$ and ($\psi_1 \in \Gamma_1$ or $\psi_1 \mathsf{R} \psi_2 \in \Gamma_2$),
5. $\neg(\psi_1 \mathsf{R} \psi_2) \in \Gamma_1$ implies $\neg\psi_2 \in \Gamma_1$ or ($\neg\psi_1 \in \Gamma_1$ and $\neg(\psi_1 \mathsf{R} \psi_2) \in \Gamma_2$).

Given an LTL formula φ, let us build the generalized Büchi automaton

$$\mathcal{A}_\varphi = (\Sigma, Q, Q_0, \delta, \{F_1, \ldots, F_k\})$$

where

- $\Sigma = \mathcal{P}(\mathrm{AT}(\varphi))$ and Q is the set of consistent and fully expanded sets.
- $Q_0 = \{\Gamma \in Q : \varphi \in \Gamma\}$.
- $\Gamma \xrightarrow{a} \Gamma' \in \delta \stackrel{\text{def}}{\Leftrightarrow} (\Gamma, \Gamma')$ is one-step consistent, $(\Gamma \cap \mathrm{AT}(\varphi)) \subseteq a$ and $\{p : \neg p \in \Gamma\} \cap a = \emptyset$.
- If the temporal operator U does not occur in φ, then $F_1 = Q$ and $k = 1$. Otherwise, suppose that $\{\psi_1 \mathsf{U} \psi'_1, \ldots, \psi_k \mathsf{U} \psi'_k\}$ is the set of U-formulae from $cl(\varphi)$. Then, for every $i \in [1, k]$, $F_i = \{\Gamma \in Q : \psi_i \mathsf{U} \psi'_i \notin \Gamma \text{ or } \psi'_i \in \Gamma\}$.

It is worth observing that $\mathrm{card}(Q) \leq 2^{|\varphi|}$ and $\mathcal{A}_\varphi$ can be built in exponential time in $|\varphi|$.

Proposition 3. *[29]* $\mathrm{Mod}(\varphi) = \mathrm{L}(\mathcal{A}_\varphi)$, *i.e. for every* $a_0 a_1 \cdots \in \Sigma^\omega$, $a_0 a_1 \cdots \in \mathrm{L}(\mathcal{A}_\varphi)$ *iff* $\mathbf{T}, 0 \models \varphi$ *where for all* $i \in \mathbb{N}$, $\mathbf{T}(i) = a_i$.

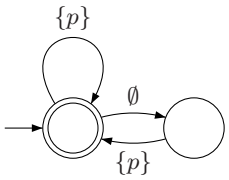

Fig. 1. Büchi automaton for models of $\mathsf{G}(\neg p \rightarrow \mathsf{X}p)$ (over the alphabet $\{\emptyset, \{p\}\}$)

Figure 1 presents a Büchi automaton recognizing the models for $\mathsf{G}(\neg p \rightarrow \mathsf{X}p)$ over the alphabet $\{\emptyset, \{p\}\}$. The automaton obtained from the above systematic construction would be a bit larger since $cl(\mathsf{G}(\neg p \rightarrow \mathsf{X}p))$ has about 2^4 subsets. However, the systematic construction has the advantage to be generic. Other translations exist with other advantages, except from simplicity, see e.g. [7]. However, herein, we need to use the following properties (apart from the correctness of the reduction): (1) the size of each state of $\mathcal{A}_\varphi$ is linear in the size of φ, (2) it can be checked if a state is initial [resp. final] in linear space in the size of φ and (3) given two subsets X, X' of $cl(\varphi)$ and $a \in \Sigma$, one can check in linear space in the size of φ whether $X \xrightarrow{a} X'$ is a transition of $\mathcal{A}_\varphi$ (each transition of $\mathcal{A}_\varphi$ can be checked in linear space in the size of φ).

These are key points towards the PSpace upper bound for LTL satisfiability since the properties above are sufficient to check the nonemptiness of $\mathcal{A}_\varphi$ in nondeterministic polynomial space in the size of φ (guess on-the-fly a prefix and a loop of length at most exponential) and then invoke Savitch Theorem [24] to eliminate nondeterminism. We will use similar arguments to establish that TEL satisfiability can be solved in ExpSpace.

4 Building TEL Models with Büchi Automata

In this section, we provide an automata-based approach to determine whether a formula φ built over the atoms $\{p_1, \ldots, p_n\}$ has a TEL model. This is the place where starts our main contribution. To do so, we build a Büchi automaton $\mathcal{B}$ over the alphabet $\Sigma = \mathcal{P}(\{p_1, \ldots, p_n\})$ such that $\mathrm{L}(\mathcal{B})$ is equal to the set of TEL models for φ. Moreover, nonemptiness can be checked in ExpSpace, which allows to answer the open problem about the complexity of determining whether a temporal formula has a TEL model.

Each model $\mathbf{M} = \langle \mathbf{H}, \mathbf{T} \rangle$ restricted to the atoms in $\{p_1, \ldots, p_n\}$ can be encoded into an LTL model $\mathbf{H}'$ over the alphabet

$$\Sigma' = \mathcal{P}(\{p_1, \ldots, p_n, p'_1, \ldots, p'_n\})$$

such that for $i \geq 0$, $\mathbf{H}'(i) = (\mathbf{T}(i) \cap \{p_1, \ldots, p_n\}) \cup \{p'_j : p_j \in \mathbf{H}(i), j \in [1, n]\}$. In that case, we write $\mathbf{H}' \approx \mathbf{M}$.

Lemma 1.

(I) *For every THT model* $\mathbf{M} = \langle \mathbf{H}, \mathbf{T} \rangle$ *restricted to atoms in* $\{p_1, \ldots, p_n\}$*, there is a unique LTL model* $\mathbf{H}'$ *such that* $\mathbf{H}' \approx \mathbf{M}$*.*

(II) *For every LTL model* $\mathbf{H}' : \mathbb{N} \to \Sigma'$ *such that* $\mathbf{H}', 0 \models \bigwedge_{i\in[1,n]} \mathsf{G}(p'_i \to p_i)$, *there is a unique THT model* $\mathbf{M} = \langle \mathbf{H}, \mathbf{T}\rangle$ *restricted to atoms such that* $\mathbf{H}' \approx \mathbf{M}$.

In (II), a THT model $\mathbf{M}$ can be built thanks to the satisfaction of the formula $\bigwedge_{i\in[1,n]} \mathsf{G}(p'_i \to p_i)$ by $\mathbf{H}'$, which guarantees that for all $i \in \mathbb{N}$, we have $\mathbf{H}(i) \subseteq \mathbf{T}(i)$. The proof is by an easy verification. This guarantees a clear isomorphism between two sets of models. In order to complete this model-theoretical correspondence, let us define the following translation f between temporal formulae:

- f is homomorphic for conjunction, disjunction and temporal operators,
- $f(\bot) \stackrel{\text{def}}{=} \bot$, $f(p_i) \stackrel{\text{def}}{=} p'_i$,
- $f(\psi \to \psi') \stackrel{\text{def}}{=} (\psi \to \psi') \wedge (f(\psi) \to f(\psi'))$.

Lemma 2. *Let* φ *be a temporal formula built over the atoms in* $\{p_1, \ldots, p_n\}$ *and* $\mathbf{M}$ *restricted to* $\{p_1, \ldots, p_n\}$ *and* $\mathbf{H}'$ *be models such that* $\mathbf{H}' \approx \mathbf{M}$. *For* $l \geq 0$, *we have* $\mathbf{H}', l \models f(\psi)$ *iff* $\mathbf{M}, l \models \psi$ *for every subformula* ψ *of* φ.

The proof is by an easy structural induction. So, there is a polynomial-time reduction from THT satisfiability into LTL satisfiability by considering the mapping $f(\cdot) \wedge \bigwedge_{i\in[1,n]} \mathsf{G}(p'_i \to p_i)$.

Let $\mathcal{A}_1$ be the Büchi automaton such that $\mathrm{L}(\mathcal{A}_1) = \mathrm{Mod}(\varphi)$, following any construction similar to [29] (see Section 3.2). The set $\mathrm{L}(\mathcal{A}_1)$ can be viewed as the set of total THT models of φ. Let φ' be the formula $f(\varphi) \wedge \bigwedge_{i\in[1,n]} \mathsf{G}(p'_i \to p_i)$.

Lemma 3. *The set of LTL models for the formula* φ' *corresponds to the set of THT models for the temporal formula* φ.

For instance, taking the formula $\varphi = \mathsf{G}(\neg p \to \mathsf{X}p)$, we can compute its THT models $\mathbf{M}$ by obtaining the corresponding LTL models (with atoms p and p') for the formula below:

$$\begin{aligned}\varphi' &= f(\ \mathsf{G}(\neg p \to \mathsf{X}p)\ )\ \wedge\ \mathsf{G}(p' \to p)\\ &= \mathsf{G}\big(\ (\neg p \to \mathsf{X}p) \wedge (\neg p \wedge \neg p' \to \mathsf{X}p')\ \big)\ \wedge\ \mathsf{G}(p' \to p)\end{aligned}$$

Figure 2 presents a Büchi automaton for the models of the formula $f(\mathsf{G}(\neg p \to \mathsf{X}p)) \wedge \mathsf{G}(p' \to p)$ over the alphabet $\{\emptyset, \{p\}, \{p'\}, \{p, p'\}\}$. Hence, we provide a symbolic representation for the THT models of $\mathsf{G}(\neg p \to \mathsf{X}p)$. For instance, reading the letter $\{p\}$ at position i corresponds to a pair $(\mathbf{H}(i), \mathbf{T}(i))$ with $p \notin \mathbf{H}(i)$ and $p \in \mathbf{T}(i)$. Similarly, reading the letter $\{p, p'\}$ at position i corresponds to a pair $(\mathbf{H}(i), \mathbf{T}(i))$ with $p \in \mathbf{H}(i)$ and $p \in \mathbf{T}(i)$. However, $\{p'\}$ cannot be read since $\mathbf{H}(i) \subseteq \mathbf{T}(i)$.

Hence, φ is THT satisfiable iff φ' is LTL satisfiable.

The map f shall be also useful to show Proposition 4 below, becoming the latter a key step to obtain PSPACE-hardness results (see e.g. Theorem 2). Proposition 4 below states that for a large class of formulae, LTL satisfiability is equivalent to TEL satisfiability.

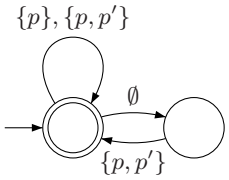

Fig. 2. Büchi automaton for models of $f(\mathsf{G}(\neg p \rightarrow \mathsf{X}p)) \wedge \mathsf{G}(p' \rightarrow p)$

Proposition 4. *Let φ be temporal formula built over the connectives $\vee$, $\wedge$, $\rightarrow$, X and U and such that $\rightarrow$ occurs only in subformulae of the form $p \rightarrow \bot$ with $p \in$ AT. The propositions below are equivalent: (I) φ is LTL satisfiable; (II) φ is THT satisfiable; (III) φ has a temporal stable model, i.e. φ is TEL satisfiable.*

Corollary 2. *THT satisfiability problem is* PSPACE*-complete.*

Proof. The translation f requires only polynomial-time and since LTL satisfiability is PSPACE-complete [25], we get that THT satisfiability is in PSPACE. It remains to show the PSPACE lower bound.

To do so, we can just observe that, as proved by Proposition 1, LTL satisfiability (which is PSPACE-complete) can be encoded into THT satisfiability using the translation from Proposition 1, which can be performed in linear time. Indeed, it just adds a formula $\mathsf{G}(p \vee \neg p)$ per each atom $p \in$ AT. □

We can strengthen the mapping φ' to obtain not only THT models of φ but also to constrain them to be strictly non-total (that is $\mathbf{H} < \mathbf{T}$) as follows

$$\varphi'' \stackrel{\text{def}}{=} \varphi' \wedge \bigvee_{i \in [1,n]} \mathsf{F}((p'_i \rightarrow \bot) \wedge p_i)$$

φ'' characterizes the non-total THT models of the formula φ. The generalized disjunction ensures that at some position j, $\mathbf{H}(j) \subset \mathbf{T}(j)$ (strict inclusion).

Lemma 4. *The set of LTL models for the formula φ'' corresponds to the set of non-total THT models for the temporal formula φ.*

The proof is again by structural induction. Let $\mathcal{A}_2$ be the Büchi automaton such that $\mathrm{L}(\mathcal{A}_2) = \mathrm{Mod}(\varphi'')$, following again any construction similar to [29] (see Section 3.2). $\mathrm{L}(\mathcal{A}_2)$ contains exactly the non-total THT models of φ.

Let $h : \Sigma' \rightarrow \Sigma$ be a map (renaming) between the two finite alphabets such that $h(a) = a \cap \{p_1, \ldots, p_n\}$. h consists in erasing the atoms from $\{p'_1, \ldots, p'_n\}$ h can be naturally extended as an homomorphism between finite words, infinite words and as a map between languages. Similary, given a Büchi automaton $\mathcal{A}_2 = (\Sigma', Q, Q_0, \delta, F)$, we write $h(\mathcal{A}_2)$ to denote the Büchi automaton $(\Sigma, Q, Q_0, \delta', F)$ such that $q \xrightarrow{a} q' \in \delta' \stackrel{\text{def}}{\Leftrightarrow}$ there is $b \in \Sigma'$ such that $q \xrightarrow{b} q' \in \delta$ and $h(b) = a$. Obviously, $\mathrm{L}(h(\mathcal{A}_2)) = h(\mathrm{L}(\mathcal{A}_2))$. Indeed, the following propositions imply each other:

1. $a_0 a_1 \cdots \in \mathrm{L}(\mathcal{A}_2)$,
2. $h(a_0)h(a_1)\cdots \in h(\mathrm{L}(\mathcal{A}_2))$ (by definition of h on languages),

3. $h(a_0)h(a_1)\cdots \in \mathrm{L}(h(\mathcal{A}_2))$ (by definition of h on $\mathcal{A}_2$).

The inclusion $\mathrm{L}(h(\mathcal{A}_2)) \subseteq h(\mathrm{L}(\mathcal{A}_2))$ can be shown in a similar way. So, $\mathrm{L}(h(\mathcal{A}_2))$ can be viewed as the set of total THT models for φ having a strictly smaller THT model.

Proposition 5. *φ has a TEL model iff* $\mathrm{L}(\mathcal{A}_1) \cap (\Sigma^\omega \setminus \mathrm{L}(h(\mathcal{A}_2))) \neq \emptyset$.

Proof. A TEL model $\mathbf{M} = (\mathbf{H}, \mathbf{T})$ for φ satisfies the following properties:

1. $\mathbf{M}, 0 \models \varphi$ and $\mathbf{H} = \mathbf{T}$.
2. For no $\mathbf{H}' < \mathbf{H}$, we have $(\mathbf{H}', \mathbf{T}), 0 \models \varphi$.

We have seen that $\mathrm{L}(\mathcal{A}_1)$ contains exactly the LTL models of φ, i.e. the total THT models satisfying φ. For taking care of condition (2.), by construction, $\mathcal{A}_2$ accepts the non-total THT models for φ whereas $\mathrm{L}(h(\mathcal{A}_2))$ contains the total THT models for φ having a strictly smaller THT model satisfying φ, the negation of (2.). Hence, $(\mathbf{T}, \mathbf{T})$ is a TEL model for φ iff $\mathbf{T} \in \mathrm{L}(\mathcal{A}_1)$ and $\mathbf{T} \notin \mathrm{L}(h(\mathcal{A}_2))$. □

Hence, the set of TEL models for a given φ forms an ω-regular language.

Proposition 6. *For each temporal formula φ, one can effectively build a Büchi automaton that accepts exactly the TEL models for φ.*

Proof. The class of languages recognized by Büchi automata (the class of ω-regular languages) is effectively closed under union, intersection and complementation. Moreover, it is obviously closed under the renaming operation. Since $\mathcal{A}_1$, $\mathcal{A}_2$, and $h(\mathcal{A}_2)$ are Büchi automata, one can build a Büchi automaton $\mathcal{A}'$ such that $\mathrm{L}(\mathcal{A}') = \Sigma^\omega \setminus \mathrm{L}(h(\mathcal{A}_2))$. Similarly, one can effectively build a Büchi automaton $\mathcal{B}_\varphi$ such that $\mathrm{L}(\mathcal{B}_\varphi) = \mathrm{L}(\mathcal{A}_1) \cap \mathrm{L}(\mathcal{A}')$. Complementation can be performed using the constructions in [26] or in [23] (if optimality is required). Roughly speaking, complementation induces an exponential blow-up. □

Figure 3 presents a Büchi automaton accepting the (unique) temporal equilibrium model for φ. The next step consists in showing that the nonemptiness check can be done in exponential space.

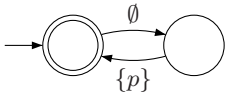

Fig. 3. Büchi automaton for stable models of $\mathsf{G}(\neg p \rightarrow \mathsf{X}p)$

Proposition 7. *Checking whether a TEL formula has a TEL model can be done in* ExpSpace.

Proof. Let φ be a temporal formula and $\mathcal{A}_1$ and $\mathcal{A}_2$ be Büchi automata such that $\mathrm{L}(\mathcal{A}_1) \cap (\Sigma^\omega \setminus \mathrm{L}(h(\mathcal{A}_2)))$ accepts exactly the TEL models for φ. We shall show that nonemptiness of the language can be tested in exponential space. With the construction of $\mathcal{A}_1$ using [29], we have seen that

1. the size of each state of $\mathcal{A}_1$ is linear in the size of φ (written $|\varphi|$),
2. it can be checked if a state is initial [resp. final] in linear space in $|\varphi|$,
3. each transition of $\mathcal{A}_1$ can be checked in linear space in $|\varphi|$,
4. $\mathcal{A}_1$ has a number of states exponential in $|\varphi|$.

Similarly, let us observe the following simple properties:

(a) φ'' is of linear size in $|\varphi|$; (b) Automaton $\mathcal{A}_2$ can be built from the formula φ'' using the construction in [29]; (c) $\mathcal{A}_2$ and $h(\mathcal{A}_2)$ have the same sets of states, initial states and final states and checking whether a transition belongs to $h(\mathcal{A}_2)$ is not more complex than checking whether a transition belongs to $\mathcal{A}_2$. So,

1. the size of each state of $h(\mathcal{A}_2)$ is linear in $|\varphi|$,
2. it can be checked if a state is initial [resp. final] in linear space in $|\varphi|$,
3. each transition of $h(\mathcal{A}_2)$ can be checked in linear space in $|\varphi|$.
4. $h(\mathcal{A}_2)$ has a number of states exponential in $|\varphi|$.

Using the complementation construction from [26] (the construction in [23] would be also fine) to complement $h(\mathcal{A}_2)$, one can obtain a Büchi automaton $\mathcal{A}'$ such that $\mathrm{L}(\mathcal{A}') = \Sigma^\omega \setminus \mathrm{L}(h(\mathcal{A}_2))$ and

1. the size of each state of $\mathcal{A}'$ is exponential in $|\varphi|$,
2. it can be checked if a state is initial [resp. final] in exponential space in $|\varphi|$,
3. each transition of $\mathcal{A}'$ can be checked in exponential space in $|\varphi|$.
4. $\mathcal{A}'$ has a number of states doubly exponential in $|\varphi|$.

Indeed, $h(\mathcal{A}_2)$ is already of exponential size in $|\varphi|$. So, using the above-mentioned property, one can check on-the-fly whether $\mathrm{L}(\mathcal{A}_1) \cap \mathrm{L}(\mathcal{A}')$ is nonempty by guessing a synchronized run of length at most double exponential (between the automata $\mathcal{A}_1$ and $\mathcal{A}'$) and check that it satisfies the acceptance conditions of both automata. At any stage of the algorithm, at most 2 product states need to be stored and this requires exponential space. Similarly, counting until a double exponential value requires only an exponential amount of bits. Details are omitted but the very algorithm is based on standard arguments for checking on-the-fly graph accessibility and checking nonemptiness of the intersection of two languages accepted by Büchi automata (similar arguments are used in [26, Lemma 2.10]). By Savitch Theorem [24], nondeterminism can be eliminated, providing the promised ExpSpace upper bound. □

Theorem 1. *Checking whether a TEL formula has a TEL model is* PSpace*-hard.*

Proof. We can use again the linear encoding in Proposition 1 and observe that any THT model $(\mathbf{T}, \mathbf{T})$ of $\psi = \varphi \wedge \bigwedge_{p \in \mathrm{AT}(\varphi)} \mathsf{G}(p \vee \neg p)$ will also be a TEL model of φ, since there are no non-total models for ψ and thus $(\mathbf{T}, \mathbf{T})$ will always be minimal. But then $\mathbf{T} \models \varphi$ in LTL iff $(\mathbf{T}, \mathbf{T}) \models \psi$ in THT iff $(\mathbf{T}, \mathbf{T})$ is a TEL model of ψ. Thus LTL satisfiability can be reduced to TEL satisfiability and so the latter problem is PSpace-hard. □

Theorem 2. *Checking whether two temporal formulae have the same TEL models is decidable in* ExpSpace *and it is* PSpace*-hard.*

5 Concluding Remarks

We have introduced an automata-based method for computing the temporal equilibrium models of an arbitrary temporal theory, under the syntax of Linear-time Temporal Logic (LTL). This construction has allowed us solving several open problems about Temporal Equilibrium Logic (TEL) and its monotonic basis Temporal Here-and-There (THT). In particular, we were able to prove that THT satisfiability can be solved in PSPACE and is PSPACE-hard whereas TEL satisfiability is decidable (something not proven before) being solvable in EXPSPACE and at least PSPACE-hard (filling the gap is part of future work). Our method consists in constructing a Büchi automaton that captures all the temporal equilibrium models of an arbitrary theory. This also implies that the set of TEL models of any theory is ω-regular.

A recent approach [2,6] has developed a tool, called `STeLP`, that also captures TEL models of a theory in terms of a Büchi automaton. Our current proposal, however, has some important advantages. First, `STeLP` restricts the input syntax to so-called *splitable temporal logic programs*, a strict subclass of a normal form for TEL that further requires the introduction of auxiliary atoms for removing U and R operators, using a structure preserving transformation. On the contrary, our current method has no syntactic restrictions and directly works on the alphabet of the original theory, for which no transformation is required prior to the automaton construction. Second, once the `STeLP` input is written in the accepted syntax, it translates the input program into LTL by the addition of a set of formulae (the so-called *loop formulae*) whose number is, in the worst case, exponential on the size of the input. Future work includes the implementation of our current method as well a comparison in terms of efficiency with respect to the tool `STeLP`.

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Proper Granularity for Atomic Sections in Concurrent Programs

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Abstract. Concurrent programming becomes more prevalent in software development, but still faces the harsh reality that writing correct and efficient programs is hard and error-prone. Race conditions are among the most frequent errors that occur in concurrent programs. Most existing static and dynamic analyses work well on low-level races but are unable to detect those that occur *at the application level*. These errors occur when an atomic section, the synchronization primitive available for the programmer, is misplaced and shared resources are exposed to other threads in an inconsistent state with respect to the design of the application. In this extended abstract, we present a framework of static analysis to deal with these high-level races in a Haskell-like language. Based on a specification that describes the consistency of the shared resources, our analysis detects related races by using symbolic execution and equational reasoning. When the program is race-free, our analysis is capable of returning a probably more efficient but still correct fine-grained program.

Keywords: concurrency, static analysis, Haskell, race condition

1 Introduction

In recent years, manufacturers of processors encountered problems to increase clock speeds and straight-line instruction throughput and have started to focus on parallel architectures [20]. This shift in hardware evolution is provoking a fundamental and necessary turn towards concurrency in software development [20]. Unfortunately, developing correct and efficient concurrent programs is hard, as the underlying programming model is more complex than it is for sequential programs [18]. Indeed, there are many opportunities for mistakes and they are often due to unexpected interference between threads. To protect parts of the code from the interference of other threads, programmers define *atomic sections*: code fragments whose execution and the data they handle must not being affected by other threads. From the programmer's point of view, these fragments will be executed atomically. In practice, to achieve atomic sections, languages offer synchronization primitives such as locks or, more recently, software transactional memories [12, 17].

The possibility to define atomic sections is mandatory, but not sufficient to ensure the development of correct concurrent programs. Indeed, once a mechanism, be it locks or transactions, is available, the programmer still has to decide where and how to use atomic sections, which is far from trivial in practice [1]. Too fine-grained sections increase the risk of errors while too coarse-grained sections is inefficient as the parallelism is not exploited optimally. The goal of our framework is to give tools to the programmer to find the adequate granularity, that is, if one disregards the overhead related to the synchronization primitives, the finest granularity which ensures the correctness of the concurrent program. In this paper, we focus on a pure Haskell-like functional language, well-recognized to be particularly well-suited for concurrent programming, notably because of its type system that explicitly distinguishes the computations that may have side effects [6, 19].

To present the problem of the granularity of atomic sections, we need to expose more precisely what kind of bad behaviour can happen when atomic sections are misplaced, which is related to the presence of *race conditions* in the program. Although there exist different definitions, a race condition is frequently defined as occurring "when two threads can access a data variable simultaneously, and at least one of two accesses is a write"[8]. We believe that this definition is limited and we denote this kind of race condition by *low-level races*. Indeed, preventing these races is not sufficient to claim that a concurrent program is correct. For example, consider the source code below, written in a Haskell-like syntax where the `do` notation refers to the IO monad [7] and `read`, resp. `write`, allows to read a value from, resp. write a value in, a shared variable, as `shTab` and `shSum`. `shTab` contains a list of integers and `shSum` contains an integer, while `n` is an integer.

```
add shTab shSum n =
  do { atomic : { tab <- read shTab
                ; write shTab (insert n tab) }
     ; atomic : { s <- read shSum
                ; write shSum (s+n) }
  }
```

As we can see, each update of a single shared variable is protected inside an atomic section – i.e. the notation `atomic`, ensuring that no low-level race condition can occur. If the values of `shTab` and `shSum` are supposed to be completely independent, using two separate atomic sections is correct and efficient. However, if there is a link between the two shared resources, as it is often the case in practice, placing the atomic section is more subtle. In this example, `shSum` is supposed to represent the sum of the integers in the list `shTab`. In this case, an inconsistent state (in which the value of `shTab` has been updated while the value of `shSum` hasn't) is exposed between the two atomic sections, which is problematic in a concurrent program. For example, consider that at this precise point, another thread doubles the value of `shSum` and of each integer of `shTab`, the whole operation being protected inside an atomic section. At the end of the execution of both threads, the sum of the integers in the list `shTab` and the value of `shSum` will be different in general, which is probably considered as

an unacceptable error in the program. This kind of error, which is corrected in Fig. 1, is what we call an *application-level race condition*, as it is related to the application logic. Like any race, it is hard to detect with testing, as its appearance depends on the interleaving of threads. In large programs, application-level races are common [13] but classic race detectors or race-free type systems, such as [2, 14], are unable to detect them. This inability is due to the fact that these analyses don't have or don't use information about the application logic, which involves the informal link between shared resources and their meaning for the programmer.

In this extended abstract, we present a framework of analysis that statically helps the programmer to find a proper granularity for atomic sections in a functional concurrent program. Based on a small and easy-to-write specification about the consistency of shared resources, the analysis, which is a work-in-progress, detects too fine-grained atomic sections by highlighting places in the code that may lead to application-level race conditions, and automatically reduces the size of too coarse-grained atomic sections in order to increase performance of race-free concurrent programs. Section 2 gives more details about the methodology and the techniques involved in our static analysis. Section 3 discusses related work and presents the prospects of our framework.

2 Analysis

We present our framework of analysis in three steps: first, we explain how we formalize what the programmer considers at the design level as a consistent state of the shared variables, the specification that is needed for our analysis to run; then, we give more details about our analysis, which is based on symbolic execution and that uses equational reasoning, by showing how we can detect application-level race conditions in a functional concurrent program; finally, we show how we can use the analysis to get finer granularity for too coarse-grained atomic sections, which potentially has the effect of improving performance while staying race-free.

2.1 Consistency Definition

An *application-level race condition*, which we simply call *race* for the remainder of the text, occurs when shared variables are exposed – i.e. unprotected by an atomic section – in a state that is considered by the programmer as inconsistent with respect to the design of his application. As this is related to the application logic, our framework requires the programmer to provide information about what he or she considers as a consistent state. For this purpose, we propose to proceed in the following way:

1. One identifies, by giving a name, the *characteristics* involved in the definition of a consistent state. For example, for a shared list of integers, it can be the sum of its elements, the fact that it is sorted or the fact that it is empty.

```
add shTab shSum n =
  do { atomic : { tab <- read shTab
                ; write shTab (insert n tab)
                ; s <- read shSum
                ; write shSum (s+n) }
  }
```

Fig. 1. An example involving two shared variables: a list of integers `shTab` and an integer `shSum`.

2. One provides a list of *axioms* indicating how these characteristics are influenced by functions that manipulate the (content of the) shared variables.
3. One defines what he considers as *a consistent state*, in the form of a set of *invariants*.

We use the corrected version of our example, depicted in Fig. 1, to describe step by step our approach. The monadic function `add` deals with two shared variables: a list of integers that is supposed to be sorted, and an integer that is supposed to be the sum of the integers in the list. The pure function `insert x xs` returns a sorted list that corresponds to the insertion of `x` in the list `xs`, supposed to be sorted. In natural language, we would define the consistency of shared variables as "the value of `shSum` must always stay equal to the sum of the integers in the list `shTab`, and this list must always stay sorted". This helps us to identify the characteristics involved in the definition: we need to talk about the *value* of a shared variable, the *sum* of elements from a list and the fact that a list is *sorted*. We denote these characteristics respectively by *val*, *sum* and *sorted*. Note that *val* is a built-in characteristic known to our analysis, whereas *sum* and *sorted* are simply names given by the programmer to refer to two different characteristics of the shared variables. Using these characteristics, we provide two axioms, (1) and (2), that will be useful to prove the consistency of states during the analysis.

$$sum(\texttt{insert x xs}) = sum(\texttt{xs})\texttt{+x} \tag{1}$$

$$sorted(\texttt{insert x xs}) = sorted(\texttt{xs}) \tag{2}$$

Finally, we can define formally what is considered as a consistent state by giving a double invariant, (3) and (4), that must be preserved outside atomic sections:

$$sum(val(\texttt{shTab})) = val(\texttt{shSum}) \tag{3}$$

$$sorted(val(\texttt{shTab})) = \texttt{True} \tag{4}$$

As they are related to the high-level design of the application, these axioms and invariants, which are sufficient to process the analysis completely automatically, must stay relatively straightforward to produce for the programmer. In the framework we propose, which is work-in-progress, the general form of axioms and invariants is equivalences involving characteristics and Haskell-like expressions.

2.2 Static Detection of Application-Level Race Conditions

Using axioms, our analysis is able to detect application-level race conditions, which is equivalent, by definition, to check whether the invariants are violated – i.e. the state is inconsistent – outside atomic sections. The analysis is based on symbolic execution where the symbolic values are represented by a set of equations, denoted by $\mathcal{S}$, that evolves with successive (monad) actions according to the function $\mathcal{A}$, which is defined thereafter. Intuitively, $\mathcal{S}$ is an abstraction of the state of shared variables and is used to represent information about the characteristics of the shared variables that hold between two actions. From each (abstraction of) state $\mathcal{S}$, we use equational reasoning to check its consistency, with the help of axioms.

The set $\mathcal{S}$ is constructed incrementally inside each atomic section, starting from an initial set that only includes the invariants, according to the following key rules for the `read` and `write` actions:

$$\begin{aligned}
\mathcal{A}(\mathcal{S}, \texttt{write}\ sh\ e) &= \mathcal{S}' \cup \{val(sh) = e\} \\
&\quad \text{where } \mathcal{S}' \text{ is obtained by removing equations of } \mathcal{S} \text{ that} \\
&\quad \text{contain } val(sh). \\
\mathcal{A}(\mathcal{S}, x\ \texttt{<-}\ \texttt{read}\ sh) &= \mathcal{S}' \cup \{val(sh) = x\} \\
&\quad \text{where } \mathcal{S}' \text{ is obtained by replacing in } \mathcal{S} \text{ every occurrence} \\
&\quad \text{of } val(sh) \text{ by } x.
\end{aligned}$$

Each action that is not explicitly inside an atomic section is considered by our analysis to be inside an implicit atomic section containing only one action.[1]

Figure 2 shows how our analysis is applied in the case of the example of Fig. 1. In particular, the annotated code shows how the function $\mathcal{A}$ allows to derive incrementally the state of the shared variables and the second part shows how the utilisation of equational reasoning allows to prove that $\mathcal{S}_{(5)}$, the state that is exposed to other threads, is consistent since it satisfies both invariants, meaning that there is no race in the function `add`. Note also that invariant (3) can not be deduced from, for example, $\mathcal{S}_{(3)}$ using equational reasoning. This depicts the fact that the atomic section could not end at that point without introducing a race. Inside the atomic section, this situation is allowed because the invariant violation is not exposed to other threads.

2.3 Program Transformation to Improve Performance

After proving that the program is race-free, our analysis is also able to split atomic sections in finer-grained sections that still satisfy the invariants. As such, it can improve parallelism without exposing inconsistent state to other threads. The idea is to examine the states inside the atomic sections in the hope of

[1] Note that this can be justified, for example, in the context of STM Haskell [6] as each action on transactional variables must be declared explicitly inside an atomic section.

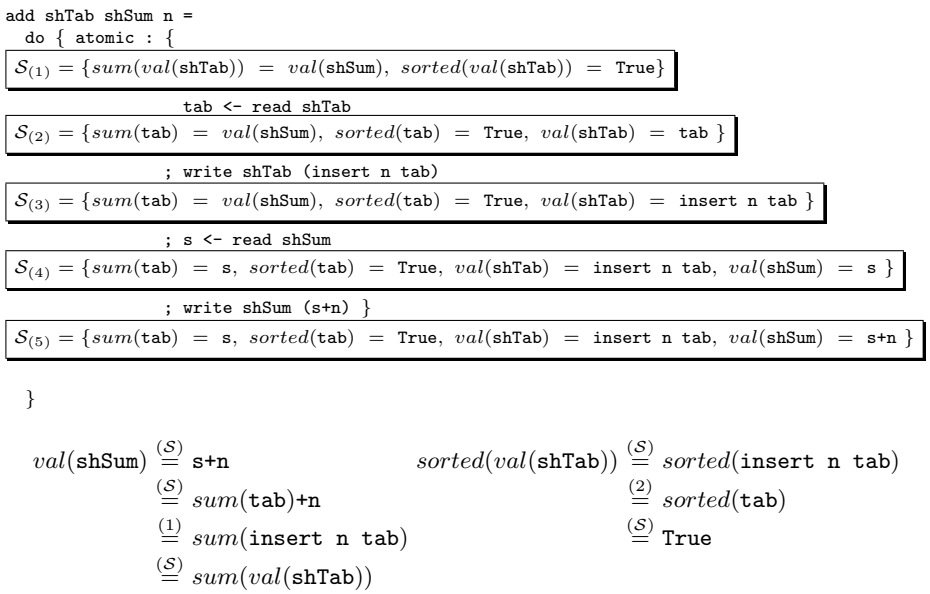

Fig. 2. Application of $\mathcal{A}$ on the example of Fig. 1 (above) and checking of invariants (3) and (4), using equational reasoning, for $\mathcal{S}_{(5)}$ (below)

finding an opportunity to split an atomic section while remaining race-free. A naïve algorithm could be as follows:

- Identification, inside the atomic section, of a state $\mathcal{S}$ that is consistent, if any.
- Splitting the atomic section at that point. The first atomic section is already proved to satisfy the invariants.
- Checking the consistency of the state at the end of the second atomic section:
  - If consistent, the splitting is confirmed and the process is run recursively for both new atomic sections.
  - If not, the splitting is cancelled and the all process is restarted for another consistent state inside the atomic section, if any.
- If there is no (more) consistent state inside the atomic section, the process ends.

Returning to the example of Fig. 2, we note that the invariants can be deduced from $\mathcal{S}_{(1)}$, $\mathcal{S}_{(2)}$ and $\mathcal{S}_{(5)}$. The fact that they can be deduced from $\mathcal{S}_{(2)}$ suggests a potential split after the first action. However, as shown in Fig. 3, the second atomic section cannot be proved to preserve the invariants, and hence the split is cancelled. Of course, it is easy to imagine a situation that would allow a split. A basic example of a such situation is depicted at Fig. 4. Indeed, given the same specification (axioms and invariants) as in the example before, we can obviously prove that the invariants are preserved at the point indicated by (X) in the code, and that thus the atomic section can be split at that point.

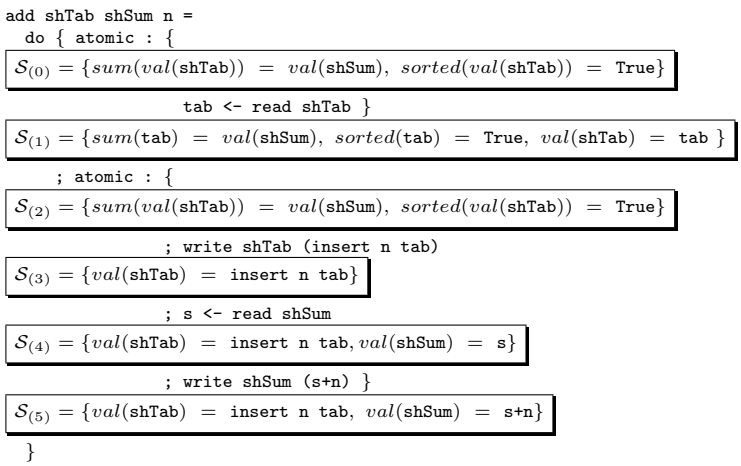

Fig. 3. An example of race: from $\mathcal{S}_{(5)}$, it is not possible to derive invariant (3) using equational reasoning, meaning that an inconsistent state is exposed to other threads.

```
add' shTab shSum shFoo n =
  do { atomic : { tab <- read shTab
                ; write shTab (insert n tab)
                ; s <- read shSum
                ; write shSum (s+n)
            (X)
                ; write shFoo "Hello"
                }
  }
```

Fig. 4. An example where a split is allowed, as the invariants are preserved by both new atomic sections.

3 Related and Ongoing Work

Despite numerous works on the analysis of concurrent programs, we are far from being able to detect all kind of errors related to concurrent programming [13, 21]. The detection of race conditions has drawn attention of a large community of researchers. In particular, model checking [9] and dynamic analysis [16, 22] has been explored. Where model checking has to cope with a computational complexity issue (the number of possible thread interleavings is exponential), dynamic analysis cannot guarantee absence of race conditions across all program executions. Static race detectors have also been developed [2, 3, 5, 14] but they tend to focus on low-level races – i.e. race condition involving a single shared variable. Although these errors can also be detected by our framework, we deal with a large range of more general races. Works closer to ours are those that introduce behavioural annotations, such as [1, 11], as they also target application-

level race conditions. Unlike our analysis, however, these works do not propose a method to split coarse-grained atomic sections. Furthermore, they focus on object-oriented languages. To fit with this paradigm, they must address specific issues, such as access permissions and unpacking methodologies, which are prevalent in these works. While we use equivalences involving self-defined characteristics and Haskell-like expressions, their systems are based on the utilisation of typestate and linear logic [1], or first-order predicate logic [11]. Unlike [11], our system does not impose any restrictions on the architecture of the application. Moreover, we feel that our annotations are well-separated from the source code, easy to write and easy to incorporate in an application in a clean and straightforward way. We use a monadic style concurrent programming language because of the clear separation of the mutable (concurrent) variables makes the analysis easier to define. Note also that the invariants we use are different from those that can be checked dynamically in STM Haskell [7], since they involve self-defined characteristics. Last, the reader can notice that, in this work, we simply declare which portion of code need to be executed atomically, without caring about how it will be done effectively. In practice, software transactional memories [6] and atomicity checkers [4, 10, 15] for lock-based systems can be used as complementary techniques.

The main contribution of this framework is a general strategy of static analysis to deal with the delicate problem of the atomic sections' granularity in concurrent programs. More specifically, our analysis detects high-level races and splits sections that are unnecessarily large. Flexibility and scalability are two important characteristics of this framework, which is a work-in-progress. In the near future, the whole process will be formalized in more details. This will be completed by an implementation of the framework and an experimental evaluation.

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