Operationally-based Program Equivalence Proofs using LCTRSs

Ștefan Ciobâcă¹, Dorel Lucanu¹, and Andrei Sebastian Buruiană²

¹ Alexandru Ioan Cuza University {stefan.ciobaca,dlucanu}@info.uaic.ro ² Bitdefender sburuiana@bitdefender.com

Abstract. We propose an operationally-based deductive proof method for program equivalence. It is based on encoding the language semantics as logically constrained term rewriting systems (LCTRSs) and the two programs as terms. The main feature of our method is its flexibility. We illustrate this flexibility in two applications, which are novel.

For the first application, we show how to encode low-level details such as stack size in the language semantics and how to prove equivalence between two programs operating at different levels of abstraction. For our running example, we show how our method can prove equivalence between a recursive function operating with an unbounded stack and its tail-recursive optimized version operating with a bounded stack. This type of equivalence checking can be used to ensure that new, undesirable behavior is not introduced by a more concrete level of abstraction.

For the second application, we show how to formalize read-sets and writesets of symbolic expressions and statements by extending the operational semantics in a conservative way. This enables the relational verification of program schemas, which we exploit to prove correctness of compiler optimizations, some of which cannot be proven by existing tools.

Our method requires an extension of standard LCTRSs with axiomatized symbols. We also present a prototype implementation that proves the feasibility of both applications that we propose.

Keywords: program equivalence \cdot compiler correctness \cdot operational semantics \cdot deductive verification \cdot term rewriting

1 Introduction

A typical transformation in optimizing recursive functions is to add an additional parameter called an accumulator, which holds the current result of the computation. The transformed function is usually tail-recursive, enabling the compiler to emit efficient code. Typically, the optimized version of a function (the tail-recursive version) is simply *assumed* to be functionally equivalent to the original function. However, as we show here, this is not necessarily the case. Consider the two functions for computing the sum of the first n positive naturals, presented in a C-like language, in Figure 1.



The programs f(n) and F(n, 0, 0) are functionally equivalent in an idealized setting. However, depending on the exact definition of functional equivalence, the equivalence may not hold. We illustrate two settings where the equivalence does not hold:

Setting 1. Consider that the two programs have a bounded stack. The program f (the left-hand side, lhs) uses O(n) stack cells, while the program F (the right-hand side, rhs) can use constant stack size, since it is tail-recursive.

In this model of computation, with a bounded stack, which is more realistic, the results of the function calls would be different for a sufficiently large input *n*: the program on the left-hand side would crash (running out of stack size), while the program on the right-hand side would work as expected.

We have confirmed this difference between the two programs on a real system. The first program (compiled on a typical Windows laptop with a recent g^{++} compiler, without optimizations) has a stack overflow when $n \geq 43340$. The second program (compiled with tail-call optimizations) exhibits no stack overflow (even for larger values of n) on the same system.

Setting 2. Also consider a variation of the two programs presented in Figure 2. Even with an unbounded stack, if the language has introspection capabilities that allow programs to query the current stack size (the function $\texttt{stack_size}$), then the *rhs* and the *lhs* behave differently, since the stack size will be large only in the *lhs*. Therefore f(n) and F(n, 0, 0) are not equivalent in this setting. We have also confirmed this difference between the two programs on a real system as well. We did this by developing a non-portable implementation of $\texttt{stack_size}()$ (for the X86 architecture, by querying the RSP register). The first program produces an error for sufficiently large n, while the second program does not, for any n.

Therefore, telling whether the optimized tail-recursive version of a function is equivalent to the original function is worth investigating in a more principled manner.

Our solution. We propose a method for proving program equivalence based on modeling the operational semantics of the language as a logically constrained term rewriting system (LCTRS). This method allows us to compare two programs for equivalence in various settings, by varying the underlying semantics defined as an LCTRS. We study the two programs in the running example above using as operational semantics an imperative language featuring integer

```
int f(int n) {
                                   int F(int n, int i, int a) {
  if (n == 0) {
                                     if (i > n) {
    if (stack_size() > 10) {
                                        if (stack_size() > 10) {
      error;
                                          error;
    7
    return 0;
                                       return a;
 } else {
                                     } else {
    return n + f(n - 1);
                                       return F(n, i + 1, a + i);
 }
                                     3
}
                                   }
```

Fig. 2: A variation of the programs in Figure 1. The only difference is in the base case.

variables, boolean conditions, if-then-else and while statements, and function calls. We call the language IMP and we introduce it formally in the subsequent sections. We propose two versions of IMP with the same syntax but with different semantics: IMP_1 has an idealized semantics, with an unbounded stack; IMP_2 has a more realistic semantics, with a bounded stack.

Our method proves that the two programs in Figure 1 are equivalent in IMP_1 , but the equivalence proof correctly fails in IMP_2 . Our method also shows that they are equivalent when the first program is interpreted in IMP_1 and the second program in IMP_2 . When the two programs query the stack size as in Figure 2, the equivalence proof correctly fails in both IMP_1 and IMP_2 . We write IMP in the cases where the exact version, IMP_1 or IMP_2 , does not matter.

We encode the operational semantics of the language as a logically constrained term rewriting system and the two programs as terms. An LCTRS consists of rewrite rules of the form $l \longrightarrow r$ if ϕ , where l, r are terms and ϕ is a first-order logical constraint. In IMP, l and r are terms of sort Cfg, representing program configurations. IMP configurations are tuples $\langle [e_1, \ldots, e_n], env, fs \rangle$ of:

- 1. a cons-list $[e_1, \ldots, e_n]$ of expressions and statements to be evaluated in order, representing the evaluation stack,
- 2. an environment env mapping identifiers to their value,
- 3. and an environment fs mapping function identifiers to the function bodies.

We use a Haskell-like notation for cons-lists: [] is the empty list, \rightarrow is the (rightassociative) list constructor, and $[e_1, e_2, \ldots, e_n]$ is a shorthand for $e_1 \rightarrow e_2 \rightarrow \ldots \rightarrow e_n \rightarrow$ []. The full order-sorted algebra defining the syntax of IMP is given in BNF-like notation in Figure 4. The operational semantics of IMP is given by logically constrained rewrite rules such as the following, which define assignments and summations:

- 1. $\langle x:=i \rightarrow es, env, fs \rangle \longrightarrow \langle es, update(env, x, i), fs \rangle;$
- 2. $\langle x := e \rightarrow es, env, fs \rangle \longrightarrow \langle e \rightarrow x := \Box \rightarrow es, env, fs \rangle$ if $\neg val(e)$;
- 3. $\langle x \rightarrow es, env, fs \rangle \longrightarrow \langle lookup(env, x) \rightarrow es, env, fs \rangle;$
- 4. $\langle e_1 + e_2 \rightarrow es, env, fs \rangle \longrightarrow \langle e_1 \rightarrow \Box + e_2 \rightarrow es, env, fs \rangle$ if $\neg val(e_1)$;

- 5. $\langle i_1 \rightarrow \Box + e_2 \rightarrow es, env, fs \rangle \longrightarrow \langle i_1 + e_2 \rightarrow es, env, fs \rangle;$
- 6. $\langle i_1 + e_2 \rightarrow e_3, env, f_5 \rangle \longrightarrow \langle e_2 \rightarrow i_1 + \Box \rightarrow e_3, env, f_5 \rangle$ if $\neg val(e_2)$;
- 7. $\langle i_2 \rightarrow i_1 + \Box \rightarrow es, env, fs \rangle \longrightarrow \langle i_1 + i_2 \rightarrow es, env, fs \rangle;$
- 8. $\langle i_1 + i_2 \rightarrow es, env, fs \rangle \longrightarrow \langle i_1 + i_2 \rightarrow es, env, fs \rangle;$
- 9. $\langle i \rightarrow x := \Box \rightarrow es, env, fs \rangle \longrightarrow \langle x := i \rightarrow es, env, fs \rangle$.

We use the following typographic conventions:

- 1. standard math font is used for meta-variables (e.g., l, r standing for terms and ϕ standing for constraints),
- 2. sans serif, red font for object-level variables (e.g., the variable symbol x, standing for program identifiers) and
- 3. **bold**, **blue font** for object-level non-variable symbols (e.g., the function symbols **update**, **val**).

The first rule defines the semantics of assigning an integer i to the program identifier x (the variables i and x are of sorts Integer and Identifier, respectively). The variable es matches the tail of the computation stack (we use the Haskell convention of using the suffix -s to denote a list). In this case, the environment is updated by using the **update** function (in the usual theory of arrays). The second rule defines assignment in the case where an expression e, which is not a value (i.e., not an integer) is assigned to the program identifier \times . In this case, the expression e is *scheduled* for evaluation, by placing it in front of the computation stack. The special constant \Box is used as a placeholder to recall which part of the statement has been promoted for evaluation. The third rule defines the evaluation rules for program identifiers (program variables), by using the lookup function in the theory of arrays. The following five rules define how additions are evaluated (left to right). Note that e, e_1, e_2 are variables of sort Exp, while i, i_1, i_2 are variables of sort Int (as Int < Exp, any term of sort Int is also a term of sort Exp, but not vice-versa). Once an expression promoted by the second rule is completely evaluated and *becomes* a term of sort Int, the last rule is allowed to fire, which places the value of the expression back into the assignment statement, which may then proceed to execute using rule 1. We use + (using teletype font) for the summation operator in the language (+ is a constructor for program expressions), and + (usual mathematication for integer summation (+ is an interpreted function symbol: summation in the usual theory of integers).

Here is how $\mathbf{x}:=\mathbf{x} + \mathbf{2}$ is executed in an initial environment $env = \mathbf{x} \mapsto \mathbf{12}$ and with an arbitrary map $fs: \langle [\mathbf{x}:=\mathbf{x} + \mathbf{2}], env, fs \rangle \longrightarrow \langle [\mathbf{x} + \mathbf{2}, \mathbf{x}:=\Box], env, fs \rangle \longrightarrow \langle [\mathbf{x}, \Box + \mathbf{2}, \mathbf{x}:=\Box], env, fs \rangle \longrightarrow \langle [\mathbf{12}, \Box + \mathbf{2}, \mathbf{x}:=\Box], env, fs \rangle \longrightarrow \langle [\mathbf{12} + \mathbf{2}, \mathbf{x}:=\Box], env, fs \rangle \longrightarrow \langle [\mathbf{14}, \mathbf{x}:=\Box], env, fs \rangle \longrightarrow \langle [\mathbf{x}:=\mathbf{14}], env, fs \rangle \longrightarrow \langle [\mathbf{1}, \mathbf{x} \mapsto \mathbf{14}, fs \rangle \not \rightarrow \rangle$. This style of giving an operational semantics to a language is called *frame* stack style according to [43], was popularized by the K framework [48] and it avoids the necessity of refocusing [16] typical of operational semantics based on evaluation contexts.

Recall the two recursive programs f and F introduced earlier (Figure 1). Formally, $f = \langle \mathbf{f}(\mathbf{n}), env, fs \rangle$ and $F = \langle \mathbf{F}(\mathbf{n}, \mathbf{0}, \mathbf{0}), env, fs \rangle$, where env is some environment and $fs = \{ \mathbf{f} \mapsto \lambda \mathbf{n}. \text{ if } \mathbf{n} = \mathbf{0} \text{ then } \mathbf{0} \text{ else } \mathbf{n} + \text{ call } \mathbf{f}(\mathbf{n} - 1), \mathbf{F} \mapsto \lambda \mathbf{n}.$

$\begin{array}{l} \text{exp.} \begin{cases} \left\langle [\mathbf{f}(3)], env, fs \right\rangle \\ \left\langle [\mathbf{f}(2), 3 + \Box], env, fs \right\rangle \\ \left\langle [\mathbf{f}(1), 2 + \Box, 3 + \Box], env, fs \right\rangle \\ \left\langle [\mathbf{f}(0), 1 + \Box, 2 + \Box, 3 + \Box], env, fs \right\rangle \\ \left\langle \left\langle [0, 1 + \Box, 2 + \Box, 3 + \Box], env, fs \right\rangle \end{cases} \end{cases}$	$ ^{*} ^{*} ^{*} ^{*} ^{*} ^{*} ^{*} ^{*} ^{*} ^{*} ^{*} ^{*} ^{*} ^{*} ^{*} ^{*} ^{*} ^{*} ^{*} ^{*} ^{*} ^{*} ^{*} ^{*} ^{*} ^{*} ^{*} ^{*} ^{*} $	$ \langle [\mathbf{F}(3,0,0)], env, fs \rangle \longrightarrow^{*} \\ \langle [\mathbf{F}(3,1,0)], env, fs \rangle \longrightarrow^{*} \\ \langle [\mathbf{F}(3,2,1)], env, fs \rangle \longrightarrow^{*} \\ \langle [\mathbf{F}(3,3,3)], env, fs \rangle \longrightarrow^{*} $
contr. phase $\begin{cases} \langle [1, 2 + \Box, 3 + \Box], env, fs \rangle \\ \langle [3, 3 + \Box], env, fs \rangle \\ \langle [6], env, fs \rangle \end{cases}$	$ ^{*} ^{*} $	$\langle [\mathbf{F}(3,4,6)], env, fs \rangle \longrightarrow^* \langle [6], env, fs \rangle \not\longrightarrow^* \not$
(a)		(b)

Fig. 3: Operational steps of f(3) (in Subfigure 3a) and of F(3,0,0) (in Subfigure 3b). Note that F has a single phase, while f has two distinct phases.

 $\lambda i.\lambda a.if i \leq n$ then call F(n, i+1, a+i) else a} is a map from identifiers to function bodies defining f and F. The fact that the two programs share the same input is represented by having the same free variable n in both symbolic configurations. We now show the main difficulty in an operational semantics-based proof of equivalence between them. To illustrate the difficulty, we use the operational behaviors of the two programs on the input 3, shown in Figure 3.

Note that f has two phases in the execution:

- 1. the stack expansion phase, before the recursive function reaches the base case and
- 2. the stack compression phase, where the actual additions take place.

Unlike this non-tail-recursive version, the tail-recursive function F has a single phase, where the second argument (the index i) increases in each step and the accumulator (the third argument) holds in turn the integers 0, 0 + 1, 0 + 1 + 2, and 0 + 1 + 2 + 3.

The method that we propose for equivalence proofs is based on two-way simulation. To prove that f and F are equivalent, we show that the configuration $\langle f(n), env, fs \rangle$ simulates $\langle F(n, 0, 0), env, fs \rangle$ and vice-versa (under the constraint $n \ge 0$). To show this, we set up a relation R that relates configurations as in the following diagram:

$\langle [\mathbf{f(3)}], env, \mathit{fs} \rangle$	$\stackrel{R}{\leftrightarrow} \langle [\mathbf{F(3,0,0)}], env, \mathit{fs} \rangle$
$\langle [{f f}(2), 3$ + $\Box], {f env}, fs angle$	$\overset{R}{\leftrightarrow} \langle [\mathbf{F}(3,0,0)], env, \mathit{fs} \rangle$
$\langle [{f f}(1), 2$ + $\Box, 3$ + $\Box], {f env}, {\it fs} angle$	$\stackrel{R}{\leftrightarrow} \langle [\mathbf{F(3,0,0)}], env, \mathit{fs} \rangle$
$\langle [\mathbf{f}(0), 1 + \Box, 2 + \Box, 3 + \Box], env, \mathit{fs} \rangle$	$\stackrel{R}{\leftrightarrow} \langle [\mathbf{F(3,0,0)}], env, \mathit{fs} \rangle$
$\langle [0, 1 + \Box, 2 + \Box, 3 + \Box], env, \mathit{fs} angle$	$\stackrel{R}{\leftrightarrow} \langle [\mathbf{F(3,1,0)}], env, \mathit{fs} \rangle$
$\langle [1,2+\Box,3+\Box],env,\mathit{fs} angle$	$\stackrel{R}{\leftrightarrow} \langle [\mathbf{F(3,2,1)}], env, \mathit{fs} angle$
$\langle [3,3+\Box],env,\mathit{fs} \rangle$	$\overset{R}{\leftrightarrow} \langle [\mathbf{F(3,3,3)}], env, \mathit{fs} \rangle$
$\langle [6], env, fs \rangle$	$\stackrel{R}{\leftrightarrow} \langle [\mathbf{F(3,4,6)}], env, \mathit{fs} \rangle$
$\langle [6], env, fs \rangle$	$\stackrel{R}{\leftrightarrow} \langle [6], env, \mathit{fs} \rangle$

That is, the relation R relates:

- 1. the configurations in the expansion phase of $\langle f(n), env, fs \rangle$ with the initial configuration $\langle \mathbf{F}(\mathbf{n}, \mathbf{0}, \mathbf{0}), \mathbf{env}, fs \rangle$ and
- 2. the configurations in contraction phase of $\langle f(n), env, fs \rangle$ with the configurations in the single phase of $\langle \mathbf{F}(n, 0, 0), env, fs \rangle$.

More formally, we would like R to relate configurations of the form

 $\langle [\mathbf{f}(\mathbf{i}), (\mathbf{i}+1) + \Box, (\mathbf{i}+2) + \Box, \dots, \mathbf{n} + \Box], \text{env}, fs \rangle$

to $\langle \mathbf{F}(\mathbf{n}, \mathbf{0}, \mathbf{0}), \mathbf{env}, fs \rangle$ and configurations of the form

$$\langle [\mathsf{s}, (\mathsf{i}+1) + \Box, (\mathsf{i}+2) + \Box, \dots, \mathsf{n} + \Box], \mathsf{env}, \mathit{fs} \rangle$$

to $\langle \mathbf{F}(\mathbf{n}, \mathbf{i}+1, \mathbf{s}), \mathbf{env}, fs \rangle$. However, in order to even express this relation R, we require a new technical development in the context of constrained term rewriting systems that we call *axiomatized symbols*. Axiomatized symbols can be used to mimic typical bigops in mathematics such as Σ, Π, \forall , etc. For our running example, we require a symbol called **reduce** axiomatized by the following constrained oriented equations:

1. reduce(i, n) \longrightarrow [] if i > n; 2. reduce(i, n) \longrightarrow (i+ \Box) \sim reduce(i + 1, n) if i \leq n.

That is, **reduce**(i, n) stands for the informally presented cons-list

 $[i + \Box, (i + 1) + \Box, \dots, n + \Box].$

By using the axiomatized symbol **reduce**, the relation R is formally defined as:

1. $(\langle [\mathbf{f}(\mathbf{n})], \mathbf{env}, fs \rangle, \langle [\mathbf{F}(\mathbf{n}, \mathbf{0}, \mathbf{0})], \mathbf{env}, fs \rangle) \in R$ if $\mathbf{0} < \mathbf{n}$;

2.
$$(\langle \mathbf{f}(\mathbf{i}) \rightsquigarrow \mathbf{reduce}(\mathbf{i}+1, \mathbf{n}), \mathsf{env}, fs \rangle, \langle \mathbf{F}(\mathbf{n}, \mathbf{0}, \mathbf{0}), \mathsf{env}, fs \rangle) \in R$$

- if $0 \le i \le n 1$; 3. $(\langle s \rightsquigarrow reduce(i, n), env, fs \rangle, \langle F(n, i, s), env, fs \rangle) \in R$ if $1 \le i \le n$,

where fs is the map defined earlier. Our algorithm checks whether R is indeed a (weak) simulation in the transition system generated by the LCTRS defining the operational semantics of IMP. To check equivalence of two symbolic program configurations P and Q (e.g., $\langle \mathbf{f}(\mathbf{n}), \ldots, \ldots \rangle$ and $\langle \mathbf{F}(\mathbf{n}, \mathbf{0}, \mathbf{0}), \ldots, \ldots \rangle$), we check that there exists simulations of P by Q and vice-versa. In practice, it is often the case that R^{-1} works for the reverse direction. Our proof method allows to conclude that f is fully simulated by F, but we can only show that F is partially simulated by f. This is because it cannot establish that the termination of Fimplies the termination of *both* phases of f.

As we have already illustrated above, an axiomatized symbol is any function symbol axiomatized by a set of oriented constrained equations. Axiomatized symbols are necessary in defining powerful relations, as shown above, but they can also be used to enable more powerful specification in LCTRSs.

For example, the symbol val used in the rewrite rules above is also an axiomatized symbol, and this symbol helps simplify the presentation of the operational semantics (otherwise, we would have had to enumerate all cases where expressions are values and non-values, respectively).

Axiomatized symbols can also simulate a form of higher-order rewriting. In order to define IMP as an LCTRS, we mix • an environment based semantics for the global store (the environment maps program identifiers to their integer value) and \bullet a substitution-based semantics for the function calls. Substitution is implemented by the symbol **subst** axiomatized as:

- 1. $\operatorname{subst}(x, e, x) \longrightarrow e$, 2. $\operatorname{subst}(x, e, y) \longrightarrow y$ if $x \neq y$,
- 3. $\operatorname{subst}(x, e, e_1 + e_2) \longrightarrow \operatorname{subst}(x, e, e_1) + \operatorname{subst}(x, e, e_2),$
- 4. $subst(x, e, y := e_1) \longrightarrow y := subst(x, e, e_1)$, etc.

Substitution-based function calls are formalized by the following rule (the function with a parameter \mathbf{x} and a body fb is called on the integer argument i):

• $\langle \text{call } \lambda x.\text{fb}(i) \rightarrow \text{es, env, fs} \rangle \longrightarrow \langle \text{subst}(x, i, \text{fb}) \rightarrow \text{es, env, fs} \rangle$.

We propose an algorithm, presented as a sound proof system, for proving simulation between symbolic program configurations. Two-way simulation is used to show equivalence. The simulation-checking algorithm relies on an oracle for the problem of *unification modulo axiomatized symbols*, which we formally define in this paper. We have implemented the equivalence-checking algorithm as a prototype in the RMT tool. Early work described here was presented, without being formally published, at the Dagstuhl seminar 18151 and the PERR 2019 workshop.

Contributions.

1. Our method is the first to allow equivalence checking in the case of bounded resources; being operationally-based, it is easy to check equivalence in various other settings (bounded versus unbounded stack, bounded versus unbounded integers, etc.) by simply varying the underlying LCTRS:

2. Unlike other relational logics, our method can easily handle structurally unrelated programs:

3. We extend our previous work on LCTRSs [13] by adding axiomatized symbols, which are critical for expressing powerful relations and we identify a new problem in rewriting, that of *unification modulo axiomatized symbols*, which is a particular type of higher-order unification, and which appears naturally in the context of program equivalence;

4. We show that our method can be used to formalize read-sets and write-sets of expressions and statements; this enables the verification of program schemas, which we take advantage of to prove compiler optimizations correct;

5. We implement the proof method in the prototype RMT tool; it can prove correctness of optimizations that are out of the reach of other verifiers.

Organization. In Section 2, we introduce the technical notations and background on LCTRSs, as well as the newly proposed notion of axiomatized symbols. In Section 3, we give the formal syntax of IMP and its formal semantics as an LCTRS (for both variations: IMP_1 and IMP_2). Section 4 contains the formalization for the definitions of full/partial simulation and equivalence and Section 5 the algorithms for checking simulations and equivalences. In Section 6 we discuss how our method can be used to formalize read/write-sets and prove compiler optimizations. In Section 7 we discuss related work before concluding in Section 8. Appendix A presents a complete example of an execution trace in IMP. Appendix B contains the proofs. Appendix C describes in detail the optimizations that we prove correct. Appendix D contains more details on the functional equivalence examples that prove.

2 LCTRSs

We consider a presentation of LCTRSs that we have introduced in our previous work [13], which we describe in this section and we extend with *axiomatized symbols*. We interpret LCTRSs in a model combining order-sorted terms with builtins such as integers, booleans, etc. Logical constraints are first-order formulae interpreted over the fixed model.

We assume an order-sorted signature $\varSigma = (S, \leq, F)$ with the following properties:

- 1. the set of sorts, $S = S^b \cup S^c$, is partitioned into a set of *builtin sorts* S^b and a set of "constructor" sorts S^c ;
- 2. in the subsorting relation, $\leq \subseteq (S^b \cup S^c) \times S^c$, builtin sorts do not have subsorts;
- 3. the set of function symbols, $F = F^b \cup F^c \cup F^a$, is partitioned into a set of builtin symbols F^b , a set of constructor symbols F^c , and a set of axiomatized symbols F^a .

If a function symbol $f \in F$ has arity $s_1 \times \ldots \times s_n \to s$, with $s_1, \ldots, s_n, s \in S$, we sometimes write $f \in F_{s_1 \ldots s_n, s}$. In particular, if n = 0 then $f \in \Sigma_{\varepsilon, s}$ is a constant of sort s.

We assume that no constructor symbol $f \in F^c$ is of arity $s_1 \times \ldots \times s_n \to s$, where $s \in S^b$ (no constructor symbol returns a builtin) and that any builtin symbol $f \in F^b$ has arity $f: s_1 \times \ldots \times s_n \to s$, with $s_1, \ldots, s_n, s \in S^b$.

We say that $\Sigma^b = (S^b, F^b)$ is the many-sorted builtin subsignature of Σ . We assume that the set of builtin sorts includes at least the sort **Bool** $\in S^b$ and that the builtin signature Σ^b has a model M^b such that $M^b_{\text{Bool}} = \{\top, \bot\}$, where the interpretation of the boolean connectives such as and $(\wedge : \text{Bool} \times \text{Bool} \to \text{Bool})$, or, etc. are standard and where the carrier set M^b_s of any builtin sort $s \in S^b$ is exactly the set of builtin constant symbols $F^b_{\epsilon,s} = M^b_s$ of the appropriate sort. By F^b_0 we denote $\cup_{s \in S^b} F^b_{\epsilon,s}$. As $M^b = F^b_0$, the set of builtin function symbols F^b might be infinite. We will assume that first-order Σ^b formulae can be decided by an oracle that is implemented in practice by a best-effort SMT solver. We let \mathcal{X} be an S-sorted set of variables. The set of Σ -terms with variables in \mathcal{X} is denoted by $T_{\Sigma}(\mathcal{X})$. Example 1. Let $S^b = \{\text{Bool}, \text{Int}, \text{Id}\}$. Let $F^b = \{0, 1, 2, \ldots :\rightarrow \text{Int}, + : \text{Int} \times \text{Int} \rightarrow \text{Int}, = : \text{Int} \times \text{Int} \rightarrow \text{Bool}, \text{true}, \text{false} :\rightarrow \text{Bool}, \wedge : \text{Bool} \times \text{Bool} \rightarrow \text{Bool}, \ldots\}$. We assume that first-order constraints over Σ^b can be solved by an SMT solver implementing integer arithmetic.

Let $S^c = \{ \text{Exp}, \text{Stack}, \text{Cfg}, \text{Env}, \text{Funcs} \}$ and $F^c = \{+, : : \text{Exp} \times \text{Exp} \rightarrow \text{Exp}, \text{ite} : \text{Exp} \times \text{Exp} \times \text{Exp} \rightarrow \text{Exp}, [] : \rightarrow \text{Stack}, \rightarrow : \text{Exp} \times \text{Stack} \rightarrow \text{Stack}, \langle \cdot, \cdot, \cdot \rangle : \text{Stack} \times \text{Env} \times \text{Funcs} \rightarrow \text{Cfg}, \ldots \}$. Let $\leq = \{ \text{Bool} \leq \text{Exp}, \text{Int} \leq \text{Exp}, \text{Id} \leq \text{Exp}, \ldots \}$. The constructors sorts and function symbols model the syntax of an imperative language with boolean and arithmetic expressions, a global environment and a function map.

Let $F^a = \{$ **val** : **Exp** \rightarrow **Bool**, **reduce** : **Int** \times **Int** \rightarrow **Bool**, ... $\}$. The axiomatized function symbols correspond to those discussed in Section 1.

The set CF of *constraint formulae* is the set of first-order formulae with equality over the signature Σ . The set CF^b of *builtin constraint formulae* is the set of first-order formulae with equality over the signature Σ^{b} .

Definition 1 (LCTRS). A logically constrained rewrite rule is a tuple (l, r, ϕ) , often written as $l \longrightarrow r$ if ϕ , where l, r are terms in $T_{\Sigma}(\mathcal{X})$ of the same sort, and $\phi \in CF$ is a first-order formula. A logically constrained term rewriting system \mathcal{R} is a set of logically constrained rewrite rules.

Definition 2 (Reduction Relation Induced by an LCTRS). Given a Σ model M, an LCTRS \mathcal{R} induces a reduction relation on the sorted carrier set of M defined by:

$$\longrightarrow_{\mathcal{R}}^{M} = \left\{ \begin{pmatrix} \rho(C[l]), \rho(C[r]) \end{pmatrix} & | \begin{array}{c} l \longrightarrow r \text{ if } \phi \in \mathcal{R} \\ \rho : \mathcal{X} \to M \text{ is a valuation s.t. } \rho(\phi) = \top \\ C \text{ is an arbitrary context} \\ \end{pmatrix} \right\}.$$

We consider the model M^a of Σ whose sorted carrier set is defined inductively by the following equations:

- 1. for any built n sort $s \in S^b$: $M_s^a = M_s^b \cup \{f(m_1, ..., m_n) \mid f \in F_{s_1...s_n,s}^a, m_1 \in M_{s_1}^a, ..., m_n \in M_{s_n}^a\} \cup \{f(m_1, ..., m_n) \mid f \in F_{s_1...s_n,s}^b, m_1 \in M_{s_1}^a, ..., m_n \in M_{s_n}^a$ and there exists $1 \le i \le n$ s.t. $m_i \notin M_{s_i}^b\}$;
- 2. for any constructor sort $s \in S^c$: $M_s^a = \{f(m_1, ..., m_n) \mid f \in F_{s_1...s_n, s}^a \cup F_{s_1...s_n, s}^c, m_1 \in M_{s_1}^a, ..., m_n \in M_{s_n}^a\}.$

The interpretation of the function symbols in M^a is defined as:

- 1. built n symbols applied to elements of M^b : the same interpretation as in M^b ;
- 2. builtin symbols applied to elements of $M^a \setminus M^b$: interpreted as free symbols;
- 3. constructor symbols and axiomatized symbols: interpreted as free symbols.

Note that, since $M_s^b = F_{\epsilon,s}^b$ for any builtin sort $s \in S^b$, ground terms over $F_0^b \cup F^c$ are elements of M^a .

We say that a LCTRS \mathcal{R}^a axiomatizes the symbols in F^a if:

- 1. the reduction relation $\longrightarrow_{R^a}^{M^a}$ induced by R^a on the model M^a defined above is convergent and
- 2. the normal form $m \downarrow$ of any element $m \in M_s^a$ w.r.t. to $\longrightarrow_{R^a}^{M^a}$ is a ground term $m \in T_{F_0^b \cup F^c}$ built from nullary builtins and constructor symbols.

In what follows, we assume that R^a is an LCTRS that axiomatizes F^a .

Example 2. Continuing the previous example, we consider $R^a = \{ reduce(i, n) \}$ $\longrightarrow [] \text{ if } i > n, \text{reduce}(i, n) \longrightarrow (i + \Box) \rightsquigarrow \text{reduce}(i + 1, n) \text{ if } i \le n, \ldots \}.$

We now fix a model M (depending on \mathbb{R}^a) defined as follows:

- 1. for any built sort $s \in S^b$: $M_s^a = M_s^b$; 2. for any constructor sort $s \in S^c$: $M_s^a = \{f(m_1, \ldots, m_n) \mid f \in F_{s_1 \ldots s_n, s}, m_1 \in$ $M_{s_1}^a,\ldots,m_n\in M_{s_n}^a\}.$

That is, the carrier set of M is the set of ground terms $T_{F_0^b \cup F^c}$ built from nullary builtins and constructor symbols. In M, the builtin symbols are interpreted as in M^b , the constructor symbols are interpreted as in M^c and axiomatized symbols $f \in F^a$ are interpreted by: $M_{f(m_1,\ldots,m_n)} = f(m_1,\ldots,m_n) \downarrow$ (the normal form w.r.t. the reduction relation induced by \mathcal{R}^a).

We call solving equations over terms $t_1, t_2 \in T_{\Sigma}(\mathcal{X})$ in the model M unification modulo axiomatized symbols (UMAS). Unification modulo axiomatized symbols is a generalization of *unification modulo builtins* (UMB) that we have introduced in our previous work [12]. Unlike usual unification problems, where a unifier is simply a substitution, in UMB (and therefore in UMAS as well) a unifier is a pair (ϕ, σ) , where $\phi \in CF^b$ is a builtin logical constraint and σ is a substitution.

A complete set of unifiers modulo axiomatized symbols of t_1, t_2 is a set $umas(t_1, t_2)$ of pairs of builtin constraints and substitutions such that:

- 1. (soundness) for any $(\phi, \sigma) \in umas(t_1, t_2)$, we have: $\rho(\sigma(t_1)) = \rho(\sigma(t_2))$ for any valuation ρ such that $\rho(\phi) = \top$.
- 2. (completeness) for any valuation $\rho: \mathcal{X} \to M$ s.t. $\rho(t_1) = \rho(t_2)$, there exists an unifier $(\phi, \sigma) \in umas(t_1, t_2)$ and a valuation ρ' such that $\rho = \rho' \circ \sigma$ and $\rho'(\phi) = \top.$

Example 3. Consider $t_1 = \langle [], env, fs \rangle$ and $t_2 = \langle reduce(i, n), env', fs' \rangle$. We have (for example) that $umas(t_1, t_2) = \{(i > n, \{env' \mapsto env, fs' \mapsto fs\})\}$. Recall that $R^a \supseteq \{ \mathbf{reduce}(i, \mathbf{n}) \longrightarrow [] \text{ if } i > \mathbf{n} \}.$

Definition 3 (Top-most LCTRSs). An LCTRS \mathcal{R} is top-most on M if

$$\longrightarrow^M_R = \left\{ \left(\rho(l), \rho(r) \right) \qquad | \qquad \begin{array}{c} l \longrightarrow r \text{ if } \phi \in \mathcal{R} \\ \rho \text{ is a valuation s.t. } \rho(\phi) = \top \end{array} \right\},$$

that is, all rewritings take place at the root.

The fact that an LCTRS \mathcal{R} is top-most can be ensured by requiring that all rewrite rules are of some sort $s \in S$ with the property that no function symbol takes elements of sort s as arguments. Therefore, terms of sort s can only be rewritten at the root. There exist techniques [47] for transforming an LCTRS into a top-most one.

Example 4. We now consider the top-most LCTRS $\mathcal{R} = \{ \langle \mathbf{x}:=i \rightarrow es, env, fs \rangle \rightarrow \langle es, update(env, \mathbf{x}, i), fs \rangle, \langle \mathbf{x}:=e \rightarrow es, env, fs \rangle \rightarrow \langle e \rightarrow \mathbf{x}:=\Box \rightarrow es, env, fs \rangle$ if $\neg val(e), \ldots \}$. Only the function symbol $\langle \cdot, \cdot, \cdot \rangle$ returns an element of sort Cfg and no function symbol takes Cfg as an argument; therefore \mathcal{R} is top-most.

Definition 4 (Constrained Terms). A constrained term φ of sort $s \in S$ is a pair (t, ϕ) (written t if ϕ), where $t \in T_{\Sigma,s}(\mathcal{X})$ and $\phi \in CF$.

We consistently use φ for constrained terms and ϕ for constraint formulae.

Definition 5 (Valuation Semantics of Constraints). The valuation semantics of a constraint ϕ is the set $\|\phi\| \triangleq \{\alpha : X \to M^{\Sigma} \mid M^{\Sigma}, \alpha \vDash \phi\}.$

Definition 6 (State Predicate Semantics of Constrained Terms). The state predicate semantics of a constrained term t if ϕ is the set $[t \text{ if } \phi] \triangleq \{\alpha(t) \mid \alpha \in ||\phi||\}.$

Definition 7 (Derivatives of Constrained Terms). The set of derivatives of a constrained term t if ϕ w.r.t. a rule $l \longrightarrow r$ if ϕ_{lr} is

$$\Delta_{l,r,\phi_{lr}}(t \text{ if } \phi) = \{\sigma'(r) \text{ if } \phi \land \phi' \land \phi_{lr} \mid (\phi',\sigma') \in umas(t,l), \\ (\phi \land \phi' \land \phi_{lr}) \text{ satisfiable} \}$$

A constrained term φ is \mathcal{R} -derivable if $\Delta_{\mathcal{R}}(\varphi) \neq \emptyset$.

We assume as usual that the rewrite rules in \mathcal{R}^a and the rewrite rules in $l \longrightarrow r$ if $\phi_{lr} \in R$ are coherent in the generalized sense [36].

Theorem 1. If t if ϕ is a constrained term, then

 $\llbracket \Delta_{\mathcal{R}}(t \text{ if } \phi) \rrbracket = \{ \gamma' \mid \gamma \longrightarrow_{\mathcal{R}}^{M} \gamma' \text{ for some } \gamma \in \llbracket t \text{ if } \phi \rrbracket \}.$

The theorem above ensures that the symbolic successors (derivatives) of a constrained term are semantically correct. We write \longrightarrow instead of $\longrightarrow_{\mathcal{R}}^{M}$ when \mathcal{R} and M can be inferred from the context.

3 Language Semantics as LCTRSs

The operational semantics of a programming language can be encoded as a topmost LCTRS. As a running example, we feature equivalence proofs for programs written in an imperative language that we call IMP. In Figure 4, we define the syntax of the IMP language. The syntax is given in a BNF-like notation, and it

$\mathbf{Exp} \qquad ::= \mathbf{Int} \mid \mathbf{Bool} \mid \mathbf{Id} \mid \mathbf{Exp}$	xp binop Exp unop Exp call FunCall skip
$Exp;Exp \mid Id:=Exp$	$\exp while Exp do Exp if Exp then Exp else Exp$
FunCall ::= Id FunCall (Exp)	FunBody ::= Exp $ \lambda$ Id . FunBody
$\mathbf{Stack} ::= [] \mid \mathbf{Exp} \rightsquigarrow \mathbf{Stack}$	$\mathbf{Cfg} ::= \langle \mathbf{Stack}, \mathbf{Env}, \mathbf{Funcs} angle$

I IG. I. IIIC SYMUAA OF III	Fig. 4:	The	syntax	of	IMF
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should be understood as defining an order-sorted term signature. The configuration is a tuple $\langle es, env, fs \rangle$, consisting of a stack *es* of program expressions and statements to be evaluated in order (as exemplified in Section 1), a map *env* from identifiers (program variables) to integers that acts as a global store, and a map *fs* from function identifiers to function bodies. In IMP, both expressions and statements are grouped under the syntactic category **Exp**, and the difference between them is encoded in the semantics: expressions are replaced by their values in the computation stack, and statements are erased after their effect is performed. The language IMP comes in two variations, IMP₁ and IMP₂, both sharing the same syntax. The difference is in the semantics: IMP₁ has an unbounded stack, while IMP₂ has a bounded stack (we use a parametric bound of *k* elements). As explained in the introduction, we write IMP instead of IMP₁ and IMP₂ when the exact variation does not matter. In Figure 5, we define the operational semantics of IMP₁ in frame stack style [43] as an LCTRS. Note the use of the axiomatized symbol **subst** in the last rule for the function calls.

The axiomatized symbol **subst** is axiomatized by the following rules:

- 1. $subst(x, e, y := e_1) \longrightarrow y := subst(x, e, e_1),$
- 2. $\operatorname{subst}(x, e, y) \longrightarrow y \text{ if } x \neq y$,
- 3. $\operatorname{subst}(x, e, e_1 + e_2) \longrightarrow \operatorname{subst}(x, e, e_1) + \operatorname{subst}(x, e, e_2),$
- 4. $\operatorname{subst}(x, e, x) \longrightarrow e$,
- 5. $\operatorname{subst}(x, e, \operatorname{not} e') \longrightarrow \operatorname{not} \operatorname{subst}(x, e, e'),$
- 6. $\operatorname{subst}(x, e, \operatorname{if} e' \operatorname{then} e_1 \operatorname{else} e_2) \longrightarrow$
- $\mathbf{if subst}(x, e, e') \mathbf{then subst}(x, e, e_1) \mathbf{else subst}(x, e, e_2),$
- 7. $\operatorname{subst}(x, e, e_1; e_2) \longrightarrow \operatorname{subst}(x, e, e_1); \operatorname{subst}(x, e, e_2).$

Note that the symbols **lookup** and **update** in the usual theory of arrays are used for handling the environment in the imperative part. The axiomatized symbol **val** returns true exactly for the values of the language: integers and booleans: 1. **val**(i) $\rightarrow \top$; 2. **val**(b) $\rightarrow \top$; 3. **val**(e₁ + e₂) $\rightarrow \bot$; 4. **val**(e₁;e₂) $\rightarrow \bot$; etc.

An example of evaluation using the operational semantics encoded as an LCTRS is shown in Appendix A. The constrained rewrite rules defining IMP_2 are presented in Figure 6. They are similar to the rules for IMP_1 , except that each rule that increases the stack size has an additional constraint. The constraint prevents the rule from firing if the stack would become too big.

4 Simulation-based Equivalence Proofs

In the following, we will assume that \mathcal{R}_L and \mathcal{R}_R are two LCTRSs modeling the semantics of two programming languages: the *left* language and the *right*

$\langle x := e \rightsquigarrow es, env, fs \rangle \longrightarrow \langle e \rightsquigarrow x := \Box \rightsquigarrow es, env, fs \rangle if \neg val(e)$	assignment
$\langle i \rightsquigarrow x := \Box \rightsquigarrow es, env, fs \rangle \longrightarrow \langle x := i \rightsquigarrow es, env, fs \rangle$	
$\langle x := i \rightarrow es, env, fs \rangle \longrightarrow \langle es, update(env, x, i), fs \rangle$	
$\langle x \sim es, env, fs \rangle \longrightarrow \langle (x, env) \sim es, env, fs \rangle$	identifier lookup
$\langle e_1 + e_2 \rightarrow es, env, fs \rangle \longrightarrow \langle e_1 \rightarrow \Box + e_2 \rightarrow es, env, fs \rangle$ if $\neg val(e_2 \rightarrow \Box + e_2 \rightarrow es, env, fs)$) binary
$\langle i_1 \rightsquigarrow \Box + e_2 \rightsquigarrow es, env, fs \rangle \longrightarrow \langle i_1 + e_2 \rightsquigarrow es, env, fs \rangle$	operations
$\langle i_1 + e_2 \rightsquigarrow es, env, fs \rangle \longrightarrow \langle e_2 \rightsquigarrow i_1 + \Box \rightsquigarrow es, env, fs \rangle \text{ if } \neg val(e_2)$)
$\langle i_2 \rightsquigarrow i_1 + \Box \rightsquigarrow es, env, fs \rangle \longrightarrow \langle i_1 + i_2 \rightsquigarrow es, env, fs \rangle$	
$\langle i_1 + i_2 \sim es, env, fs \rangle \longrightarrow \langle i_1 + i_2 \sim es, env, fs \rangle$	
$\langle not e \rightsquigarrow es, env, fs \rangle \longrightarrow \langle e \rightsquigarrow not \Box \rightsquigarrow es, env, fs \rangle if \neg val(e)$	unary
$\langle b \rightsquigarrow \mathbf{not} \Box \rightsquigarrow es, env, fs \rangle {\longrightarrow} \langle \mathbf{not} b \rightsquigarrow es, env, fs \rangle$	operations
$\langle \operatorname{\mathbf{not}} b \rightsquigarrow es, env, fs \rangle \longrightarrow \langle \overline{b} \rightsquigarrow es, env, fs \rangle$	
$\langle \mathbf{if} \top \mathbf{then} \mathbf{e}_2 \mathbf{else} \mathbf{e}_3 \sim \mathbf{es}, \mathbf{env}, \mathbf{fs} \rangle \longrightarrow \langle \mathbf{e}_2 \sim \mathbf{es}, \mathbf{env}, \mathbf{fs} \rangle$	if-then-else
$\langle \mathbf{if} \perp \mathbf{then} e_2 \mathbf{else} e_3 \rightsquigarrow es, env, fs \rangle {\longrightarrow} \langle e_3 \rightsquigarrow es, env, fs \rangle$	
$\langle \text{if } e_1 \text{ then } e_2 \text{ else } e_3 \sim \text{es}, \text{env}, \text{fs} \rangle \longrightarrow \langle e_1 \sim \text{if } \Box \text{ then } e_2 \text{ else} \rangle$	$ e_3 \sim es, env, fs \rangle$
	if $\neg val(e_1)$
$\langle b \sim if \square then e_2 else e_3 \sim es, env, fs \rangle \longrightarrow \langle if b then e_2 else es \rangle$	$_{3} \sim es, env, fs \rangle$
$\langle while e_1 do e_2 \sim es, env, fs \rangle \longrightarrow$	while loop
$\langle ext{if e}_1 ext{ then } (ext{e}_2; ext{while e}_1 ext{ do e}_2) ext{ else skip} \sim ext{ es, env, fs} angle$	
$\langle e_1; e_2 \rightsquigarrow es, env, fs \rangle \longrightarrow \langle e_1 \rightsquigarrow e_2 \rightsquigarrow es, env, fs \rangle$	sequence
$\langle skip \rightsquigarrow es, env, fs \rangle \longrightarrow \langle es, env, fs \rangle$	skip
$\langle \operatorname{call} f \rightsquigarrow es, env, fs \rangle \longrightarrow \langle \operatorname{lookup}(f, fs) \rightsquigarrow es, env, fs \rangle$	function calls
$\langle \operatorname{call} f(e) \rightsquigarrow es, env, fs \rangle \longrightarrow \langle \operatorname{call} f \rightsquigarrow \operatorname{call} \Box(e) \rightsquigarrow es, env, fs \rangle$	
$\langle \lambda x. fb \sim call \ \Box(e) \sim es, env, fs \rangle \longrightarrow \langle call \ \lambda x. fb(e) \sim es, env \rangle$	∕, fs⟩
$\langle \operatorname{call} \lambda x.\operatorname{fb}(e) \rightsquigarrow \operatorname{es}, \operatorname{env}, \operatorname{fs} \rangle \longrightarrow \langle e \rightsquigarrow \operatorname{call} \lambda x.\operatorname{fb}(\Box) \rightsquigarrow \operatorname{es}, \operatorname{env} \rangle$	$\langle fs \rangle$ if $\neg val(e)$
$\langle i \sim call \ \lambda x.fb(\Box) \sim es, env, fs \rangle \longrightarrow \langle call \ \lambda x.fb(i) \sim es, env,$	fs〉
$\langle \mathbf{call} \ \boldsymbol{\lambda} x.\mathbf{fb}(i) \sim \mathbf{es}, \mathbf{env}, \mathbf{fs} \rangle \longrightarrow \langle \mathbf{subst}(x, i, \mathbf{fb}) \sim \mathbf{es}, \mathbf{env}, \mathbf{fs} \rangle$	

Fig. 5: The small-step operational semantics of IMP_1 encoded as an LCTRS in frame stack style. The language IMP_1 has an unbounded stack. The variables have the following sorts: x : Id, e : Exp, es : Stack, env : Env, fs : Funcs, i : Int, b : Bool, f : Id, fb : FunBody.

language. We assume that the sorts CfgL and CfgR are the sorts of configurations of the left language and of the right language, respectively. The LCTRSs \mathcal{R}_L and \mathcal{R}_R induce transition relations on the interpretations of CfgL and CfgR, transition relations that capture the operational semantics of the two languages. The languages might be the same, or they might be different; all our results are parametric in \mathcal{R}_L and \mathcal{R}_R . In the following examples we take $\mathcal{R}_L = \mathcal{R}_R = IMP$ and CfgL = CfgR = Cfg.

Formally, we define equivalence not between programs, but between *program* configurations. Program configurations typically contain both a program and additional information such as program counter, heap information, stack information or others, depending on the particular programming language. In our examples, the program configuration is a tuple $\langle [e_1, \ldots, e_n], env, fs \rangle$ consisting of a stack e_1, \ldots, e_n of expressions to be evaluated in this order, an environment

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 \begin{array}{ll} \langle \mathsf{x} := \mathsf{e} \sim \mathsf{es}, \mathsf{env}, \mathsf{fs} \rangle \longrightarrow \langle \mathsf{e} \sim \mathsf{x} := \Box \sim \mathsf{es}, \mathsf{env}, \mathsf{fs} \rangle & \text{if } \neg \mathsf{val}(\mathsf{e}) \land \mathsf{len}(\mathsf{es}) < k \\ \langle \mathsf{e}_1 + \mathsf{e}_2 \sim \mathsf{es}, \mathsf{env}, \mathsf{fs} \rangle \longrightarrow \langle \mathsf{e}_1 \sim \Box + \mathsf{e}_2 \sim \mathsf{es}, \mathsf{env}, \mathsf{fs} \rangle & \text{if } \neg \mathsf{val}(\mathsf{e}_1) \land \mathsf{len}(\mathsf{es}) < k \\ \langle \mathsf{i}_1 + \mathsf{e}_2 \sim \mathsf{es}, \mathsf{env}, \mathsf{fs} \rangle \longrightarrow \langle \mathsf{e}_2 \sim \mathsf{i}_1 + \Box \sim \mathsf{es}, \mathsf{env}, \mathsf{fs} \rangle & \text{if } \neg \mathsf{val}(\mathsf{e}_1) \land \mathsf{len}(\mathsf{es}) < k \\ \langle \mathsf{not} \, \mathsf{e}_1 \sim \mathsf{es}, \mathsf{env}, \mathsf{fs} \rangle \longrightarrow \langle \mathsf{e}_1 \sim \mathsf{not} \, \Box \sim \mathsf{es}, \mathsf{env}, \mathsf{fs} \rangle & \text{if } \neg \mathsf{val}(\mathsf{e}_1) \land \mathsf{len}(\mathsf{es}) < k \\ \langle \mathsf{if} \, \mathsf{e}_1 \, \mathsf{then} \, \mathsf{e}_2 \, \mathsf{else} \, \mathsf{e}_3 \sim \mathsf{es}, \mathsf{env}, \mathsf{fs} \rangle & \text{if } \neg \mathsf{val}(\mathsf{e}_1) \land \mathsf{len}(\mathsf{es}) < k \\ \langle \mathsf{if} \, \mathsf{e}_1 \, \mathsf{then} \, \mathsf{e}_2 \, \mathsf{else} \, \mathsf{e}_3 \sim \mathsf{es}, \mathsf{env}, \mathsf{fs} \rangle & \text{if } \neg \mathsf{val}(\mathsf{e}_1) \land \mathsf{len}(\mathsf{es}) < k \\ \langle \mathsf{eif} \, \mathsf{e}_1 \, \mathsf{then} \, \mathsf{e}_2 \, \mathsf{else} \, \mathsf{e}_3 \sim \mathsf{es}, \mathsf{env}, \mathsf{fs} \rangle & \text{if } \neg \mathsf{val}(\mathsf{e}_1) \land \mathsf{len}(\mathsf{es}) < k \\ \langle \mathsf{e}_1; \mathsf{e}_2 \sim \mathsf{es}, \mathsf{env}, \mathsf{fs} \rangle \longrightarrow \langle \mathsf{e}_1 \sim \mathsf{e}_2 \sim \mathsf{es}, \mathsf{env}, \mathsf{fs} \rangle & \text{if } \mathsf{len}(\mathsf{es}) < k \\ \langle \mathsf{e}_1; \mathsf{e}_2 \sim \mathsf{es}, \mathsf{env}, \mathsf{fs} \rangle \longrightarrow \langle \mathsf{e}_1 \sim \mathsf{e}_2 \sim \mathsf{es}, \mathsf{env}, \mathsf{fs} \rangle & \text{if } \mathsf{len}(\mathsf{es}) < k \\ \langle \mathsf{call} \, \mathsf{f}(\mathsf{e}) \sim \mathsf{es}, \mathsf{env}, \mathsf{fs} \rangle \longrightarrow \langle \mathsf{el} \, \mathsf{call} \, \mathsf{f} \sim \mathsf{call} \, \mathsf{I} \circ \mathsf{call} \, \mathsf{I} \circ \mathsf{call} \, \mathsf{I} \circ \mathsf{call} \, \mathsf{I} \circ \mathsf{es}, \mathsf{env}, \mathsf{fs} \rangle & \text{if } \mathsf{len}(\mathsf{es}) < k \\ \langle \mathsf{call} \, \lambda \mathsf{x}.\mathsf{fb}(\mathsf{e}) \sim \mathsf{es}, \mathsf{env}, \mathsf{fs} \rangle \longrightarrow \langle \mathsf{e} \sim \mathsf{call} \, \lambda \mathsf{x}.\mathsf{fb}(\Box) \sim \mathsf{es}, \mathsf{env}, \mathsf{fs} \rangle \\ & \text{if } \neg \mathsf{val}(\mathsf{e}) \land \mathsf{len}(\mathsf{es}) < k \end{cases} \end{cases}
```

Fig. 6: The small-step operational semantics of IMP_2 . The language IMP_2 has a stack bounded to k + 1 elements, where k is a parameter of the semantics. Only the rules different from the rules in IMP_1 are presented. The constraint len(es) < k ensures that the stack is of length at most k + 1 in the rhs.

env mapping global program variables to integers, and a map fs from identifiers to function bodies.

We sometimes distinguish between *symbolic program configurations* (terms of sort CfgL or CfgR, possibly with variables) and *ground program configurations* (elements of the interpretation of the sorts CfgL and CfgR). Due to the definition of the fixed model in which we work, any ground program configuration is also a symbolic program configuration with 0 variables. Our proof method shows equivalence between two symbolic program configurations. The fact that the same variable occurs in both symbolic configurations models that the two programs take the same input.

For our motivating example, we show the equivalence of the symbolic program configurations

 $\langle [\text{call } f(N)], \text{env}, fs \rangle$ and $\langle [\text{call } F(N, 0, 0)], \text{env}, fs \rangle$ for $N \geq 0$,

where fs is the map containing the function bodies corresponding to the function identifiers f and F. We use F(N, 0, 0) as an abbreviation for the syntactic construct F(N)(0)(0) of sort FunCall. Note that N is a variable of sort Intand env is a variable of sort Env(map from program identifiers to integers). The fact that both N and env occur in the two symbolic configurations models that we want the two programs to take the same input N and to start in the same environment env. In the initial configuration, the helper arguments of F are fixed to 0.

Sometimes two programs perform the same computation, but record the results in slightly different places. For example, an imperative program might store its result in a global variable **result**, while a functional program would simply reduce to its final value. We still want to consider these programs equivalent. Therefore, we parameterize our definition for equivalence by a set of *base cases*, which define the pairs of terminal ground configurations that are known to be equivalent. We denote by \mathbb{B} (for base) the set of pairs of ground terminal program configurations that are known to be equivalent. In our motivating example, $\mathbb{B} = \{(\langle [i], env, fs \rangle, \langle [i'], env', fs' \rangle) \mid i = i' \land i, i' \in \mathbb{Z}\}$ (both configurations have been reduced to the same integer i = i', the environments are allowed to be different: env on the lhs and env' on the rhs, and the function maps are also allowed to be different). See Example 4 in Appendix D for a more complex example.

We propose two definitions for the notion of functional equivalence of programs, based on two-way simulations. In the following, P denotes a symbolic configuration of sort CfgL, Q denotes a symbolic configuration of sort CfgR and ϕ denotes a first-order constraint. In the following definitions, by a complete path $\rho(P) \longrightarrow_{\mathcal{R}_{I}}^{\ast} P'$, we mean that no further reduction step is possible for P'.

Definition 8 (Full Simulation). We say that a symbolic program configuration P is fully simulated by a symbolic program configuration Q under constraint ϕ with a set of base cases \mathbb{B} (denoted by $\mathbb{B} \models P \prec Q$ if ϕ) if, for any valuation ρ such that $\rho(\phi) = \top$ and for any complete path $\rho(P) \longrightarrow_{\mathcal{R}_L}^* P'$, there exists a complete path $\rho(Q) \longrightarrow_{\mathcal{R}_R}^* Q'$ such that $(P', Q') \in \mathbb{B}$;

This intuitively states that for any terminating run of the left hand side on some input, there is a terminating run of the right hand side on the same input, such that the results are part of \mathbb{B} (e.g., the results are equal). The notion of *full simulation* is inspired from the usual notion of *full equivalence* in the relational program verification literature. It can be seen as a lopsided version of full equivalence. Full simulation is a transitive relation (assuming the base cases are defined consistently).

Definition 9 (Partial Simulation). We say that a symbolic program configuration P is partially simulated by a symbolic program configuration Q under constraint ϕ with a set of base cases \mathbb{B} (denoted by $\mathbb{B} \models P \preceq Q$ if ϕ) if, for any valuation ρ such that $\rho(\phi) = \top$ and for any complete path $\rho(P) \longrightarrow_{\mathcal{R}_L}^* P'$, one of the following holds: • there exists a complete path $\rho(Q) \longrightarrow_{\mathcal{R}_R}^* Q'$ s. t. $(P', Q') \in \mathbb{B}$; • there exists an infinite path $\rho(Q) \longrightarrow_{\mathcal{R}_R} \ldots$

Intuitively, a terminating run of the left hand side on some input is considered simulated by either (1) a terminating run of the right hand side on the same input with the same output or (2) by an infinite run of the right hand side on the same input. The notion of *partial simulation* is inspired from the usual notion of *partial equivalence* in the relation program verification literature. It can be seen as a lopsided version of partial equivalence. Partial simulation is not a transitive relation (even for consistently defined sets of base cases). Note that $\prec \subseteq \preceq$ (for a fixed \mathbb{B}), which justifies the notation.

Definition 10 (Full Equivalence). Two symbolic program configurations Pand Q are fully equivalent under constraint ϕ with a set of base cases \mathbb{B} , written $\mathbb{B} \models P \sim Q$ if ϕ , if $\mathbb{B} \models P \prec Q$ if ϕ and $\mathbb{B}^{-1} \models Q \prec P$ if ϕ .

Two-way full simulation gives the usual notion of full equivalence (for determinate programs). **Definition 11 (Partial Equivalence).** Two symbolic program configurations P and Q are partially equivalent under constraint ϕ with a set of base cases \mathbb{B} , written $\mathbb{B} \models P \simeq Q$ if ϕ , if $\mathbb{B} \models P \preceq Q$ if ϕ and $\mathbb{B}^{-1} \models Q \preceq P$ if ϕ .

Two-way partial simulation is the usual notion of partial equivalence (for determinate programs). Partial equivalence is not an equivalence relation (hence the name *partial*). The notation is justified by the fact that $\sim \subseteq \simeq$ (for a fixed \mathbb{B}).

5 Proof Systems

In this section, we give proof systems for partial and full simulation. We work with simulation formulae of the form $P \prec Q$ if ϕ for full simulation and of the form $P \preceq Q$ if ϕ for partial simulation, where P is a symbolic configuration of sort CfgL, Q is a symbolic configuration of sort CfgR and ϕ is a first-order logical constraint. We first present the proof system for full simulation. For a set R of simulation formulae $P \prec Q$ if ϕ , its denotation is

$$\llbracket R \rrbracket = \{ (\rho(P), \rho(Q)) \mid (P \prec Q \text{ if } \phi) \in R \text{ and } \rho \vDash \phi \}$$

i.e., the pairs of instances of P and Q that satisfy ϕ .

We fix a set B of simulation formulae that under-approximates the set \mathbb{B} of base cases: $\llbracket B \rrbracket \subseteq \mathbb{B}$. We also consider a set G (for *goals*) consisting of simulation formulae to be proven. The set G usually includes the actual goal, but also a set of intermediate helper goals that are needed for the proof that we call *circularities*.

Example 5. For our motivating example, we use the language IMP_1 and the following set of base cases: $B = \{\langle [i], env, fs \rangle \prec \langle [i'], env', fs' \rangle$ if $i = i' \}$. Thus, the set of base cases includes only pairs of identical terminal configurations where the stack of expressions contains the same integer. The set of goals includes the actual goal to be proven and two helper circularities:

$$G = \begin{cases} \langle [\text{call } \mathbf{f}(\mathsf{N})], \mathsf{env}, fs \rangle \prec \langle [\text{call } \mathbf{F}(\mathsf{N}, \mathbf{0}, \mathbf{0})], \mathsf{env}, fs \rangle \text{ if } \mathbf{0} \leq \mathsf{N}, \\ \langle \text{call } \mathbf{f}(\mathsf{I} - \mathbf{1}) \rightsquigarrow reduce(\mathsf{I}, \mathsf{N}), \mathsf{env}, fs \rangle \prec \langle [\text{call } \mathbf{F}(\mathsf{N}, \mathbf{0}, \mathbf{0})], \mathsf{env}, fs \rangle \\ \text{ if } \mathbf{0} \leq \mathsf{I} \leq \mathsf{N}, \\ \langle \mathsf{S} \rightsquigarrow reduce(\mathsf{I}, \mathsf{N}), \mathsf{env}, fs \rangle \prec \langle [\text{call } \mathbf{F}(\mathsf{N}, \mathsf{I}, \mathsf{S})], \mathsf{env}, fs \rangle \text{ if } \mathbf{1} \leq \mathsf{I} \leq \mathsf{N}, \end{cases} \end{cases}$$

where $fs = \{ f \mapsto \lambda n. \text{ if } n = 0 \text{ then } 0 \text{ else } n + \text{ call } f(n - 1), F \mapsto \lambda n.\lambda i.\lambda a. \text{ if } i \leq n \text{ then call } F(n, i + 1, a + i) \text{ else } a \}$ is the function map, n, i, a, f, F are constants of sort Id (program identifiers), and where N, I, S: Int are variables.

The proof system for full simulation, presented in Figure 7, manipulates sequents of the form $G, B \vdash^{g} P \prec Q$ if ϕ , where $g \in \{0, 1\}$, G is the set of goals and B is the set of base cases. The superscript g to the turnstile is a boolean flag (representing a *guard*) that denotes whether circularities are enabled or not, as formalized in the proof rules.

The AXIOM rule states that any P is simulated by any Q under the constraint \perp (false). The BASE rule handles the case when the right hand side Q can take

Notation: $sub((P,Q),R) \triangleq \bigvee_{P' \prec Q' \text{ if } \phi' \in R} \exists var(P',Q',\phi') \cdot (\phi' \land P = P' \land Q = Q')$

$$\begin{array}{c} \operatorname{AXIOM} & \overline{G, B \vdash^g P \prec Q \text{ if } \bot} \\ \operatorname{BASE} \frac{G, B \vdash^g P \prec Q \text{ if } \phi \land \neg \phi_B}{G, B \vdash^g P \prec Q \text{ if } \phi} \vDash \phi_B \rightarrow & \bigvee \quad \phi' \rightarrow sub\Big((P, Q'), B\Big) \\ \operatorname{CIRC} & \frac{G, B \vdash^1 P \prec Q \text{ if } \phi \land \neg \phi_G}{G, B \vdash^1 P \prec Q \text{ if } \phi} \vDash \phi_G \rightarrow & \bigvee \quad \phi' \rightarrow sub\Big((P, Q'), G\Big) \\ \operatorname{STEP} & \frac{G, B \vdash^1 P^i \prec Q \text{ if } \phi^i (\text{for all } 1 \leq i \leq n)}{G, B \vdash^g P \prec Q \text{ if } \phi} & \Delta_{\mathcal{R}_L}(P \text{ if } \phi) = \{P^i \text{ if } \phi^i | 1 \leq i \leq n\} \end{array}$$

Fig. 7: The proof system for full simulation.

a number of steps into Q' so that the base cases are reached (the pair (P, Q') is part of the base cases). The constraint sub((P,Q), R) expresses that $P \prec Q$ is an instance of R. The CIRC rule handles the case when Q reaches in a number of steps a configuration Q' such that the pair P, Q' is subsumed by some goal in G. In order to ensure soundness, this rule can only be applied when the superscript for the turnstile, g, is 1. The superscript becomes 1 only in rule STEP, which intuitively takes a step in the left-hand side. Therefore, when the rule CIRC is actually used, it means that there was progress on the lhs (by a *previous* STEP on the lhs). This ensures soundness.

Finally, rule STEP can be used to take a symbolic step in the left-hand side. Recall that Δ computes the symbolic successors of a configuration. Note that all possible symbolic steps from P are taken. This corresponds to the fact that in our notion of simulation, *every* run of P must have a corresponding run in Q. The constraint $\neg \phi^1 \land \ldots \land \neg \phi^n$ describes the instances of P where no step can be taken, and therefore these configurations must be solved by some other rule, hence the second line in the hypotheses of STEP.

We write $G, B \vdash^{g} G'$ if $G, B \vdash^{g} P \prec Q$ if ϕ for any formula $P \prec Q$ if $\phi \in G'$ (that is, all formulae in G' are provable from G, B). We are now ready to give the main soundness theorem of our result for full simulation.

Theorem 2 (Soundness for full simulation). If $G, B \vdash^0 G$ and $[\![B]\!] \subseteq \mathbb{B}$, then for any simulation formula $P \prec Q$ if $\phi \in G$, we have that $\mathbb{B} \models P \prec Q$ if ϕ .

The theorem requires that *all formulae* in G be proved in order to trust *any* of them. If a formula in G is not provable then even if the others are provable, they cannot be trusted to hold semantically. The starting superscript of the turnstile must be 0 in order not to allow the CIRC rule to fire immediately (otherwise the CIRC rule could be used to prove a circularity by itself, leading to unsoundness).

Example 6. Continuing Example 5, we have $G, B \vdash^0 G$. To save space, we sometimes abbreviate $\langle [call f(N)], env, fs \rangle$ by f and $\langle [call F(N, 0, 0)], env, fs \rangle$ by F.

Notation: $sub((P,Q),R) \triangleq \bigvee_{P' \preceq Q' \text{ if } \phi' \in R} \exists var(P',Q',\phi').(\phi' \land P = P' \land Q = Q')$

$$\begin{array}{c} \operatorname{Axiom} \overline{G, B \vdash^{g} P \preceq Q \text{ if } \bot} \\ \operatorname{Base} \frac{G, B \vdash^{g} P \preceq Q \text{ if } \phi \land \neg \phi_{B}}{G, B \vdash^{g} P \preceq Q \text{ if } \phi} \vDash \phi_{B} \rightarrow \bigvee \phi' \rightarrow sub\Big((P, Q'), B\Big) \\ \operatorname{Circ} \frac{G, B \vdash^{g} P \preceq Q \text{ if } \phi \land \neg \phi_{G}}{G, B \vdash^{g} P \preceq Q \text{ if } \phi} \vDash \phi_{G} \rightarrow \bigvee \phi' \rightarrow sub\Big((P, Q'), G\Big) \\ \operatorname{Circ} \frac{G, B \vdash^{g} P \preceq Q \text{ if } \phi \land \neg \phi_{G}}{G, B \vdash^{g} P \preceq Q \text{ if } \phi} \vDash \phi_{G} \rightarrow \bigvee \phi' \rightarrow sub\Big((P, Q'), G\Big) \\ \operatorname{Step} \frac{G, B \vdash^{1} P^{i} \preceq Q \text{ if } \phi^{i} (\text{ for all } 1 \leq i \leq n)}{G, B \vdash^{g} P \preceq Q \text{ if } \phi} \vartriangle_{\mathcal{A} = 1}^{R} \Delta_{\mathcal{R}_{L}}(P \text{ if } \phi) = \{P^{i} \text{ if } \phi^{i} | 1 \leq i \leq n\} \end{array}$$

Fig. 8: The proof system for partial simulation.

As $G, B \vdash^0 G$, $\mathbf{f} \prec \mathbf{F}$ for $\mathbb{N} \geq \mathbf{0}$. As explained in the introduction, our proof system cannot establish the other direction, $G^{-1}, B^{-1} \vdash^0 G^{-1}$, intuitively because it cannot prove that the termination of \mathbf{F} (one phase) implies the termination of \mathbf{f} (two phases). The full simulation relation would require an operationally-based termination argument [9] for the second phase of \mathbf{f} , which we leave for future work.

Proving partial simulation. We adopt the same notation as above for a set of base cases B and a set of goals G, but replacing \prec by \preceq . The proof system for partial simulation, presented in Figure 8, manipulates sequents of the form $G, B \vdash^{g} P \preceq Q$ if ϕ , where G is the set of goals (with \preceq instead of \prec), B is the set of base cases (with \preceq instead of \prec), and $g \in \{0, 1\}$. The meaning of g is different: g = 1 enables the CIRC rule to not make progress on the rhs.

The proof rules for partial simulation are similar to those for full simulation, and therefore we only underline the main differences. The rules AXIOM and BASE are identical to those in the proof system for full simulation (except for \leq instead of \prec). The rule CIRC is also very similar, but progress is required on the rhs unless g = 1. Therefore, for partial simulation, it is allowed to discharge a goal directly by CIRC, without taking any step in the left hand side, but with progress on the rhs (note the superscript $\geq 1 - g$). This corresponds to the case where a terminal configuration is partially simulated by an infinite loop. Finally, another difference is that once rule STEP is applied to make progress on the lhs, circularities can be applied even if there no progress on the rhs. This corresponds potentially to the case where the left-hand side loops forever and the right hand side finishes. As for full simulation, we write $G, B \vdash G'$ if $G, B \vdash P \preceq Q$ if ϕ for any formula $P \preceq Q$ if $\phi \in G'$ (that is, all formulae in G' are provable from G, B). We now give the main soundness theorem of our result for partial simulation.

Theorem 3 (Soundness for partial simulation). If $G, B \vdash^0 G$ and $\llbracket B \rrbracket \subseteq \mathbb{B}$, then for any formula $P \preceq Q$ if $\phi \in G$, we have that $\mathbb{B} \models P \preceq Q$ if ϕ .

Note that still all goals in G must be proven to trust any of them.

Example 7. Continuing Example 5, we have shown that $G, B \vdash^0 G$ and that $G^{-1}, B^{-1} \vdash^0 G^{-1}$ in the sense of partial simulation (with \prec changed to \preceq in G and B) and therefore $\mathbf{f} \preceq \mathbf{F}$ and $\mathbf{F} \preceq \mathbf{f}$ for $N \geq \mathbf{0}$ (i.e., \mathbf{f} and \mathbf{F} are partially equivalent).

Implementation. We have a prototype implementation of the two proof systems in the RMT tool (http://profs.info.uaic.ro/~stefan.ciobaca/rmteq). RMT implements order-sorted logically constrained term rewriting, that is rewriting of mixed terms, which contains both free symbols and symbols in some theory solvable by an SMT solver. RMT relies on Z3, and therefore any combination of theories solvable by Z3 can be used (e.g., bitvectors, arrays, LIA, etc.). RMT already supported reachability proofs [13]. In this paper, we extend it with axiomatized symbols and we implement the algorithms for checking partial and full simulation in Section 5. To prove equivalence, we check two-way simulation. The implementation for checking partial/full simulation works in two phases:

• the *left* phase implements the STEP rule: to prove $L \prec R$ if ϕ ($L \preceq R$ if ϕ), RMT finds all symbolic successors of L and, for each successor L' if ϕ' , attempts to prove $L' \prec R$ if $\phi \land \phi'$ ($L' \preceq R$ if $\phi \land \phi'$). If L' unifies with the lhs of either a base case or a circularity goal (e.g., there is a chance to reach the base case or a circularity), the algorithm moves to the *right* phase.

• the *right* phase implements the BASE and CIRC proof rules: to prove $L \prec R$ if ϕ $(L \preceq R \text{ if } \phi)$, the symbolic successors of R are searched, in order to find a constraint ϕ^1 s.t. $L \prec R'$ if $\phi \land \phi^1$ $(L \preceq R' \text{ if } \phi \land \phi^1)$ are either base cases or circularities for some symbolic successor R' of R if ϕ . If ϕ^1 is valid, the proof is done. Otherwise, the *left* phase resumes, limiting the search space to $\neg \phi^1$.

In both phases, we fix a user-settable bound on the number of symbolic steps (by default, 100). If the bound is reached, then the current branch of the proof fails. Unification modulo axiomatized symbols is not fully implemented. Instead, we use a couple of heuristics to handle it the cases of interest: 1. in order to compute symbolic successors of a term (possibly containing axiomatized symbols), we first unroll the definition of the axiomatized symbols and 2. in order to check whether the current goal is an instance of the base cases or of a circularity (rules BASE and CIRC), we perform a bounded search with the equations of the symbol.

Examples. We use the IMP language defined in Section 3. We have worked out the following equivalence examples using our method: • We show that $f(N) \prec F(N, 0, 0), f(N) \preceq F(N, 0, 0)$ and that $F(N, 0, 0) \preceq f(N)$ under the constraint $N \ge 0$ for our running example in the language IMP₁. Our method is not sufficiently powerful to show $F(N, 0, 0) \prec f(N)$ if $N \ge 0$. • In IMP₂, none of $f(N) \prec F(N, 0, 0), f(N) \preceq F(N, 0, 0), F(N, 0, 0) \preceq f(N), F(N, 0, 0) \preceq f(N)$ hold under the constraint $N \ge 0$, and therefore the proofs of these goals (correctly) fail. • Our method can prove programs in two different languages as well. We show that f(N), interpreted in IMP₁, is partially equivalent to F(N, 0, 0), interpreted in IMP₂, when $N \ge 0$. For one direction $(f \prec F)$, we establish full

simulation; for the other direction, just partial simulation. • We show that a while loop is partially equivalent to a recursive function, when both compute the sum of the first N naturals. • We prove full equivalence for an instance of loop unswitching, showing that our method can handle programs that are structurally unrelated. More details on these examples can be found in Appendix D.

6 Proving Equivalence of Program Schemas

The method that we have introduced in Section 5 can be used to show full/partial simulations between *symbolic program configurations*. Symbolic program configurations can contain variables. In our running example, we prove twoway simulations between the symbolic configurations $\langle [call f(N)], env, fs \rangle$ and $\langle [call F(N, 0, 0)], env, fs \rangle$, under the constraint $N \geq 0$. The variables env and N occur in both configurations, denoting the fact that their value is shared in both configurations, and fs is the map defined in Example 5.

It is also possible to use variables of sort **Exp** (variables standing for program expressions or statements) in a symbolic configuration. For example, we might want to prove that $\langle [e], env, fs \rangle$ and $\langle [e], env, fs \rangle$ (both configurations are the same) are equivalent. The variable e of sort **Exp** denotes a program expression. We call such variables, which stand for parts of the program (such as e), *structural variables*, in constrast to other variables (such as N or env).

Our proof method fails when trying to prove equivalence between symbolic configuration containing structural variables³. The issue is in the STEP rule, which tries to compute the possible symbolic successors of $\langle [e], env, fs \rangle$. When computing all successors, a case analysis on the structural variable **e** is performed: **e** might be an addition $e_1 + e_2$, an ite statement if e_0 then e_1 else e_2 , etc. This case analysis occurs ad-infinitum, and no real progress is made in the proof.

We call such symbolic program configurations, with variables denoting program parts, *program configuration schemas* or simply *configuration schemas*. We also use *program schema* when we refer just to the part of the configuration holding the program. The naming is because such a program schema denotes several programs, depending on how the structural variables are instantiated.

Therefore, even if our proof system can technically handle program configuration schemas, it cannot be used directly to show interesting properties of such schemas. In particular, it is not possible to *directly use* our proof system to show the correctness of program optimizations such as the constant propagation optimization presented in Figure 9. However, our proof system *can directly prove* instances of this optimization (i.e., for particular instantiations of e_1, st_1).

We show how our method can be easily extended to prove simulations between program schemas. This extension crucially relies on the fact that our proof method is parametric in the operational semantics. We consider two configuration schemas. In order to prove their equivalence, we transform the structural variables into fresh constants. We give semantics to the new constants by *adding*

³ It may seem surprising that our system cannot prove an expression equivalent to itself, but our method is *operational*, not axiomatic – there is no rule for reflexivity.

Initial Program	Optimized Program
$x_1 := e_1 ; st_1 ; x_2 := e_1$	$x_1 := e_1 ; st_1 ; x_2 := x_1$

Fig. 9: Two program schemas, where: $\mathbf{x}_1, \mathbf{x}_2$: Id are two identifiers, \mathbf{e}_1 : Exp is an expression, and \mathbf{s}_1 : Exp is a statement. The optimization is valid assuming that \mathbf{s}_1 does not change \mathbf{x}_1 or the program variables in \mathbf{e}_1 .

new rules to the operational semantics of the language. These rules capture the read-set of expressions and the read-set and write-set of statements.

We explain this encoding on the example in Figure 9. We create fresh constants $\mathbf{e_1}$ and $\mathbf{st_1}$ of sort \mathbf{Exp} . The constants are not considered values of the language: $\mathbf{val}(\mathbf{e_1}) \longrightarrow \bot, \mathbf{val}(\mathbf{st_1}) \longrightarrow \bot$. In the two programs schemas above, we replace the structural variables $\mathbf{e_1}$ and $\mathbf{st_1}$ by the new constants $\mathbf{e_1}$ and $\mathbf{st_1}$, respectively. We say that the constant $\mathbf{e_1}$ ($\mathbf{st_1}$) abstracts the variable $\mathbf{e_1}$ ($\mathbf{st_1}$). After this abstraction, we obtain the following configurations that we would like to prove equivalent:

```
\langle [\mathbf{x}_1 := \mathbf{e}_1; \mathbf{s}_1; \mathbf{x}_2 := \mathbf{e}_1], \mathbf{env}, \mathbf{fs} \rangle and \langle \mathbf{x}_1 := \mathbf{e}_1; \mathbf{s}_1; \mathbf{x}_2 := \mathbf{x}_1, \mathbf{env}, \mathbf{fs} \rangle.
```

A new problem when proving such abstracted configurations is that they block whenever $\mathbf{e_1}$ or $\mathbf{st_1}$ reach the top of the evaluation stack, as there is no operational rule that describes their semantics. Thus, a configuration like $\langle \mathbf{e_1} \sim \dots, \dots, \dots \rangle$ is stuck. We take advantage of the fact that our proof systems for showing simulation and equivalence are *parametric* in the operational semantics and we add semantic rules that specify the behaviors of $\mathbf{e_1}$ and $\mathbf{st_1}$.

The new rules formalize in a rigorous manner the notions of *read-set* and *write-set*. The read-set of an expression is the set of program variables that the expression is allowed to depend on. In addition to a *read-set*, a statement, such as st_1 , also has a *write-set*, that is a set of program variables that the statement is allowed to write to. Assume that the read-set of e_1 is $\{y_2, x_2\}$. We formalize this read-set by adding to the semantics the rule

 $\langle e_1 \rightsquigarrow \mathsf{es}, \mathsf{env}, \mathsf{fs} \rangle \longrightarrow \langle ie_1(lookup(\mathsf{env}, y_2), lookup(\mathsf{env}, x_2)) \rightsquigarrow \mathsf{es}, \mathsf{env}, \mathsf{fs} \rangle,$

where $\mathbf{ie_1} : \mathbf{Int} \times \mathbf{Int} \to \mathbf{Int}$ is a fresh builtin uninterpreted function symbol. This rule models the fact that $\mathbf{e_1}$ terminates, is deterministic, and evaluates to a value $\mathbf{ie_1}(\mathbf{lookup}(\mathbf{env}, \mathbf{y_2}), \mathbf{lookup}(\mathbf{env}, \mathbf{x_2}))$ that only depends on the program variables $\mathbf{y_2}$ and $\mathbf{x_2}$. In general, for an expression having read-set x_1, \ldots, x_n , we add a fresh *n*-ary builtin symbol and we use it in a rule such as the one above.

To model write-sets of statements, we add rules that modify in the environment only the program variables that are written to. For example, assume that the read-set of \mathbf{st}_1 is $\mathbf{y}_1, \mathbf{y}_2, \mathbf{x}_1, \mathbf{x}_2$ and that the write-set of \mathbf{st}_1 is \mathbf{y}_1 . We add the following rule: $\langle \mathbf{st}_1 \sim \mathbf{es}, \mathbf{env}, \mathbf{fs} \rangle \longrightarrow \langle \mathbf{s}, \mathbf{update}(\mathbf{env}, \mathbf{y}_1, nv), \mathbf{fs} \rangle$, where $nv = \mathbf{ist}_1(\mathbf{env}[\mathbf{y}_1], \mathbf{env}[\mathbf{y}_2], \mathbf{env}[\mathbf{x}_1], \mathbf{env}[\mathbf{x}_2])$, the symbol $\mathbf{ist}_1 : \mathbf{Int}^4 \rightarrow \mathbf{Int}$ is a fresh builtin and env[x] is short for $\mathbf{lookup}(env, x)$. This rule models that \mathbf{st}_1 terminates, is deterministic, writes to \mathbf{y}_1 only and the value computed and

New constructors:	$\mathbf{e_1}: \mathbf{Exp}, \mathbf{st_1}: \mathbf{Exp}$
New builtins:	$\mathbf{ie_1}:\mathbf{Int}^2 ightarrow\mathbf{Int},\mathbf{ist_1}:\mathbf{Int}^4 ightarrow\mathbf{Int}$
New rules:	$\langle \mathbf{e_1} \rightsquigarrow es, env, fs \rangle {\longrightarrow} \langle \mathbf{ie_1}(env[\mathbf{y_2}], env[\mathbf{x_2}]) \rightsquigarrow es, env, fs \rangle$
$\langle \mathbf{st_1} \rightsquigarrow es, env, fs \rangle \longrightarrow$	$\hspace{1.5cm} \hspace{0.5cm} \langle \mathbf{s}, env[\mathbf{y_1} \mapsto ist_1(env[\mathbf{y_1}], env[\mathbf{y_2}], env[\mathbf{x_1}], env[\mathbf{x_2}])], fs \rangle \\$

Fig. 10: Abstraction process required to prove the optimization described in Figure 9. The notation env[x] and $env[x \mapsto w]$ are short for lookup(env, x) and update(env, x, w), respectively.

written to $\mathbf{y_1}$ only depends on $\mathbf{y_1}, \mathbf{y_2}, \mathbf{x_1}, \mathbf{x_2}$. We summarize the abstraction process in Figure 10.

With the encoding in Figure 10, our proof system and RMT can show the equivalence of the two programs in Figure 9 and therefore the correctness of this optimization in the context of IMP. Comparison with CORK and PEC. We show that our approach also generalizes to a number of compiler optimizations previously discussed in the context of the CORK [33] and PEC [31] optimization correctness verification tools. The comparison is shown Figure 11. We use two annotations for special cases: 1. the mark \bigcirc denotes that, even if the two programs schemas are functionally equivalent, there is no simulation of one by the other – instead, we prove two different simulations, one for each of the two output variables; 2. \Box denotes that we have used an upper bound on one of the program variables – the bound is not a weakness of RMT or of our proof method, but of the fact that the SMT solver that we use, Z3, does not handle non-linear arithmetic well enough. Using another SMT solver for non-linear integer arithmetic, like CVC4, could potentially allow us to prove these examples, marked with \Box , in the unbounded case as well. In comparison with existing approaches, we can prove the correctness of an optimization (Loop flattening) that the two previous approaches [31,33] cannot. However, our tool is not automated when loops are involved and must be guided by helper circularities, as explained in Example 5 on Page 16. We describe the proof of each optimization in turn in Appendix C. In this appendix, we also develop a methodology that help us find such helper circularities, giving evidence that our equivalence/simulation checker could be automated for optimization correctness verification purposes.

7 Related Work

• In the series of papers [40,41,42,43], Pitts was one of the first to propose the use of operationally-based notions of contextual equivalence. The differences to our work is that we only consider functional equivalence, and not contextual equivalence, but in our approach the operational semantics can be varied. We also explicitly allow for nondeterminism and there is no need to define explicitly a logical relation for the entire language: instead, the user defines a simulation relation that depends only on the particular programs to be shown equivalent. In [43], the *frame stack* approach for small-step semantics that we use is introduced. The same style of using a frame stack was popularized by the K framework [48] in

Optimization	PEC	CORK	RMT	Optimization	PEC	CORK	RMT
Code hoisting	\checkmark	0.32s	0.41s	Software pipelining	\checkmark	8.02s	3.56s
Constant propagation	\checkmark	0.33s	0.31s	Loop fission	\checkmark_p	23.45s	\bigcirc 10.40s
Copy propagation	\checkmark	0.33s	0.26s	Loop fusion	\checkmark_p	23.34s	\bigcirc 9.67s
If-conversion	\checkmark	0.34s	0.48s	Loop interchange	\checkmark_p	29.30s	\Box 108.63s
Partial redundancy	\checkmark	0.34s	0.75s	Loop reversal	\checkmark_p	8.41s	2.70s
elimination				Loop skewing	\checkmark_p	8.50s	7.68s
Loop invariant	\checkmark	3.48s	3.79s	Loop flattening	\times	×	□ 8.14s
code motion				Loop strength	\times	5.63s	5.26s
Loop peeling	\checkmark	3.26s	0.97s	reduction			
Loop unrolling	\checkmark	12.17s	7.09s	Loop tiling 01		10.04a	25.41s
Loop unswitching	\checkmark	8.19s	4.71s	Loop tiling 02	×	10.948	\Box 21.58s

Fig. 11: Optimizations on which we compare the tools PEC, CORK, and RMT (our prototype). Columns one-three are due to Lopes and Monteiro [33] (\checkmark_p means PEC needs a heuristic called *permute*). The third column is based on our own benchmark. The annotations \bigcirc and \square are described in the main text.

the rewriting based semantics of several large languages [21,8]. We make extensive use of this frame-stack technique, which enables simpler equivalence proofs. • Logical relations and bisimulation can be used to prove contextual equivalence. Bisimulation techniques such as [46] are usually language dependent and proofs of congruence and other properties need to be established independently. Language features such as higher-order functions are handled by enhancing the bisimulation with an *environment* holding the current knowledge of the observer. Instead, by reducing the scope to functional equivalence instead of contextual equivalence, we allow to use simpler simulation relations that depend only on the particular pair of programs to be proven equivalent (there is no need to prove congruence in our case). Logical relations techniques such as [19] can be used to prove contextual equivalences for various languages. Logical relations can also used in mechanized frameworks for separation logic such as Iris [28] in order to handle contextual equivalence in the presence of state (see [50]) or continuations (see [49]). However, logical relations may be difficult to adapt to different languages and may require additional indexing to account for language features. Mechanized proofs may be quite long and tedious. Game semantics can be used to reason denotationally (see, e.g., [37]) about contextual equivalence, but it does not enjoy good algorithmic properties [38]; however, proof search can be implemented for languages with higher-order functions and effects, as shown by Jaber [27]. • Several relational Hoare logics were proposed (e.g., [6,7,1]) for reasoning about pairs of programs. Typically, such logics are developed for a particular language and can usually be used to prove equivalence of syntactically similar programs. For example, they usually assume that two matching while loops will both take the same number of steps. In contract, the logic that we propose can also be used to reason about structurally dissimilar programs. Relational higher-order logic, introduced in [1], allows both synchronous and

asynchronous reasoning about pairs of programs in a higher-order lambda calculus. It can be used to show functional equivalence, but also for other properties such as relational cost analysis. In contrast to RHOL, the logic that we propose here is formally less expressive (RHOL is as expressive as HOL). However, unlike RHOL, it is simpler to use and mechanize. Relational separation logic [52] enhances relational Hoare logic with the ability to reason about the heap. In [4], the authors propose a relational logic with a framing rule that enables a SMTfriendly encoding of the heap, but also enhances the ability to reason about less structurally related programs. Unlike these logics, we do not currently handle the heap, but our proof system is much simpler, because most of the complexity of reasoning about the language features goes to the LCTRS encoding the language semantics. Also, in our case, it is much simpler to experiment with variations of the language semantics, as explained in Sections 5 and 6. A concept close to relational Hoare logic is that of product-program [5], which are programs that mimic the behavior of two programs; they allow to reduce relational reasoning to reasoning about a single program. In our work, there is no need to construct such product programs. Such a product construction is possible in a rewritingbased scenario as well [11,14]. Compared to all approaches above, the logic that we introduce in this paper has the advantage that the underlying operational semantics of the language can be easily changed. This makes it easy to experiment with various settings. In our examples, we show how we go from a semantics with an unbounded stack to a semantics with a bounded stack, but other variations of interest could be using fixed-size integers (bitvectors) instead of unbounded integers, enabling or disabling language features such as exceptions, introspection, etc. in order to check how each affects functional equivalence. In [31], an implementation of a parametrized equivalence prover is presented and we compare against the tool in Section 6. Grimm et al. [26] propose a general method for relational proofs based on encoding the state transformation as a monad in the F* proof assistant. After encoding, relational proofs then require user interaction, although significant parts are solved directly by an SMT solver. Maillard et al. [35] show how to generalize this to arbitrary monadic effects. • In [10], Chaki et al. propose a new definition of equivalence suitable for nondeterministic programs, extending the usual definition of partial equivalence for deterministic programs, and introduce sound proof rules for regression verification of multithreaded programs. Our definition of equivalence, defined as two-way simulation, is implied by the definition of partial equivalence proposed here – the difference is that our notion of equivalence allows a terminating execution on some input to be simulated by an infinite execution of the other program on the same input. However, we also additionally propose a definition for full equivalence suitable for a non-deterministic setting; this definition is more involved than the usual definition of full equivalence as partial equivalence plus mutual termination as outlined in [20], since a non-deterministic program could have both terminating and non-terminating runs starting with the same input. Felsing et al. [24] propose an automated method for regression verification. Lahiri et al. [32] present a method based on translation into the intermediate verification language Boogie for checking semantical differences between programs. A technique for automated discovery of simulation relations is proposed in [23]. Their technique is automated using Z3 as a solver. Techniques based on an efficient encodings of the relational property as a set of constrained Horn clause are described in [18]. Another technique for automatic proving of equivalences for procedural programs that is also based on LCTRSs is proposed in [25]. Unlike our approach, in [25] the two C-like programs are translated by a tool called C2LCTRS into LCTRSs. An advantage of their approach is automation by using a constrained version of the well-known technique of rewriting induction. However, the C2LCTRS tool contains an implicit semantics of the C-like language and therefore, unlike in our work, variations of the semantics that change various language features (like stack size, integer semantics, etc.) require changing the tool. Moreover, in [25], the two programs are also assumed to be deterministic. Even if we changed the C2LCTRS program to explicitly model a stack, constrained rewriting induction would fail in general to find an equivalence proof between two programs such as example in Section 1, as the simulation relation requires axiomatized symbols to state. • Early ideas on adding logical constraints to deduction rules in general date back to the 1990s, in work like [29] and [17]. Logically constrained term rewriting systems, which combine term rewriting and SMT constraints are introduced in [30]. LCTRSs generalize previous formalisms like TRSs enriched with numbers and Presburger constraints (e.g., as in [22]) by allowing arbitrary theories that can be handled by SMT solvers. Rewriting modulo SMT is introduced in [45] for analyzing open systems. In [3], the authors introduce guarded terms, which generalize logically constrained terms. A narrowing calculus for constrained rewriting is introduced in [2]. In [39], an approach to proving *inequalities* based on constrained rewriting induction is proposed. Finally, logically constrained rewriting enjoys completion procedures, as shown in [51]. • Our own related work. We first considered semantics-based equivalence in [34] for symbolic programs in the context of the K framework in [48], but for a notion of behavioural equivalence of deterministic programs. In [15], we give a semantics-based proof system for full equivalence. Our present work improves on this by adding axiomatized symbols, using different notions of equivalence that handle non-determinism and are more modular (we now also test for one-way simulation) and providing a working implementation based on LCTRSs with several novel examples. Most of the infrastructure required for LCTRSs is based on our earlier work on proving reachability in LCTRSs [13] and solving unification modulo builtins [12]. However, the present work includes axiomatized symbols, which pose new technical challenges.

8 Conclusion and Future Work

We have introduced and implemented in RMT a new method for proving simulation and equivalence in languages whose semantics are defined by LCTRSs in frame stack style. Our method allows to easily check program equivalence in various settings, such as unbounded versus bounded stack, arbitrary precision versus fixed size integers, etc. To express simulation relations, we enrich standard LCTRSs with *axiomatized symbols*, which raise new research questions such as *unification modulo axiomatized symbols*. We also generalize existing definitions for full/partial equivalence. Our approach allows for nondeterminism in the definitions and in the proofs, but we currently do not exploit this, as we only have simple examples. We also show an advantage of an operational semantics-based approach: we can easily model read-sets and write-set and prove simulation/e-quivalence of program schemas.

As future work, we would like to apply our methods to more challenging concurrent programs and to realistic language definitions, available as part of the K framework [21,8]. We would also like to integrate an external termination checker to handle full equivalence better. Other directions for future work include relational cost analysis, as in [44], possibly by simply using an appropriate set \mathbb{B} of base cases, and generalizing to contextual equivalence, possibly by extending the techniques in Section 6.

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A Example of Program Execution

Here is an example of how evaluation proceeds for the program

 $x = \operatorname{call} f(0)$

in an initial environment mapping the program identifier \mathbf{x} to $\mathbf{12}$, and a function map fs, mapping the program identifier \mathbf{f} to

 $(\lambda y. \text{ if } y > 5 \text{ then } y + x \text{ else } 0)$

according to the semantics of IMP introduced in Section 3:

- 1. $\langle [\mathbf{x} := \operatorname{call} \mathbf{f}(10)], \mathbf{x} \mapsto \mathbf{12}, \mathbf{fs} \rangle \longrightarrow$
- 2. $(\text{call } f(10) \rightsquigarrow x := \Box \rightsquigarrow [], x \mapsto 12, f_s) \longrightarrow$
- 3. $\langle \text{call } f \rightsquigarrow \text{call } \Box(10) \rightsquigarrow x \coloneqq \Box \rightsquigarrow [], x \mapsto 12, fs \rangle \longrightarrow$
- 4. $(\text{lookup}(f, fs) \rightsquigarrow \text{call } \Box(10) \rightsquigarrow x := \Box \rightsquigarrow [], x \mapsto 12, fs) =$
- 5. $\langle (\lambda y. \text{ if } y > 5 \text{ then } y + x \text{ else } 0) \sim \text{ call } \Box(10) \sim x := \Box \sim [], x \mapsto 12, fs \rangle$
- 6. $(\operatorname{call}(\lambda y, \operatorname{if} y > 5 \operatorname{then} y + x \operatorname{else} 0)(10) \rightsquigarrow x := \Box \rightsquigarrow [], x \mapsto 12, f_s) \longrightarrow$
- 7. $(\operatorname{subst}(y, 10, (\operatorname{if} y > 5 \operatorname{then} y + x \operatorname{else} 0)) \longrightarrow x := \Box \longrightarrow [], x \mapsto 12, f_{\mathcal{S}} \longrightarrow$
- 8. $\langle \text{if } 10 > 5 \text{ then } 10 + x \text{ else } 0 \rightsquigarrow x := \Box \rightsquigarrow [], x \mapsto 12, fs \rangle \longrightarrow$
- 9. $(10 > 5 \rightsquigarrow \text{ if } \Box \text{ then } 10 + x \text{ else } 0 \rightsquigarrow x := \Box \rightsquigarrow [], x \mapsto 12, fs) \longrightarrow$
- 10. $\langle \top \rightsquigarrow \text{ if } \Box \text{ then } 10 + x \text{ else } 0 \rightsquigarrow x := \Box \rightsquigarrow [], x \mapsto 12, fs \rangle \longrightarrow$
- 11. $(\text{if} \top \text{then } 10 + x \text{ else } 0 \rightsquigarrow x := \Box \rightsquigarrow [], x \mapsto 12, f_s) \longrightarrow$
- 12. $\langle 10 + x \rightsquigarrow x := \Box \rightsquigarrow [], x \mapsto 12, fs \rangle \longrightarrow$
- 13. $\langle \mathbf{x} \rightsquigarrow \mathbf{10} + \Box \rightsquigarrow \mathbf{x} := \Box \rightsquigarrow [], \mathbf{x} \mapsto \mathbf{12}, fs \rangle \longrightarrow$
- 14. $(\text{lookup}(\mathbf{x}, \mathbf{x} \mapsto \mathbf{12}) \rightsquigarrow \mathbf{10} + \Box \rightsquigarrow \mathbf{x} := \Box \rightsquigarrow [], \mathbf{x} \mapsto \mathbf{12}, fs = \mathbf{10}$
- 15. $\langle 12 \rightarrow 10 + \Box \rightarrow x + \Box \rightarrow [], x \mapsto 12, fs \rangle \longrightarrow$
- 16. $\langle 10 + 12 \rightarrow x := \Box \rightarrow [], x \mapsto 12, f_s \rangle \longrightarrow$
- 17. $\langle 22 \rightsquigarrow x := \Box \rightsquigarrow [], x \mapsto 12, fs \rangle \longrightarrow$
- 18. $\langle [\mathbf{x} := \mathbf{22}], \mathbf{x} \mapsto \mathbf{12}, fs \rangle \longrightarrow$
- 19. $\langle [], \mathbf{x} \mapsto \mathbf{22}, fs \rangle \not\longrightarrow$.

B Proofs

This section includes the proof for the soundness theorems. The proof principle used is a kind of parametric coinduction. We start with two lemmas that state coinductive characterizations for full simulation and partial simulation, respectively.

Lemma 1. $\mathbb{B} \models P \prec Q$ if ϕ iff $[\![P \prec Q \text{ if } \phi]\!] \subseteq \nu S$. fsim(S), where

$$fsim(S) = \{ (\mathbf{P}, \mathbf{Q}) \mid \mathbf{P} \Downarrow \rightarrow \exists \mathbf{Q}'. \mathbf{Q} \longrightarrow_{\mathcal{R}_L}^* \mathbf{Q}' \land (\mathbf{P}, \mathbf{Q}') \in \mathbb{B} \land$$
$$\neg \mathbf{P} \Downarrow \rightarrow \forall \mathbf{P}'. \mathbf{P} \longrightarrow_{\mathcal{R}_L} \mathbf{P}' \rightarrow$$
$$\exists \mathbf{Q}'. \mathbf{Q} \longrightarrow_{\mathcal{R}_R}^* \mathbf{Q}' \land (\mathbf{P}', \mathbf{Q}') \in S \}$$

and $P \Downarrow$ means that P is a $\longrightarrow_{\mathcal{R}_{\overline{R}}}$ irreducible configuration, i.e., $\forall P' . P \longrightarrow_{\mathcal{R}_{L}}^{*} P' \rightarrow P = P'$.

Proof. We first notice that we have $\mathbb{B} \models P \prec Q$ if ϕ iff $[\![P \prec Q \text{ if } \phi]\!] \subseteq S \prec$, where

$$S^{\prec} = \{ (\mathbf{P}, \mathbf{Q}) \mid \forall \mathbf{P}'. \mathbf{P} \longrightarrow_{\mathcal{R}_{L}}^{*} \mathbf{P}' \land \mathbf{P}' \Downarrow \rightarrow \\ \exists \mathbf{Q}'. \mathbf{Q} \longrightarrow_{\mathcal{R}_{R}}^{*} \mathbf{Q}' \land (\mathbf{P}', \mathbf{Q}') \in \mathbb{B} \}$$

⇒. We show that $S \prec$ is post-fixed point for fsim, i.e., $S \prec \subseteq fsim(S \prec)$. Let $(P, Q) \in S \prec$. There are two cases:

- 1. P \Downarrow . Then $\exists Q' . Q \longrightarrow_{\mathcal{R}_L}^* Q' \land (P, Q') \in \mathbb{B}$ by the definition of S^{\prec} .
- 2. $\neg P \Downarrow$. Let P' be such that $P \longrightarrow_{\mathcal{R}_L} P'$. We show that $(P', Q) \in S^{\prec}$. Let P'' be such that $P' \longrightarrow_{\mathcal{R}_L} P'' \land P'' \Downarrow$. Then $P \longrightarrow_{\mathcal{R}_L} P'' \land P'' \Downarrow$, which implies $\exists Q'. Q \longrightarrow_{\mathcal{R}_L}^* Q' \land (P'', Q') \in \mathbb{B}$ (recall that $(P, Q) \in S^{\prec}$). Hence $(P', Q) \in S^{\prec}$. Since P' is arbitrary, it follows that $\forall P'. P \longrightarrow_{\mathcal{R}_L} P' \rightarrow (P', Q) \in S^{\prec}$.

From the above case analysis we may conclude $(P, Q) \in fsim(S^{\prec})$. \Leftarrow . We show that if S is a post-fixed point for fsim then $S \subseteq S^{\prec}$. Let $(P, Q) \in S$ and assume that $P \longrightarrow_{\mathcal{R}_L}^* P' \wedge P' \Downarrow$. In order to show that $(P, Q) \in S^{\prec}$ we have to prove that $\exists Q'. Q \longrightarrow_{\mathcal{R}_L}^* Q' \wedge (P', Q') \in \mathbb{B}$. We have two cases:

- 1. P = P'. Then $\exists Q' . Q \longrightarrow_{\mathcal{R}_L}^* Q' \land (P, Q') \in \mathbb{B}$ by the first part of the definition of *fsim*, which implies $(P, Q) \in S \checkmark$.
- 2. $P \neq P'$ (which implies $\neg P \Downarrow$). Let P'_1 be s.t. $P \longrightarrow_{\mathcal{R}_L} P'_1 \longrightarrow_{\mathcal{R}_L}^* P'$. We obtain $(P'_1, Q'_1) \in S$ by the second part of the definition of *fsim*. We repeat the same reasoning until we obtain $P'_n = P'$ and $(P'_n, Q'_n) \in S$. Then $\exists Q' . Q'_n \longrightarrow_{\mathcal{R}_L}^* Q' \land (P'_n, Q') \in \mathbb{B}$ is proved in a similar way to the first case. Since P'_1 is arbitrarily chosen, it follows that

$$\forall P'. P \longrightarrow_{\mathcal{R}_{L}}^{*} P' \land P' \Downarrow \rightarrow \exists Q'. Q \longrightarrow_{\mathcal{R}_{B}}^{*} Q' \land (P', Q') \in \mathbb{B},$$

which implies $(\mathbf{P}, \mathbf{Q}) \in S^{\prec}$.

Corollary 1. 1. $S \prec = \nu S \cdot fsim(S)$. 2. \mathbb{B} is a post-fixed point of fsim, i.e., $\mathbb{B} \subseteq fsim(\mathbb{B})$.

Lemma 2. $\mathbb{B} \models P \preceq Q$ if ϕ iff $[\![P \preceq Q]$ if $\phi]\!] \subseteq \nu S$. psim(S), where

$$psim(S) = \{ (\mathbf{P}, \mathbf{Q}) \mid (\mathbf{P} \Downarrow \rightarrow \exists \mathbf{Q}'. \mathbf{Q} \longrightarrow_{\mathcal{R}_R}^* \mathbf{Q}' \land (\mathbf{P}, \mathbf{Q}') \in \mathbb{B} \land$$
$$\neg \mathbf{P} \Downarrow \rightarrow \forall \mathbf{P}'. \mathbf{P} \longrightarrow_{\mathcal{R}_L} \mathbf{P}' \rightarrow$$
$$\exists \mathbf{Q}'. \mathbf{Q} \longrightarrow_{\mathcal{R}_R}^* \mathbf{Q}' \land (\mathbf{P}', \mathbf{Q}') \in S$$
$$) \lor$$
$$\exists \mathbf{Q}'. \mathbf{Q} \longrightarrow_{\mathcal{R}_R} \mathbf{Q}' \land (\mathbf{P}, \mathbf{Q}') \in S$$
$$\}$$

Proof. We have $\mathbb{B} \models P \preceq Q$ if ϕ iff $[\![P \preceq Q \text{ if } \phi]\!] \subseteq S \preceq$, where

$$S \stackrel{\checkmark}{=} \{ (\mathbf{P}, \mathbf{Q}) \mid \forall \mathbf{P}'. \mathbf{P} \stackrel{*}{\longrightarrow} _{\mathcal{R}_{L}}^{*} \mathbf{P}' \wedge \mathbf{P}' \Downarrow \rightarrow \\ \exists \mathbf{Q}'. \mathbf{Q} \stackrel{*}{\longrightarrow} _{\mathcal{R}_{R}}^{*} \mathbf{Q}' \wedge (\mathbf{P}', \mathbf{Q}') \in \mathbb{B} \\ \lor \mathbf{Q} \Uparrow \}$$

and $Q\uparrow$ means that there is an infinite execution starting from Q, i.e., $\exists Q_1, Q_2, \ldots$ such that $Q \longrightarrow_{\mathcal{R}_R} Q_1 \longrightarrow_{\mathcal{R}_R} Q_2 \longrightarrow_{\mathcal{R}_R} \cdots$. \Rightarrow . We show that $S \stackrel{\checkmark}{\rightharpoonup}$ is post-fixed point for psim, i.e., $S \stackrel{\checkmark}{\rightharpoonup} \subseteq psim(S \stackrel{\checkmark}{\rightharpoonup})$. Let

 $(P, Q) \in S \preceq$. There are three cases:

- 1. $P \Downarrow$ and $\exists Q'. Q \longrightarrow_{\mathcal{R}_R}^* Q' \land (P, Q') \in \mathbb{B}$. 2. $\neg P \Downarrow$ and $\forall P''. P \longrightarrow_{\mathcal{R}_L}^* P'' \land P'' \Downarrow \rightarrow \exists Q'. Q \longrightarrow_{\mathcal{R}_R}^* Q' \land (P'', Q') \in \mathbb{B}$. Let $P \longrightarrow_{\mathcal{R}_L} P'$ arbitrary. Then $\forall P''. P' \longrightarrow_{\mathcal{R}_L}^* P'' \land P'' \Downarrow \rightarrow \exists Q'. Q \longrightarrow_{\mathcal{R}_R}^* Q' \land (P'', Q') \in \mathbb{B}$. Hence $(\mathbf{P}', \mathbf{Q}') \in S \preceq$.
- 3. $Q\uparrow$, i.e., $\exists Q_1, Q_2, \ldots$ such that $Q \longrightarrow_{\mathcal{R}_L} Q_1 \longrightarrow_{\mathcal{R}_R} Q_2 \longrightarrow_{\mathcal{R}_R} \cdots$. Then (P, Q' = $Q_1 \in S^{\preceq}$.

The above case-analysis shows that $(P, Q) \in psim(S^{\leq})$ in all the cases. \Leftarrow . We show that if S is a post-fixed point for *psim* then $S \subseteq S^{\preceq}$. Let $(P, Q) \in$ $S \subseteq psim(S)$. We have the following cases:

1. $P \Downarrow$ and $\exists Q'. Q \longrightarrow_{\mathcal{R}_R}^* Q' \land (P, Q') \in \mathbb{B}$. We obviously have $(P, Q) \in S \preceq$. 2. $\exists Q_1. Q \longrightarrow_{\mathcal{R}_R} Q_1 \land P_1 = P \land \land (P_1, Q_1) \in S$. 3. $\forall P_1. \exists Q_1. P \longrightarrow_{\mathcal{R}_L}^* P_1 \land Q \longrightarrow_{\mathcal{R}_R}^* Q_1 \land (P_1, Q_1) \in S$.

The steps 2 and 3 are repeated until for each P_n with $P \longrightarrow_{\mathcal{R}_I}^* P_n \wedge P_n \Downarrow$ either exists Q_{n+1} such that $Q \longrightarrow_{\mathcal{R}_R}^* Q_n \wedge (P_n, Q_n) \in \mathbb{B}$ and $(P_i, Q_i) \in S$ for $i \in \{1, \ldots, n\}$, or we obtain an infinite sequence $Q \longrightarrow_{\mathcal{R}_R} Q_1 \longrightarrow_{\mathcal{R}_R} Q_2, \ldots$ with $(\mathbf{P}, \mathbf{Q}_i) \in S$. In both cases we obtain $(\mathbf{P}, \mathbf{Q}) \in S \stackrel{\checkmark}{\rightharpoonup}$. П

Corollary 2. 1. $S \stackrel{\checkmark}{=} \nu S . psim(S)$. 2. \mathbb{B} is a post-fixed point of psim, i.e., $\mathbb{B} \subseteq psim(\mathbb{B})$.

Theorem 2 (Soundness for full simulation). If $G, B \vdash^0 G$ and $[\![B]\!] \subseteq \mathbb{B}$, then for any simulation formula $P \prec Q$ if $\phi \in G$, we have that $\mathbb{B} \models P \prec Q$ if ϕ .

Before proving Theorem 2, we introduce the following notations, where P and Q denote ground configurations , \mathbb{C} and S a set of pairs of ground configurations:

$$\begin{split} &CoReach((\mathbf{P},\mathbf{Q}),\mathbb{C}) \equiv \exists \, Q' \,. \, \mathbf{Q} \longrightarrow_{\mathcal{R}_R}^* Q' \wedge (\mathbf{P},Q') \in \mathbb{C}, \\ &Reach^+((\mathbf{P},\mathbf{Q}),S) \equiv \neg \mathbf{P} \Downarrow \wedge \forall \, \mathbf{P}' \,. \, \mathbf{P} \longrightarrow_{\mathcal{R}_L} \mathbf{P}' \rightarrow \exists \, Q' \,. \, \mathbf{Q} \longrightarrow_{\mathcal{R}_R}^* Q' \wedge (\mathbf{P}',Q') \in S, \\ &f_{\mathbb{C}}(S) = \{(\mathbf{P},\mathbf{Q}) \mid CoReach((\mathbf{P},\mathbf{Q}),\mathbb{C}) \lor Reach^+((\mathbf{P},\mathbf{Q}),S)\}. \end{split}$$

Lemma 3. 1. $f_{\mathbb{C}}$ is monotonic. 2. If $\mathbb{C} \subseteq \mathbb{D}$ then $f_{\mathbb{C}}(S) \subseteq f_{\mathbb{D}}(S)$ for any S. 3. $f_{\mathbb{C} \cup \mathbb{D}}(S) = f_{\mathbb{C}}(S) \cup f_{\mathbb{D}}(S)$.

Proof. The conclusions of the lemma are direct consequences of the definition. $\hfill \Box$

Lemma 4. Let \mathbb{C} and $S_{\mathbb{C}}$ be such that $\mathbb{C} = \{(P', Q') \mid Reach^+((P', Q'), S_{\mathbb{C}})\}$. Then

$$\vDash CoReach((\mathbf{P},\mathbf{Q}),\mathbb{C}) \rightarrow Reach^+((\mathbf{P},\mathbf{Q}),S_{\mathbb{C}})$$

Proof.

$$CoReach((\mathbf{P},\mathbf{Q}),\mathbb{C}) \leftrightarrow \exists \mathbf{Q}'' \cdot \mathbf{Q} \longrightarrow_{\mathcal{R}_{R}} \mathbf{Q}'' \wedge (\mathbf{P},\mathbf{Q}'') \in \mathbb{C}$$

$$\leftrightarrow \exists \mathbf{Q}'' \cdot \mathbf{Q} \longrightarrow_{\mathcal{R}_{R}} \mathbf{Q}'' \wedge \neg \mathbf{P} \Downarrow \wedge$$

$$\forall \mathbf{P}' \cdot \mathbf{P} \longrightarrow_{\mathcal{R}_{L}} \mathbf{P}' \rightarrow$$

$$\exists \mathbf{Q}' \cdot \mathbf{Q}'' \longrightarrow_{\mathcal{R}_{R}}^{*} \mathbf{Q}' \wedge (\mathbf{P}',\mathbf{Q}') \in S_{\mathbb{C}}$$

$$\rightarrow \neg \mathbf{P} \Downarrow \wedge \forall \mathbf{P}' \cdot \mathbf{P} \longrightarrow_{\mathcal{R}_{L}} \mathbf{P}' \rightarrow$$

$$\exists \mathbf{Q}' \cdot \mathbf{Q} \longrightarrow_{\mathcal{R}_{R}}^{*} \mathbf{Q}' \wedge (\mathbf{P}',\mathbf{Q}') \in S_{\mathbb{C}}$$

$$\leftrightarrow Reach^{+}((\mathbf{P},\mathbf{Q}),S_{\mathbb{C}})$$

Corollary 3. If $\mathbb{C} = \{(P', Q') \mid Reach^+((P', Q'), S_{\mathbb{C}})\}$ then $f_{\mathbb{C}}(S) \subseteq f_{\emptyset}(S \cup S_{\mathbb{C}})$.

Proof.

$$f_{\mathbb{C}}(S) = \{(P,Q) \mid CoReach((P,Q),\mathbb{C}) \lor Reach^{+}((P,Q),S)\}$$
$$\subseteq \{(P,Q) \mid Reach^{+}((P,Q),S_{\mathbb{C}}) \lor Reach^{+}((P,Q),S)\}$$
$$= \{(P,Q) \mid Reach^{+}((P,Q),S \cup S_{\mathbb{C}})\}$$
$$= f_{\emptyset}(S \cup S_{\mathbb{C}})$$

Lemma 5. $f_{\mathbb{B}}(S) = fsim(S)$.

Proof. We first notice that the following fact holds:

$$\vDash (V \rightarrow W) \rightarrow ((U \rightarrow V) \land (\neg U \rightarrow W) \leftrightarrow V \lor (\neg U \land W))$$

We have

$$fsim(S) = \{(\mathbf{P}, \mathbf{Q}) \mid \mathbf{P} \Downarrow \rightarrow CoReach((\mathbf{P}, \mathbf{Q}), \mathbb{B}) \land \neg \mathbf{P} \Downarrow \rightarrow Reach^{(}(\mathbf{P}, \mathbf{Q}), S)\} \\ = \{(\mathbf{P}, \mathbf{Q}) \mid CoReach((\mathbf{P}, \mathbf{Q}), \mathbb{B}) \lor Reach^{(}(\mathbf{P}, \mathbf{Q}), S)\} \\ = f_{\mathbb{B}}(S)$$

by applying the above fact, where $U \equiv P \Downarrow, V \equiv CoReach((P,Q), \mathbb{B})$, and $W \equiv \forall P' . (P \longrightarrow_{\mathcal{R}_L} P') \rightarrow (\exists Q' . Q \longrightarrow_{\mathcal{R}_R}^* Q' \land (P',Q') \in S_{\mathbb{B}}).$

Lemma 6. Let PT the set of the proof trees of $G, B \vdash^0 G$ and let S be the union of all the sets $\llbracket \varphi \rrbracket$ with φ occurring in PT. Then $\llbracket \varphi \rrbracket \subseteq f_{\mathbb{B} \cup \mathbb{G}}(S)$ for each φ occurring in PT.

Proof (Sketch). We proceed by induction on the height of PT and case analysis on the rule applied in the root.

AXIOM. We have $\llbracket \varphi \rrbracket = \emptyset$.

BASE. $\phi' \rightarrow sub((P,Q'), B)$ means $\phi' \rightarrow \llbracket (P,Q') \rrbracket \subseteq \llbracket B \rrbracket \subseteq \mathbb{B}$, which implies $\phi' \rightarrow \forall P \in \llbracket P \text{ if } \phi' \rrbracket \cdot P \Downarrow \wedge \forall Q' \in \llbracket Q' \text{ if } \phi' \rrbracket \cdot Q' \Downarrow \text{ (i.e. } \phi' \text{ implies that P and } Q'$ are terminal). Since ϕ' is a path condition derived from Q', it follows that it does not affect the termination of P, i.e. we have $\vDash \forall P \in \llbracket P \text{ if } \top \rrbracket \cdot P \Downarrow$. It follows that $\vDash \forall (P,Q) \in \llbracket P \prec Q \text{ if } \phi \rrbracket \cdot CoReach((P,Q), \mathbb{B})$, which implies $\llbracket P \prec Q \text{ if } \phi \rrbracket \subseteq f_{\mathbb{B}}(\emptyset) \cup f_{\mathbb{B} \cup \mathbb{G}}(\llbracket P \prec Q \text{ if } \phi \land \neg \phi_B \rrbracket) \subseteq f_{\mathbb{B} \cup \mathbb{G}}(S)$ by the definition of $f_{\mathbb{B}}$, Lemma 3, and the inductive hypothesis.

CIRC. $\phi' \rightarrow sub((P,Q'), G)$ means $\phi' \rightarrow \llbracket (P,Q') \rrbracket \subseteq \mathbb{G}$, which implies $\vDash \forall (P,Q) \in \llbracket (P,Q) \rrbracket$. *CoReach*((P,Q), \mathbb{G}). We obtain

$$\llbracket P \prec Q \text{ if } \phi \rrbracket \subseteq f_{\mathbb{G}}(\llbracket P \prec Q \text{ if } \phi \rrbracket) \cup f_{\mathbb{B} \cup \mathbb{G}}(\llbracket P \prec Q \text{ if } \phi \land \neg \phi_B \rrbracket) \subseteq f_{\mathbb{B} \cup \mathbb{G}}(S)$$

by the definition of $f_{\mathbb{G}}$, Lemma 3, and the inductive hypothesis. STEP. We have $\llbracket P \prec Q$ if $\phi \rrbracket = \llbracket P \prec Q$ if $\phi \land (\phi_1 \lor \cdots \lor \phi_n) \rrbracket \cup \llbracket P \prec Q$ if $\phi \land \neg \phi_1 \land \cdots \land \neg \phi_n \rrbracket$. We obtain $\llbracket P \prec Q$ if $\phi \land \neg \phi_1 \land \cdots \land \neg \phi_n \rrbracket \subseteq f_{\mathbb{B} \cup \mathbb{G}}(S)$ by the inductive hypothesis. We have $\{P' \mid P \longrightarrow_{\mathcal{R}_L} P', P \in \llbracket P \text{ if } \phi \rrbracket\} = \llbracket \Delta_{\mathcal{R}_L}(P \text{ if } \phi) \rrbracket$ (by Theorem 1) and $\{(P', Q) \mid P \longrightarrow_{\mathcal{R}_L} P', P \in \llbracket P \text{ if } \phi \rrbracket, Q \in \llbracket Q \text{ if } \phi \rrbracket\} = \{(P', Q) \mid P' \in \llbracket \Delta_{\mathcal{R}_L}(P \text{ if } \phi) \rrbracket, Q \in \llbracket Q \text{ if } \phi \rrbracket\} = \llbracket \{P^i \prec Q \text{ if } \phi^i \mid 1 \leq i \leq n\} \rrbracket$, which implies

$$\vDash \forall (\mathbf{P}, \mathbf{Q}) . (\mathbf{P}, \mathbf{Q}) \in \llbracket P \prec Q \text{ if } \phi \land (\phi_1 \lor \cdots \lor \phi_n) \rrbracket \rightarrow Reach^+((\mathbf{P}, \mathbf{Q}), \llbracket \{ P^i \prec Q \text{ if } \phi^i \mid 1 \le i \le n \} \rrbracket)$$

We obtain

$$\begin{bmatrix} P \prec Q \text{ if } \phi \end{bmatrix} \subseteq f_{\mathbb{B} \cup \mathbb{G}}(\llbracket \{P^i \prec Q \text{ if } \phi^i \mid 1 \le i \le n\} \rrbracket) \cup \llbracket P \prec Q \text{ if } \phi \land \neg \phi_1 \land \ldots \land \neg \phi_n \rrbracket \subseteq f_{\mathbb{B} \cup \mathbb{G}}(S)$$

by the definition of $f_{\mathbb{G}}$, Lemma 3, and the inductive hypothesis.

Proof (Theorem 2). Let PT the set of the proof trees of $G, B \vdash^0 G$ and let S be the union of all the sets $\llbracket P \prec Q \text{ if } \phi \rrbracket$ with $P \preceq Q \text{ if } \phi$ occurring in PT. We obtain $S \subseteq f_{\mathbb{B} \cup \mathbb{G}}(S)$ by Lemma 6 and Lemma 3. Let (G_0, G_1) denote the partition of G such that the proof trees corresponding to G_i uses only instances of inference rules $G, B \vdash^g \varphi$ with $g \leq i$. Let \mathbb{G}_i denote $\llbracket G_i \rrbracket$. For G_0 we have $f_{\mathbb{G}_0}(S) \subseteq f_{\mathbb{B}}(S)$ since only BASE AXIOM rules are applied in the proof of G_0 .

We obtain $S \subseteq f_{\mathbb{B}\cup\mathbb{G}}(S) = f_{\mathbb{B}}(S) \cup f_{\mathbb{G}_0}(S) \cup f_{\mathbb{G}_1}(S) \subseteq f_{\mathbb{B}}(S) \cup f_{\emptyset}(S_{\mathbb{G}_1}) = f_{\mathbb{B}}(S \cup S_{\mathbb{G}_1}) = f_{\mathbb{B}}(S) = fsim(S)$ by Lemma 3, Corollary 3, and Lemma 5. Hence $S \subseteq \nu Y$. fsim(Y), which implies the conclusion of the theorem by Lemma 1. \Box

Theorem 3 (Soundness for partial simulation). If $G, B \vdash^0 G$ and $\llbracket B \rrbracket \subseteq \mathbb{B}$, then for any formula $P \preceq Q$ if $\phi \in G$, we have that $\mathbb{B} \models P \preceq Q$ if ϕ .

We first introduce the following additional notations:

 $CoReach^+((\mathbf{P},\mathbf{Q}),\mathbb{C}) \equiv \exists \mathbf{Q}' . \mathbf{Q} \longrightarrow_{\mathcal{R}_R} \mathbf{Q}' \land (\mathbf{P},\mathbf{Q}') \in \mathbb{C}, \\ p_{\mathbb{C}}(S) = \{(P,Q) \mid CoReach((P,Q),\mathbb{C}) \lor CoReach^+((P,Q),S) \lor Reach^+((P,Q),S)\}.$

The function $p_{\mathbb{C}}$ has properties similar to those of $f_{\mathbb{C}}$:

Lemma 7. 1. $p_{\mathbb{C}}$ is monotonic. 2. If $\mathbb{C} \subseteq \mathbb{D}$ then $p_{\mathbb{C}}(S) \subseteq p_{\mathbb{D}}(S)$ for any S. 3. $p_{\mathbb{C}\cup\mathbb{D}}(S) = p_{\mathbb{C}}(S) \cup p_{\mathbb{D}}(S)$. 4. If $\mathbb{C} = \{(P',Q') \mid Reach^+((P',Q'),S_{\mathbb{C}})\}$ then $p_{\mathbb{C}}(S) \subseteq p_{\emptyset}(S \cup S_{\mathbb{C}})$.

Proof. It follows directly from the definition.

Lemma 8. $p_{\mathbb{B}}(S) = psim(S)$.

Proof. The first member of the disjunction from the definition of *psim* is equivalent to $CoReach((P,Q), \mathbb{C}) \vee Reach^+((P,Q), S)$ by Lemma 5 and the second one is equivalent to $CoReach^+((P,Q), S)$.

Lemma 9. Let PT the set of the proof trees of $G, B \vdash^0 G$ and let S be the union of all the sets $\llbracket \varphi \rrbracket$ with φ occurring in PT. Then $\llbracket \varphi \rrbracket \subseteq p_{\mathbb{B} \cup \mathbb{G}}(S)$ for each φ occurring in PT.

Proof (Sketch). We proceed by induction on the height of PT and case analysis on the rule applied in the root. For AXIOM and BASE the proofs are similar to those of Lemma 6. For the rest of rules we let (G_0, G_1) denote the partition of G such that the proof trees corresponding to G_i uses only instances of inference rules $G, B \vdash^g \varphi$ with $g \leq i$. We also use \mathbb{G}_i to denote $\llbracket G_i \rrbracket$. CIRC. Let φ denote $P \prec Q$ if ϕ .

Subcase g = 1. We have $\{(\mathbf{P}, \mathbf{Q}) \in \llbracket \varphi \rrbracket \mid CoReach^+((\mathbf{P}, \mathbf{Q}), \mathbb{G}_1)\} = \{(\mathbf{P}, \mathbf{Q}) \in \llbracket \varphi \rrbracket \mid Reach^+((\mathbf{P}, \mathbf{Q}), S_{\mathbb{G}_1})\} \subseteq p_{\emptyset}(S_{\mathbb{G}_1}) \subseteq p_{\mathbb{B}}(S)$ by Lemma 4 and the definition of p; the inclusion $S_{\mathbb{G}_1} \subseteq S$ follows by the fact there is an instance of STEP in PT for each formula in G_1 . Since there is no an instance of STEP in PT for any

formula in G_0 , $(\mathbf{P}, \mathbf{Q}) \in \mathbb{G}_0$ implies $CoReach((\mathbf{P}, \mathbf{Q}), \mathbb{B}) \vee CoReach^+((\mathbf{P}, \mathbf{Q}), S)$ (corresponding to BASE and CIRC, respectively). We obtain

 $\mathbb{G} = \mathbb{G}_0 \cup \mathbb{G}_1$ implies $\{(\mathbf{P}, \mathbf{Q}) \in \llbracket \varphi \rrbracket \mid CoReach((\mathbf{P}, \mathbf{Q}), \mathbb{G})\} \subseteq p_{\mathbb{B}}(S)$. Subcase g = 0. We have

Now the two cases are finished. From the definition of the rule we obtain

$$\llbracket \varphi \rrbracket \subseteq \{(\mathbf{P}, \mathbf{Q}) \mid CoReach^+((\mathbf{P}, \mathbf{Q}), \mathbb{G})\} \cup \llbracket P \preceq Q \text{ if } \phi \land \neg \phi_G \rrbracket \subseteq p_{\mathbb{B}}(S) \cup p_{\mathbb{B} \cup \mathbb{G}}(S) \subseteq p_{\mathbb{B} \cup \mathbb{G}}(S)$$

by the definition, the properties of p and the inductive hypothesis. STEP. Let φ denote $P \preceq Q$ if ϕ . We have

$$\begin{split} \llbracket \varphi \rrbracket &\subseteq \\ \{ (\mathbf{P}, \mathbf{Q}) \mid Reach^+((\mathbf{P}, \mathbf{Q}), \varDelta_{\mathcal{R}_l}(P \text{ if } \phi)) \} \cup \llbracket P \preceq Q \text{ if } \phi \land \neg \phi_1 \land \cdots \land \neg \phi_n \rrbracket \subseteq \\ p_{\mathbb{B} \cup \mathbb{G}}(S) \end{split}$$

by the inductive hypothesis and the definition of P.

Proof (Theorem 3). Let PT the set of the proof trees of $G, B \vdash^0 G$ and let S be the union of all the sets $\llbracket \varphi \rrbracket$ with φ occurring in PT. We obtain $S \subseteq p_{\mathbb{B}\cup\mathbb{G}}(S)$ by Lemma 9. We have $S \subseteq p_{\mathbb{B}\cup\mathbb{G}}(S) = p_{\mathbb{B}}(S) \cup p_{\mathbb{G}_0}(S) \cup p_{\mathbb{G}_1}(S) \subseteq p_{\mathbb{B}}(S) \cup p_{\emptyset}(S_{\mathbb{G}_1}) =$ $p_{\mathbb{B}}(S \cup S_{\mathbb{G}_1}) = p_{\mathbb{B}}(S) = psim(S)$ by Lemma 7, Lemma 9, and Lemma 8. Hence $S \subseteq \nu Y \cdot psim(Y)$, which implies the conclusion of the theorem by Lemma 2.

\mathbf{C} **Examples of Optimization Correctness Proofs**

We present these examples in a C-like language, denoting symbolic expressions and sequences by suggestive identifiers (e.g., E1, S1). We go through all examples worked out in CORK [33]. The read-sets and write-sets of these expressions/sequences are given in a .wp (weakest precondition) file. We encode these read/write-sets as explained in Section 6. In this section, we will use the term equivalence and we will mean two-way simulation. When proving equivalence, we prove the simulation of the rhs by the lhs and vice-versa. The base cases and the goals used for the reverse direction are always symmetric. These examples are all implemented in the RMT tool (http://profs.info.uaic.ro/~stefan.ciobaca/rmteq).

The base equivalence \mathbb{B} we consider has two terminal programs, under the constraint that output variables have equal values in the two resulting environments.

In this section we list each of the optimizations individually, analyze them, and present how our method can be applied to prove the equivalences. For consistency, we will always present the original program on the left and the optimized one on the right.

In order for RMT to successfully prove equivalences involving loops, it requires helper equivalences (circularities). We describe a methodology, which we call snapshotting the two programs at certain points, that allows us to easily find these helper circularities for proving optimizations.

By taking a *snapshot* of a program at a certain point, we mean running it until it reaches that point and saving its form once that point is reached. RMT provides a run query, which can be used to make the process of taking these snapshots easier.

In general, in order to obtain a helpful circularity, the snapshot needs to happen at a point in which the structure of the program remains similar after some program steps are executed (e.g., inside loops). In addition, the two snapshots of the programs still need to be equivalent. Usually, this only happens under some constraint.

-	
V1 = 0;	V1 = 0;
while (V1 < V2) {	while (V1 < V2) {
S1;	S1;
V1 = V1 + 1;	V1 = V1 + 1;
}	}

Consider a simple example in which we want to prove the equivalence of a program with itself:

For this example, no matter how many program steps we execute, the program will never be structurally similar to the initial one, due to the initial assignment is *erased* after being executed. However, we snapshot the program at the beginning of the loop (just after the initial assignment was executed). In order to prove the initial equivalence, we use the following helper equivalence found by snapshotting:

while (V1 < V2) {	while (V1 < V2) {
S1;	S1;
V1 = V1 + 1;	V1 = V1 + 1;
}	}

Intuitively, because the snapshot reaches a configuration having a form similar to itself, this new equivalence can be used to prove itself (hence why we call these equivalences *circularities*). In addition, the original equivalence can be easily reduced to this second one.

Since the first assignment is missing from these new programs, we must specify that this equivalence only holds true if the value of V1 in the left-hand-side program is equal to the value of V1 in the right-hand-side program. We add this as a logical constraint of the circularity. In the next examples, we will always assume equality of variables with the same name, unless otherwise specified.

Note that this is not the only way to specify a helper circularity. For example, we could snapshot the programs at S1, at V1 = V1 + 1, or even at different points inside the loop, under proper constraints.

Code hoisting Program sequences which appear on both branches of a conditional branch can be hoisted out of the if-else statement. On modern CPUs, this could potentially help with pipelining and branch prediction, improving run-time performance.

if (B1) {	
S1;	S1;
S2;	if (B1) {
} else {	S2;
S1;	} else {
S3;	S3;
}	}

In this example, B1 is a symbolic boolean expression and S1 is a symbolic sequence which does not write to the read set of B1. There are no restrictions on the read/write-sets of symbolic sequences S2 and S3. RMT is able to prove the equivalence of the two programs with no additional circularities (as expected, since helper circularities are generally only needed when programs contain loops). The name of the file corresponding to this examples is imp-hoisting.rmt.

Constant propagation The goal of constant propagation is to eliminate the need to evaluate certain expressions multiple times, if these expressions remain constant thorough the program's execution. We have already discussed this example in Section 6.

V1 = E1;	V1 = E1;
S1;	S1;
V2 = E1;	V2 = V1;

In the original program, we can see that the result of E1 is stored in variable V1. On line 3, expression E1 is evaluated again. Provided that the evaluation of E1 does not need the value of V1 or any variables which S1 modifies, we could avoid this re-evaluation and use the memorized value, stored in V1. Depending on the complexity of E1, this could greatly improve run-time performance.

V1 = E1;	V1 = E1;
S1;	V2 = V1;
V2 = E1;	S1;

If additionally S1 does not use the value of V2, the order in which the last two lines are executed becomes irrelevant, as illustrated in the example above. Modern CPUs could pick up on this and execute the lines in parallel, further improving performance.

RMT is able to prove both of these equivalences, with no helper circularities. The names of the two files corresponding to this examples are of the form imp-constant-propagation*.rmt.

Copy propagation In compiler theory, copy propagation is the process of replacing the occurrences of targets of direct assignments with their values. Copy propagation is a useful *clean up* optimization frequently used after other optimizations have already been run. Some optimizations, such as elimination of common sub expressions, require that copy propagation be run afterwards in order to achieve an increase in efficiency.

V1 = V2;	V1 = V2;
V3 = V1;	V3 = V2;

The two programs above illustrate an example of a copy propagation optimization. Proving the equivalence of the two is similar to proving equivalence in the case of constant propagation. As expected, RMT was able to prove this equivalence as well, without the need for additional circularities. The name of the file corresponding to this examples is imp-copy-propagation.rmt.

If-conversion If-conversion is an optimization which deletes a branch around an instruction and replaces it with a predicate on the instruction. This optimization can be described as a transformation which converts control dependencies into data dependencies, and it may be required for software pipelining.

	if (B1) {
if (B1) {	V1 = E1;
V1 = E1;	} else {
}	V1 = V1;
	}

The programs above illustrate an example of if-conversion. Using the ternary operator from the C language, the optimized program could also be expressed in a single line as V1 = B1? E1 : V1;. It is assumed that neither B1 nor E1 have any side effects.

RMT is able to prove this equivalence as well, with no helper circularities. The name of the file corresponding to this examples is imp-if-conversion.rmt.

Partial redundancy elimination Partial redundancy elimination (PRE) is a compiler optimization that eliminates expressions that are redundant on some but not necessarily all paths through a program. PRE is a form of common subexpression elimination.

An expression is called partially redundant if the value computed by the expression is already available on some but not all paths through a program to that expression. An expression is fully redundant if the value computed by the expression is available on all paths through the program to that expression. PRE can eliminate partially redundant expressions by inserting the partially redundant expression on the paths that do not already compute it, thereby making the partially redundant expression fully redundant.

if (B1) {	if (B1) {
S1;	S1;
V1 = E1;	V1 = E1;
S2;	S2;
	V2 = V1;
} else {	} else {
S3;	S3;
}	V2 = E1;
V2 = E1;	}

Here, it is assumed that B1 and E1 have no side effects, E1 does not read from V1 and S1 does not write to V1 or V2 and, in addition, S1 does not write to any variables read by E1.

Under these assumptions, it can be observed that E1 is partially redundant: its value is already available at the end of the if branch, but not at the end of the else branch. PRE inserts this expression on the else branch, whereas on the if branch it uses the value stored in V1, avoiding the re-evaluation of E1.

As before, RMT is able to prove the equivalence of the two programs without the need for helper circularities. The following examples all have loops and therefore helper circularities are required. The name of the file corresponding to this examples is imp-pre.rmt. Loop invariant code motion Loop invariant code consists of statements and/or expressions inside a loop body that do not depend on the contents of the loop itself, and as such could be moved outside the loop without affecting the results of the program. Loop invariant code motion (LICM) is the compiler optimization which identifies such statements and moves them outside the loop automatically. This results in a single evaluation of the loop invariant code, as opposed to multiple ones, which could significantly improve performance.

	if (V1 < V2) {
while (V1 < V2) {	S2;
S1;	while (V1 < V2) {
S2;	S1;
V1 = V1 + 1;	V1 = V1 + 1;
}	}
	}

In this example, S2 is a symbolic statement, which does not read from and does not write to any variables modified inside the loop (i.e. V1 and the write-set of S1). The if instruction added in the optimized program ensures that S2 is only evaluated if the initial loop was going to be entered into at least once, thus preserving program semantics.

As explained, since the right-hand-side program does not preserve its structure (the conditional statement *disappears* after a few steps), we need a helper circularity. We created such a circularity by snapshotting the optimized program at the start of the loop. With this new circularity, RMT is indeed able to successfully prove the desired equivalence. The name of the file corresponding to this examples is imp-licm.rmt.

Loop peeling Loop splitting is a compiler optimization technique that attempts to simplify a loop or eliminate dependencies by breaking it into multiple loops which have the same bodies but iterate over different contiguous portions of the index range. Loop peeling is a special case of loop splitting which splits any potentially problematic first (or last) few iterations from the loop and performs them outside of the loop body.

	if (V1 < V2) {
	S1;
	V1 = V1 + 1;
while (V1 < V2) {	while (V1 < V2) {
S1;	S1;
V1 = V1 + 1;	V1 = V1 + 1;
}	}
	}

In this example, one loop step from the initial program is *peeled* outside the loop in the optimized one.

Interestingly, even though the second program begins with an if instruction, which will be eliminated after some steps, RMT does not require an additional circularity in order to prove this example. This is because of the definition of the language semantics we used. In the semantics, while(B) S; is rewritten to if(B) {S; while(B) S;}. It can be observed that, by applying this transformation, the inner loop of the optimized program translates into a program which structurally matches the initial one. If the semantics were defined differently, we might have had to build an auxiliary circularity in order for RMT to successfully prove the equivalence. The name of the file corresponding to this examples is imp-loop-peeling.rmt.

Loop unrolling Loop unrolling is an optimization that attempts to improve the execution speed of a program at the expense of code size. It involves repeating the loop body multiple times inside a single iteration, eliminating some of the loop overhead, such as unnecessary termination condition checks.

while (V1 < V2) {	while (V1+1 < V2) {
51,	υ1,
V1 = V1 + 1;	V1 = V1 + 1;
}	S1;
	V1 = V1 + 1;
	}
	if (V1 < V2) {
	S1;
	V1 = V1 + 1;
	}

In this example, the loop body of the optimized program corresponds to two iterations of the initial loop. This means that the termination condition will be checked in the optimized program roughly half the number of times compared to the original one. This assumes that S1 does not write to V1 and V2. The final if statement from the optimized program is needed for when the original loop would execute S1 an odd number of times.

As before, since the optimized program does not preserve structure (the final conditional statement is pushed on the computation stack before the loop is executed), we need an additional circularity. We created a new circularity by snapshotting the second program before the loop. RMT is able to use this circularity and prove the equivalence of the two programs.

V1 = 0;	V1 = 0;
while (V1 < V2) {	while (V1 < V2) {
S1;	S1;
V1 = V1 + 1;	V1 = V1 + 1;
}	S1;
	V1 = V1 + 1;
	}

In this second example of unrolling, we illustrate that if we know a priori that the loop executes an even number of times (i.e. that the value of V2 is an even number), we can omit the final if statement, simplifying the optimized program.

As with previous examples, we use a helper circularity, which consists of the two programs snapshotted at the start of the loops. With this circularity in place, RMT is able to successfully prove this equivalence as well. The names of the two files corresponding to this examples are of the form imp-loop-unrolling*.rmt.

Loop unswitching Loop unswitching is a compiler optimization that moves a conditional inside a loop outside of it, by duplicating the body of loop and placing a version of the body in each of the two branches of the conditional statement. Despite roughly doubling the code size, this optimization not only allows the conditional expression to be evaluated only once (as opposed to on each iteration of the loop), but also allows each conditional branch to be further optimized separately.

	if (B1) {
while (V1 < V2) {	while (V1 < V2) {
if (B1) {	S1;
S1;	V1 = V1 + 1;
} else {	}
S2;	} else {
}	while (V1 < V2) {
V1 = V1 + 1;	S2;
}	V1 = V1 + 1;
	}
	}

In this example, we assume that B1 does not depend on V1, V2, or on any variable in the write-sets of S1 and S2. In other words, it does not change its value thorough the execution of the loop.

As with previous examples, since the optimized program starts with an if instruction, which disappears after some program steps, we need additional circularities. Interestingly, since the if statement has two branches, we need two new circularities (one for each branch). In other words, in the two new circularities, the left program will remain unchanged, whereas the right program will respectively turn into the two programs below:

while (V1 < V2) {	while (V1 < V2) {
S1;	S2;
V1 = V1 + 1;	V1 = V1 + 1;
}	}

Of course, we can only prove the first additional equivalence under the constraint that B1 evaluates to true and the second one under the constraint that B1 evaluates to false. RMT is able to successfully prove these equivalences. The name of the file corresponding to this examples is imp-loop-unswitch.rmt.

Software pipelining Software pipelining is a technique used to optimize loops, in a manner that enables better parallelization via hardware pipelining. This optimization is a type of out-of-order execution, which is done by the compiler (or by the programmer).

	if (V1 < V2) {
	S1;
while (V1 < V2) {	while (V1 < V2-1) {
S1;	S2;
S2;	V1 = V1 + 1;
V1 = V1 + 1;	S1;
}	}
	S2;
	V1 = V1 + 1;
	}

In this example, if we compare the loop bodies of the two programs, we can see that statements S1 and S2 are executed in a different order. This could lead to performance improvements if the processor considers it easier to parallelize the second loop compared to the first one.

As with previous examples, since the second program does not preserve structure, we use a helper circularity, in which the second program is snapshotted just before the S1 instruction. With this helper circularity, RMT is able to successfully prove the equivalence of the two programs. The name of the file corresponding to this examples is imp-software-pipelining.rmt.

Loop fission and fusion Loop fission (or loop distribution) is a compiler optimization in which a loop is broken into multiple loops over the same index range with each taking only a part of the original body of loop. The goal is to break down a large loop body into smaller ones for better locality.

Conversely, loop fusion (or loop jamming) is the loop transformation that replaces multiple loops with a single one.

	V1 = E1;
V1 = E1;	while (V1 < V2) {
	S1;
while (V1 < V2) {	V1 := V1 + 1;
S1;	}
S2;	V1 = E1;
V1 = V1 + 1;	while (V1 < V2) {
}	S2;
	V1 = V1 + 1;
	}

The programs above represent an example of loop fission. If the order of the programs were reversed, it would be an example of loop fusion. It is assumed that S1 and S2 write to disjoint sets of variables (let us denote these sets by C1 and C2 respectively), and none of the two sequences read from variables written to by the other. In addition, E1 does not read from C1, C2, or V1.

In order to solve this example, we need two separate simulation proofs, with two different base equivalences. Usually, we consider the base equivalence to be two terminal programs in which *all* relevant variables have equal values. For this example, we first consider them equivalent (1) if *only* variables in C1 have equal values, and then (2) if *only* variables in C2 have equal values. In other words, we track the results of S1 and S2 separately.

For (1), we construct a helper circularity by snapshotting the left-hand-side program just before the **while** loop and the right-hand-side program just before the *first* **while** loop. We construct another helper circularity by snapshotting the first program at its termination point and the second program just before the *second* **while** loop. Intuitively, this last circularity has the role of ensuring that the final loop of the second program does not modify variables written to by **S1**. Because this circularity contains a terminal program configuration, we can only prove the *partial* equivalence of the two programs.

For (2), we construct a helper circularity by snapshotting the left-hand-side program just before the while loop and the right-hand-side program just before the second while loop. We construct another helper circularity consisting of the first program (unchanged) and the second program snapshotted just before the *first* while loop. When proving this final circularity, the left-hand-side program does not advance; only the right-hand side program advances, ensuring that the first loop does not modify the variables written to by S2. Because the first program must not make progress, we can only prove *partial* simulation for this case as well.

The names of the four files corresponding to this examples are of the form imp-loop-fission*.rmt and imp-loop-fusion*.rmt.

Loop interchange Loop interchange is the process of exchanging the order of two iteration variables used by a nested loop. The variable used in the inner loop switches to the outer loop, and vice versa. It is often done to ensure that the elements of a multi-dimensional array are accessed in the order in which they are present in memory, improving locality of reference.

V1 = 0;	V1 = 0;
V3 = 0;	V3 = 0;
if (V3 < V4) {	if (V1 < V2) {
while (V1 < V2) {	while (V3 < V4) {
V3 = 0;	V1 = 0;
while (V3 < V4) {	while (V1 < V2) {
S1;	S1;
V3 = V3 + 1;	V1 = V1 + 1;
}	}
V1 = V1 + 1;	V3 = V3 + 1;
}	}
}	}

In this example, we assume that S1 does not modify the values of variables V1 through V4 and does not read the values of V1 and V3.

Similarly to previous examples, we take a snapshot of each of these programs just before the execution of S1.

In order for the programs in the new circularity to truly be equivalent, we need to add the constraint that S1 was executed the same number of times on both sides. We note that, in the left-hand-side program, when the flow reaches the inner loop, S1 was executed $V1 \times V4 + V3$ times. Similarly, in the right-hand-side program, S1 was executed $V3 \times V2 + V1$ times. Therefore, the equality of these two quantities is the required constraint.

In addition, since our circularity snapshots the program at S1, we need to add to the constraint the conditions necessary for the programs to actually reach S1 (i.e., that all loop conditions evaluate to true).

With this helper circularity under the discussed constraints, we can prove the equivalence of the two programs. However, the constraint $V1 \times V4 + V3 = V3 \times V2 + V1$ introduces a component of non-linear integer algebra into the proof. As discussed in Section 6, the SMT solver that we use (Z3) does not handle non-linear integer algebra well. Because of this, RMT can only successfully prove the equivalence of the two programs if the loop limits (i.e., the values of V2 and V4) are bounded. Our prover does not use this bound explicitly, but it is required for the SMT solver to solve the non-linear integer algebra problems. The name of the file corresponding to this examples is imp-loop-interchange.rmt.

Loop reversal Loop reversal is an optimization that reverses the order in which values are assigned to the loop variable, essentially changing the direction in which the loop is iterated. In some cases, this might improve cache efficiency and enable other optimizations.

```
V1 = E1;
while (V1 < V2) {
    S1;
    V1 = V1 + 1;
}

if (E1 < V2) {
    V1 = V2 - 1;
while (V1 >= E1) {
    S1;
    V1 = V1 - 1;
}
V1 = V2;
}
else {
    V1 = E1;
}
```

Here, we assume that S1 does not write to V1, and E1 does not depend on V1, or to any variables that S1 writes to. The else branch of the second program ensures equivalence if E1 is greater than V2. The final assignment inside the if branch of the second program ensures that the value of V1 is the same at the end of the executions of the two programs.

In a similar manner to previous examples, we create a new circularity by snapshotting each program at the start of the loop execution.

In this new circularity, we note that the programs are equivalent only if the value of V1 in the left program is equal to the value of V2 - 1 - V1 in the right one. With this helper circularity, RMT is able to successfully prove the equivalence of the two programs. The name of the file corresponding to this examples is imp-loop-reversal.rmt.

Loop skewing This optimization skews the execution of an inner loop relative to an outer one, which could be useful if the inner loop has a dependence on the outer loop which prevents it from running in parallel. This optimization is often combined with loop interchanging in order to improve parallelization.

while (V1 < V2) {	while (V1 < V2) {
	V5 = E1 + V6;
V3 = E1;	V3 = V5 - V6;
	if (V5 < V4 + V6) {
while (V3 < V4) {	while (V5 < V4 + V6) {
	V3 = V5 - V6;
S1;	S1;
V3 = V3 + 1;	V5 = V5 + 1;
}	}
	V3 = V4;
	}
V1 = V1 + 1;	V1 = V1 + 1;
}	}

As with previous examples, we use an additional circularity which consists of both programs snapshotted once they have reached S1. We need the constraint under which the two programs in the new circularity truly are equivalent (i.e., some relationship between the variables in the two programs). By analyzing the programs, we see that when both programs have reached S1, the values of V3 are equal and the value of V5 (in the right-hand-side program) is the sum of the values of V3 and V6. We also need to add the condition that the program flows truly reach S1, which is that all loop conditions evaluate to true.

With this new circularity, under the described constraints, RMT is able to successfully prove the equivalence of the two programs. The name of the file corresponding to this examples is imp-loop-skewing.rmt.

Loop strength reduction Strength reduction is a compiler optimization that replaces expensive operations by equivalent but less expensive ones. For example, converting multiplications inside a loop into repeated additions, which can often be used, for example, to improve the performance of array addressing.

	V5 = V1 * V4;
while (V1 < V2) {	while (V1 < V2) {
V3 = V1 * V4;	V3 = V5;
	V5 = V5 + V4;
S1;	S1;
V1 = V1 + 1;	V1 = V1 + 1;
}	}

In these examples, S1 is a symbolic sequence that does not write to variables V1 through V4. We can see that the original program executes a multiplication at every loop iteration, whereas the optimized program executes the multiplication only once, and instead replaces the original multiplications by additions.

As in previous examples, we need to use an additional circularity. Though multiple options are possible, we chose to snapshot the first program just before S1, and the second program just before the line V5 = V5 + V4. At these points, we notice that the value of V3 is the same on both sides. In addition, V3 = V1 * V4 on the left side, and V3 = V5 on the right side. Using these constraints, RMT is able to prove this additional circularity and, therefore, the original equivalence as well.

Interestingly, even though we are dealing with multiplications and therefore non-linear integer algebra, unlike Loop Interchange, the required formula is properly solved by Z3. The name of the file corresponding to this examples is imp-strength-reduction.rmt.

Loop tiling Loop tiling is a technique that partitions the iteration space of a loop into smaller chunks or blocks, often with the purpose of locality optimization or parallelization.

```
V3 = V1;

while (V3 < V2) {

V1 = V3;

while (V1 < V2) {

S1;

V1 = V1 + 1;

}

V3 = V1 + 1;

}

V3 = V3 + V4;

}

V3 = V3 + V4;

}
```

In this example, S1 is a symbolic statement that cannot write to the variables V1 through V4. The two programs are similar, except that in the second one the outer loop is broken down into smaller chunks of size V4. The call to min inside the loop condition ensures that the programs are equivalent even if the outer loop cannot be broken down into an exact number of full chunks, by potentially cutting the final chunk short.

As in previous examples, we use a helper circularity, which consists of the two programs snapshotted at S1. The only constraints that we need are the conditions needed for both programs to reach S1 (i.e., that all loop conditions evaluate to true).

RMT is able to successfully prove the equivalence of the two programs.

V1 = 0;	V1 = 0;	
	while (V1 < V2) {	
	V3 = 0;	
while (V1 < V2) {	while (V3 < V4) {	
S1;	S1;	
V1 = V1 + 1;	V3 = V3 + 1;	
}	}	
	V1 = V1 + V4;	
	}	

This second example of loop tiling is similar to the first one, except we assume that V2 is a multiple of V4. This allows avoiding the overhead of treating the case in which the outer loop cannot be broken into an exact number of full chunks.

Even though the code in this second example is simpler than the first one, the fact that we have to consider that V2 is a multiple of V4 introduces a component of non-linear integer algebra, which Z3 cannot properly handle. Because of this, as explained in Section 6, this example can currently be proven by RMT only when the loop limit (the value of V2) is bounded. Again, the bound is not a limitation of RMT itself. It might be possible to use another SMT solver, such as CVC4, as an oracle that can handle this case of non-linear integer algebra. We leave this for future work. The names of the two files corresponding to this examples are of the form imp-loop-tiling*.rmt.

D Examples

In this section, we describe in greater detail all functional equivalence examples that we prove in IMP.

Example 1: recursive functions with and without an accumulator This example corresponds to the motivating example in Section 1, of showing the equivalence of function with and without accumulators. We use the language IMP_1 (unbounded stack). We prove the following goal:

 $\langle \operatorname{call} f(\mathsf{N}) \rightsquigarrow [], \operatorname{env}, fs \rangle \rangle \prec \langle \operatorname{call} F(\mathsf{N}, 0, 0) \rightsquigarrow [], \operatorname{env}, fs \rangle \text{ if } 0 \leq \mathsf{N},$

where $fs = \{f \mapsto \lambda x. \text{ if } 0 \leq x \text{ then } x + \text{ call } f(x-1) \text{ else } 0\}, F \mapsto \lambda n.\lambda i.\lambda a.$ if $i \leq n \text{ then call } F(n, i+1, a+i) \text{ else } a\}.$

Note that \mathbf{F} , \mathbf{f} , \mathbf{n} , \mathbf{i} , \mathbf{a} are identifiers (program variables), while N and \mathbf{env} are variables of type Int and Env (from identifiers to integers). The fact that the programs run with the same input is implemented by the fact that the same variable N appears in both the lhs (... call $\mathbf{f}(N)$...) and the rhs (... call $\mathbf{F}(N, \mathbf{0}, \mathbf{0})$...). The two programs configurations have the same environment *env*, although, as there are no global variables in the examples, the environment does not matter.

For the set *B* of base cases, we use $B = \{\langle [s], env, fs \rangle \prec \langle [s], env, fs \rangle \}$, where s is a variable of sort Int (recall that [s] is a notation for the one-element cons-list $s \rightsquigarrow []$). That is, two terminal configurations are considered equivalent if the programs are reduced to the same integer s and the environments are the same.

As explained in the introduction, in order to express the circularities, we create a defined function **reduce**, axiomatized by the following constrained rules:

- 1. reduce(I, N) \longrightarrow [] if I > N;
- 2. reduce $(I, N) \longrightarrow (I + \Box) \sim reduce (I + 1, N)$ if $I \leq N$.

We use two helper circularities to prove the goal:

$$\begin{array}{l} \langle \operatorname{call} f(\mathsf{I}-\mathsf{1}) \\ & \sim \operatorname{reduce}(\mathsf{I},\mathsf{N}), \operatorname{env}, \mathit{fs} \rangle \\ \\ \langle \mathbf{S} \sim \operatorname{reduce}(\mathsf{I},\mathsf{N}), \underset{\mathsf{env}, \mathit{fs} \rangle}{\langle \operatorname{call} F(\mathsf{N},\mathsf{I},\mathsf{S})], \\ & \operatorname{env}, \mathit{fs} \rangle \\ \end{array} \quad \text{if } \mathsf{0} \leq \mathsf{I} \leq \mathsf{N},$$

The first circularity represents the expansion phase of the left-hand side program, while the second circularity corresponds to the contraction phase, as explained in the introduction. Our prover can establish using the circularities above that $\mathbf{f} \prec \mathbf{F}$ and that $\mathbf{f} \preceq \mathbf{F}$ under the constraint $N \ge 0$. By \mathbf{f} we formally mean $\langle [\operatorname{call} \mathbf{f}(N)], \operatorname{env}, fs \rangle$ and by \mathbf{F} we formally mean $\langle [\operatorname{call} \mathbf{F}(N, \mathbf{0}, \mathbf{0})], \operatorname{env}, fs \rangle$, as introduced above (we use this shorthand in the following two examples as well). By reversing the lhs and rhs of the circularities, our algorithm can also show $\mathbf{F} \preceq \mathbf{f}$ under the constraint $N \ge \mathbf{0}$. However, it cannot show $\mathbf{F} \prec \mathbf{f}$ under the same constraint, because the circularity for the second phase of \mathbf{f} cannot be established due to lack of progress on the left-hand side. **Therefore, our tool** establishes partial equivalence of f and F and half of what is necessary for full equivalence. As future work, in order to enable the complete proof of full equivalence, we will add termination measures to the proof system as in [9] – the termination measure for the second phase of f will enable $\mathbf{F} \prec \mathbf{f}$ to be proven. The names of the four files corresponding to this example are of the form example1*.rmt.

Example 2: recursive functions in the presence of a bounded stack. In this example, we work in the language IMP_2 , which has a bounded stack of length 10.. The equivalence between **f** and **F** does not hold in IMP_2 (because for a sufficiently high input, **F** will work as expected, while **f** will crash with a stack overflow). Our tool correctly fails to prove, in the operational semantics IMP_2 , any of the cases $\mathbf{f} \prec \mathbf{F}, \mathbf{F} \prec \mathbf{f}, \mathbf{f} \prec \mathbf{F}, \mathbf{F} \prec \mathbf{f}$ (under the constraint $N \ge \mathbf{0}$). We used the same base cases and circularities as above. The names of the four files corresponding to this examples are of the form example2*.rmt.

Example 3: two different semantics. As explained in Section 5, our algorithm for functional equivalence works even for two programs written in different languages. We exploit this to prove that \mathbf{f} , interpreted in IMP_1 , is partially equivalent to \mathbf{F} , interpreted in IMP_2 . The equivalence works because \mathbf{F} uses constant stack space, so it works properly in IMP_2 . The only simulation which the tools fails to prove in this setting is $\mathbf{F} \prec \mathbf{f}$, for the same reasons as above. The names of the four files corresponding to this example are of the form example3*.rmt.

Example 4: imperative and functional style. This example shows that our proof method allows proofs of structurally different programs. We show that a recursive function is equivalent to a while loop (both computing the sum of the first N numbers). We prove:

$$\langle \text{call f}(\mathsf{N}) \\ \sim \langle \text{[], env, } fs \rangle \stackrel{\leq}{\prec} \frac{ \substack{\text{s} = 0; \\ \text{s} = 0; \\ \text{while}(i \leq \mathsf{N}) \\ \text{s} := \text{s} + i; \\ i := i + 1 \\ \sim \langle \text{[], env, } fs \rangle } \text{ if } 0 \leq \mathsf{N}$$

and vice-versa (rhs partially simulated by lhs and lhs partially simulated by rhs), where $fs = \{ \mathbf{f} \mapsto \lambda \mathbf{x}. \text{ if } \mathbf{0} \leq \mathbf{x} \text{ then } \mathbf{x} + \text{ call } \mathbf{f}(\mathbf{x} - \mathbf{1}) \text{ else } \mathbf{0} \}$. We can also show full simulation for one of the direction (the other direction fails for the same reason as in the first example). The fact that both programs take the same input is represented by the integer variable N appearing in both sides. The same variable env is also used on both sides, meaning that the two programs start with the same set of values associated to the global variables (however, as the programs do not depend on the value of the globals, the equivalence proof would also work when starting with two different environments).

An interesting observation in this example is that the first program is written in a functional style and therefore it will reduce to a value without modifying the environment. The imperative program will hold the result in the environment, associated to the program identifier s. Additionally, the second program will modify in the environment the variable i, whose value should not considered to be part of the result of the program. Therefore, the set of base cases we use is

 $B = \{ \langle [x], env_1, fs \rangle \prec \langle [], env_2, fs \rangle \text{ if } x = lookup(s, env_2) \}.$

The files corresponding to this example are of the form example4*.rmt.

Example 5: loop unswitching We prove:

$$\begin{array}{ll} & \langle \mathbf{a} := \mathsf{A}; \\ \mathbf{y} := \mathsf{Y}; \\ \text{if even(a) then} \\ & \text{while}(\mathbf{y} \leq \mathsf{N}) \\ & \mathbf{y} := \mathbf{y} + 1 \\ \text{else} \\ & \text{while}(\mathbf{y} \leq \mathsf{N}) \\ & \mathbf{y} := \mathbf{y} + 2 \\ & \sim [], \mathsf{env}, f_S \rangle \end{array} \begin{array}{ll} & \langle \mathbf{a} := \mathsf{A}; \\ & \mathbf{y} := \mathsf{Y}; \\ & \text{while}(\mathbf{y} \leq \mathsf{N}) \\ & \text{if even(a) then} \\ & \mathbf{y} := \mathbf{y} + 1 \\ & \text{else} \\ & \mathbf{y} := \mathbf{y} + 2 \\ & \sim [], \mathsf{env}, f_S \rangle \end{array}$$

and vice-versa, where fs is arbitrary. For this, we require two circularities:

$$\begin{array}{ll} \langle \text{while}(\text{y} \leq \mathbb{N}) & \text{if even(a) then} \\ \text{y:=y+1} & \prec & \text{y:=y+1} \\ \sim [], \text{env}, fs \rangle & \text{y:=y+2} \\ & & \swarrow [], \text{env}, fs \rangle \end{array} \text{ if even(lookup(\text{env}, a))}$$

and

We use the base cases

$$B = \{ \langle [], \mathsf{env}_1, f_s \rangle \prec \langle [], \mathsf{env}_2, f_s \rangle \text{ if } \mathsf{lookup}(\mathsf{env}_1, \mathbf{y}) = \mathsf{lookup}(\mathsf{env}_2, \mathbf{y}) \}.$$

That is, we consider two terminal configurations to be equivalent when the corresponding environments map the program variable **y** to the same value. The names of the files corresponding to this example are of the form example5*.rmt.