Proof-Producing Translation of Functional Programs into a Time & Space Reasonable Model

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Abstract. We present a semi-automated framework to construct and reason about programs in a deeply-embedded while-language. The while-language we consider is a simple computation model that can simulate (and be simulated by) Turing Machines with a quadratic time and constant space blow-up. Our framework derives while-programs from functional programs written in a subset of Isabelle/HOL, namely tail-recursive functions with first-order arguments and algebraic datatypes. As far as we are aware, it is the first framework targeting a computation model that is reasonable in time and space from a complexity-theoretic perspective.

Keywords: Program synthesis \cdot Certified compilation \cdot Interactive theorem proving \cdot Complexity theory \cdot Computation models

1 Introduction

A large array of mathematical results has been formlised in interactive theorem provers. One example is theoretical computer science, where extensive results on algorithm correctness and computational objects, such as reductions, were proven. Nonetheless, one type of results has proved to be particularly hard to formalise: the construction and verification of algorithms modelled within a deeply embedded computation model, such as a Turing machine. These constructions, however, are crucial to formalise the theory of efficient algorithms and computational complexity theory as understood by practitioners of theoretical computing. In these fields, most results show that an algorithm runs in polynomial time (worst-case, average case, etc.) when implemented as a program within a reasonable computation model, i.e. a model that can simulate Turing machines with a polynomial time and constant space overhead for all computations [36]. Previous work on reasoning about concrete programs within a deeply embedded computation model did so in one of two ways:

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- (1) Automated synthesis of deeply embedded programs from functional programs in the theorem prover's logic along with equivalence proofs [11,30]. In the context of formalising complexity theory, this approach was only used for a lambda calculus model so far [10]. In practical verification contexts, it was used for a lambda calculus model [30] and assembly [29].
- (2) Interactively proving properties of deeply embedded programs, mainly using Hoare or other program logics. This approach is used in many practical verification settings [16, 18, 20] and has been applied to imperative languages, including toy languages [32], C, Java, and Rust. In the context of formalising theoretical computer science, this approach was mainly used for Turing machines [4, 13, 39], with few applications to lambda calculus [14, 34] and partial recursive functions [6].

To formalise the theory of efficient algorithms and complexity theory, we suggest the synthesis into a simple, imperative, and reasonable computation model.

Why? As others have noted [11, 15], reasoning about programs in a theorem prover's native language is significantly easier than reasoning about deeply embedded programs. This is crucial when verifying complex algorithms. For example, Gäher and Kunze [15] proved the Cook-Levin theorem with native Coq programs, benefiting from existing tools and automation. In contrast, Balbach [5] directly reasoned about Turing machines in Isabelle/HOL, requiring extensive low-level reasoning. Others [27] note difficulties when reasoning about deeply-embedded programs, e.g. missing warning messages and no static type checking.

Although automated synthesis methods exist for lambda calculi, we believe it is worthwhile to develop them for an imperative model. The main reason is that the lambda calculi used in previous work are *less equivalent* to Turing machines than imperative models: they are only reasonable for computations solving decision problems but not reasonable in space in general [12]. This limits their applicability when analysing complexity-theoretic questions.

Finally, while there exists a synthesis-based method for x86-assembly in Coq [29], it does not support user-defined datatypes, only allows pattern matching and recursion with fixed recursion schemes, and its target language's semantics are vastly more complicated than needed for complexity-theoretic questions.

Contribution We present a framework that synthesises verified programs in a simple while-language that is reasonable ($\mathsf{IMP}^{\mathsf{W}}$) w.r.t. time and space in Isabelle/HOL. Our framework takes tail-recursive, first-order functions¹ with algebraic datatypes as input. We call this fragment $\mathsf{HOL}^{\mathsf{TC}}$. Given a $\mathsf{HOL}^{\mathsf{TC}}$ function f, our proof-producing metaprogram synthesises a related $\mathsf{HOL}^{\mathsf{TC}}$ function which only operates on natural numbers. We call this $\mathsf{HOL}^{\mathsf{TC}}$ fragment $\mathsf{HOL}^{\mathsf{TCN}}$.

The resulting $\mathrm{HOL^{TC\mathbb{N}}}$ function $f^{\mathrm{TC\mathbb{N}}}$ is compiled into a program p of our deeply embedded, imperative language $\mathrm{IMP^{TC}}$, which supports function calls and tail-recursion. We provide automation to interactively prove the correspondence

¹ Although the framework does not support higher-order functions, each first-order instance of such a function can be compiled as described in Section 4.

$$\begin{array}{c} \text{HOL}^{\text{TC}} & \xrightarrow{\text{proof-producing metaprogram}} \text{HOL}^{\text{TCN}} \\ \text{verified compilers} & & \downarrow \text{interactive deep embedding} \\ \text{IMP}^{-} & \longleftarrow & \text{IMP}^{\text{W}} & \longleftarrow & \text{IMP}^{\text{TC}} \end{array}$$

Fig. 1: Compilation pipeline from HOL^{TC} functions to IMP⁻ programs.

between f^{TCN} and p. In all examples we tried, the proofs were automatic. Finally, a verified chain of compilers in Isabelle/HOL translates IMP^{TC} programs into programs in our target computation model IMPW. Fig. 1 gives an overview. The blow-up introduced by each compiler is linear in the execution time.

Furthermore, we verify a compiler for IMP^W programs that compiles them into programs in IMP⁻, a computation model with fixed bit-width registers. This is a step towards showing that our framework and computation model are suited for formalising significant theorems in complexity theory, like the Cook-Levin Theorem, many of which need bit-blasting into a bounded bit-width computation model as a major proof step. We show that this compilation step is correct and leads to a running blow-up linear in the product of the IMP^W program running time and the size of the input.

The target language only has one-bit-wide registers and only allows comparison to zero as well as bit assignments. Both operations take constant time. This is in addition to the regular program constructs of if-then-else and while-loops. Hence it is clear that IMP⁻ is reasonable with respect to memory and time.

Availability This article's supplementary material² includes the formalisation and a guide linking all definitions, results, and examples to their counterpart in the formalisation. Theorems 1 and 6-8 and all underlying sub-results are formalised in Isabelle/HOL. Other proofs are provided in the appendix.

$\mathbf{2}$ **Preliminaries**

We built our framework in Isabelle/HOL [33], but our approach could be followed in any simple type theory (higher-order logic) [7] or more expressive foundation. We use standard lambda calculi syntax, i.e. $t := \lambda x \cdot t \mid t_1 t_2 \mid x \mid f$, where $\lambda x \cdot t$ denotes function abstractions, $t_1 t_2$ function applications, x bound variables, and f functions with defining equations $f = \lambda \vec{x} \cdot t$. We write $t : \alpha$ for "t has type α ". We use vector notation for n-ary applications, abstractions, and inputs:

$$f \vec{x} \equiv f x_1 \cdots x_n \qquad \lambda \vec{x} \cdot t \equiv \lambda x_1 \cdots x_n \cdot t \qquad (1)$$

$$\overrightarrow{f_i x_i} \equiv (f_1 x_1) \cdots (f_n x_n) \qquad \overrightarrow{\alpha} \Rightarrow \alpha \equiv \alpha_1 \Rightarrow \cdots \alpha_n \Rightarrow \alpha \qquad (2)$$

$$\overrightarrow{f_i} \overrightarrow{x_i} \equiv (f_1 x_1) \cdots (f_n x_n)$$
 $\overrightarrow{\alpha} \Rightarrow \alpha \equiv \alpha_1 \Rightarrow \cdots \alpha_n \Rightarrow \alpha$ (2)

A function $f: \vec{\alpha} \Rightarrow \alpha$ is called *higher-order* if some α_i is a function type. Otherwise, it is called *first-order*. An application $f \vec{x} : \alpha$ is called *higher-order*

 $[\]frac{1}{2}$ swh:1:dir:0885d0653246b8b2e81f168ed4a596d29200deed

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t ::= \operatorname{let} x = t_1 \operatorname{in} t_2 \qquad \qquad (\operatorname{bind} t_1 \text{ to } x \text{ in } t_2)
\mid (\operatorname{case}_d t \text{ of } \overrightarrow{x_1} \Rightarrow t_1 \mid \cdots \mid \overrightarrow{x_n} \Rightarrow t_n) \qquad (\operatorname{case \ combinator \ of \ ADT \ } \overrightarrow{\alpha} d)
\mid h \overrightarrow{t} \qquad \qquad (\operatorname{first-order \ application})
h ::= x \mid g \mid f \qquad (\operatorname{bound \ variable} x, \operatorname{function} g, \operatorname{or} f \operatorname{ itself})
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Fig. 2: Grammar for body t of a first-order function $f = \lambda \vec{x} \cdot t$ with ADTs.

if α is a function type. Otherwise, it is called *first-order*. An algebraic datatype (ADT) $\overrightarrow{\alpha} d = C_1 \overrightarrow{\alpha_1} \mid \cdots \mid C_n \overrightarrow{\alpha_n}$ is a possibly recursive sum type of product types with constructors $C_i : \overrightarrow{\alpha_i} \Rightarrow \overrightarrow{\alpha} d$ and case combinator $\mathsf{case}_d : (\overrightarrow{\alpha_1} \Rightarrow \alpha) \Rightarrow \cdots \Rightarrow (\overrightarrow{\alpha_n} \Rightarrow \alpha) \Rightarrow \overrightarrow{\alpha} d \Rightarrow \alpha$.

Our framework takes as an *input language* tail-recursive, first-order functions $f = \lambda \vec{x} \cdot t$, where \vec{x} are the *arguments* bound in the *body t*. The body may use other such functions and ADT functions in first-order applications. Fig. 2 shows the grammar for recursive, first-order function bodies. Our input language HOL^{TC} is the subset where each recursive call f \vec{t} is in tail-position.

We use several deeply-embedded, deterministic languages based on the *imperative language* IMP from Winskel's book [38], which is well-studied in formal verification [31,35]. Our IMP languages operate on a *state* of type string \Rightarrow val. Terms of type string are called *registers* and terms of type val are called *values*. The registers in a program p are denoted by regs p. As a computation model, IMP allows simple reasoning about space since there is no indirect memory addressing – only registers occurring in a program can be accessed. In our final model, IMP⁻, values are single bits, making the space usage bounded by regs p. We define IMP⁻ in Section 5.3, and a summary of all IMP languages can be found in Appendix D. Here, we describe the intermediate languages used during compilation. They use values of type $\mathbb N$ and consist of atoms, (arithmetic) expressions and (imperative) commands. Every atom is also an arithmetic expression.

We now define the *semantics*. With $[\![A]\!]_s$ and $[\![a]\!]_s$ we denote the evaluation (returning a natural number) of an atom A and expression a, respectively, under state s, defined by the rules in Figs. 3(a) and 3(b). With $tp \vdash (p,s) \Rightarrow_R^n s'$ we denote that in context of the program tp, tp the program tp started from tp terminates in at most tp steps with state tp such that tp is tp for all tp in tp.

$$(tp \vdash (p,s) \Rightarrow_{R}^{n} s') \equiv \exists n' s''. tp \vdash (p,s) \Rightarrow^{n'} s'' \land \forall r \in R. s' r = s'' r \land n' \le n,$$

where \Rightarrow^n is the (big-step) execution relation, defined inductively using the rules from Fig. 3(c) along with the language-specific rules specified in their respective sections. In rule ASSIGN, the state s is updated at register r using the state update notation $s(r := v) \equiv \lambda r'$. if r = r' then v else s r'. If we are only interested in a single return register r, we write

$$(tp \vdash (p,s) \Rightarrow_r v) \equiv \exists s'. (tp \vdash (p,s) \Rightarrow s' \land s' r = v).$$

³ The context is only relevant for recursive calls in Section 4.

$$[\![\mathbb{C} \, n]\!]_s \equiv n, \quad [\![\mathbb{R} \, r]\!]_s \equiv s \, r \qquad \qquad [\![A_1 \otimes A_2]\!]_s \equiv [\![A_1]\!]_s \otimes [\![A_2]\!]_s, \text{ for } \otimes \in \{+,-\}$$

(a) Evaluation of atoms A. (b) Ev

(b) Evaluation rules for arithmetic expressions.

(c) Execution relation for commands, where each \mathcal{C} is a fixed, non-negative constant.

Fig. 3: Semantics shared by our IMP-languages, excluding the final IMP⁻.

To simplify notation, we omit "... \vdash " if the context is irrelevant, R if the program terminates exactly with state s', and n if the number of steps is irrelevant.

One may question why rule ASSIGN only takes constant, and not logarithmic, time. This is merely for simplicity and makes no difference for polynomial time considerations since logarithmic space usage (i.e. space usage in a binary encoding of \mathbb{N}) is bounded by time in all intermediate IMP languages, as shown in Theorem 1. For this, let a_{max} denote the largest constant in an expression a, p_{max} the largest constant in a program p, and $s_{\text{max}} \equiv \max\{s \ r \mid r : \text{string}\}$.

Theorem 1. If
$$max\{s_{max}, p_{max}\} < 2^w$$
 and $(p, s) \Rightarrow^n s'$, then $s'_{max} < 2^{w+n}$.

Proof sketch. The proof is by induction over the execution relation. In case of an assignment, the maximum size can at most double. In other cases, the claim holds by applying the induction hypothesis, followed by algebraic manipulation. \Box

3 $HOL^{(TC)}$ to $HOL^{(TC)N}$

This section describes the proof-producing translation of $\mathrm{HOL^{TC}}$ functions into equivalent $\mathrm{HOL^{TCN}}$ functions. More generally, our translation applies to any HOL function f with ADTs, producing a $\mathrm{HOL^{N}}$ function $f^{\mathbb{N}}$ that operates only on natural numbers while preserving tail-recursiveness and first-order applications.

Intuitively, the function f and its translation $f^{\mathbb{N}}$ should compute the same values for the same inputs, up to encoding and decoding. Our method is based on a technique called transport, which, intuitively, takes objects of one type and derives that "corresponding" objects exist of another type, synthesising the latter objects as necessary. To formalise this correspondence, we first review some concepts on relations.

Definition 1. A relation on α and β is a function of type $\alpha \Rightarrow \beta \Rightarrow \text{bool}$. Two functions f, g are related from R to S if they map R-related inputs to S-related

outputs, written $(R \Rightarrow S)$ $f g \equiv \forall x y. R x y \longrightarrow S(f x)(g y)$. Repeated relations are abbreviated as $(R^n \Rightarrow S) \equiv (R \Rightarrow \cdots \Rightarrow R \Rightarrow S)$, i.e. R repeated n-times.

We can now define the desired relation between f and $f^{\mathbb{N}}$.

Definition 2. A type α is encodable if there are functions natify: $\alpha \Rightarrow \mathbb{N}$ and denatify: $\mathbb{N} \Rightarrow \alpha$ such that denatify (natify x) = x for all x.

We say that $n:\mathbb{N}$ and $x:\alpha$ are (RN-)related if they represent the same value: RN $nx\equiv n=$ natify x. A number n is well-encoded (with respect to α) if RN nx holds for some $x:\alpha$. We lift this relation to functions and say that $f^{\mathbb{N}}:\alpha^{\mathbb{N}}$ and $f:\alpha$ are RN-related if $\alpha^{\mathbb{R}\mathbb{N}}f^{\mathbb{N}}f$, where $\alpha^{\mathbb{N}},\alpha^{\mathbb{R}\mathbb{N}}$ are defined recursively:

$$(\alpha \Rightarrow \beta)^{\mathbb{N}} \equiv \alpha^{\mathbb{N}} \Rightarrow \beta^{\mathbb{N}}, \quad \alpha^{\mathbb{N}} \equiv \mathbb{N}, \qquad (\alpha \Rightarrow \beta)^{\mathbb{R}\mathbb{N}} \equiv \alpha^{\mathbb{R}\mathbb{N}} \Rightarrow \beta^{\mathbb{R}\mathbb{N}}, \quad \alpha^{\mathbb{R}\mathbb{N}} \equiv \mathbb{R}\mathbb{N}.$$

Objective 1. Given a HOL function f, synthesise a \mathbb{RN} -related $\mathrm{HOL}^{\mathbb{N}}$ term $f^{\mathbb{N}}$. Moreover, the synthesis preserves tail-recursiveness and first-order applications on well-encoded inputs.

We achieve this in two steps: First, we encode the datatypes used by f (Section 3.1). Second, we synthesise a HOL^N term f^N related to f (Section 3.2).

3.1 Encoding of Datatypes

Let $\overrightarrow{\alpha} d = C_1 \overrightarrow{\alpha_1} \mid \cdots \mid C_n \overrightarrow{\alpha_n}$ be an ADT with $a_i \equiv |\overrightarrow{\alpha_i}|$. We want to encode $\overrightarrow{\alpha} d$ according to Def. 2. Assuming that all $\alpha \in \overrightarrow{\alpha_1} \cup \cdots \cup \overrightarrow{\alpha_n}$ are encoded or $\alpha = \overrightarrow{\alpha} d$, the existence of suitable en- and decoding functions is straightforward. Following Gordon's approach [17] to encode the type of lists, each value $C_i \overrightarrow{x}$ is encoded as a tagged and nested pair. Datatypes are encoded recursively this way, using natural numbers as the base type:

Definition 3. Fix an injective pairing function pair : $\mathbb{N}^2 \Rightarrow \mathbb{N}$ with inverses fst, snd, i.e. fst (pair nm) = n and snd (pair nm) = m. We define $C_i^{\mathbb{N}} : \mathbb{N}^{a_i} \Rightarrow \mathbb{N}$ by $C_i^{\mathbb{N}} \overrightarrow{x} \equiv \text{pair } i$ (if $a_i = 0$ then 0 else (pair x_1 (pair $x_2(\cdots (\text{pair } x_{a_{i-1}} x_{a_i}) \cdots))$). For each i, j, we define the selector select_{i,j} $x \equiv (\text{if } j < i \text{ then fst else id}) (\text{snd}^j x)$. Using the selector, we can define a companion $\text{case}_d^{\mathbb{N}}$ for the case combinator case_d using a nested if-then-else construction. Details can be found in Appendix A.1.

These functions suffice to show that $\vec{\alpha} t$ is encodable:

Theorem 2. $\overrightarrow{\alpha} d = C_1 \overrightarrow{\alpha_1} \mid \cdots \mid C_n \overrightarrow{\alpha_n}$ is encodable if all $\alpha \in \overrightarrow{\alpha_1} \cup \cdots \cup \overrightarrow{\alpha_n}$ are encoded or $\alpha = \overrightarrow{\alpha} d$. Also, for all $1 \leq i \leq n$, $1 \leq j \leq a_i$ and relations R, we have

$$\begin{split} \left(\mathsf{R}\mathbb{N}^{a_i} \Rrightarrow \mathsf{R}\mathbb{N}\right) C_i^{\mathbb{N}} \, C_i, & \mathsf{R}\mathbb{N} \, n \, (C_i \, \overrightarrow{x}) \implies \mathsf{R}\mathbb{N} \, (\mathsf{select}_{a_i,j} n) \, x_j, \\ \left(\left(\mathsf{R}\mathbb{N}^{a_1} \Rrightarrow R\right) \Rrightarrow \cdots \Rrightarrow \left(\mathsf{R}\mathbb{N}^{a_n} \Rrightarrow R\right) \Rrightarrow \mathsf{R}\mathbb{N} \Rrightarrow R\right) \mathsf{case}_d^{\mathbb{N}} \, \mathsf{case}_d. \end{split}$$

The described pipeline is fully automatic in our framework. An example application can be found in Appendix A.1. We note that our underlying pairing function is the Cantor pairing function, which results in a number computable in time polynomial in the sizes of the two numbers in the encoded pair.

⁴ In the formalisation, natify, denatify are overloaded as part of a typeclass.

3.2 Synthesis of $HOL^{\mathbb{N}}$ Functions

Let $f = \lambda \vec{x} \cdot t$ be a HOL function of type α . We aim for Objective 1. For this, we can assume that all ADTs in α are encoded and every user-specified function $g \neq f$ in t is already compiled – and thus RN-related to some $g^{\mathbb{N}}$.

Our approach combines black-box and white-box transports [19, 22, 37] in a novel way, to the best of our knowledge. Both kinds of transport take a term $t:\alpha$ and a relation R as input and synthesise a term t' together with a proof that Rt't. While black-box transports do so using only the structure of α and R, white-box transports also use the structure of t.

Our approach is as follows: (1) Use black-box transport to obtain a function $f^{\mathbb{N}}$ that is RN-related to f. (2) Use white-box transport to obtain a term $(\lambda \vec{x}.t)^{\square}$ that uses $f^{\mathbb{N}}$ and which is also RN-related to f. (3) Derive the recursive equation $f^{\mathbb{N}} = (\lambda \vec{x}.t)^{\square}$ using that RN is left-unique. The use of black-box transports relies on the fact that RN can be used as a relation by TRANSPORT [22]:

Theorem 3 (Blackbox-Transport [22]). RN, natify, and denatify form a partial Galois equivalence. Thus, there is some $f^{\mathbb{N}}$ that is RN-related to f.

In the formalisation, we use the Transport prototype [21] to obtain $f^{\mathbb{N}}$. Since the black-box transport disregards the structure of t, Theorem 3 may not preserve tail-recursiveness and first-order applications. To derive an equation $f^{\mathbb{N}} = \lambda \overrightarrow{x^{\mathbb{N}}}$. $t^{\mathbb{N}}$ structurally related to the one of f, we use white-box transport:

Definition 4. The white-box-transport of $\lambda \vec{x}$. t replaces every subterm by its RN-related companion. It is defined recursively by

$$(\lambda \overrightarrow{x}.s)^{\square} \equiv \lambda \overrightarrow{x^{\mathbb{N}}}.s^{\square}, \qquad (t_1\,t_2)^{\square} \equiv t_1^{\square}t_2^{\square}, \qquad x_i^{\square} \equiv x_i^{\mathbb{N}}, \qquad g^{\square} \equiv g^{\mathbb{N}}, \qquad f^{\square} \equiv f^{\mathbb{N}}.$$

Theorem 4 (Whitebox-Transport [19]). $(\lambda \vec{x}.t)^{\square}$ and $\lambda \vec{x}.t$ are RN-related and white-box transports preserve tail-recursiveness and first-order applications.

Theorem 5. If
$$\overrightarrow{\mathsf{RN}} \overrightarrow{x_i^{\mathbb{N}}} x_i$$
 then $f^{\mathbb{N}} \overrightarrow{x^{\mathbb{N}}} = t^{\square}$.

Proof. We have $\mathbb{RN}(f^{\mathbb{N}}\overrightarrow{x^{\mathbb{N}}})(f\overrightarrow{x})$ and $\mathbb{RN}(t^{\square})(f\overrightarrow{x})$ by Theorems 3 and 4. Moreover, \mathbb{RN} is left-unique by Def. 2. Thus $f^{\mathbb{N}}\overrightarrow{x^{\mathbb{N}}} = t^{\square}$.

Theorems 3–5 show that we have achieved Objective 1. The described synthesis is fully automatic in our framework. An example is shown in Fig. 4.

4 HOL^{TCN} to IMP^{TC}

We next describe the deep embedding from HOL^{TCN} to IMP^{TC} . Fig. 5 shows the IMP^{TC} -specific commands and their semantics, extending those in Fig. 3(c). Notably, IMP^{TC} supports calls of IMP^{W} programs (defined in Section 5.2) and

Listing 1.1 Input function from the user. Listing 1.2 Constant $\mathtt{count}^{\mathbb{N}}$ and related-count \mathtt{a} xs \mathtt{n} = case xs of [] \Rightarrow \mathtt{n} ness theorem from black-box transport. | x # xs \Rightarrow count \mathtt{a} xs (RN \Rightarrow RN \Rightarrow RN) count $^{\mathbb{N}}$ count (if x = a then Suc n else n)

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Listing 1.3 White-box transport theorem. Listing 1.4 Final tail-recursive equation.  (\mathsf{R}\mathbb{N} \Rightarrow \mathsf{R}\mathbb{N} \Rightarrow \mathsf{R}\mathbb{N} \Rightarrow \mathsf{R}\mathbb{N}) \qquad \qquad \mathsf{R}\mathbb{N} \Rightarrow \mathsf{R}\mathbb{N} \Rightarrow \mathsf{R}\mathbb{N}) \qquad \qquad \mathsf{R}\mathbb{N} \Rightarrow \mathsf{R} \Rightarrow \mathsf{R}\mathbb{N} \Rightarrow \mathsf{R}\mathbb{N} \Rightarrow \mathsf{R}\mathbb{N} \Rightarrow \mathsf{R}\mathbb{N} \Rightarrow \mathsf{R}\mathbb{N} \Rightarrow \mathsf{R} \Rightarrow \mathsf{R
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Fig. 4: For the user-specified function⁵ count in Listing 1.1, we obtain a related constant $count^{\mathbb{N}}$ in Listing 1.2 using Theorem 3. Using Theorem 4, we obtain a second term related to count in Listing 1.3. Using that RN is left-unique (cf. Theorem 5), we derive the desired equation for $count^{\mathbb{N}}$ in Listing 1.4.

$$\operatorname{Call} \frac{(pc,s) \Rightarrow_r^n v \qquad s' = s(r \coloneqq v)}{p \vdash (\operatorname{CALL} pc \ \operatorname{RETURN} r,s) \Rightarrow_r^n s'} \qquad \operatorname{REC} \frac{p \vdash (p,s) \Rightarrow_r^n s'}{p \vdash (\operatorname{RECURSE},s) \Rightarrow_r^{n+\mathcal{C}} s'}$$

Fig. 5: Execution relation of IMP^{TC}-specific commands.

tail-recursion. It also supports if-then-elses but no case combinators. Since every $\mathsf{case}_d^{\mathbb{N}}$ is defined as a nested if-then-else construction (Def. 3), this is sufficient.

To relate a HOL^{TCN} function f^{TCN} , with its conditional (recursive) equation $\overline{\text{RN}} \, x_i^{\mathbb{N}} \, x_i \implies f^{\text{TCN}} \, \overline{x^{\mathbb{N}}} = t^{\text{TCN}}$, to an IMP^{TC} program p, we presume injective functions arg, ret such that (1) $\arg_{f,i}$ returns a unique name for the i-th argument of f and (2) ret_f returns a unique name for the result computed by f.

We focus on total, functional correctness of p in this work (proving concrete time bounds for p is left as future work, see Section 6): From any state s with well-encoded inputs \overrightarrow{s} arg $_{f,i}$, the program p terminates and the value in return register ret $_f$ is equal to f^{TCN} \overrightarrow{s} arg $_{f,i}$. Formally, our objective is:

Objective 2. Given a HOL^{TCN} function f^{TCN} , compile it to an IMP^{TC} program p such that $p \vdash (p, s) \Rightarrow_{\mathsf{ret}_f} f^{\text{TCN}} \overrightarrow{s} \, \mathsf{arg}_{f,i}$ whenever $\overline{\mathsf{RN}} \, (s \, \mathsf{arg}_{f,i}) \, x_i$.

The deep embedding has two steps: (1) Compile f^{TCN} into an IMP^{TC} program p (Section 4.1) and (2) prove the equivalence between f^{TCN} and p using custom-built automation (Section 4.2). The automation uses symbolic execution,

⁵ There is a commmand in Isabelle/HOL that turns functions specified by multiple equations into an equivalent definition consisting of only one equation.

normalises the (otherwise incomprehensible) program state such that it becomes amenable to automatic proof, and discharges well-encodedness side-conditions.

Note on Higher-Order Functions Since IMP^{TC} does not support higher-order functions, we assume first-order functions as input for our framework. Nevertheless, each first-order instance of a higher-order function can be compiled systematically with our framework. We demonstrate this by means of an example. More cases can be found in the formalisation:

Example 1. Consider the iteration function of type $(\alpha \Rightarrow \alpha) \Rightarrow \mathbb{N} \Rightarrow \alpha \Rightarrow \alpha$:

$$f^n x \equiv \operatorname{case} n \text{ of } 0 \Rightarrow x \mid n+1 \Rightarrow f^n (f x).$$
 (3)

This function cannot be compiled as it is. However, every first-order instance, e.g. snd^j as used in the definition of $\operatorname{select}_{i,j}$ (Def. 3), can be compiled. To do so, we define $\operatorname{powsnd} n \equiv \operatorname{snd}^n$. We then instantiate Eq. (3) with $f = \operatorname{snd}$ and fold the definition of powsnd to obtain $\operatorname{powsnd} n x = \operatorname{case} n$ of $0 \Rightarrow x \mid n+1 \Rightarrow \operatorname{powsnd} n (\operatorname{snd} x)$. This equation can then be compiled with our framework.

4.1 Compilation to IMP^{TC}

We compile $f^{\text{TCN}} \overrightarrow{x^{\mathbb{N}}} = t^{\text{TCN}}$ to an IMP^{TC} program p in two steps. For ease of notation, we drop the superscript and just write f and t below.

First, we parse t into a metaprogram data type resembling HOL^{TCN}. Second, we compile the parsed term to an IMP^{TC} program, as shown in Fig. 6. We denote the compilation by $[\![t]\!]_r^b$, where b is a list of registers holding values of terms bound by enclosing **Let** bindings and r is the register that will hold the program's result.

For a call $\operatorname{Call} g[t_1, \ldots, t_m]$, the compiler retrieves the registered IMP^W implementation g^{IMP} of g. For the primitives equality, addition, and subtraction, manual implementations must be provided to the compiler. The compiler generates fresh register names when needed, namely to compile Let bindings, to store the value of If conditions, and to save function arguments in temporary registers to prevent them from being overwritten. For example, in $\operatorname{Call} g[t_1, \ldots, t_m]$, argument registers could be overwritten if another call of g appears within t_1, \ldots, t_m .

In summary, we parse t into a term t' of the metaprogram datatype and compile t' to the $\mathsf{IMP}^{\mathsf{TC}}$ program $p \equiv \llbracket t' \rrbracket_{\mathsf{ret}_s}^{\rrbracket}$.

4.2 Correctness Proofs

Since the compiler to $\mathsf{IMP}^{\mathsf{TC}}$ is a metaprogram, its correctness cannot be proven in Isabelle/HOL. Instead, the correctness of each compiled program p must be verified individually through automation (a process sometimes called "certified extraction"), which we describe next.

⁶ While the datatype allows recursive calls in non-tail positions, the compiler rejects such terms using a syntactic check.

Fig. 6: The compiler from the HOL^{TCN} representation to IMP^{TC} . Term t_1 in If $t_1 t_2 t_3$ denotes the condition $t_1 \neq 0$, Let $t_1 t_2$ binds t_1 to the first de Bruijn index in t_2 , LetBound i denotes the variable bound by the i-th enclosing Let, and Arg i the i-th argument of f, i.e. x_i .

$$\begin{aligned} &\text{Update } \frac{[\![a]\!]_s \leadsto v}{s(r \coloneqq [\![a]\!]_s) \leadsto s(r \coloneqq v)} & \text{Const } \frac{1}{[\![\mathbf{C}\,n]\!]_s \leadsto n} & \text{Reg } \frac{s\,r \leadsto v}{[\![\mathbf{R}\,r]\!]_s \leadsto v} \end{aligned}$$

$$\text{Hit } \frac{r = r'}{s(r \coloneqq v)\,r' \leadsto v} & \text{Cont } \frac{r \neq r' \qquad s\,r' \leadsto v'}{s(r \coloneqq v)\,r' \leadsto v'} & \text{Arith } \frac{[\![A_1]\!]_s \leadsto v_1 \qquad [\![A_2]\!]_s \leadsto v_2}{[\![A_1]\!]_s \leadsto v_1 \otimes v_2}$$

Fig. 7: State normalisation rules.

First, p is normalised such that no recursive constructor (sequences and ifthen-elses) appears on the left of a sequence. This simplifies the implementation, but shall not concern us any further (for details see Appendix B.2). The automation proceed as follows:

- (1) If f is recursive, start an induction proof on \vec{x} using the induction rule of f.
- (2) Symbolically run p to completion or until a recursive call is encountered. Let s' be the end state.
- (3) Run f^{TCN} to completion with result r or until a recursive call $f^{\text{TCN}} \vec{y}$ is encountered.
- (4) If both computations ran to completion, prove $s' \operatorname{ret}_f = r$. Otherwise, prove $\overrightarrow{s' \operatorname{arg}_{f,i}} = \overrightarrow{y}$ and conclude using the inductive hypothesis.

To run p, we use the execution rules from Figs. 3(c) and 5 (specialised to single return registers)⁷ and the correctness theorems of subprograms. Each update

⁷ The specialisation is routine and can be found in Appendix B.2.

Fig. 8: Step-by-step correctness proof for $count^{\mathbb{N}}$, described in Example 2.

RN (s "a") a \land RN (select_{2,2} (s "xs")) xs \land RN (Suc (s "n")) (Suc n)

to the IMP^{TC} state is normalised with the rules from Fig. 7 to (1) to simplify the proof state for interactive proofs and (2) to speed up the automation. The automation eliminates cases where p and f^{TCN} took different execution branches.

Since our correctness theorems are conditional, the inductive hypothesis and the subprograms' correctness theorems are conditional too. Whenever they are used, goals of the form $\mathbb{RN}\,x^{\mathbb{N}}\,x$ must be solved. This is done automatically by a resolution-based method that uses Def. 1, the relatedness theorems of ADTs and functions (Theorems 2 and 3), and local assumptions. Note that this is essentially a form of type-checking, making sure that all involved terms are well-encoded.

Example 2. We continue with the example from Fig. 4 and show the correctness of $\mathtt{count}^{\mathbb{N}}$. The goal states are shown in Fig. 8. First, the induction rule of \mathtt{count} is applied, creating cases for [] and (#). We focus on the latter. Running $\mathtt{count}^{\mathsf{IMP}}$ and $\mathtt{count}^{\mathbb{N}}$ produces two subcases: one for $\mathtt{x} = \mathtt{a}$ and one for $\mathtt{x} \neq \mathtt{a}$. We consider the former. The new state $\mathtt{s'} = \mathtt{s(r1} := \mathtt{x1,...}$) is obtained from \mathtt{s} by normalised state updates. Due to normalisation, we immediately get:

```
s' "a" = s "a" \wedge s' "xs" = select_{2,2}(s "xs") \wedge s' "n" = Suc(s "n")
```

Thus, the inductive hypothesis can be applied, leaving a set of relatedness goals. These are solved automatically, using the local assumptions, the selector relatedness theorems for lists, and the relatedness theorem for Suc.

Case Studies We applied our framework to typical functional programs, including standard datatype functions (map, fold, ...), the bisection method for square

$$\text{WHF} \ \frac{s \, r = 0}{\text{(WHILE} \ r \ \text{DO} \ p, s) \Rightarrow^{\mathcal{C}} s} \ \text{WHT} \ \frac{s \, r \neq 0 \quad (p, s) \Rightarrow^{n_1} s' \quad \text{(WHILE} \ r \ \text{DO} \ p, s') \Rightarrow^{n_2} s''}{\text{(WHILE} \ r \ \text{DO} \ p, s) \Rightarrow^{n_1 + n_2 + \mathcal{C}} s''}$$

Fig. 9: Execution relation for WHILE.

roots, and problems from complexity theory – such as reductions from SAT to 3SAT and 3SAT to independent sets. The examples can be found in the formalisation. All proofs were automatic, but functions using hundreds of registers had to be split due to inefficient retrievals for the tracked IMP^{TC} state in the current implementation. Performance improvements are future work. We conjecture that our method is complete when applied to programs compiled from HOL^{TC} using our framework, but a formal proof is out of scope.

5 IMP^{TC} to IMP⁻

In this section, we describe the verified chain of compilers from IMP^{TC} to IMP⁻:

Objective 3. For every IMP^{TC} program p, compile an IMP^{-} program p' such that (up to encoding and decoding), for the same input, (1) p and p' compute the same output and (2) the number of steps p' takes is at most polynomially more than the number of steps p takes.

Note that since the size of the values stored in registers is governed by Theorem 1, if the above objective is satisfied, the memory used by the final IMP^- program is polynomial in the size of p and its running time.

The compilation proceeds in several steps: First, we compile recursive calls into while-loops of an intermediate language IMP^{WC} (Section 5.1), Second, we eliminate calls to other programs (Section 5.2). Finally, we use bit blasting to compile into our final language IMP⁻ (Section 5.3).

5.1 IMP^{TC} to IMP^{WC}

In the first step, we replace tail-recursive calls by while-loops, whose semantics are given in Fig. 9. In rule WHT, the loop-condition $r \neq 0$ is checked before stepping into the WHILE. In contrast, tail-recursive calls occur at the end of the program. To bridge this gap, we prove the following rules for IMP^{TC}.

Lemma 1. Let $(p,s) \Rightarrow^n (s',b)$ denote the modified execution relation shown in Fig. 10 that runs p but stops and flags whenever a tail-recursive call is encountered using $b \in \{0,1\}$ Then the following rules are admissible:

$$\frac{(p,s)\Rightarrow^n(s',0)}{tp\vdash(p,s)\Rightarrow^ns'} \qquad \frac{(p,s_1)\Rightarrow^{n_1}(s_2,1) \qquad tp\vdash(tp,s_2)\Rightarrow^{n_2}s_3}{tp\vdash(p,s_1)\Rightarrow^{n_1+n_2}s_3}$$

$$\frac{s \ r \neq 0 \qquad (p_1,s) \Rightarrow^n (s',b)}{(\text{IF } r \text{ THEN } p_1 \text{ ELSE } p_2,s) \Rightarrow^{n+\mathcal{C}} (s',b)} \qquad \frac{(p_1,s) \Rightarrow^{n_1} (s',0) \qquad (p_2,s') \Rightarrow^{n_2} (s'',b)}{(p_1 \ ; \ p_2,s) \Rightarrow^{n_1+n_2+\mathcal{C}} (s'',b)} \\ \frac{s' = s(r \coloneqq \llbracket a \rrbracket_s)}{(r \leftarrow a,s) \Rightarrow^{\mathcal{C}} (s',0)} \qquad \cdots$$

Fig. 10: Execution relation from Lemma 1 that halts with a flag when encountering a tail-recursive call. Omitted rules are routine and listed in Appendix C.1.

Note the similarity between these rules and those for WHT and WHF. These rules suggest a straightforward translation from p to an IMP^{WC} program by using a loop that continues as long as a recursive call would have occurred:

Theorem 6. Let cnt be a fresh register with respect to regs p. Let p[t/x] denote the syntactic substitution of any occurrence of x by t in a program p. Define

$$(p)_{\circlearrowleft} \equiv \text{cnt} \leftarrow 1 \; ; \; \text{WHILE cnt DO cnt} \leftarrow 0 \; ; \; p[(\text{cnt} \leftarrow 1)/\text{RECURSE}].$$

Then it holds that
$$p \vdash (p,s) \Rightarrow_{\mathsf{regs}\, p}^n s'$$
 if and only if $((p)_{\circlearrowleft}, s) \Rightarrow_{\mathsf{regs}\, p}^{n+\mathcal{C}} s'$.

Since we use an additional register, we only get partial equivalence of states in the correctness theorem. This is sufficient for our purposes nonetheless.

5.2 IMPWC to IMPW

We next eliminate calls to IMP^W programs. We simply inline every call to a program p^w by copying its used registers to fresh memory locations, executing the program there, and copying the result register back:

Definition 5. Let regs $p^w = \{r_1, \dots, r_n\}$ and m be a renaming to fresh registers. We define the inlining of a call to program p^w with return register r as

$$(CALL \ p^w \ RETURN \ r)_* \equiv m r_1 \leftarrow r_1 \ ; \cdots \ ; m r_n \leftarrow r_n \ ; p^w [m x/x] \ ; r \leftarrow m r.$$

For an $\mathsf{IMP}^{\mathrm{WC}}$ program p, we let $(p)_{\star}$ denote the $\mathsf{IMP}^{\mathrm{W}}$ program obtained from p by inlining all calls.

Note that called programs must already be compiled to IMP^W and hence do not contain further calls. Arguing about a program in a different memory location requires the obvious substitution lemma:

Lemma 2. $(p[(m x)/x], s) \Rightarrow^n s' \text{ implies } (p, s \circ m) \Rightarrow^n s' \circ m \text{ for injective } m.$

The inlining induces a blow-up that is dependent on the program size (but not the input), as shown below.

Theorem 7. $(p,s) \Rightarrow_{\mathsf{regs}\ p}^n s' \ if ((p)_{\star}, s) \Rightarrow_{\mathsf{regs}\ p}^{f(n,p)} s' \ where \ f(n,p) \ is \ linear \ in \ n \cdot |p|. \ Moreover, \ if ((p)_{\star}, s) \Rightarrow_{\mathsf{regs}\ p}^n s' \ then \ (p,s) \Rightarrow_{\mathsf{regs}\ p}^n s'.$

$$\frac{b \in \{0,1\} \quad s' = s(r \coloneqq b)}{(r \leftarrow b,s) \Rightarrow^1 s'} \qquad \frac{s \, r \neq 0 \quad (p_1,s) \Rightarrow^n s'}{(\operatorname{IF} \, r \, \operatorname{THEN} \, p_1 \, \operatorname{ELSE} \, p_2,s) \Rightarrow^{n+1} s'} \\ \frac{(p_1,s) \Rightarrow^{n_1} s' \quad (p_2,s') \Rightarrow^{n_2} s''}{(p_1\,;\, p_2,s) \Rightarrow^{n_1+n_2+1} s''} \qquad \frac{s \, r = 0 \quad (p_2,s) \Rightarrow^n s'}{(\operatorname{IF} \, r \, \operatorname{THEN} \, p_1 \, \operatorname{ELSE} \, p_2,s) \Rightarrow^{n+1} s'} \\ \frac{s \, r = 0}{(\operatorname{WHILE} \, r \, \operatorname{DO} \, p,s) \Rightarrow^1 s} \qquad \frac{s_1 \, r \neq 0 \quad (p,s_1) \Rightarrow^{n_1} s_2 \quad (\operatorname{WHILE} \, r \, \operatorname{DO} \, p,s_2) \Rightarrow^{n_2} s_3}{(\operatorname{WHILE} \, r \, \operatorname{DO} \, p,s_1) \Rightarrow^{n_1+n_2+2} s_3}$$

Fig. 11: Execution relation for IMP⁻.

Note that the fact that IMP^W is reasonable w.r.t. time and space follows from standard reductions in computability theory. A good exposition is in Erk and Priese's book [9]. There it is shown that While-programs can be simulated by Goto-programs with constant space (one-to-one-correspondence between registers) and polynomial time overheads (Theorem 12.4.3), and Goto-programs can be simulated with constant space (one tape per register) and polynomial time overheads by k-tape Turing Machines (Theorem 11.4.1), and k-tape TMs can be simulated by single-tape TMs in constant space (2k tuple letters per cell) and quadratic running time overheads (Theorem 7.4.5). The other direction, showing that TMs can be simulated by While-programs is obvious.

5.3 IMPW to IMP

Our programs so far operate on arbitrary-size natural numbers. In contrast, our final language IMP⁻ operates on single bits, represented as 0 and 1. The commands of IMP⁻ and their semantics are shown in Fig. 11. There are no arithmetic expressions, and all registers represent a single bit.

We use bit-blasting to compile IMP^W programs to IMP^- programs. The bit-blasting is parametrised with a number w, indicating the bit-width of the compilation. Each IMP^W register r is represented as w+1 fresh IMP^- registers r_0,\ldots,r_w : The IMP^- register r_i corresponds to the i-th bit of the IMP^W register r, and the register r_0 indicates whether all bits are 0. Arithmetic expressions of IMP^W are bit-blasted to IMP^- programs. We showcase the bit-blasting for addition here. The addition of x and y in register r is compiled to

$$\operatorname{add}^{w} x \, y \, r \equiv \operatorname{copy}^{w} a \, x \, ; \operatorname{copy}^{w} b \, y \, ; \operatorname{adder}^{w} r, \tag{4}$$

where a, b are fresh, fixed IMP^W registers. The function copies the first w bits of x and y to a_1, \ldots, a_w and b_1, \ldots, b_w , respectively, which are then added by the function $\mathsf{adder}^w r$. The function $\mathsf{adder}^w r$ puts the result of the addition in registers r_0, \ldots, r_w . It is implemented as follows:

$$\mathsf{adder}^w \, r \equiv \mathsf{fullAdder}^1 \, r; \cdots; \mathsf{fullAdder}^w \, r; carry \leftarrow 0; zero \leftarrow 0, \tag{5}$$

where fullAdderⁱr is a program that implements a standard full adder with zero check. It adds the bits a_i and b_i and the carry register carry, storing the result in r_i , the new carry value in carry, and stores in zero whether the result and the previous zero value were 0. The full adder is called for all bits of the addends. Then r_0 is written, and the carry and zero registers are reset.

We bit-blast all other arithmetic expressions of $\mathsf{IMP}^{\mathsf{W}}$ in a similar way; details are in the formalisation. In the next definition, we fix a maximum bit-width w:

Definition 6. We denote with $(a)_r^w$ the bit-blasted version of arithmetic expression a stored in register r. For an IMP^W state s, we denote with $(s)_r^w$ its corresponding IMP^- state, i.e. $(s)_r^w r_i = (s\,r)_i$ for all registers r and i < w, where n_i denotes the i-th bit of n.

The functional correctness can now be stated as follows:

Lemma 3. If $\max\{a_{max}, \llbracket a \rrbracket_s, s_{max}\} < 2^w$ then $(\langle a \rangle_r^w, \langle s \rangle^w) \Rightarrow^{f(w)} \langle s(r := \llbracket a \rrbracket_s) \rangle^w$, where f(w) is linear in w.

Lastly, we show that the overall runtime blow-up of the bit-blasted program is polynomial. We first lift the bit-blasting of expressions to IMP^W programs p, denoted by $(p)^w$. In $(p)^w$, arithmetic expressions are replaced with their bit-blasted version and all other constructs are mapped to their corresponding constructs in the obvious way. For functional correctness, we get:

Theorem 8. If
$$(p,s) \Rightarrow^n s'$$
 and $n < w$ and $max\{s_{max}, p_{max}\} \cdot 2^n < 2^w$, then $((p)^w, (s)^w) \Rightarrow^{f(n,w)} (s')^w$ where $f(n,w)$ is linear in $n \cdot w$.

Proof sketch. The proof is by structural induction on the IMP^- program p. There are two interesting cases. The first is the case of assignment, where the theorem follows from Lemma 3. The other case is that of composition, in which case the theorem follows from Theorem 1. All other cases follow from basic properties of program composition and algebraic manipulation of exponents.

6 Discussion

Our work touches the areas of formalised computability and complexity theory, algorithm refinements and program synthesis, and certified compilation.

Notable work in the first area includes Norrish's [34] formalisation results, like Rice's theorem, in a lambda calculus model. Xu et al. [39] and Asperti and Ricciotti [4] proved basic results on Turing machines, using Hoare-like logics to reason about deeply-embedded machines. Carneiro [6] proved basic results using partial recursive functions. The richest line of work is by Forster [10], modelling the call-by-value lambda calculus, Turing machines, and other models, and proving simulations between them. Forster and Kunze [11] introduced a largely automated synthesis framework from native Coq functions to said lambda calculus model, including semi-automated time bound proofs. This was used for serious algorithms, like the Cook-Levin theorem [15]. However, their model is not

reasonable in space in general. Our contribution is the first synthesis method into a simple computation model that is reasonable in time and space.

To make our method practical, we used ideas from algorithm refinements and transport-based program synthesis [19,22,37], introducing a novel synthesis for recursive functions in Section 3.2. Other related approaches are algorithm refinements, which were deeply studied by Lammich [23–26].

In the area of certified compilation, most substantial developments geared towards practical compilers, such as CakeML [30] and CompCert [28]. We, on the other hand, we were mainly inspired by the simple and elegant use of IMP languages [38] in educational material [31,35], which is sufficient to formalise the theory of efficient algorithms and complexity theory.

Future Work Our framework can be extended in several ways, such as proving time and memory bounds of synthesised programs with respect to some sensible semantics for Isabelle/HOL functions [3], generalising from tail-recursion to general recursion, reducing the time and memory overhead of the compilers for finer analyses needed in efficient algorithms, and extending it to richer models of computation, e.g. probabilistic computation, interactive computation, or online computation. We plan to improve the framework's performance such that it can be applied to the verification of serious computational objects, e.g. reductions, like the Cook-Levin theorem [8] or Karp's 21 NP-complete problems, and the verification of running time bounds of complex algorithms in general, e.g. flow algorithms [2, 25] or matching algorithms [1]. A challenge with our framework, as in any system that synthesises programs using natural numbers as the sole datatype, is the computational overhead from encoding/decoding datatypes into natural numbers. Without special care, unsuspecting users may discrepancies between the expected and actual running time of synthesised programs. Methods to smoothly handle that discrepancy would greatly improve the usability of our framework and are a possible future direction.

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A $HOL^{(TC)}$ to $HOL^{(TC)N}$

A.1 Compilation of Datatypes

Let $\overrightarrow{\alpha} t = C_1 \overrightarrow{\alpha_1} | \cdots | C_n \overrightarrow{\alpha_n}$ be an algebraic datatype with $a_i \equiv |\overrightarrow{\alpha_i}|$. Recall that we require an injective pairing function pair : $\mathbb{N}^2 \Rightarrow \mathbb{N}$ and functions fst, snd : $\mathbb{N} \Rightarrow \mathbb{N}$ with

$$fst(pair n m) = n$$
 and $snd(pair n m) = m$. (6)

Our construction proceeds as follows:

(a) We define $C_i^{\mathbb{N}}: \mathbb{N}^{a_i} \Rightarrow \mathbb{N}$ by

$$C_i^{\mathbb{N}} \overrightarrow{x} \equiv \begin{cases} \operatorname{pair} i \left(\operatorname{pair} x_1 \left(\operatorname{pair} x_2 \left(\cdots \left(\operatorname{pair} x_{a_i - 1} x_{a_i} \right) \cdots \right), & \text{if } a_i > 0 \\ \operatorname{pair} i \, 0, & \text{otherwise} \end{cases}. \tag{7}$$

(b) For each i, j, we define the selector select_{i,j}: $\mathbb{N} \Rightarrow \mathbb{N}$ as

$$select_{i,j} x \equiv (if j < i then fst else id) (snd^j x).$$
 (8)

(c) We define $\mathsf{case}^{\mathbb{N}} : ((\mathbb{N}^{a_1} \Rightarrow \alpha) \Rightarrow \cdots \Rightarrow (\mathbb{N}^{a_n} \Rightarrow \alpha) \Rightarrow \mathbb{N} \Rightarrow \alpha)$ by

$$\operatorname{case}^{\mathbb{N}} \overrightarrow{f} \, x \equiv \begin{cases} f_i \, (\operatorname{select}_{a_i,1} \, x) \cdots (\operatorname{select}_{a_i,a_i} \, x), & \text{if } i = \operatorname{fst} \, x, 1 \leq i \leq n-1 \\ f_n \, (\operatorname{select}_{a_n,1} \, x) \cdots (\operatorname{select}_{a_n,a_n} \, x), & \text{otherwise.} \end{cases}$$

(9)

(d) We define natify: $\overrightarrow{\alpha} t \Rightarrow \mathbb{N}$ and denatify: $\mathbb{N} \Rightarrow \overrightarrow{\alpha} t$ by

$$\operatorname{natify}(C_i \overrightarrow{x}) \equiv C_i^{\mathbb{N}} \overrightarrow{\operatorname{natify}} x_j, \tag{10}$$

denatify
$$(C_i^{\mathbb{N}} \overrightarrow{x}) \equiv C_i \overrightarrow{\text{denatify } x_j}$$
. (11)

Note that natify, denatify are overloaded and Eqs. (10) and (11) well-defined if all $\alpha \in \overrightarrow{\alpha_1} \cup \cdots \cup \overrightarrow{\alpha_n}$ are already encoded or $\alpha = \overrightarrow{\alpha} t$.

Theorem. $\overrightarrow{\alpha} d = C_1 \overrightarrow{\alpha_1} \mid \cdots \mid C_n \overrightarrow{\alpha_n}$ is encodable if all $\alpha \in \overrightarrow{\alpha_1} \cup \cdots \cup \overrightarrow{\alpha_n}$ are encoded or $\alpha = \overrightarrow{\alpha} d$. Also, for all $1 \leq i \leq n$, $1 \leq j \leq a_i$ and relations R, we have

$$\begin{split} \left(\mathsf{R}\mathbb{N}^{a_i} \Rrightarrow \mathsf{R}\mathbb{N}\right) C_i^{\mathbb{N}} C_i, \qquad & \mathsf{R}\mathbb{N} \, n \, (C_i \, \overrightarrow{x}) \implies \mathsf{R}\mathbb{N} \, (\mathsf{select}_{a_i,j} n) \, x_j, \\ \left(\left(\mathsf{R}\mathbb{N}^{a_1} \Rrightarrow R\right) \Rrightarrow \cdots \Rrightarrow \left(\mathsf{R}\mathbb{N}^{a_n} \Rrightarrow R\right) \Rrightarrow \mathsf{R}\mathbb{N} \Rrightarrow R\right) \mathsf{case}_d^{\mathbb{N}} \, \mathsf{case}_d. \end{split}$$

Proof. We have to show that denatify (natify x) = x for all x. This follows directly by definition of denatify, natify and the fact that fst, snd are inverse to pair and all $\alpha \in \overrightarrow{\alpha_1} \cup \cdots \cup \overrightarrow{\alpha_n}$ are encoded (and hence have inverse functions natify, denatify).

The relatedness statements follow similarly by definition and the relatedness properties of the type arguments en- and decoding functions. \Box

Example 3. For the type of lists, 'a list = Nil | Cons 'a "'a list", the following constants are defined

```
definition Nil_nat = pair_nat 1 0 definition Cons_nat x xs = pair_nat 2 (pair_nat x xs) definition case_list_nat f1 f2 n = if fst n = 1 then f1 else f2 (select<sub>2,1</sub> n) (select<sub>2,2</sub> n) definition denatify = case_list_nat Nil (\lambdax xs. Cons (denatify x) (denatify xs)) definition natify = case_list Nil_nat (\lambdax xs. Cons_nat (natify x) (natify xs)) and the following theorems are proven:
```

```
lemma "RN Nil_nat Nil"
lemma "(RN \Rightarrow RN \Rightarrow RN) Cons_nat Cons"
lemma "(R \Rightarrow (RN \Rightarrow RN \Rightarrow R) \Rightarrow RN \Rightarrow R)
case_list_nat case_list"
lemma "RN ns (x # xs) \Longrightarrow RN (select<sub>2,1</sub> ns) x"
lemma "RN ns (x # xs) \Longrightarrow RN (select<sub>2,2</sub> ns) xs"
```

A.2 Synthesis of $HOL^{\mathbb{N}}$ Functions

Theorem. \mathbb{RN} , natify, and denatify form a partial Galois equivalence. Thus, there is some $f^{\mathbb{N}}$ that is \mathbb{RN} -related to f.

```
t ::= \mathbf{If} t_1 \, t_2 \, t_3 (if-then-else with natural number condition t_1)

| \, \mathbf{Let} \, t_1 \, t_2 \,  (bind t_1 to the first de Bruijn index in t_2)

| \, \mathbf{LetBound} \, i \,  (variable bound by i-th enclosing \mathbf{Let})

| \, \mathbf{Arg} \, i \,  (i-th argument of f, i.e. x_i)

| \, \mathbf{Number} \, n \,  (natural number n \in \mathbb{N})

| \, \mathbf{Call} \, g \, [t_1, \ldots, t_m] \,  (call to g : \mathbb{N}^m \Rightarrow \mathbb{N} with arguments t_1, \ldots, t_m)

| \, \mathbf{Recurse} \, [t_1, \ldots, t_k] \,  (recursion with arguments t_1, \ldots, t_k)
```

Fig. 12: Datatype representation of HOL^{TCN} in the metaprogramming language.

Proof. Due to [22, Lemma 2], it suffices to show that (1) RN is right-total and right-unique, (2) RN nx implies denatify n=x, and (3) RN (natify x) x for all n,x. By Def. 2, RN is right-total and RN (natify x) x. Since natify is injective (Def. 2), RN is also right-unique and RN nx implies denatify n=x.

The existence of $f^{\mathbb{N}}$ now follows from [22, Theorem 1 and 2].

Theorem (Whitebox-Transport [19]). $(\lambda \vec{x}.t)^{\square}$ and $\lambda \vec{x}.t$ are RN-related and white-box transports preserve tail-recursiveness and first-order applications.

Proof. The former is shown by structural induction on t, using that f is RN-related to $f^{\mathbb{N}}$ by Theorem 3 and all other functions g are RN-related to $g^{\mathbb{N}}$ by assumption.

The latter follows immediately from Def. 4 and structural induction on t. \square

B HOL^{TCN} to IMP^{TC}

B.1 Compilation to IMP^{TC}

Fig. 12 shows the data type representation of HOL^{TCN} as used in the compiler to IMP^{TC} , shown in Fig. 13.

B.2 Correctness Proofs

Our goal is to show that $p \vdash (p,s) \Rightarrow_{\mathsf{ret}_f} f^{\mathsf{TCN}} \, \overline{s\,\mathsf{arg}_{f,i}}$, i.e. we are interested in the single return register ret_f . Fig. 14 shows the execution relation for $\mathsf{IMP}^{\mathsf{TC}}$ specialised to single return registers. Note that for sequences $(p_1\,;\,p_2,s) \Rightarrow_r v$, the standard execution relation " \Rightarrow " (and not " \Rightarrow_r ") must be used for p_1 , that is $(p_1,s) \Rightarrow s'$.

This is the reason why each compiled $\mathsf{IMP}^{\mathsf{TC}}$ program p is normalised such that no recursive constructor (sequences and if-then-elses) appears on the left of a sequence. This way, all goals involving recursive constructors use the execution relation " \Rightarrow_r ", saving us from implementing separate recursive automation for " \Rightarrow ".

Fig. 13: The compiler from the HOL^{TCN} representation in Fig. 12 to IMP^{TC} .

$$\begin{aligned} & \operatorname{Assign_1} \frac{s(r \coloneqq \llbracket a \rrbracket_s) \, r' = v}{(r \leftarrow a, s) \Rightarrow_{r'} v} & \operatorname{IfT_1} \frac{s \, r \neq 0 \quad (p_1, s) \Rightarrow_r v}{(\operatorname{IF} \, r \, \operatorname{THEN} \, p_1 \, \operatorname{ELSE} \, p_2, s) \Rightarrow_r v} \\ & \operatorname{SEQ_1} \frac{(p_1, s) \Rightarrow s' \quad (p_2, s') \Rightarrow_r v}{(p_1 \, ; \, p_2, s) \Rightarrow_r v} & \operatorname{IfF_1} \frac{s \, r = 0 \quad (p_2, s) \Rightarrow_r v}{(\operatorname{IF} \, r \, \operatorname{THEN} \, p_1 \, \operatorname{ELSE} \, p_2, s) \Rightarrow_r v} \\ & \operatorname{Call_1} \frac{(pc, s) \Rightarrow_r v \quad s(r \coloneqq v) \, r' = v'}{(\operatorname{Call} \, pc \, \operatorname{RETURN} \, r, s) \Rightarrow_{r'} v'} & \operatorname{Rec_1} \frac{p \vdash (p, s) \Rightarrow_r v}{p \vdash (\operatorname{RECURSE}, s) \Rightarrow_r v} \end{aligned}$$

Fig. 14: Execution relation of IMP^{TC} for single return registers.

C IMP^{TC} to IMP⁻

C.1 IMP^{TC} to IMP^{WC}

Lemma. Let $(p,s) \Rightarrow^n (s',b)$ denote the modified execution relation shown in Fig. 15 that runs p but stops and flags whenever a tail-recursive call is encountered using $b \in \{0,1\}$ Then the following rules are admissible:

$$\frac{(p,s)\Rightarrow^n(s',0)}{(p,s)\Rightarrow^ns'} \qquad \frac{(p,s_1)\Rightarrow^{n_1}(s_2,1) \qquad tp\vdash (tp,s_2)\Rightarrow^{n_2}s_3}{tp\vdash (p,s_1)\Rightarrow^{n_1+n_2}s_3}$$

Proof sketch. By induction over the execution rules.

$$\frac{s' = s(r \coloneqq \llbracket a \rrbracket_s)}{(r \leftarrow a, s) \Rightarrow^{\mathcal{C}}(s', 0)} \qquad \frac{s \, r \neq 0 \qquad (p_1, s) \Rightarrow^n (s', b)}{(\mathsf{IF} \, r \, \mathsf{THEN} \, p_1 \, \mathsf{ELSE} \, p_2, s) \Rightarrow^{n+\mathcal{C}}(s', b)}$$

$$\frac{(p_1, s) \Rightarrow^{n_1}(s', 0) \qquad (p_2, s') \Rightarrow^{n_2}(s'', b)}{(p_1 \, ; \, p_2, s) \Rightarrow^{n_1+n_2+\mathcal{C}}(s'', b)} \qquad \frac{s \, r = 0 \qquad (p_2, s) \Rightarrow^n (s', b)}{(\mathsf{IF} \, r \, \mathsf{THEN} \, p_1 \, \mathsf{ELSE} \, p_2, s) \Rightarrow^{n+\mathcal{C}}(s', b)}$$

$$\frac{(pc, s) \Rightarrow^n_r \, v \qquad s' = s(r \coloneqq v)}{(\mathsf{CALL} \, pc \, \mathsf{RETURN} \, r, s) \Rightarrow^{n+\mathcal{C}}(s', 0)} \qquad \overline{(\mathsf{RECURSE}, s) \Rightarrow^{\mathcal{C}}(s, 1)}$$

Fig. 15: Auxiliary execution relation used in Lemma 1.

Theorem. Let cnt be a fresh register with respect to regs p. Let p[t/x] denote the syntactic substitution of any occurrence of x by t in a program p. Define

$$\{p\}_{\circlearrowleft} \equiv \mathtt{cnt} \leftarrow \mathtt{1} \; ; \; \mathtt{WHILE} \; \mathtt{cnt} \; \mathtt{DO} \; \mathtt{cnt} \leftarrow \mathtt{0} \; ; \; p[(\mathtt{cnt} \leftarrow \mathtt{1})/\mathtt{RECURSE}].$$

Then it holds that $p \vdash (p,s) \Rightarrow_{\mathsf{regs}\,p}^n s'$ if and only if $((p)_{\circlearrowleft}, s) \Rightarrow_{\mathsf{regs}\,p}^{n+\mathcal{C}} s'$.

Proof sketch. We show that $\vdash (p,s) \Rightarrow^n (s',b)$ holds if and only if

$$\exists s''. (p[(\mathtt{cnt} \leftarrow 1)/\mathtt{RECURSE}], s) \Rightarrow^n s'' \land s'' \mathtt{cnt} = b \land \forall r \in \mathtt{regs} \ p. \ s' \ p = s'' \ p$$

by induction over the execution rules, generalising over S such that $\operatorname{regs} p \subseteq S$ and $\operatorname{cnt} \notin S$. Then the semantics for the while-loop with rules from Fig. 9 are equivalent to the semantics of the compiled program with rules from Lemma 1 by straightforward induction over the respective rules.

C.2 IMPWC to IMPW

Lemma. $(p[m x/x], s) \Rightarrow^n s' \text{ implies } (p, s \circ m) \Rightarrow^n s' \circ m \text{ for injective } m.$

Proof sketch. By induction over the execution of p.

The inlining induces a blow-up that is dependent on the program size (but not the input), as shown below.

П

Theorem. $(p,s) \Rightarrow_{\mathsf{regs}\ p}^n s' \text{ if and only if } ((p)_{\star}, s) \Rightarrow_{\mathsf{regs}\ p}^{f(n)} s', \text{ where } f(n) \text{ is linear in } n \cdot |p|.$

Proof sketch. The inlining is correct by Lemma 2, so correctness follows by a simple induction. \Box

C.3 IMPW to IMP-

Lemma. Assume that $\max\{a_{max}, \llbracket a \rrbracket_s, s_{max}\} < 2^w$. Then it holds that $((a)_r^w, (s)^w) \Rightarrow^{f(w)} (s(r := \llbracket a \rrbracket_s))^w$, where f(w) is linear in w.

$$[\![\mathbb{C} \, n]\!]_s \equiv n, \quad [\![\mathbb{R} \, r]\!]_s \equiv s \, r \qquad \qquad [\![A_1 \otimes A_2]\!]_s \equiv [\![A_1]\!]_s \otimes [\![A_2]\!]_s, \text{ for } \otimes \in \{+,-\}$$

(a) Evaluation of atoms A.

(b) Evaluation rules for arithmetic expressions.

$$\operatorname{Assign} \frac{s' = s(r \coloneqq \llbracket a \rrbracket_s)}{(r \leftarrow a, s) \Rightarrow^{\mathcal{C}} s'} \qquad \operatorname{IfT} \frac{s \, r \neq 0 \quad (p_1, s) \Rightarrow^n s'}{(\operatorname{IF} \, r \, \operatorname{THEN} \, p_1 \, \operatorname{ELSE} \, p_2, s) \Rightarrow^{n+\mathcal{C}} s'}$$

$$\operatorname{SeQ} \frac{(p_1, s) \Rightarrow^{n_1} s' \quad (p_2, s') \Rightarrow^{n_2} s''}{(p_1 \; ; \; p_2, s) \Rightarrow^{n_1+n_2+\mathcal{C}} s''} \qquad \operatorname{IfF} \frac{s \, r = 0 \quad (p_2, s) \Rightarrow^n s'}{(\operatorname{IF} \, r \, \operatorname{THEN} \, p_1 \, \operatorname{ELSE} \, p_2, s) \Rightarrow^{n+\mathcal{C}} s'}$$

$$\operatorname{Call} \frac{(pc, s) \Rightarrow^n_r v \quad s' = s(r \coloneqq v)}{(\operatorname{Call} \, pc \, \operatorname{RETURN} \, r, s) \Rightarrow^n s'} \qquad \operatorname{Rec} \frac{p \vdash (p, s) \Rightarrow^n s'}{p \vdash (\operatorname{RECURSE}, s) \Rightarrow^{n+\mathcal{C}} s'}$$

(c) Execution relation for commands.

Fig. 16: Semantics of IMP^{TC}.

$$\begin{aligned} & \text{WHF} \; \frac{s \, r = 0}{(\text{WHILE} \; r \; \text{DO} \; p, s) \Rightarrow^{\mathcal{C}} s} \\ & \text{WHT} \; \frac{s_1 \, r \neq 0}{(\text{WHILE} \; r \; \text{DO} \; p, s_1) \Rightarrow^{n_1} s_2} \; \; (\text{WHILE} \; r \; \text{DO} \; p, s_2) \Rightarrow^{n_2} s_3}{(\text{WHILE} \; r \; \text{DO} \; p, s_1) \Rightarrow^{n_1 + n_2 + \mathcal{C}} s_3} \end{aligned}$$

Fig. 17: Execution relation for WHILE from IMP^{WC} and IMP^W.

Proof Sketch. The proof is based on showing an upper bound on the running time of each of the functions $\operatorname{copy}^a b y$ and $\operatorname{adder}^w v$, which in turn depends on the running time of fullAdderⁱ r. The running time of fullAdderⁱ r is a constant. The running times of adder and copy are shown to be linear in w by induction on w.

D IMP-Definitions

Fig. 16 shows the complete specification of IMP^{TC}, Fig. 17 the rule for WHILE, and Fig. 18 the complete specification of IMP⁻.

$$\frac{b \in \{0,1\} \quad s' = s(r \coloneqq b)}{(r \leftarrow b,s) \Rightarrow^{1} s'} \qquad \frac{s \, r \neq 0 \quad (p_{1},s) \Rightarrow^{n} s'}{(\text{IF r THEN p_{1} ELSE $p_{2},s)} \Rightarrow^{n+1} s'}$$

$$\frac{(p_{1},s) \Rightarrow^{n_{1}} s' \quad (p_{2},s') \Rightarrow^{n_{2}} s''}{(p_{1};p_{2},s) \Rightarrow^{n_{1}+n_{2}+1} s''} \qquad \frac{s \, r = 0 \quad (p_{2},s) \Rightarrow^{n} s'}{(\text{IF r THEN p_{1} ELSE $p_{2},s)} \Rightarrow^{n+1} s'}$$

$$\frac{s \, r = 0}{(\text{WHILE r DO $p,s)} \Rightarrow^{1} s} \qquad \frac{s_{1} \, r \neq 0 \quad (p,s_{1}) \Rightarrow^{n_{1}} s_{2} \quad (\text{WHILE r DO $p,s_{2})} \Rightarrow^{n_{2}} s_{3}}{(\text{WHILE r DO $p,s_{1})} \Rightarrow^{n_{1}+n_{2}+2} s_{3}}$$

Fig. 18: Execution relation for IMP^- .