

# Exact Flow Analysis by Higher-Order Model Checking

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**Abstract.** We propose a novel control flow analysis for higher-order functional programs, based on a reduction to higher-order model checking. The distinguished features of our control flow analysis are that, unlike most of the control flow analyses like  $k$ -CFA, it is *exact* for simply-typed  $\lambda$ -calculus with recursion and finite base types, and that, unlike Mossin’s exact flow analysis, it is indeed runnable in practice, at least for small programs. Furthermore, under certain (arguably strong) assumptions, our control flow analysis runs in time cubic in the size of a program. We formalize the reduction of control flow analysis to higher-order model checking, prove the correctness, and report preliminary experiments.

## 1 Introduction

Control flow analysis (CFA) is among the most important and popular static analyses for functional programs. It computes a set of functions that may be called from each call site, and the result of CFA is used as a basis of more complex static analyses and also for compiler optimizations. Various CFA methods, with varying degrees of precision and efficiency, have been proposed, including Shiver’s  $k$ -CFA [23]. Most of the existing CFA algorithms compute an *over-approximation* of the control flow set, even when the target language is restricted to a decidable fragment. To our knowledge, the only exception is Mossin’s exact analysis [18], which is however impractical and not runnable in practice.

We propose a novel control flow analysis based on *higher-order model checking* [19, 9]. We reduce CFA to a decision problem on the tree generated by a simply-typed, higher-order functional program, which can be decided by using higher-order model checking. Our method has the following nice properties. First, like Mossin’s analysis [18] (and unlike other CFAs), our CFA is *exact* for simply-typed  $\lambda$ -calculus with recursion and *finite* base types.<sup>1</sup> Secondly, unlike Mossin’s [18], our CFA is runnable despite its extreme precision, thanks to the recent advances in higher-order model checking [7, 11]. Thus, even if our analysis is still too slow compared with the state-of-the-art CFA methods, it may be useful for evaluating and comparing the precision of other methods. Thirdly, under the (rather strong) assumptions that the largest size of types is fixed and

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<sup>1</sup> With infinite base types like integers, our CFA is of course inexact, as the language becomes Turing-complete.

that the nesting depth of function definitions is fixed, our CFA runs in time cubic in the size of a program. Lastly, like Heintze and McAllester’s subtransitive CFA [6], our CFA is on-demand, in the sense that it can answer each flow query: “May a function created at  $\ell_1$  be called at the call site  $\ell_2$ ?” in linear time (with the same assumptions as above). Thus, one can invoke our CFA only for critical flow queries that cannot be answered by a faster (but more imprecise) CFA.

Our CFA based on higher-order model checking has been already hinted by Kobayashi [9, 10], but it has not been formalized before. The contributions of the present paper include the formalization, a proof of its correctness, implementation and preliminary experiments.

The rest of this paper is structured as follows. Section 2 reviews higher-order model checking, specialized for the purpose of this paper. Section 3 introduces the source language and defines CFA. Section 4 shows the reduction from CFA to higher-order model checking. Section 5 describes extensions of our CFA. Section 6 reports experiments. Section 7 discusses related work, and Section 8 concludes.

## 2 Review of Higher-Order Model Checking

This section briefly reviews (a subclass of) higher-order model checking problems (HO model checking, for short) [19, 9], to which we reduce CFA in Section 4. The aim of HO model checking is to check whether the tree generated by a given program satisfies a given property. The usual HO model checking uses *higher-order recursion schemes* [19] as the target, but we consider here a simply-typed  $\lambda$ -calculus with recursion and tree constructors, called  $\lambda_T$ . For tree-generating programs,  $\lambda_T$  has the same expressive power as higher-order recursion schemes.

Let  $\Sigma$  be a finite set of tree constructors. We write  $\mathbf{a}$  for an element of  $\Sigma$ , and  $\Sigma(\mathbf{a})$  for its arity (which is a non-negative integer). The set of  $\lambda_T$ -terms is given by the following grammar:

$$e ::= \mathbf{a} \mid x \mid \mathbf{fun}(f, x, e) \mid e_1 e_2$$

where  $f$  and  $x$  range over variables. The term  $\mathbf{fun}(f, x, e)$  represents a recursive function  $f$  defined by the equation  $f(x) = e$ . The term constructor  $\mathbf{fun}(f, x, -)$  binds  $f$  and  $x$ . As usual, we implicitly rename bound variables as necessary. We write  $\lambda x.e$  for  $\mathbf{fun}(f, x, e)$  if  $f$  does not occur in  $e$ .

We assume that the terms are well-typed in the standard simple type system, which has only one base type  $o$  for trees. The typing rules for tree constructors and recursive function definitions are given by:

$$\frac{}{\Gamma \vdash \mathbf{a} : \underbrace{o \rightarrow \cdots \rightarrow o}_{\Sigma(\mathbf{a})} \rightarrow o} \quad \frac{\Gamma, f : \tau \rightarrow \sigma, x : \tau \vdash e : \sigma}{\Gamma \vdash \mathbf{fun}(f, x, e) : \tau \rightarrow \sigma}$$

The other rules are standard, which are given in [12]. We call a closed term (i.e. a term containing no free variables) of type  $o$  a *tree-generating program*.

The operational semantics of  $\lambda_T$  is the standard call-by-name semantics, which evaluates a program to a (possibly infinite) tree: see [12]. Actually we are only concerned with the set of *paths* of the tree generated by a program. Thus, we introduce an alternative semantics for describing the paths. We define  $e \xrightarrow{l} e'$  as the least relation satisfying (i)  $(\mathbf{fun}(f, x, e))e' \xrightarrow{\epsilon} [e'/x, \mathbf{fun}(f, x, e)/f]e$ , (ii)  $\mathbf{a} e_1 \cdots e_{\Sigma(\mathbf{a})} \xrightarrow{\mathbf{a}} e_i$  for every  $i \in \{1, \dots, \Sigma(\mathbf{a})\}$ , and (iii)  $e_1 \xrightarrow{l} e'_1$  implies  $e_1 e_2 \xrightarrow{l} e'_1 e_2$ .

The *path language* generated by a program  $e$ , written  $Path(e)$ , is defined by:

$$Path(e) = \{l_1 \cdot \dots \cdot l_m \mid e \xrightarrow{l_1} e_1 \xrightarrow{l_2} \dots \xrightarrow{l_m} e_m\}.$$

Here,  $\cdot$  denotes the concatenation and  $\epsilon$  is treated as an empty sequence.

*Example 1.* Let  $F$  be  $\mathbf{fun}(f, x, \mathbf{a} x (f(\mathbf{b} x)))$  and  $e$  be  $F c$ . Types for tree constructors and variables are given by  $\mathbf{a}: \mathbf{o} \rightarrow \mathbf{o} \rightarrow \mathbf{o}$ ,  $\mathbf{b}: \mathbf{o} \rightarrow \mathbf{o}$ ,  $\mathbf{c}: \mathbf{o}$ ,  $f: (\mathbf{o} \rightarrow \mathbf{o})$ , and  $x: \mathbf{o}$ . Then  $e$  has the following reduction sequence:

$$e = F c \xrightarrow{\epsilon} \mathbf{a} c (F(\mathbf{b} c)) \xrightarrow{\mathbf{a}} F(\mathbf{b} c) \xrightarrow{\epsilon} \mathbf{a}(\mathbf{b} c) (F(\mathbf{b}(\mathbf{b} c))) \xrightarrow{\mathbf{a}} \mathbf{b} c \xrightarrow{\mathbf{b}} c.$$

Thus  $\epsilon, \mathbf{a}, \mathbf{aa}, \mathbf{aab} \in Path(e)$ . The path language  $Path(e)$  is  $\{\mathbf{a}^n \mathbf{b}^m \mid n > m \geq 0\} \cup \{\epsilon\}$ , where  $\mathbf{a}^n$  is a sequence of length  $n$  consisting of  $\mathbf{a}$ .  $\square$

We are interested in the decision problem: “given a program  $e$  and a regular language  $R$ , is  $Path(e)$  a subset of  $R$ ?” It can be considered an instance of higher-order model checking, and its decidability follows from Ong’s result [19].

**Theorem 1.** *Let  $e$  be a tree-generating program and  $R$  a regular word language. Then whether  $Path(e) \subseteq R$  is decidable.*

In the rest of this paper, we just call the decision problem  $Path(e) \stackrel{?}{\subseteq} R$  above a *HO model checking problem*. It can be solved by using existing higher-order model checkers [7, 11, 16].<sup>2</sup> Note that higher-order model checking [19, 9] is a generalization of conventional (finite-state or pushdown) model checking, and that finite state model checkers can’t. The worst-case complexity is in general non-elementary [19, 13]. Under certain assumptions, however, it is linear time in the program size [9]. It is rephrased for our language as follows.

**Theorem 2.** *Suppose (i)  $R$  is fixed and (ii) the largest type size of a variable in  $e$  and the nesting depth of function definitions are bounded above by a constant. Then,  $Path(e) \stackrel{?}{\subseteq} R$  can be decided in time linear in the size of  $e$ .*

The constant factor is, however, huge: It is non-elementary in the parameters that have been assumed to be bounded by constants above.

<sup>2</sup> Higher-order model checking [19, 9] should not be confused with ordinary (finite state) model checking. The former can be considered a generalization of the latter.

### 3 Source Language and CFA Problem

This section defines the source language, called  $\lambda_S$ , and the control-flow analysis (CFA) for its programs.

#### 3.1 Source Language $\lambda_S$

Our source language  $\lambda_S$  is a simply-typed  $\lambda$ -calculus extended with recursions and non-deterministic branches. Its syntax is defined by:

$$\begin{aligned} t \text{ (terms)} &::= () \mid x \mid \mathbf{fun}^\ell(f, x, t) \mid t_1 @^\ell t_2 \mid \mathbf{if}^* t_1 t_2 \\ v \text{ (value)} &::= () \mid \mathbf{fun}^\ell(f, x, t) \\ T \text{ (types)} &::= \mathbf{Unit} \mid T_1 \rightarrow T_2. \end{aligned}$$

Here,  $\mathbf{fun}^\ell(f, x, t)$  describes a recursion function  $f$  given by  $f(x) = t$ . We often write  $\lambda^\ell x.t$  for  $\mathbf{fun}^\ell(f, x, t)$  when  $f$  does not occur in  $t$ . The term  $t_1 @^\ell t_2$  applies the function  $t_1$  to  $t_2$ , and  $\mathbf{if}^* t_1 t_2$  reduces to  $t_1$  or  $t_2$  in a non-deterministic manner. The non-determinism will be used to abstract values in Section 5. To talk about flows of functions, we attach a label  $\ell$  to each function and application. We use a special dummy label  $\ell_*$  for an unimportant label and often omit it. We write  $\mathcal{L}$  for the set of all labels, and  $\mathcal{L}^-$  for  $\mathcal{L} \setminus \{\ell_*\}$ .

The evaluation strategy of  $\lambda_S$  is call-by-value<sup>3</sup>. The evaluation context ( $E$ ) and the reduction relation ( $\longrightarrow$ ) are defined by:

$$E \text{ (evaluation contexts)} ::= [] \mid E@^\ell t \mid v@^\ell E.$$

$$\begin{aligned} E[\mathbf{fun}^\ell(f, x, t_1)@^\ell v_2] &\longrightarrow E[[v_2/x, \mathbf{fun}^\ell(f, x, t_1)/f]t_1] \\ E[\mathbf{if}^* t_1 t_2] &\longrightarrow E[t_1] \quad E[\mathbf{if}^* t_1 t_2] \longrightarrow E[t_2]. \end{aligned}$$

Here,  $E[t]$  is the expression obtained by replacing the hole  $[]$  in  $E$  with  $t$ , and  $[t_1/x_1, \dots, t_k/x_k]t$  denotes the term obtained by replacing every free occurrence of  $x_i$  in  $t$  with  $t_i$ . We write  $\longrightarrow^+$  for the transitive closure and  $\longrightarrow^*$  for the reflexive and transitive closure of  $\longrightarrow$ .

As usual, the type judgment relation  $\Gamma \vdash t : T$  is defined as the least relation closed under the rules below. We call a closed  $\lambda_S$ -term of type  $\mathbf{Unit}$  (i.e., a term  $t$  such that  $\emptyset \vdash t : \mathbf{Unit}$ ) a *source program*.

$$\frac{}{\Gamma \vdash () : \mathbf{Unit}} \quad \frac{}{\Gamma, x : T \vdash x : T} \quad \frac{\Gamma \vdash t_1 : T_1 \quad \Gamma \vdash t_2 : T_1}{\Gamma \vdash \mathbf{if}^* t_1 t_2 : T_1} \\ \frac{\Gamma, f : T_1 \rightarrow T_2, x : T_1 \vdash t_1 : T_2}{\Gamma \vdash \mathbf{fun}^\ell(f, x, t_1) : T_1 \rightarrow T_2} \quad \frac{\Gamma \vdash t_1 : T_1 \rightarrow T_2 \quad \Gamma \vdash t_2 : T_2}{\Gamma \vdash t_1 @^\ell t_2 : T_2}$$

<sup>3</sup> We can also deal with CFA for call-by-name languages, just by changing the CPS transformation in Section 4.1

### 3.2 CFA Problem

We define CFA as a decision problem to check whether a given function may be called at a given call site.

**Definition 1 (Control-flow relation and CFA problem).** *For a source program  $t$ , the control-flow relation  $CF(t)$  is given by:*

$$CF(t) = \{(\ell_1, \ell_2) \in \mathcal{L}^- \times \mathcal{L}^- \mid \exists t_1, v_2, f, x, E. t \longrightarrow^* E[(\mathbf{fun}^{\ell_2}(f, x, t_1))@^{\ell_1}v_2]\}.$$

*CFA is the problem of deciding whether  $(\ell_1, \ell_2) \in CF(t)$ , for a given program  $t$  and labels  $\ell_1, \ell_2 \in \mathcal{L}^-$ .*

A usual flow analysis aims to compute an *over-approximation* of the set  $CF(t)$ . In the next section, we shall give an *exact* flow analysis algorithm for solving the above decision problem. It is non-trivial even for  $\lambda_S$ , as it has recursion and non-determinism.

*Example 2.* Consider the program  $t_p = (\lambda^1 x. x@^2())@^3(\lambda^4 z.())$ . It is evaluated as follows:

$$(\lambda^1 x. x@^2())@^3(\lambda^4 z.()) \longrightarrow (\lambda^4 z.())@^2() \longrightarrow ().$$

The function (labeled by) 1 is applied at the call site 3, and the function 4 is applied at the call site 2. By the definition,  $CF(t_p) = \{(3, 1), (2, 4)\}$ .

*Remark 1.* The CFA problem above is defined only for closed programs. CFA is undecidable for open programs containing higher-order variables [20].

## 4 Reduction from CFA to HO Model Checking

This section reduces CFA to the HO model checking problem reviewed in Section 2. By combining the reduction with a HO model checking algorithm we obtain a sound and complete algorithm for CFA. The reduction consists of two steps: we first reduce CFA to *call-sequence analysis* (CSA), which is the problem of analyzing the order of function call. We then reduce CSA to HO model checking, i.e., a verification problem for a tree-generating program.

### 4.1 From CFA to CSA

We first define the CSA problem.

**Definition 2 (CSA problem).** *For a term  $t$ , we define the call-sequence relation  $CS(t)$  by:*

$$CS(t) = \{(\ell_1, \ell_2) \in \mathcal{L}^- \times \mathcal{L}^- \mid t \longrightarrow^* E_1[(\mathbf{fun}^{\ell_1}(f_1, x_1, t_1))@v_1] \longrightarrow E_2[(\mathbf{fun}^{\ell_2}(f_2, x_2, t_2))@v_2]\}.$$

*CSA is the problem of deciding whether  $(\ell_1, \ell_2) \in CS(t)$ , for a given term  $t$  and labels  $\ell_1, \ell_2 \in \mathcal{L}^-$ .*

*Example 3.* Let us consider the following program  $t_0$ .

$$t_0 = (\lambda^3 b. (\lambda^1 x. \lambda k_1. (\lambda^2 a. x a k_1) () ) b (\lambda m. m)) (\lambda^4 z. \lambda k_2. k_2 ()).$$

We have omitted symbols  $@$  and their labels for readability.  $t_0$  is reduced as:

$$\begin{aligned} & (\lambda^3 b. (\lambda^1 x. \lambda k_1. (\lambda^2 a. x a k_1) () ) b (\lambda m. m)) (\lambda^4 z. \lambda k_2. k_2 () ) \\ & \longrightarrow (\lambda^1 x. \lambda k_1. (\lambda^2 a. x a k_1) () ) (\lambda^4 z. \lambda k_2. k_2 () ) (\lambda m. m) \\ & \longrightarrow^* (\lambda^2 a. (\lambda^4 z. \lambda k_2. k_2 () ) a (\lambda m. m)) () \\ & \longrightarrow (\lambda^4 z. \lambda k_2. k_2 () ) () (\lambda m. m) \longrightarrow^* (). \end{aligned}$$

Thus,  $CS(t_0) = \{(3, 1), (2, 4)\}$ . □

To reduce CFA to CSA, it suffices to apply the following call-by-value continuation-passing-style (CPS) transformation  $\llbracket \cdot \rrbracket$  [2, 21].

$$\begin{aligned} \llbracket () \rrbracket &= \lambda^{\ell^*} k. k @^{\ell^*} () \\ \llbracket x \rrbracket &= \lambda^{\ell^*} k. k @^{\ell^*} x \\ \llbracket \mathbf{fun}^\ell(f, x, t) \rrbracket &= \lambda^{\ell^*} k. k @^{\ell^*} (\mathbf{fun}^\ell(f, x, \llbracket t \rrbracket)) \\ \llbracket [t_1 @^{\ell} t_2] \rrbracket &= \lambda^{\ell^*} k. \llbracket t_1 \rrbracket @^{\ell^*} (\lambda^{\ell^*} f. \llbracket t_2 \rrbracket @^{\ell^*} (\lambda^\ell z. (f @^{\ell^*} z) @^{\ell^*} k)) \quad (f, z \text{ are fresh}) \\ \llbracket \mathbf{if}^* t_1 t_2 \rrbracket &= \lambda^{\ell^*} k. (\mathbf{if}^* (\llbracket t_1 \rrbracket @^{\ell^*} k) (\llbracket t_2 \rrbracket @^{\ell^*} k)). \end{aligned}$$

By the CPS transformation, every term is converted to a function that takes a continuation (i.e., the rest of the computation) and passes the evaluation result to it. The CPS transformation above is the same as the standard (simplest) one [21], except for the treatment of labels. In the third rule, the label  $\ell$  of the function  $\mathbf{fun}(f, x, t)$  is retained in the result  $\mathbf{fun}^\ell(f, x, \llbracket t \rrbracket)$ . In the fourth rule, the label  $\ell$  of the function application is moved to the continuation argument for  $\llbracket t_2 \rrbracket$ . Dummy labels are attached to all the other functions introduced by the transformation. Note that the CPS transformation above is type-preserving [17]. If  $t$  is a source program (of type  $\mathbf{Unit}$ ), then  $\llbracket t \rrbracket$  has type  $(\mathbf{Unit} \rightarrow \mathbf{Unit}) \rightarrow \mathbf{Unit}$ .

The transformation rule for  $t_1 @^{\ell} t_2$  above is the key for the reduction from CFA to CSA. In  $\llbracket t_1 @^{\ell} t_2 \rrbracket$ ,  $\ell$  is attached to  $\lambda z. f @ z @ k$ , which is the continuation to call the function  $f$  obtained by evaluating  $t_1$ . Thus, if the value of  $t_1$  is labeled by  $\ell_1$  in a source program, then  $\ell_1$  is called immediately after the continuation function  $\lambda z. f @ z @ k$  in the target program. Figure 1 shows a rough correspondence between reduction sequences of a source program and its target program.<sup>4</sup> The left-hand side shows a reduction sequence of a source program  $t$  that leads to a call of function  $\ell_2$  from a call site  $\ell_1$ .  $t$  is first evaluated to  $E[t_1 @^{\ell_1} t_2]$ , and then  $t_1$  is evaluated to a function  $\lambda^{\ell_1} x. t_3$  (see the term marked by (i)).  $t_2$  is then evaluated to a value  $v_4$ , and the function  $\ell_2$  is called at  $\ell_1$  (see (ii)). The corresponding reduction sequence after the CPS transformation is shown on the right-hand side. The term (i) shows the state after  $t_1$  has been evaluated and before  $t_2$  is evaluated. The term (ii) shows the state after  $t_2$  has

<sup>4</sup> For the sake of simplicity, we show here an inaccurate reduction sequence on the right-hand side. See [12] for the exact correspondence.

$$\begin{array}{l|l}
t & \llbracket t \rrbracket @ (\lambda m. m) \\
\hline
\longrightarrow^* E[t_1 @^{\ell_1} t_2] & \longrightarrow^* \llbracket t_1 @^{\ell_1} t_2 \rrbracket @ K \\
\longrightarrow^* E[(\lambda^{\ell_2} x. t_3) @^{\ell_1} t_2] \text{ (i)} & \longrightarrow^* \llbracket t_2 \rrbracket @ (\lambda^{\ell_1} z. ((\lambda^{\ell_2} x. \llbracket t_3 \rrbracket) @ z) @ K) \text{ (i)} \\
\longrightarrow^* E[(\lambda^{\ell_2} x. t_3) @^{\ell_1} v_4] \text{ (ii)} & \longrightarrow^* (\lambda^{\ell_1} z. ((\lambda^{\ell_2} x. \llbracket t_3 \rrbracket) @ z @ K)) @ \llbracket v_4 \rrbracket \text{ (ii)} \\
& \longrightarrow (\lambda^{\ell_2} x. \llbracket t_3 \rrbracket) @ \llbracket v_4 \rrbracket @ K
\end{array}$$

**Fig. 1.** Evaluation of an application on source and CPS programs

been evaluated and its value being passed to the continuation. After that,  $\ell_1$  and  $\ell_2$  are consecutively called.

From the correspondence above, the following theorem should be intuitively clear. A proof is given in [12].

**Theorem 3 (Correctness of the Reduction from CFA to CSA).** *Let  $t$  be a source program and  $\ell_1, \ell_2$  labels in  $t$ . Then,  $(\ell_1, \ell_2) \in CF(t)$  if and only if  $(\ell_1, \ell_2) \in CS(\llbracket t \rrbracket @ (\lambda m. m))$ .*

*Example 4.* Recall the program  $t_p$  in Example 2. After the CPS transformation, the program is reduced as follows (where  $K = \lambda m. m$ ):

$$\begin{aligned}
& \llbracket (\lambda^1 x. x @^2 ()) @^3 (\lambda^4 y. ()) \rrbracket @ K \longrightarrow^* (\lambda^3 z. ((\lambda^1 x. \llbracket x @^2 () \rrbracket) @ z) @ K) @ (\lambda^4 y. \llbracket () \rrbracket) \\
& \longrightarrow ((\lambda^1 x. \llbracket x @^2 () \rrbracket) @ (\lambda^4 y. \llbracket () \rrbracket)) @ K \longrightarrow^* (\lambda^2 z'. ((\lambda^4 y. \llbracket () \rrbracket) @ z') @ K) @ () \\
& \longrightarrow ((\lambda^4 y. \llbracket () \rrbracket) @ ()) @ K \longrightarrow^* ().
\end{aligned}$$

Thus,  $CS(\llbracket t_p \rrbracket @ K) = \{(3, 1), (2, 4)\} (= CF(t_p))$ .

## 4.2 From CSA to HO Model Checking

To reduce CSA to HO model checking, we transform the output of the CPS transformation into a tree-generating program having tree constructors:  $\Sigma = \{\ell \mapsto 1 \mid \ell \in \mathcal{L}\} \cup \{\mathbf{br} \mapsto 2, \mathbf{e} \mapsto 0\}$ . Here,  $\ell$  is a tree constructor for a label, and  $\mathbf{br}$  is a tree constructor for conditionals. The translation  $\langle\langle \cdot \rangle\rangle$  to the tree-generating program is given by:

$$\begin{aligned}
\langle\langle () \rangle\rangle &= \mathbf{e} & \langle\langle x \rangle\rangle &= x & \langle\langle t_1 @^{\ell} t_2 \rangle\rangle &= \langle\langle t_1 \rangle\rangle @ \langle\langle t_2 \rangle\rangle & \langle\langle \mathbf{if} * t_1 t_2 \rangle\rangle &= \mathbf{br} \langle\langle t_1 \rangle\rangle \langle\langle t_2 \rangle\rangle. \\
\langle\langle \mathbf{fun}^{\ell}(f, x, \lambda k. t) \rangle\rangle &= \mathbf{fun}(f, x, \lambda k. \ell @ \langle\langle t \rangle\rangle) & & & & & & \text{(if } t \text{ has type Unit)} \\
\langle\langle \lambda^{\ell} x. t \rangle\rangle &= \lambda x. \ell @ \langle\langle t \rangle\rangle & & & & & & \text{(if } t \text{ has type Unit)}
\end{aligned}$$

Note that the translation above is well-defined for the image of the CPS transformation: A function occurs only in the form: (i)  $\mathbf{fun}^{\ell}(f, x, \lambda k. t)$  (which comes from a function in a source program) where  $t$  has type **Unit**, or (ii)  $\lambda^{\ell} x. t$  (which is a continuation function) where  $t$  has type **Unit**. The translation is also type-preserving, turning the base type **Unit** to **o**.

Whenever a function  $\text{fun}^\ell(f, x, \lambda k.t)$  or  $\lambda^\ell x.t$  is called in a program in CPS, a tree node labeled with  $\ell$  is created in the corresponding  $\lambda_T$ -program obtained by the above translation. From this observation, it should be clear that CSA has now been reduced to HO model checking, as stated below without a proof.

**Theorem 4 (Correctness of the Reduction from CSA to HOMC).** *Let  $t$  be a  $\lambda_S$ -program,  $t_C$  be  $\llbracket t \rrbracket @(\lambda z.z)$ , and  $\ell_1, \ell_2$  be labels in  $t$ . Then,  $(\ell_1, \ell_2) \in CS(\llbracket t \rrbracket @(\lambda z.z))$  if and only if  $\exists w_1, w_2. w_1 \ell_1 \ell_2 w_2 \in \text{Path}(\llbracket t_C \rrbracket)$ .*

From Theorems 3 and 4, we obtain the following corollary.

**Corollary 1 (Correctness of the Reduction from CFA to HOMC).** *Let  $t$  be a source program and  $\ell_1, \ell_2$  labels in  $t$ . Then,  $(\ell_1, \ell_2) \in CF(t)$  if and only if  $\exists w_1, w_2. w_1 \ell_1 \ell_2 w_2 \in \text{Path}(\llbracket t \rrbracket @(\lambda m.m))$ .*

### 4.3 Complexity

We now discuss the time complexity of our flow analysis with respect to the program size. We assume below that both (i) the largest size of the type of a variable and (ii) the nesting depth of function definitions are bounded above by a constant. These are rather strong assumptions, but in realistic programs, these parameters do not seem to depend much on the program size, so that it would be reasonable to assume that they are constants when we discuss the parameterized complexity with respect to the program size. Heintze and McAllester [6] also assume that the largest type size is bounded by a constant. Without the assumptions above, the time complexity of our CFA is non-elementary in the program size. We write  $|t|$  for the size of a program  $t$ .

**Theorem 5.** *Given a program  $t$  and labels  $\ell_1, \ell_2$ , the query  $(\ell_1, \ell_2) \stackrel{?}{\in} CF(t)$  can be answered in time  $O(|t|)$ , under the assumption above. Under the same assumption, the control flow set  $CF(t)$  can be computed in time  $O(|t|^3)$ .*

*Proof.* Under the assumption, the reductions from CFA to CSA and from CSA to HO model checking can be carried out in time linear in the size of  $t$ , and the size of the tree-generating program is  $O(|t|)$ . The resulting HO model checking problem satisfies the assumption of Theorem 2, hence solved in linear time. The flow set  $CF(t)$  can be computed by deciding  $(\ell_1, \ell_2) \stackrel{?}{\in} CF(t)$  for every pair  $(\ell_1, \ell_2)$  of labels. As the number of pairs is  $O(|t|^2)$ , the total cost is  $O(|t|^3)$ .  $\square$

The control flow set  $CF(t)$  is often sparse, and its size is much smaller than  $|t|^2$ . In such a case, we can use a binary search to compute  $CF(t)$  in time  $O(m|t| \log |t|)$ , where  $m$  is the size of  $CF(t)$ . For that purpose, we consider the following extended CFA problem:

“Given  $L_1, L_2 (\subseteq \mathcal{L}^-)$  and a program  $t$ , is  $(L_1 \times L_2) \cap CF(t)$  empty?”



```

enumCF () = subCF( $L_{\textcircled{}}$ ,  $L_{\lambda}$ )
subCF( $L_1, L_2$ ) = if  $L_1 \times L_2 \cap CF(t) = \emptyset$  then ()
                  else if  $(L_1 = \{\ell_1\}) \wedge (L_2 = \{\ell_2\})$  then output  $(\ell_1, \ell_2)$ 
                  else if  $|L_1| \leq |L_2|$  then
                    let  $(L_{21}, L_{22}) = \text{div}(L_2)$  in subCF( $L_1, L_{21}$ ); subCF( $L_1, L_{22}$ )
                    else let  $(L_{11}, L_{12}) = \text{div}(L_1)$  in subCF( $L_{11}, L_2$ ); subCF( $L_{12}, L_2$ )

```

**Fig. 2.** Algorithm `enumCF` for CFA with the binary search technique.

The algorithm for the extended CFA can be obtained by slightly modifying our algorithm for CFA: in the last step from CSA to HO model checking, we just need to replace all the labels in  $L_1$  with the same tree constructor  $\ell_1$  and those in  $L_2$  with  $\ell_2$ . Under the same assumption as for CFA, the extended CFA query can be answered in time  $O(|t|)$ .

Figure 2 shows an algorithm to output all elements of  $CF(t)$  by using the extended CFA. In the figure,  $L_{\textcircled{}}$  ( $L_{\lambda}$ , resp.) is the set of all labels attached to call sites (functions, resp.) in  $t$ . The function `div` splits a set  $L$  into two disjoint sets  $L_1$  and  $L_2$  such that  $L = L_1 \cup L_2$  and  $|L_2| \leq |L_1| \leq |L_2| + 1$ . `subCF`( $L_1, L_2$ ) outputs all the elements of  $(L_1 \times L_2) \cap CF(t)$ . It first checks whether  $(L_1 \times L_2) \cap CF(t)$  is empty. If  $(L_1 \times L_2) \cap CF(t)$  is non-empty and  $L_1$  and  $L_2$  are singleton sets, then `subCF`( $L_1, L_2$ ) just outputs the flow pair. Otherwise, it divides  $L_1$  or  $L_2$  and calls `subCF` recursively. For each  $(\ell_1, \ell_2) \in CF(t)$ , the algorithm checks the emptiness of  $(L_1 \times L_2) \cap CF(t)$  for some  $L_1, L_2$  such that  $(\ell_1, \ell_2) \in L_1 \times L_2$   $O(\log |t|)$  times. Thus, the whole algorithm runs in time  $O(m|t| \log |t|)$ , provided  $m > 0$ .

## 5 Extensions

We have so far considered a simple language having only functions and the unit value. In this section, we discuss how to extend our CFA to deal with other data and control structures. We also discuss an extension to compute *data* flow.

### 5.1 Booleans and Control Structures

We can extend our exact CFA to deal with booleans and control structures such as (a restricted form of) exceptions and call/cc, without losing the exactness.

To deal with booleans, we just need to extend the reduction from CFA to CSA, by combining the CPS transformation with Church encoding to enumerate booleans. The extended transformation is given as follows.

$$\begin{aligned}
\llbracket \text{true} \rrbracket &= \lambda k.k \textcircled{\text{}} (\lambda t.\lambda f.t) & \llbracket \text{false} \rrbracket &= \lambda k.k \textcircled{\text{}} (\lambda t.\lambda f.f) \\
\llbracket \text{if } t_1 \text{ then } t_2 \text{ else } t_3 \rrbracket &= \lambda k.(\llbracket t_1 \rrbracket \textcircled{\text{}} (\lambda b.b \textcircled{\text{}} (\llbracket t_2 \rrbracket \textcircled{\text{}} k) \textcircled{\text{}} (\llbracket t_3 \rrbracket \textcircled{\text{}} k))).
\end{aligned}$$

In the above transformation, we apply the standard CPS transformation (e.g. to transform `true` to  $\lambda k.k \text{true}$ ) and then encode booleans into functions (e.g.

`true` to  $\lambda t. \lambda f. t$ ). The result of the transformation is a well-typed  $\lambda_S$ -program: an expression of type `Bool` is transformed to that of type  $((\circ \rightarrow \circ \rightarrow \circ) \rightarrow \circ) \rightarrow \circ$ .

As our analysis is precise for higher-order functions, we can also deal with control structures such as (i) a finite number of exceptions that do not carry values and (ii) (the simply-typed version of) `call/cc` of type  $((\tau \rightarrow \mathbf{Unit}) \rightarrow \tau) \rightarrow \tau$  by encoding them in  $\lambda_S$ . Exceptions can be encoding by using auxiliary continuations [1]. For `call/cc`, it suffices to extend the transformation by:

$$\llbracket \text{call/cc } t \rrbracket = \lambda k. \llbracket t \rrbracket @ (\lambda f. f @ (\lambda x. \lambda k'. k @ x) @ k).$$

## 5.2 Infinite Data Domains

If  $\lambda_S$  is extended with infinite data domains such as integers and lists, the CFA problem becomes undecidable. Thus, we have to give up the exact analysis and apply some abstraction to compute an over-approximation of the actual flow set. The simplest solution is to ignore all the values except functions and booleans and replace them with unit values, before applying our CFA. Such a translation  $\llbracket \cdot \rrbracket_S$  from the extended language to  $\lambda_S$  is given by:

$$\begin{aligned} \llbracket \mathbf{Int} \rrbracket_S &= \mathbf{Unit} & \llbracket \tau_1 \rightarrow \tau_2 \rrbracket_S &= \llbracket \tau_1 \rrbracket_S \rightarrow \llbracket \tau_2 \rrbracket_S & \llbracket \tau \text{ List} \rrbracket_S &= \mathbf{Unit} \rightarrow \llbracket \tau \rrbracket_S \\ \llbracket n \rrbracket_S &= () \text{ if } n \text{ is an integer} \\ \llbracket + \rrbracket_S &= \lambda x. \lambda y. () & \llbracket =_{\mathbf{Int}} \rrbracket_S &= \lambda x. \lambda y. \text{if* true false} \\ \llbracket \mathbf{nil} \rrbracket_S &= \mathbf{fun}(f, x, f @ x) & \llbracket \mathbf{cons} \rrbracket_S &= \lambda x. \lambda l. \lambda z. \text{if* } x (l @ ()) \\ \llbracket \mathbf{hd} \rrbracket_S &= \lambda l. l @ () & \llbracket \mathbf{tl} \rrbracket_S &= \lambda l. l \\ \llbracket x \rrbracket_S &= x & \llbracket t_1 @^\ell t_2 \rrbracket_S &= \llbracket t_1 \rrbracket_S @^\ell \llbracket t_2 \rrbracket_S & \llbracket \mathbf{fun}^\ell(f, x, t) \rrbracket_S &= \mathbf{fun}^\ell(f, x, \llbracket t \rrbracket_S) \end{aligned}$$

Here, a list of elements of type  $\tau$  is represented by a non-deterministic function that takes the unit value as an argument and returns an element of the list.

*Example 5.* Let  $t_l$  be  $(\mathbf{hd}(\mathbf{cons}(\lambda^1 x. ())(\mathbf{cons}(\lambda^2 y. y) \mathbf{nil}))) @^3 ()$ .  $\llbracket t_l \rrbracket_S$  is reduced to  $(\text{if*}(\lambda^1 x. ())((\lambda u. \text{if*}(\lambda^2 y. y)(\mathbf{fun}(f, x, f @ ()))) @ ())) @^3 ()$ , which is then non-deterministically reduced to one of the following terms:

$$(\lambda^1 x. ()) @^3 () \quad (\lambda^2 y. y) @^3 () \quad (\mathbf{fun}(f, x, f @ ())) @^3 ()$$

Thus,  $CF(\llbracket t_l \rrbracket_S) = \{(3, 1), (3, 2)\}$ , which is an over-approximation of the actual flow set  $CF(t_l) = \{(3, 1)\}$ .  $\square$

Though information about the order of list elements is lost, our analysis is still very precise compared with OCFA, as demonstrated in the following example.

*Example 6.* Consider the following program:

$$\mathbf{let } app = \lambda(f, x). f @ x \mathbf{ in } \mathbf{map } app [(f_1, g_1); \dots; (f_n, g_n)]$$

where  $f_i = \lambda h. h @^{\ell_i} ()$ . Our method (extended to handle pairs) can infer that only  $g_i$  (not  $g_j$  for  $j \neq i$ ) may be called at  $\ell_i$ .  $\square$

The abstraction above completely throws away information about values other than functions and booleans. A more precise analysis can be obtained by using predicate abstractions [14].

### 5.3 Data Flow Analysis

We can extend our CFA to *data* flow analysis (DFA), which computes (an over-approximation of) the flow of not only functions but other data. We add a label to each sub-expression of the program. The DFA problem is then defined as a decision problem: “Given a program  $t$  and labels  $\ell_1, \ell_2$ , may an expression labeled by  $\ell_2$  evaluate to a value created at program point  $\ell_1$ ?”. We write  $DF(t)$  for the set of all pairs  $(\ell_1, \ell_2)$  that satisfies the condition. The DFA problem is undecidable in general in the presence of infinite data domains. Thus the goal here is to compute an over-approximation of the set  $DF(t)$ .

*Example 7.* Consider the program:  $(\lambda x.\lambda y.x^{\ell_{d,0}} + y^{\ell_{d,1}})@1^{\ell_{s,0}}@2^{\ell_{s,1}}$ . Here, we have given a label  $\ell_{s,i}$  for a source of data flow, and  $\ell_{d,j}$  for a destination.  $DF(t) = \{(\ell_{s,0}, \ell_{d,0}), (\ell_{s,1}, \ell_{d,1})\}$ .  $\square$

(An over-approximation of)  $DF(t)$  can be computed by a reduction to CFA, encoding all data into functions. For integers, we modify the encoding  $\llbracket \cdot \rrbracket_S$  in Section 5.2 as follows.

$$\begin{aligned} \llbracket \text{Int} \rrbracket_{S'} &= \text{Unit} \rightarrow \text{Unit} \\ \llbracket n^{\ell_s} \rrbracket_{S'} &= \lambda x^{\ell_s}. () \text{ if } n \text{ is an integer} & \llbracket +^{\ell_s} \rrbracket_{S'} &= \lambda x.\lambda y.\lambda z^{\ell_s}. () \\ \llbracket e^{\ell_d} \rrbracket_{S'} &= \text{let } x = \llbracket e \rrbracket_{S'} \text{ in } (x@^{\ell_d} (); x) \text{ (} e \text{ has type Int)} \end{aligned}$$

Here, both  $\text{let } x = e_1 \text{ in } e_2$  and  $e_1; e_2$  are abbreviations for  $(\lambda x.e_2)@e_1$  where the latter is a special case of the former, when  $x$  does not occur in  $e_2$ . The label  $\ell_s$  attached to  $+$  expresses the value created by the operation. An integer is turned into a function labelled by its creation point. For an expression with a destination label  $\ell_d$ , we insert an application labeled with  $\ell_d$ . Then, it should be obvious that if  $(\ell_s, \ell_d) \in DF(t)$  then  $(\ell_d, \ell_s) \in CF(\llbracket t \rrbracket_{S'})$ .

*Example 8.* Recall the program in Example 7. It is translated to the following  $\lambda_S$ -program  $\llbracket t \rrbracket_{S'}$ :

$$(\lambda x.\lambda y.\underbrace{(\lambda x' . \lambda y' . \lambda z^{\ell_{s,2}}. ())}_{+} \underbrace{(x@^{\ell_{d,0}} (); x)}_{x^{\ell_{d,0}}} \underbrace{(y@^{\ell_{d,1}} (); y)}_{y^{\ell_{d,1}}})@ \underbrace{(\lambda x^{\ell_{s,0}}. ())}_{1^{\ell_{s,0}}} @ \underbrace{(\lambda x^{\ell_{s,1}}. ())}_{2^{\ell_{s,1}}}$$

Here we have inlined let-expressions in  $\llbracket x^{\ell_{d,0}} \rrbracket_{S'}$  and  $\llbracket y^{\ell_{d,1}} \rrbracket_{S'}$ . By using our CFA, we obtain  $CF(\llbracket t \rrbracket_{S'}) = \{(\ell_{d,0}, \ell_{s,0}), (\ell_{d,1}, \ell_{s,1})\}$ . Thus, we know  $DF(t) \subseteq \{(\ell_{s,0}, \ell_{d,0}), (\ell_{s,1}, \ell_{d,1})\}$ .

## 6 Experiments

We have implemented our flow analysis for the extension of  $\lambda_S$  with integers and lists, as discussed in Section 5. The current implementation analyzes the flow of functions and integers. For data flow analysis, argument positions of integer

operations (+, =, <, ...) are taken as destinations of data flow. TRECS [7, 8] is used as the underlying model checker.<sup>5</sup>

The results of preliminary experiments are summarized in Table 1. In the table, the column OS shows the largest order of types in a source program, where the order of a type is defined by:  $order(\mathbf{Unit}) = order(\mathbf{Int}) = 0$  and  $order(T_1 \rightarrow T_2) = \max(order(T_1) + 1, order(T_2))$ . OT shows the largest order of types in the tree-generating program (represented in the form of higher-order recursion schemes [19]) obtained by the two step reductions. For comparison, the column “OCFA” shows the number of flow queries for which OCFA answered yes. As OCFA outputs an over-approximation of the actual flow set, it is always greater than or equal to the number in the column “Flow”. The numbers in parentheses show the number of queries among them for which TRECS timed out. The first five programs `fib-tak` have been taken (and slightly modified) from the benchmark set of MLton (<http://mlton.org/Performance>), and `callcc` has been taken from [26], obtained by encoding `call/cc`. The other programs have been handcrafted by ourselves. For space restriction, we explain only some of the programs below: see [12] for more details. `app` defines an apply function, and uses it twice for different pairs of functions and arguments:

```
let apply = fun f -> fun g -> f g in
let f1 = .. in let f2 = .. in let g1 = .. in let g2 = .. in
(apply f1 g1)+(apply f2 g2)
```

Our analysis is able to infer that `f1` is applied to `g1` and `f2` is applied to `g2`, unlike OCFA. `app_div` is the same as above, except that the definition of `apply` has been replaced by:

```
let rec apply' = fun f -> fun g -> (f g; apply' f g) in ...
```

Our analysis respects the call-by-value semantics and correctly infers that `f2` is never called. `map` creates a list of integers and applies a function to each element. `map_pair` is the program discussed in Example 6. `map_pair2` is the same as `map_pair`, except that the definition of `map` is optimized to:

```
let map f l = if null(l) then nil else f(car(l)),
```

by taking into account our encoding of list primitives: note that, due to the over-approximation introduced by our encoding, the flow set remains the same.

Some observations from the results in Table 1 follow. First, as expected, the analysis is very slow, compared with the state-of-the-art control flow analyzer (e.g., see [22]). In fact, our naive implementation of OCFA terminated in less than 0.1 second for all the benchmark programs. This point may however be improved by refining higher-order model checkers and the reduction from CFA to higher-order model checking. Secondly, for many of the tested programs, all the flow queries were answered by TRECS, which is encouraging given the extremely high worst-case complexity (i.e.,  $k$ -EXPTIME-completeness for order- $k$

<sup>5</sup> There are a few other higher-order model checkers [11, 16] to date, but TRECS appears to be the fastest for this type of application.

Program	OS	OT	Call	Fun	Dest	Op	Const	Time	Flow	No Flow	TimeOut	OCFA
<code>fib</code>	1	4	7	3	20	8	7	5.56	42	279	0	42
<code>merge</code>	1	8	20	10	29	13	6	85.38	60	690	1	62 (1)
<code>mandelbrot</code>	1	8	18	12	49	22	8	276.94	83	1603	0	83
<code>tailfib</code>	1	8	13	8	17	7	7	3.33	36	306	0	36
<code>tak</code>	1	8	19	6	14	6	6	125.34	58	222	2	60 (2)
<code>callcc</code>	4	5	3	2	7	3	2	0.16	0	41	0	—
<code>imp_for</code>	2	9	33	17	8	3	4	13.63	47	570	0	61
<code>app_div</code>	3	8	9	6	4	2	2	0.14	6	64	0	15
<code>map</code>	2	8	6	3	8	4	4	1.25	21	61	0	21
<code>map_imflist</code>	2	8	9	6	3	2	4	1.30	13	59	0	13
<code>map_rand</code>	2	10	13	5	15	7	3	15.91	36	179	0	36
<code>map_pair</code>	5	13	15	12	3	2	2	5.80	19	173	0	22
<code>map_pair2</code>	5	13	13	12	3	2	2	0.88	17	151	0	20

Machine spec.: Intel(R) Core(TM)2 Duo 3.16GHz CPU and 3.21GB memory. Columns OS and OT: the order of the source and target programs. Call and Fun: the number of call sites and functions. Dest: the number of destinations of data flow. Op and Const: the number of (occurrences of) integer operations and constants. Time: the total running time (second) of the flow analysis. Flow: the number of flow queries answered “yes”. No Flow: the number of flow queries answered “no”. TimeOut: the number of flow queries for which TRECS could not answer in 10 seconds. OCFA: the number of flow queries for which OCFA answers “yes”.

**Table 1.** Results of experiments.

programs) of higher-order model checking [19]. TRECS [7] does not always suffer from the  $k$ -EXPTIME bottleneck, and tends to terminate quickly if there is a small certificate for a verified property. The result suggests that for our benchmark programs, certificates of flow or non-flow are small enough. Three flow queries timed out: one for `merge` and two for `tak`. These are due to a limitation of the current TRECS, rather than that of our approach. In fact, for `tak`, those queries are answered “yes” if a parameter of the model checker TRECS is manually adjusted. The query for `merge` is answered “no” by another higher-order model checker under development. For `imp_for`, `app_div`, and `map_pair2`, we can confirm that our analysis is more accurate than OCFA. Experimental comparison with more precise analyses such as  $k$ -CFA and CFA2 is left for future work.

## 7 Related Work

A number of methods for control flow analysis have been studied, including  $k$ -CFA [23], polymorphic splitting [27], type-based flow analyses [6, 18, 4], and CFA2 [26, 25]. To our knowledge, ours is the first implementation of a flow analysis that is *exact* for the simply-typed  $\lambda$ -calculus with recursion. Except Mossin’s

exact flow analysis [18], the previous methods are not exact even for  $\lambda_S$  in Section 3. An advantage brought by the exactness of our analysis for higher-order functions is that various control structures can be easily handled via encoding without losing any precision, as discussed in Section 5.1. This is in contrast with CFA2, which needed to be adapted to deal with call/cc [26]. Our reduction from CFA to CSA uses CPS transformation. Incidentally, usefulness of CPS transformation in flow analysis has been already pointed out by Shivers [24].

Mossin’s analysis [18] based on intersection types is exact for the simply-typed  $\lambda$ -calculus with recursion under the full reduction semantics (i.e.,  $\beta$ -reductions can be applied inside  $\lambda$ -abstractions). To our knowledge, his algorithm has never been implemented. Given a term  $e$ , his algorithm unfolds recursion a certain (huge) number of times to obtain a recursion-free (thus strongly normalizing) term  $e'$  that has the same flow set as  $e$ , and then fully reduces  $e'$  to obtain the flow set. Both the number of required unfoldings is huge, so that his algorithm would not be runnable even for the small benchmark programs in Section 6.

Vardoulakis and Shivers [26, 25], and Earl et al. [3] have recently proposed new control flow analyses, where programs are modeled as *first-order* pushdown systems. Our CFA based on HO model checking may have some connection to their methods, since we model programs (via the two-step encodings) as higher-order recursion schemes, which are equivalent to *higher-order* (collapsible) pushdown systems [5]. It would be interesting to consider something between our CFA (based on higher-order pushdown in the sense above) and theirs, like “CFA based on 2nd-order pushdown systems”.

Ong and Tzevelekos [20] studied the (un)decidability of control flow analysis of *open* higher-order functional programs (i.e. programs that may have unknown arguments), and shown that the CFA problem in that setting is undecidable in general but that it is decidable for a certain fragment. In the present paper, we considered only closed programs.

Our CFA benefits from recent advances in higher-order model checking [19, 9, 7]. Kobayashi ([10], Section 3.3.2) sketched the reduction from CFA to HO model checking, but have neither formalized nor implemented it. Kobayashi et al. [9, 15, 14] have also applied higher-order model checking to other program analysis/verification problems for functional programs, and implemented tools for tree-processing programs [15] and reachability verification [14].

## 8 Conclusions

We have formalized a new method for control flow analysis based on HO model checking, and proved its correctness. It is exact for the simply-typed  $\lambda$ -calculus with recursion. We have also implemented the method and carried out preliminary experiments, to show that it is indeed runnable at least for small programs. We have to wait for further advances of HO model checking to judge its practicality, but we believe that the present work expands the design space for control flow analyses, by providing an analysis with the extreme precision.

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## Appendix

### A Syntax and Semantics of $\lambda_T$ and Tree-Generating Programs

This section gives a complete description of the language  $\lambda_T$  and tree-generating programs introduced in Section 2. After giving the syntax and reduction semantics of  $\lambda_T$ , we define the *value tree* of a tree-generating program, which is a possibly infinite tree defined as a “limit” of an infinite reduction sequence. A path of the value tree corresponds to a word in the path language defined in Section 2.

In the following, we fix a ranked alphabet  $\Sigma$ , ranged over by **a** and **b**. We assume that  $\Sigma$  has a distinguished element  $\perp$  whose arity is 0 (i.e.,  $\Sigma(\perp) = 0$ ), which indicates a tree that is “not yet determined” or “undefined”.

#### A.1 Syntax, Type System and Reduction Semantics

The language  $\lambda_T$  is a call-by-name simply-typed  $\lambda$ -calculus extended with recursion and tree constructors. The syntax of its *terms* and *types* is given by the following grammar:

$$\begin{array}{l} \text{Types } \tau, \sigma ::= o \mid \tau_1 \rightarrow \tau_2 \\ \text{Terms } e ::= \mathbf{a} \mid \mathbf{fun}(f, x, e) \mid e_1 e_2 \mid x \end{array}$$

where  $f$  and  $x$  range over variables. The unique base type  $o$  is for trees. The type  $\tau \rightarrow \sigma$  is for functions from  $\tau$  to  $\sigma$ , as usual.

A *type environment*  $\Gamma$  is a set of type bindings of the form  $x : \tau$ , which contains at most one binding for each variable. The typing rules are given as follows.

$$\begin{array}{c} \frac{}{\Gamma \vdash \mathbf{a} : \underbrace{o \rightarrow \cdots \rightarrow o \rightarrow o}_{\Sigma(\mathbf{a})}} \\ \\ \frac{\Gamma, f : \tau \rightarrow \sigma, x : \tau \vdash e : \sigma}{\Gamma \vdash \mathbf{fun}(f, x, e) : \tau \rightarrow \sigma} \\ \\ \frac{\Gamma \vdash e_1 : \sigma \rightarrow \tau \quad \Gamma \vdash e_2 : \sigma}{\Gamma \vdash e_1 e_2 : \tau} \\ \\ \frac{x : \tau \in \Gamma}{\Gamma \vdash x : \tau} \end{array}$$

A *tree-generating program* is a closed term (i.e., a term containing no free variables) of type  $o$ .

The operational semantics of  $\lambda_T$  is call-by-name. *Evaluation contexts* are defined by:

$$E ::= [] \mid E e \mid \mathbf{a} e_1 \dots e_{j-1} E e_{j+1} \dots e_{\Sigma(\mathbf{a})} ,$$

where  $1 \leq j \leq \Sigma(\mathbf{a})$ . The *reduction relation* is defined by:

$$E[\mathbf{fun}(f, x, e) e'] \longrightarrow E[e'/x, \mathbf{fun}(f, x, e)/f]e],$$

where  $[e'/x]e$  is capture-avoiding substitution of  $x$  by  $e'$  for  $e$ . We write  $\longrightarrow^*$  for the reflexive and transitive closure of  $\longrightarrow$ .

The reduction of  $\lambda_T$  is non-deterministic, since the evaluation order for arguments of a tree constructor is not determined. For example, let  $\mathbf{a} \in \Sigma$  with  $\Sigma(\mathbf{a}) = 2$  and  $e = \mathbf{a} e_1 e_2$  and assume  $e_1 \longrightarrow e'_1$  and  $e_2 \longrightarrow e'_2$ . We can reduce  $e$  in two ways:  $e \longrightarrow \mathbf{a} e'_1 e_2$  and  $e \longrightarrow \mathbf{a} e_1 e'_2$ .

It is easy to see that the reduction relation of  $\lambda_T$  is confluent. In the above example, a witness of confluence is  $\mathbf{a} e'_1 e'_2$ . We can show confluence in the general case in a similar way, since only tree constructors cause non-deterministic reduction.

## A.2 Trees

First we give some auxiliary definitions. For a given set  $A$ ,  $A^*$  is the set of all finite sequences of elements of  $A$ . We write  $\varepsilon$  for the empty sequence. For a partial function  $f : A \rightarrow B$ ,  $\text{dom}(f)$  is the domain of  $f$ , i.e.,  $\text{dom}(f) = \{a \in A \mid f(a) \text{ is defined}\}$ . If  $f : A \rightarrow B$  is a total function, then  $\text{dom}(f) = A$ .  $\mathbb{N} = \{1, 2, \dots\}$  is the set of all natural numbers.

A  $\Sigma$ -labeled tree is a partial function  $r : \mathbb{N}^* \rightarrow \Sigma$  which satisfies the following conditions:

1.  $\varepsilon \in \text{dom}(r)$  and
2.  $pi \in \text{dom}(r)$  if and only if  $p \in \text{dom}(r)$  and  $1 \leq i \leq \Sigma(r(p))$ .

$\mathcal{T}_\Sigma$  is the set of all  $\Sigma$ -labeled trees.

For  $\Sigma$ -labeled trees  $r$  and  $r'$ , we write  $r \sqsubseteq r'$  if  $\text{dom}(r) \subseteq \text{dom}(r')$  and for all  $p \in \text{dom}(r)$ ,  $r(p) = r'(p)$  or  $r(p) = \perp$ . Then the set  $\mathcal{T}_\Sigma$  of all  $\Sigma$ -labeled trees with the ordering  $\sqsubseteq$  is a complete partial order. So every directed subset<sup>6</sup>  $A$  of  $\mathcal{T}_\Sigma$  has the least upper bound in  $\mathcal{T}_\Sigma$ , written as  $\bigsqcup A$ .

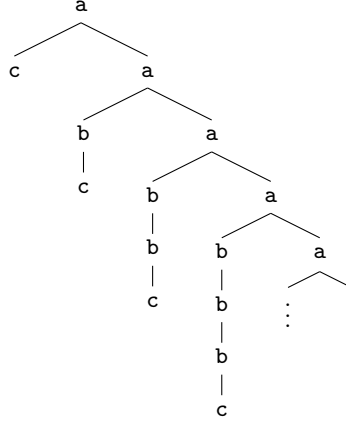
## A.3 Value Tree of Tree-Generating Program

Intuitively, the value tree of a tree-generating program is the limit of possibly infinite reduction sequences. For a given tree-generating program  $e$ , its *approximation*  $e^\perp$  is a tree inductively defined by

$$\begin{aligned} (\mathbf{a} e_1 \dots e_{\Sigma(\mathbf{a})})^\perp &= \hat{\mathbf{a}}(e_1^\perp, e_2^\perp, \dots, e_{\Sigma(\mathbf{a})}^\perp) \\ (\mathbf{fun}(f, x, e) e_1 \dots e_n)^\perp &= \perp , \end{aligned}$$

<sup>6</sup> A subset  $A$  of a partially ordered set is *directed* if for any  $a, b \in A$ , there exists  $c \in A$  such that  $a \preceq c$  and  $b \preceq c$ .





**Fig. 3.** The value tree of  $e$ .

are divided into three classes: the set  $\mathcal{L}_{@}$  of labels for applications, the set  $\mathcal{L}_{\text{fun}}$  of labels for functions and the dummy label  $\ell_{\star}$ , which is introduced by the CPS transformation. In a CPS-transformed program, all of them are attached to a function.

A *well-formed continuation* is a counterpart of a evaluation context of a source program. To define it, we need an auxiliary function  $\Psi(v)$  from values to terms defined inductively as follows:

$$\begin{aligned} \Psi(c) &= c \\ \Psi(\text{fun}^{\ell}(f, x, t)) &= \text{fun}^{\ell}(f, x, \llbracket t \rrbracket) , \end{aligned}$$

where  $c$  represents a constant value (e.g.,  $()$ ) and  $\llbracket \cdot \rrbracket$  is the CPS transformation in Section 4.1. If  $\Gamma \vdash v : T$ , then  $\Gamma^{\sharp} \vdash \Psi(v) : T^{\sharp}$ , where  $\sharp$  is the transformation of types in CPS transformation given by:

$$\begin{aligned} \text{Unit}^{\sharp} &= \text{Unit} \\ (T_1 \rightarrow T_2)^{\sharp} &= T_1^{\sharp} \rightarrow (T_2^{\sharp} \rightarrow \text{Unit}) \rightarrow \text{Unit} \\ (\Gamma, x : T)^{\sharp} &= \Gamma^{\sharp}, x : T^{\sharp} . \end{aligned}$$

The set of well-formed continuations, which is a subset of closed  $\lambda_S$ -terms, is defined by the following grammar.

$$\begin{aligned} K \text{ (well-formed continuation)} &::= \lambda m. m \\ &| (\lambda^{\ell_{\star}} f. \llbracket t \rrbracket @ (\lambda^{\ell} z. (f @ z) @ K)) \\ &| (\lambda^{\ell} z. (\Psi(v) @ z) @ K) , \end{aligned}$$

where  $f$  and  $z$  are fresh variables and  $\ell$  ranges over labels for *applications* (because  $\lambda z$ , which is a part of a CPS-transformed program, corresponds to an

application in a source program). A relation  $\simeq$  between evaluation contexts and well-formed continuations is inductively defined by the following rules:

$$\begin{aligned} [] &\simeq \lambda m.m \\ E[[]@^\ell t_2] &\simeq \lambda^{\ell_*} f. \llbracket t_2 \rrbracket @(\lambda^\ell z.(f@z)@K) \quad \text{if } E \simeq K \text{ (where } f \text{ and } z \text{ are fresh)} \\ E[v_1@^\ell []] &\simeq \lambda^\ell z. (\Psi(v_1)@z)@K \quad \text{if } E \simeq K \text{ (where } z \text{ is fresh).} \end{aligned}$$

The relation  $\simeq$  is one-to-one as in the next lemma.

**Lemma 1.** *For each evaluation context  $E$ , there exists a unique  $K$  such that  $E \simeq K$ . For each well-formed continuation  $K$ , there exists a unique evaluation context  $E$  such that  $E \simeq K$ .*

*Proof.* Easy induction on the structure of  $E$  and  $K$  respectively.  $\square$

Next we introduce a variant of Plotkin's colon-translation [21]. It is similar to CPS transformation, but easier to relate to a source program. For a closed  $\lambda_S$ -term  $t$  and a well-form continuation  $K$ , the *colon-translation*  $t : K$  is defined as follows:

$$\begin{aligned} v : K &= K@^\Psi(v) \\ (t_1@^\ell t_2) : K &= t_1 : (\lambda f. \llbracket t_2 \rrbracket @(\lambda^\ell z.(f@z)@K)) \quad (\text{where } t_1 \notin \mathbf{Value}) \\ (v_1@^\ell t_2) : K &= t_2 : (\lambda^\ell z. (\Psi(v_1)@z)@K) \\ (\mathbf{if} * t_1 t_2) : K &= \mathbf{if} * (\llbracket t_1 \rrbracket @K) (\llbracket t_2 \rrbracket @K) . \end{aligned}$$

If  $t$  has type  $T$  and  $K$  has type  $T^\# \rightarrow \mathbf{Unit}$ , then  $t : K$  is well-typed and has type  $\mathbf{Unit}$ . In the following, only well-typed colon-translations are examined. Our colon-translation differs from Plotkin's one [21] in that ours does not distinguish whether  $t_2$  is a value and that ours deals with recursions and non-deterministic choice.

We slightly modify the notation of reduction by annotating it with labels. The (new) reduction relation is defined by the following rules.

$$\begin{aligned} E[\mathbf{fun}^\ell(f, x, t)@v] &\xrightarrow{\ell} E[\mathbf{fun}^\ell(f, x, t)/f, v/x] t \\ E[\mathbf{if} * t_1 t_2] &\xrightarrow{1} E[t_1] \\ E[\mathbf{if} * t_1 t_2] &\xrightarrow{2} E[t_2] \end{aligned}$$

We write  $t \xrightarrow{\ell_1 \dots \ell_k} u$  if  $t \xrightarrow{\ell_1} \dots \xrightarrow{\ell_k} u$ . For a set  $S$  of finite sequences over labels, we write  $t \xrightarrow{S} t'$  if  $t \xrightarrow{w} t'$  for some  $w \in S$ . We omit  $\ell$ ,  $w$  and  $S$  if it is not important. So  $t \xRightarrow{} u$  is equivalent to  $t \xrightarrow{*} u$ .

Reduction  $t \xrightarrow{\ell} t'$  with  $\ell \in \mathcal{L}_@ \cup \{1, 2\}$  is called *principal* and one with  $\ell \in \mathcal{L}_{\mathbf{fun}} \cup \{\ell_*\}$  is called *administrative*. Intuitively, principal reduction of a CPS-transformed program corresponds to a reduction of a source program and administrative reduction is additional one introduced by the CPS-transformation.

The following lemma is trivial by the definition above.

**Lemma 2.** For any  $\ell_1, \ell_2 \in \mathcal{L}^- = \mathcal{L}_@ \cup \mathcal{L}_{\text{fun}}$ ,  $(\ell_1, \ell_2) \in CS(t)$  if and only if  $\exists t' \exists w. t \xrightarrow{w\ell_1\ell_2} t'$ .

We write  $|w|$  for the length of  $w$ , and  $w \downarrow_S$  for the projection of the sequence  $w$  on  $S$ . For example,  $(\ell_* 1 \ell_*) \downarrow_{\{1,2\}} = 1$ . We write  $w_1 \preceq w_2$  and call  $w_1$  a *prefix* of  $w_2$ , if there exists  $w_3$  such that  $w_2 = w_1 w_3$ . If  $|w_3| > 0$  and  $w_2 = w_1 w_3$ , we write  $w_1 \prec w_2$ . The following lemma states that the reduction is deterministic except non-determinism introduced by if-expressions.

**Lemma 3.** Suppose  $t \xrightarrow{w_1} t_1$  and  $t \xrightarrow{w_2} t_2$ . Then the following conditions hold.

- (I) If  $w_1 \downarrow_{\{1,2\}} = w_2 \downarrow_{\{1,2\}}$ , then  $w_1 \preceq w_2$  or  $w_2 \preceq w_1$ .
- (II) If  $w_1 \downarrow_{\{1,2\}} \prec w_2 \downarrow_{\{1,2\}}$ , then  $w_1 \prec w_2$ .
- (III) If  $w_1 = w'_1 \ell_1$  and  $w_2 = w'_2 \ell_2$  with  $w'_1, w'_2 \in \ell_*^*$  and  $\ell_1, \ell_2 \neq \ell_*$ , then (i)  $\ell_1 = \ell_2 \notin \{1, 2\}$  or (ii)  $\ell_1, \ell_2 \in \{1, 2\}$ .

*Proof.* The first two properties follow by easy induction on the length of  $w_1$ . (III) follows from (I) and (II). Suppose  $\ell_1, \ell_2 \notin \{1, 2\}$ . Then, by (I), either  $w_1 \preceq w_2$  or  $w_2 \preceq w_1$  holds. As  $\ell_1, \ell_2 \neq \ell_*$ , we have  $w'_1 = w'_2$  and  $\ell_1 = \ell_2$ . Suppose  $\ell_1 \in \{1, 2\}$  but  $\ell_2 \notin \{1, 2\}$ . Then by (II),  $w_2 \prec w_1$ , which implies  $w_2 \preceq w'_1$ . This cannot happen, however, since  $w'_1 \in \ell_*^*$  but  $w_2 \notin \ell_*^*$ . By the same argument, it cannot be the case that  $\ell_2 \in \{1, 2\}$  but  $\ell_1 \notin \{1, 2\}$ .  $\square$

We abbreviate induction hypothesis as I.H. in the following proofs.

**Lemma 4.** Let  $t$  be a closed  $\lambda_S$ -term,  $K$  a well-formed continuation. Then

$$\llbracket t \rrbracket @ K \xrightarrow{\ell_*^+} t : K .$$

*Proof.* By induction on  $t$ .

Case  $t = c$  for some constant value  $c$ .

$$\begin{aligned} \llbracket c \rrbracket @ K &= (\lambda^{\ell_*} k. k @ c) @ K \\ &\xrightarrow{\ell_*} K @ c \\ &= K @ \Psi(c) \\ &= c : K . \end{aligned}$$

Case  $t = \text{fun}^\ell(f, x, t_1)$ .

$$\begin{aligned} \llbracket \text{fun}^\ell(f, x, t_1) \rrbracket @ K &= (\lambda^{\ell_*} k. k @ (\text{fun}^\ell(f, x, \llbracket t_1 \rrbracket))) @ K \\ &\xrightarrow{\ell_*} K @ (\text{fun}^\ell(f, x, \llbracket t_1 \rrbracket)) \\ &= K @ \Psi(\text{fun}^\ell(f, x, t_1)) \\ &= (\text{fun}^\ell(f, x, t_1)) : K . \end{aligned}$$

Case  $t = t_1 @^\ell t_2$ , where  $t_1$  is not a value.

$$\begin{aligned} \llbracket t_1 @^\ell t_2 \rrbracket @ K &= (\lambda^{\ell_*} k. \llbracket t_1 \rrbracket @ (\lambda^{\ell_*} f. \llbracket t_2 \rrbracket @ (\lambda^{\ell_*} z. (f @ z) @ k))) @ K \\ &\xrightarrow{\ell_*} \llbracket t_1 \rrbracket @ (\lambda^{\ell_*} f. \llbracket t_2 \rrbracket @ (\lambda^{\ell_*} z. (f @ z) @ K)) \\ &\xrightarrow{\ell_*^+} t_1 : (\lambda^{\ell_*} f. \llbracket t_2 \rrbracket @ (\lambda^{\ell_*} z. (f @ z) @ K)) && \text{(by I.H.)} \\ &= (t_1 @^\ell t_2) : K . \end{aligned}$$

Case  $t = v_1 @^\ell t_2$ .

$$\begin{aligned}
\llbracket v_1 @^\ell t_2 \rrbracket @K &= (\lambda^{\ell_*} k. \llbracket v_1 \rrbracket @(\lambda^{\ell_*} f. \llbracket t_2 \rrbracket @(\lambda^\ell z. (f @z) @k))) @K \\
&\xrightarrow{\ell_*} \llbracket v_1 \rrbracket @(\lambda^{\ell_*} f. \llbracket t_2 \rrbracket @(\lambda^\ell z. (f @z) @K)) \\
&\xRightarrow{\ell_*^+} v_1 : (\lambda^{\ell_*} f. \llbracket t_2 \rrbracket @(\lambda^\ell z. (f @z) @K)) && \text{(by I.H.)} \\
&= (\lambda^{\ell_*} f. \llbracket t_2 \rrbracket @(\lambda^\ell z. (f @z) @K)) @\Psi(v_1) \\
&\xrightarrow{\ell_*} \llbracket t_2 \rrbracket @(\lambda^\ell z. (\Psi(v_1) @z) @K) \\
&\xRightarrow{\ell_*^+} t_2 : (\lambda^\ell z. (\Psi(v_1) @z) @K) && \text{(by I.H.)} \\
&= (t_1 @^\ell t_2) : K .
\end{aligned}$$

Case  $t = \text{if} * t_1 t_2$ .

$$\begin{aligned}
\llbracket \text{if} * t_1 t_2 \rrbracket @K &= (\lambda k. (\text{if} * (\llbracket t_1 \rrbracket @k) (\llbracket t_2 \rrbracket @k))) @K \\
&\xrightarrow{\ell_*} \text{if} * (\llbracket t_1 \rrbracket @K) (\llbracket t_2 \rrbracket @K) \\
&= (\text{if} * t_1 t_2) : K .
\end{aligned}$$

□

**Lemma 5.** *Let  $t$  be a closed  $\lambda_S$ -term,  $K$  be a well-formed continuation and  $E$  be an evaluation context such that  $E \simeq K$ .*

1. *If  $t$  is not a value, then  $E[t] : (\lambda m. m) = t : K$ .*
2.  *$t : K \xRightarrow{\ell_*^+} E[t] : (\lambda m. m)$ .*

*Proof.* By well-founded induction with respect to the ordering  $\prec$  over evaluation contexts such that  $E[] \prec E[v @ []] \prec E[[] @ t]$ . If  $E = []$ , then  $K = \lambda m. m$  and the proposition trivially stands.

Assume  $E = E_0[[] @^\ell t_2]$ . Then  $K = \lambda^{\ell_*} f. \llbracket t_2 \rrbracket @(\lambda^\ell z. (f @z) @K_0)$ , where  $E_0 \simeq K_0$ . If  $t$  is not a value, then we have

$$\begin{aligned}
E_0[t @^\ell t_2] &: (\lambda m. m.) \\
&= (t @^\ell t_2) : K_0 && \text{(by I.H.)} \\
&= t : (\lambda^{\ell_*} f. \llbracket t_2 \rrbracket @(\lambda^\ell z. (f @z) @K_0)) && \text{(since } t \text{ is not a value).}
\end{aligned}$$

So (1) holds. As a consequence, if  $t$  is not a value, then we have  $t : K \xrightarrow{*} E[t] : (\lambda m. m)$  and thus (2) stands. Now consider a case in which  $t$  is a value, say  $v$ . Then

$$\begin{aligned}
v &: K \\
&= K @\Psi(v) \\
&= (\lambda^{\ell_*} f. \llbracket t_2 \rrbracket @(\lambda^\ell z. (f @z) @K_0)) @\Psi(v) \\
&\xrightarrow{\ell_*} \llbracket t_2 \rrbracket @(\lambda^\ell z. (\Psi(v) @z) @K_0) \\
&\xRightarrow{\ell_*^+} t_2 : (\lambda^\ell z. (\Psi(v) @z) @K_0) && \text{(by Lemma 4).}
\end{aligned}$$

Here we can apply the induction hypothesis for the last term, since the well-formed continuation  $(\lambda^\ell z.(\Psi(v)@z)@K_0)$  corresponds to the evaluation context  $E_0[v@[]]$ , which is “smaller” than  $E_0[[]@t_2]$ , and we complete the proof of this case.

The case  $E = E_0[v@[]]$  can be proved in a similar way.  $\square$

**Lemma 6.** *Let  $t$  be a  $\lambda_S$ -term,  $v$  a value and  $x$  a variable. Then*

$$\llbracket [v/x]t \rrbracket = [\Psi(v)/x]\llbracket t \rrbracket.$$

*Proof.* By induction on  $t$ .

Case  $t = c$  for some constant value  $c$ .

$$\begin{aligned} \llbracket [v/x]c \rrbracket &= \llbracket c \rrbracket \\ &= [\Psi(v)/x]\llbracket c \rrbracket. \end{aligned}$$

Case  $t = x$ . Let  $k$  be a fresh variable.

$$\begin{aligned} \llbracket [v/x]x \rrbracket &= \llbracket v \rrbracket \\ &= \lambda k.k@[\Psi(v)] \\ &= [\Psi(v)/x](\lambda k.k@x) \\ &= [\Psi(v)/x]\llbracket x \rrbracket. \end{aligned}$$

Case  $t = y$  for some  $y \neq x$ .

$$\begin{aligned} \llbracket [v/x]y \rrbracket &= \llbracket y \rrbracket \\ &= [\Psi(v)/x]\llbracket y \rrbracket. \end{aligned}$$

Case  $t = \mathbf{fun}^\ell(f, y, t_1)$  for some  $y \neq x$ . Let  $k$  be a fresh variable.

$$\begin{aligned} \llbracket [v/x](\mathbf{fun}^\ell(f, y, t_1)) \rrbracket &= \llbracket \mathbf{fun}^\ell(f, y, [v/x]t_1) \rrbracket \\ &= \lambda k.k@(\mathbf{fun}^\ell(f, y, \llbracket [v/x]t_1 \rrbracket)) \\ &= \lambda k.k@(\mathbf{fun}^\ell(f, y, [\Psi(v)/x]\llbracket t_1 \rrbracket)) \quad (\text{by I.H.}) \\ &= [\Psi(v)/x](\lambda k.k@(\mathbf{fun}^\ell(f, y, \llbracket t_1 \rrbracket))) \\ &= [\Psi(v)/x]\llbracket (\mathbf{fun}^\ell(f, y, t_1)) \rrbracket. \end{aligned}$$

Case  $t = t_1@^\ell t_2$ . Let  $k, f$  and  $z$  be fresh variables.

$$\begin{aligned} &\llbracket [v/x](t_1@^\ell t_2) \rrbracket \\ &= \llbracket ([v/x]t_1)@^\ell([v/x]t_2) \rrbracket \\ &= \lambda k.\llbracket [v/x]t_1 \rrbracket@(\lambda f.\llbracket [v/x]t_2 \rrbracket@(\lambda z.(f@z)@k)) \\ &= \lambda k.([\Psi(v)/x]\llbracket t_1 \rrbracket)@(\lambda f.([\Psi(v)/x]\llbracket t_2 \rrbracket)@(\lambda z.(f@z)@k)) \quad (\text{by I.H.}) \\ &= [\Psi(v)/x](\lambda k.([\Psi(v)/x]\llbracket t_1 \rrbracket)@(\lambda f.([\Psi(v)/x]\llbracket t_2 \rrbracket)@(\lambda z.(f@z)@k))) \\ &= [\Psi(v)/x]\llbracket (t_1@^\ell t_2) \rrbracket. \end{aligned}$$



Case  $t = \mathbf{if}^* t_1 t_2$ . Let  $k$  be a fresh variable.

$$\begin{aligned}
& \llbracket [v/x](\mathbf{if}^* t_1 t_2) \rrbracket \\
&= \llbracket \mathbf{if}^* ([v/x]t_1) ([v/x]t_2) \rrbracket \\
&= \lambda k. (\mathbf{if}^* (\llbracket [v/x]t_1 \rrbracket @k) (\llbracket [v/x]t_2 \rrbracket @k))) \\
&= \lambda k. (\mathbf{if}^* ((\llbracket \Psi(v)/x \rrbracket [t_1]) @k) ((\llbracket \Psi(v)/x \rrbracket [t_2]) @k))) \quad (\text{by I.H.}) \\
&= \llbracket \Psi(v)/x \rrbracket (\lambda k. (\mathbf{if}^* (\llbracket [t_1] \rrbracket @k) (\llbracket [t_2] \rrbracket @k))) \\
&= \llbracket \Psi(v)/x \rrbracket \llbracket \mathbf{if}^* t_1 t_2 \rrbracket.
\end{aligned}$$

□

We write  $t \overset{w}{\rightsquigarrow} u$  if  $t \xrightarrow{w} u$  and  $w$  is of the form  $1\ell_\star^+$ ,  $2\ell_\star^+$ , or  $\ell_1\ell_2\ell_\star^+$  with  $\ell_1, \ell_2 \notin \{1, 2, \ell_\star\}$ . The two lemmas below (Lemma 7 and Lemma 9) establish a relationship between reduction ( $\longrightarrow$ ) of a source program and reduction ( $\rightsquigarrow$ ) of a CPS-transformed program. Intuitively, they state that

$$t_1 \longrightarrow t_2 \longrightarrow \dots \longrightarrow t_n$$

if and only if

$$t_0 : (\lambda m.m) \overset{w_1}{\rightsquigarrow} t_2 : (\lambda m.m) \overset{w_2}{\rightsquigarrow} \dots \overset{w_{n-1}}{\rightsquigarrow} t_n : (\lambda m.m)$$

for some  $w_1, \dots, w_{n-1}$ . Moreover,  $w_i$  is determined by the shape of  $t$ .

**Lemma 7.** *Let  $t$  and  $t'$  be source programs. If  $t \xrightarrow{\ell} t'$ , then  $t : (\lambda m.m) \overset{w}{\rightsquigarrow} t' : (\lambda m.m)$  for some  $w$ . Moreover,*

- If  $\ell \in \{1, 2\}$ , then  $t = E[\mathbf{if}^* t_1 t_2]$  and  $w \in \ell\ell_\star^+$ .
- If  $\ell \notin \{1, 2\}$ , then  $t = E[\mathbf{fun}^\ell(f, x, t_0) @^\ell v]$  and  $w \in \ell'\ell_\star^+$ .

*Proof.* By a case-analysis on  $\ell$ . Let  $K$  be a well-formed continuation such that  $E \simeq K$ .

Case  $\ell \in \{1, 2\}$ : The reduction  $t \xrightarrow{\ell} t'$  must be of the form  $E[\mathbf{if}^* t_1 t_2] \xrightarrow{\ell} E[t_\ell]$ . We have the following reduction sequence.

$$\begin{aligned}
& E[\mathbf{if}^* t_1 t_2] : (\lambda m.m) \\
&= (\mathbf{if}^* t_1 t_2) : K && (\text{by Lemma 5}) \\
&= \mathbf{if}^* (\llbracket [t_1] \rrbracket @K) (\llbracket [t_2] \rrbracket @K) \\
&\xrightarrow{\ell} \llbracket [t_\ell] \rrbracket @K \\
&\xrightarrow{\ell_\star^+} t_\ell : K && (\text{by Lemma 4}) \\
&\xrightarrow{\ell_\star^*} E[t_\ell] : (\lambda m.m) && (\text{by Lemma 5})
\end{aligned}$$

So  $E[\mathbf{if}^* t_1 t_2] : (\lambda m.m) \overset{\ell\ell_\star^+}{\rightsquigarrow} E[t_1] : (\lambda m.m)$ .

Case  $\ell \notin \{1, 2\}$ :  $t \xrightarrow{\ell} t'$  must be of the form  $E[\mathbf{fun}^\ell(f, x, t_0)@^{\ell'} v] \xrightarrow{\ell} E[[\mathbf{fun}^\ell(f, x, t_0)/y, v/x] t_0]$ : We have the following reduction sequence.

$$\begin{aligned}
& E[\mathbf{fun}^\ell(f, x, t_0)@^{\ell'} v] : (\lambda m.m) \\
&= (\mathbf{fun}^\ell(f, x, t_0)@^{\ell'} v) : K && \text{(by Lemma 5)} \\
&= v : (\lambda^{\ell'} z.(\mathbf{fun}^\ell(f, x, [t_0]) @z)@K) \\
&= (\lambda^{\ell'} z.(\mathbf{fun}^\ell(f, x, [t_0]) @z)@K)@Psi(v) \\
&\xrightarrow{\ell'} (\mathbf{fun}^\ell(f, x, [t_0]) @Psi(v))@K \\
&\xrightarrow{\ell} ([\mathbf{fun}^\ell(f, x, [t_0])/f, Psi(v)/x] [t_0])@K \\
&= [[\mathbf{fun}^\ell(f, x, t_0)/f, v/x] t_0]@K && \text{(by Lemma 6)} \\
&\xrightarrow{\ell_*^+} [[\mathbf{fun}^\ell(f, x, t_0)/f, v/x] t_0] : K && \text{(by Lemma 4)} \\
&\xrightarrow{\ell_*^*} E[[\mathbf{fun}^\ell(f, x, t_0)/f, v/x] t_0] : (\lambda m.m) && \text{(by Lemma 5)}
\end{aligned}$$

□

**Lemma 8.** If  $t : (\lambda m.m) \xrightarrow{\ell_*^* \ell} u$  with  $\ell \neq \ell_*$ , then there exist  $t'$ ,  $\ell'$  and  $w$  such that (i)  $t \xrightarrow{\ell'} t'$  and (ii)  $t : (\lambda m.m) \xrightarrow{w} t' : (\lambda m.m)$  with  $w \downarrow_{\{1,2\}} = \ell \downarrow_{\{1,2\}}$ .

*Proof.* This follows by easy case analysis on  $t$ . If  $t$  is a constant value, say  $c$ , then

$$c : (\lambda m.m) = (\lambda m.m)@Psi(c) = (\lambda m.m)@c \xrightarrow{\ell_*} c .$$

(Recall that an omitted label is  $\ell_*$ .) Therefore the assumption does not hold. If  $t = E[\mathbf{fun}^{\ell_1}(f, x, t_1)@^{\ell_2} v]$ , then we have  $t \xrightarrow{\ell'} t'$  for  $t' = E[[\mathbf{fun}^{\ell_1}(f, x, t_1)/f, v/x] t_1]$  and  $\ell_1 = \ell'$ . Furthermore, by Lemma 7,  $t : (\lambda m.m) \xrightarrow{w} t' : (\lambda m.m)$  with  $w \in \ell_2 \ell' \ell_*^+$ . By the determinism of reductions (Lemma 3), we have  $\ell = \ell_2$  and  $\ell \downarrow_{\{1,2\}} = w \downarrow_{\{1,2\}}$ .

If  $t = E[\mathbf{if}^* t_1 t_2]$ , then we have  $t \xrightarrow{\ell'} t_{\ell'}$  for each  $\ell' \in \{1, 2\}$ . Furthermore, by Lemma 7,  $t : (\lambda m.m) \xrightarrow{w_{\ell'}} t_{\ell'} : (\lambda m.m)$  with  $w_{\ell'} \in \ell' \ell_*^+$ . By Lemma 3, we have  $\ell \in \{1, 2\}$ . Thus, the required conditions hold for  $t' = t_{\ell}$ ,  $\ell' = \ell$ , and  $w = w_{\ell}$ . □

**Lemma 9.** If  $t : (\lambda m.m) \xrightarrow{w \ell} u$  with  $\ell \neq \ell_*$ , then there exist  $t_1, \dots, t_k, w_1, \dots, w_k$  such that

$$t \longrightarrow t_1 \cdots \longrightarrow t_k,$$

and

$$t : (\lambda m.m) \xrightarrow{w_1} t_1 : (\lambda m.m) \xrightarrow{w_2} \cdots \xrightarrow{w_k} t_k : (\lambda m.m)$$

and  $w \ell \preceq w_1 w_2 \dots w_k$ .

*Proof.* This follows by induction on the length of  $w$ . Let  $\ell_1$  be the first non- $\ell_*$  label in  $w \ell$ . By Lemma 8, there must exist  $t_1$  such that (i)  $t \xrightarrow{\ell'} t_1$  and (ii)

$t : (\lambda m.m) \xrightarrow{w_1} t_1 : (\lambda m.m)$  with  $w_1 \downarrow_{\{1,2\}} = \ell_1 \downarrow_{\{1,2\}}$ . By the last condition, we have  $w_1 \downarrow_{\{1,2\}} \preceq w\ell \downarrow_{\{1,2\}}$ . By the determinism of reductions (Lemma 3), either  $w_1 \preceq w\ell$  or  $w\ell \preceq w_1$ . If  $w\ell \preceq w_1$ , then we are done (with  $k = 1$ ). Otherwise,  $w = w_1 w'$  and  $|w'| < |w|$ . Thus, the result follows from the induction hypothesis.  $\square$

### Proof of Theorem 3

(only if case:) Assume that  $(\ell_1, \ell_2) \in CF(t)$ . Then

$$t \longrightarrow^* E[\mathbf{fun}^{\ell_2}(f, x, t_1) @^{\ell_1} v_2] \longrightarrow E[t']$$

for some  $\pi$  and  $\pi'$ , where  $t' = [\mathbf{fun}^{\ell_2}(f, x, t_1)/f, v_2/x] t_1$ . Then we have

$$\begin{aligned} & \llbracket t \rrbracket @(\lambda m.m) \\ \longrightarrow^* & t : (\lambda m.m) && \text{(by Lemma 4)} \\ \longrightarrow^* & E[\mathbf{fun}^{\ell_2}(f, x, t_1) @^{\ell_1} v_2] : (\lambda m.m) && \text{(by iteratively applying Lemma 7)} \\ \xrightarrow{w} & E[t'] : (\lambda m.m) && \text{(by Lemma 7)}. \end{aligned}$$

By Lemma 7,  $w \in \ell_1 \ell_2 \ell_\star^+$ . Thus by Lemma 2,  $(\ell_1, \ell_2) \in CS(\llbracket t \rrbracket @(\lambda m.m))$ .

(if case:) Assume that  $(\ell_1, \ell_2) \in CS(\llbracket t \rrbracket @(\lambda m.m))$ . By Lemma 2, we have a reduction sequence  $\llbracket t \rrbracket @(\lambda m.m) \xrightarrow{w\ell_1 \ell_2} t'$  for some  $t'$ . By determinacy of reduction (Lemma 3) and Lemma 9 and Lemma 4, then there exists  $t_1, \dots, t_k, w_1, \dots, w_k$  such that

$$t \longrightarrow t_1 \cdots \longrightarrow t_k,$$

and

$$\llbracket t \rrbracket @(\lambda m.m) \xrightarrow{\ell_\star^*} t : (\lambda m.m) \xrightarrow{w_1} t_1 : (\lambda m.m) \xrightarrow{w_2} \cdots \xrightarrow{w_k} t_k : (\lambda m.m)$$

and  $w\ell_1 \ell_2$  is a prefix of  $w_1 w_2 \dots w_k$ . Thus, there exists  $i$  such that  $w_i \in \ell_1 \ell_2 \ell_\star^+$ . By Lemma 7 and Lemma 3, it must be the case that  $t_{i-1} = E[\mathbf{fun}^{\ell_2}(f, x, t') @_1^{\ell_1} v]$ . We have therefore  $(\ell_1, \ell_2) \in CF(t)$  as required.  $\square$