

Defunctionalization at Work *

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Abstract

Reynolds's defunctionalization technique is a whole-program transformation from higher-order to first-order functional programs. We study practical applications of this transformation and uncover new connections betw een seemingly unrelated higher-order and first-order specifications and between their correctness proofs. Defunctionalization therefore appearsboth as a springboard for rev ealing new connections and as a bridge for transferring existing results betw een the first-order world and the higher-order world.

Categories and Subject Descriptors

D.1.1 [**Programming Tec hniques**]: Applicative (functional) programming; D.3.3 [**Programming Languages**]: Language Constructs and Features—A bstact data typ es, Control structur es, Data types and structures, Procedures, functions, and subroutines, Recursion; E.1 [**Data**]: Data Structures—R eords; F.3.3 [**Logics and Meanings of Programs**]: Studies of Program Constructs—F unctional constructs; F.4.1 [**Mathematical Logic and Formal Languages**]: Lambda calculus and related systems; I.2.2 [**Artificial Intelligence**]: Automatic Programming—Program transformation.

Keywords

Church encoding, closure conversion, con tinuations, cotinuation-passing style (CPS), CPS transformation, defunctionalization, direct-style transformation, first-order programs, higher-order programs, lambda-lifting, ML, regular expressions, Sc heme, supercombinator conversion, syntactic theories.

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1. Background and Introduction

In first-order programs, all functions are named and each call refers to the callee by its name. In higher-order programs, functions may be anonymous, passed as arguments, and returned as results. As Strachey put it [49], functions are *second-class* denotable values in a first-order program, and *first-class* expressible values in a higher-order program. One may then w onder how first-class functions are represented at run time.

- First-class functions are often represented with *closures*, i.e., expressible values pairing a code pointer and the denotable values of the variables occurring free in that code, as proposed by Landin in the mid-1960's [30]. Today, closures are the most common representation of first-class functions in the world of eager functional programming [1, 17, 32], as well as a standard representation for implementing object-oriented programs [23]. They are also used to implement higher-order logic programming [8].
- Alternatively, higher-order programs can be *defunctionalize d* into first-order programs, as proposed by Reynolds in the early 1970's [43]. In a defunctionalized program, first-class functions are represented with first-order data types: a first-class function is introduced with a constructor holding the values of the free v ariables of a function abstraction, and it is eliminated with a case expression dispatching over the corresponding constructors.
- First-class functions can also be dealt with by translating functional programs into *combinators* and using graph reduction, as proposed by Turner in the mid-1970's [51]. This implementation technique has been investigated extensively in the world of lazy functional programming [27, 29, 37, 38].

Compared to closure conversion and to combinator conversion, defunctionalization has been used very little. The goal of this article is to study practical applications of it.

We first illustrate defunctionalization with two concrete examples (Sections 1.1 and 1.2). In the first program, two function abstractions are instantiated once, and in the second program, one function abstraction is instantiated repeatedly .We then characterize defunctionalization in a nutshell (Section 1.3) before reviewing related work (Section 1.4). Finally, we raise questions to which defunctionalization provides answers (Section 1.5).

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1.1 A sample higher-order program with a static number of closures

In the following ML program, aux is passed a first-class function, applies it to 1 and 10, and sums the results. The main function calls aux twice and multiplies the results. All in all, two function abstractions occur in this program, in main.

```
(* aux : (int -> int) -> int *)
fun aux f
    = f 1 + f 10
(* main : int * int * bool -> int *)
fun main (x, y, b)
    = aux (fn z => x + z) *
        aux (fn z => if b then y + z else y - z)
```

Defunctionalizing this program amounts to defining a data type with two constructors, one for each function abstraction, and its associated apply function. The first function abstraction contains one free variable (x, of type integer), and therefore the first data-type constructor requires an integer. The second function abstraction contains two free variables (y, of type integer, and b, of type boolean), and therefore the second data-type constructor requires an integer and a boolean.

In main, the first first-class function is thus introduced with the first constructor and the value of x, and the second with the second constructor and the values of y and b.

In aux, the functional argument is passed to a secondclass function apply that eliminates it with a case expression dispatching over the two constructors.

1.2 A sample higher-order program with a dynamic number of closures

A reviewer wondered what happens for programs that "dynamically generate" new closures, and whether such programs lead to new constants and thus require extensible case expressions. The following example illustrates such a situation and shows that no new constants and no extensible case expressions are needed.

In the following ML program, aux is passed two arguments and applies one to the other. The main function is given a number i and a list of numbers [j1, j2, ...] and returns the list of numbers [i+j1, i+j2, ...]. One function abstraction, fn i => i + j, occurs in this program, in main, as the second argument of aux. Given an input list of length n, the function abstraction is instantiated n times in the course of the computation.

Defunctionalizing this program amounts to defining a data type with only one constructor, since there is only one function abstraction, and its associated apply function. The function abstraction contains one free variable (j, of type integer), and therefore the data-type constructor requires an integer.

In main, the first-class function is introduced with the constructor and the value of j.

In aux, the functional argument is passed to a secondclass function apply that eliminates it with a case expression dispatching over the constructor.

Given an input list of length n, the constructor LAM is used n times in the course of the computation.

1.3 Defunctionalization in a nutshell

In a higher-order program, first-class functions arise as instances of function abstractions. All these function abstractions can be enumerated in a whole program. Defunctionalization is thus a whole-program transformation where function types are replaced by an enumeration of the function abstractions in this program.

Defunctionalization therefore takes its roots in type theory. Indeed, a function type hides typing assumptions from the context, and, as pointed out by Minamide, Morrisett, and Harper in their work on typed closure conversion [32], making these assumptions explicit requires an existential type. For a whole program, this existential type can be represented with a finite sum together with the corresponding injections and case dispatch, and this representation is precisely what defunctionalization achieves.

These type-theoretical roots do not make defunctionalization a straitjacket, to paraphrase Reynolds about Algol [42]. For example, one can use several apply functions, e.g., grouped by types, as in Bell, Bellegarde, and Hook's work [4]. One can also defunctionalize a program selectively, e.g., only its continuations, as in Section 3. One can even envision a lightweight defunctionalization similar to Steckler and Wand's lightweight closure conversion [47], as in Banerjee, Heintze, and Riecke's recent work [2].

1.4 Related work

Originally, Reynolds devised defunctionalization to transform a higher-order interpreter into a first-order one [43]. He presented it as a programming technique, and never used it again [44].

Since then, defunctionalization has not been used much, though when it has, it was as a full-fledged implementation technique: Bondorf uses it to make higher-order programs amenable to first-order partial evaluation [5]; Tolmach and Oliva use it to compile ML programs into Ada [50]; Fegaras uses it in his object-oriented database management system, lambda-DB [18]; Wang and Appel use it in type-safe garbage collectors [54]; and defunctionalization is an integral part of MLton [7] and of Boquist's Haskell compiler [6].

Only lately has defunctionalization been formalized: Bell, Bellegarde, and Hook showed that it preserves types [4]; Nielsen proved its partial correctness using denotational semantics [35, 36]; and Banerjee, Heintze and Riecke proved its total correctness using operational semantics [2].

1.5 This work

Functional programming encourages fold-like recursive descents, typically using auxiliary recursive functions. Often, these auxiliary functions are higher order in that their codomain is a function space. For example, if an auxiliary function has an accumulator of type α , its co-domain is $\alpha \rightarrow \beta$, for some β . For another example, if an auxiliary function has a continuation of type $\alpha \rightarrow \beta$, for some β , its co-domain is $(\alpha \rightarrow \beta) \rightarrow \beta$. How do these functional programs compare to programs written using a first-order, data-structure oriented approach?

Wand's classical work on continuation-based program transformations [53] was motivated by the question "What is a data-structure continuation?". Each of the examples considered in Wand's paper required a eureka step to design a data structure for representing a continuation. Are such eureka steps always necessary?

Continuations are variously presented as a functional representation of the rest of the computation and as a functional representation of the context of a computation [20]. Wand's work addressed the former view, so let us consider the latter one. For example, in his PhD thesis [19], Felleisen developed a syntactic approach to semantics relying on the first-order notions of 'evaluation context' and of 'plugging expressions into contexts'. How do these first-order notions compare to the notion of continuation?

In the rest of this article, we show that defunctionalization provides a single answer to all these questions. All the programs we consider perform a recursive descent and use an auxiliary function. When this auxiliary function is higherorder, defunctionalization yields a first-order version with an accumulator (e.g., tree flattening in Section 2.1 and list reversal in Section 2.2). When this auxiliary function is firstorder, we transform it into continuation-passing style; defunctionalization then yields an iterative first-order version with an accumulator in the form of a data structure (e.g., string parsing in Section 3.1 and regular-expression matching in Section 5). We also consider a definitional interpreter for a syntactic theory and we identify that it is written in a defunctionalized form. We then "refunctionalize" it and obtain a continuation-passing definitional interpreter whose continuations represents the evaluation contexts of the syntactic theory (Section 4).

In addition, we observe that defunctionalization and Church encoding have dual purposes, since Church encoding is a classical way to represent data structures with higher-order functions. What is the result of defunctionalizing a Churchencoded data structure? And what does one obtain when Church-encoding the result of defunctionalization?

Similarly, we observe that backtracking is variously implemented in a first-order setting with one or two stacks, and in a higher-order setting with one or two continuations. It is natural enough to wonder what is the result of Churchencoding the stacks and of defunctionalizing the continuations. One can wonder as well about the correctness proofs of these programs—how do they compare?

In the rest of this article, we also answer these questions. We defunctionalize two programs using Hughes's higherorder representation of intermediate lists and obtain two efficient and traditional first-order programs (Section 2.2). We also clarify the extent to which Church encoding and defunctionalization can be considered as inverses of each other (Sections 2.3, 2.4, and 2.5). Finally, we compare and contrast a regular-expression matcher and its proof before and after defunctionalization (Section 5).

2. Defunctionalization of List- and of Tree-Processing Programs

We consider several canonical higher-order programs over lists and trees and we defunctionalize them. In each case, defunctionalization yields a known, but unrelated solution. We then turn to Church encoding, which provides a uniform higher-order representation of data structures. We consider the result of defunctionalizing Church-encoded data structures, and we consider the result of Church-encoding the result of defunctionalization.

2.1 Flattening a binary tree into a list

To flatten a binary tree into a list of its leaves, we choose to map a leaf to a curried list constructor and a node to function composition, homomorphically. In other words, we map a list into the monoid of functions from lists to lists. This definition hinges on the built-in associativity of function composition.

```
datatype 'a bt = LEAF of 'a
              | NODE of 'a bt * 'a bt
(* cons : 'a -> 'a list -> 'a list *)
fun cons x xs
    = x :: xs
(*
  flatten : 'a bt -> 'a list
      walk : 'a bt -> 'a list -> 'a list *)
(*
fun flatten t
    = let fun walk (LEAF x)
              = cons x
            walk (NODE (t1, t2))
              = (walk t1) o (walk t2)
      in walk t nil
      end
```

Eta-expanding the result of walk and inlining cons and o yields a curried version of the fast flatten function with an accumulator.

```
(* flatten_ee : 'a bt -> 'a list *)
(* walk : 'a bt -> 'a list -> 'a list *)
```

It is also instructive to defunctionalize flatten. Two functional values occur—one for the leaves and one for the nodes and therefore they give rise to a data type with two constructors. Since flatten is homomorphic, the new data type is isomorphic to the data type of binary trees, and therefore the associated apply function could be made to work directly on the input tree, e.g., using deforestation [52]. At any rate, we recognize this apply function as an uncurried version of the fast flatten function with an accumulator.

```
datatype 'a lam = LAM1 of 'a
                | LAM2 of 'a lam * 'a lam
(* apply : 'a lam * 'a list -> 'a list *)
fun apply (LAM1 x, xs)
    = x :: xs
  | apply (LAM2 (f1, f2), xs)
    = apply (f1, apply (f2, xs))
(* cons_def : 'a -> 'a lam *)
fun cons_def x
    = LAM1 x
(* o_def : 'a lam * 'a lam -> 'a lam *)
fun o_def (f1, f2)
    = LAM2 (f1, f2)
(* flatten_def : 'a bt -> 'a list *)
(*
          walk : 'a bt -> 'a lam
                                    *)
fun flatten_def t
    = let fun walk (LEAF x)
              = cons_def x
            walk (NODE (t1. t2))
              = o_def (walk t1, walk t2)
      in apply (walk t, nil)
      end
```

The monoid of functions from lists to lists corresponds to Hughes's novel representations of lists [28], which we treat next.

2.2 Higher-order representations of lists

In the mid-1980's, Hughes proposed to represent intermediate lists as partially applied concatenation functions [28], so that instead of constructing a list xs, one instantiates the function abstraction fn $ys \Rightarrow xs @ ys$. The key property of this higher-order representation is that lists can be concatenated in constant time. Therefore, the following naive version of reverse operates in linear time instead of in quadratic time, as with the usual linked representation of lists, where lists are concatenated in linear time.

Let us defunctionalize this program. First, like Hughes, we recognize that appending the empty list is the identity function and that appending a single element amounts to consing it.

```
(* id : 'a list -> 'a list *)
fun id ys
    = vs
(* cons : 'a -> 'a list -> 'a list *)
fun cons x xs
   = x :: xs
(* reverse : 'a list -> 'a list
     walk : 'a list -> 'a list -> 'a list *)
(*
fun reverse xs
    = let fun walk nil
             = id
            | walk (x :: xs)
             = (walk xs) o (cons x)
      in walk xs nil
      end
```

The function space 'a list -> 'a list arises because of three functional values: id, in one conditional branch; and, in the other, the results of consing an element and of calling walk.

We thus defunctionalize the program using a data type with three constructors and its associated apply function.

This data type makes it plain that in Hughes's monoid of intermediate lists, concatenation is performed in constant time (here with LAM2).

The rest of the defunctionalized program reads as follows.

```
(* id_def : 'a lam *)
val id_def = LAM0
(* cons_def : 'a -> 'a lam *)
fun cons_def x = LAM1 x
(* o_def : 'a lam * 'a lam -> 'a lam *)
fun o_def(f, g) = LAM2(f, g)
  reverse_def : 'a list -> 'a list *)
(*
(*
          walk : 'a list -> 'a lam
                                     *)
fun reverse_def xs
   = let fun walk nil
             = id_def
            | walk (x :: xs)
             = o_def (walk xs, cons_def x)
      in apply (walk xs, nil)
      end
```

The auxiliary functions are only aliases for the data-type constructors. We also observe that LAM1 and LAM2 are always used in connection with each other. Therefore, they can be fused in a single constructor LAM3 and so can their treatment in apply_lam. The result reads as follows.

```
datatype 'a lam_alt = LAMO
                    | LAM3 of 'a lam_alt * 'a
(* apply_lam_alt : 'a lam_alt * 'a list -> 'a list *)
fun apply_lam_alt (LAM0, ys)
     уs
  | apply_lam_alt (LAM3 (f, x), ys)
    = apply_lam_alt (f, x :: ys)
   reverse_def_alt : 'a list -> 'a list
                                              *)
(*
               walk : 'a list -> 'a lam_alt
(*
                                              *)
fun reverse_def_alt xs
    = let fun walk nil
              = I.AMO
            | walk (x :: xs)
              = LAM3 (walk xs, x)
      in apply_lam_alt (walk xs, nil)
      end
```

As in Section 2.1, we can see that reverse_def_alt embeds its input list into the data type lam_alt, homomorphically. The associated apply function could therefore be made to work directly on the input list. We also recognize apply_lam_alt as an uncurried version of the fast reverse function with an accumulator.

Hughes also uses his representation of intermediate lists to define a 'fields' function that extracts words from strings. His representation gives rise to an efficient implementation of the fields function. And indeed, as for reverse above, defunctionalizing this implementation gives the fast implementation that accumulates words in reverse order and reverses them using a fast reverse function once the whole word has been found. Defunctionalization thus confirms the effectiveness of Hughes's representation.

2.3 Defunctionalizing Church-encoded non-recursive data structures

Church-encoding a value amounts to representing it by a λ -term in such a way that operations on this value are carried out by applying the representation to specific λ -terms [3, 9, 24, 33].

A data structure is a sum in a domain. (When the data structure is inductive, the domain is recursive.) A sum is defined by its corresponding injection functions and a case dispatch [55, page 133]. Church-encoding a data structure consists in (1) combining injection functions and case dispatch into λ -terms and (2) operating by function application.

In the rest of this section, for simplicity, we only consider Church-encoded data structures that are uncurried. This way, we can defunctionalize them as a whole.

For example, monotyped Church pairs and their selectors are defined as follows.

A pair is represented as a λ -term expecting one argument. This argument is a selector corresponding to the first or the second projection. In general, each of the injection functions defining a data structure has the following form.

$$inj_i = \lambda(x_1, ..., x_n) . \lambda(s_1, ..., s_m) . s_i (x_1, ..., x_n)$$

So what happens if one defunctionalizes a Church-encoded data structure, i.e., the result of the injection functions? Each injection function gives rise to a data-type constructor whose arguments correspond to the free variables in the term underlined just above. These free variables are precisely the parameters of the injection functions, which are themselves the parameters of the original constructors that were Church encoded.

Therefore defunctionalizing Church-encoded data structures (i.e., the result of their injection functions) gives rise to the same data structures, prior to Church encoding. These data structures are accessed through the auxiliary apply functions introduced by defunctionalization.

For example, monotyped Church pairs and their selectors are defunctionalized as follows.

• The selectors are closed terms and therefore the corresponding constructors are parameterless. By definition, a selector is passed a tuple of arguments and returns one of them.

• There is one injection function for pairs, and therefore it gives rise to a data type with one constructor for the values of the two free variables of the result of Church_pair. The corresponding apply function performs a selection. (N.B: apply_pair calls apply_sel, reflecting the curried type of Church_pair.)

• Finally, constructing a pair amounts to constructing a pair, à la Tarski one could say [21], and selecting a component of a pair is achieved by calling apply_pair, which in turns calls apply_sel.

An optimizing compiler would inline both apply functions. The resulting selectors, together with the defunctionalized pair constructor, would then coincide with the original definition of pairs, prior to Church encoding.

2.4 Defunctionalizing Church-encoded recursive data structures

Let us briefly consider Church-encoded binary trees. Two injection functions occur: one for the leaves, and one for the nodes. A Church-encoded tree is a λ -term expecting two arguments. These arguments are the selectors corresponding to whether the tree is a leaf or whether it is a node.

Due to the recursive nature of binary trees, Church-node propagates the selectors to the subtrees.

In general, each of the injection functions defining a data structure has the following form.

$$\begin{split} \mathrm{inj}_i &= \frac{\lambda(x_1, \, ..., \, x_n).}{\lambda(s_1, \, ..., \, s_m).s_i \, (x_1, \, ..., \, x_j \, (s_1, \, ..., \, s_m), \, ..., \, x_n) } \end{split}$$

where x_j (s_1 , ..., s_m) occurs for each x_j that is in the data type.

So what happens if one defunctionalizes a Church-encoded recursive data structure, i.e., the result of the injection functions? Again, each injection function gives rise to a datatype constructor whose arguments correspond to the free variables in the term underlined just above. These free variables are precisely the parameters of the injection functions, which are themselves the parameters of the original constructors that were Church encoded.

Therefore defunctionalizing Church-encoded recursive data structures (i.e., the result of their injection functions) also gives rise to the same data structures, prior to Church encoding. These data structures are accessed through the auxiliary apply functions introduced by defunctionalization.

Let us get back to Church-encoded binary trees. Since defunctionalization is a whole-program transformation, we consider a whole program. Let us consider the function computing the depth of a Church-encoded binary tree. This function passes two selectors to its argument. The first is the constant function returning 0, and accounting for the depth of a leaf. The second is a function that will be applied to the depth of the subtrees of each node, and computes the depth of the node by taking the max of the depths of the two subtrees and adding one.

```
fun Church_depth t
= t (fn x => 0,
fn (d1, d2) => 1 + Int.max (d1, d2))
```

This whole program is defunctionalized as follows.

• The selectors give rise to two constructors, SEL_LEAF and SEL_NODE, and the corresponding two apply functions, apply_sel_leaf and apply_sel_node.

```
datatype sel_leaf = SEL_LEAF
fun apply_sel_leaf (SEL_LEAF, x)
        = 0
datatype sel_node = SEL_NODE
fun apply_sel_node (SEL_NODE, (d1, d2))
        = Int.max (d1, d2) + 1
```

• As for the injection functions, as noted above, they give rise to two constructors, LEAF and NODE, and the corresponding apply function.

• Finally, the defunctionalized main function applies its argument to the two selectors.

Again, an optimizing compiler would inline both apply functions and SEL_LEAF and SEL_NODE would then disappear. The result would thus coincide with the original definition of binary trees, prior to Church encoding.

2.5 Church-encoding the result of defunctionalization

As can be easily verified with the Church pairs and the Church trees above, Church-encoding the result of defunctionalizing a Church-encoded data structure gives back this Church-encoded data structure: the apply functions revert to simple applications, the main data-structure constructors become injection functions, and the auxiliary data-structure constructors become selectors.

In practice, however, one often inlines selectors during Church encoding if they only occur once—which Shivers refers to as "super-beta" [45]. Doing so yields an actual inverse to defunctionalization, as illustrated in Section 4.3. This "refunctionalization" is used, e.g., in Danvy, Grobauer, and Rhiger's work on goal-directed evaluation [13]. We also illustrate it in Section 4.3.

In Church-encoded data structures, selectors have the flavor of a continuation. In the next section, we consider how to defunctionalize continuations.

3. Defunctionalization of CPS-Transformed First-Order Programs

As functional representations of control, continuations provide a natural target for defunctionalization. In this section, we investigate the process of transforming direct-style programs into continuation-passing style (CPS) programs [12, 48] and defunctionalizing their continuation. We then compare this process with Wand's continuation-based programtransformation strategies [53].

3.1 String parsing

We consider a recognizer for the language $0^n 1^n$. We write it as a function of type int list -> bool. The input is a list of integers, and the recognizer checks whether it is the concatenation of a list of n 0s and of a list of n 1s (and therefore of length 2n).

We start with a recursive-descent parser traversing the input list.

The auxiliary function walk traverses the input list. Every time it encounters 0, it calls itself recursively. When it meets something else than 0, it returns the rest of the list, and expects to find 1 at every return. In case of mismatch (i.e., a list element other than 1 for returns, or a list that is too short or too long), an exception is raised.

Let us write walk in continuation-passing style [12, 48].

The auxiliary function walk traverses the input list tailrecursively (and thus does not need any exception). If it meets something else than 0, it sends the current list to the current continuation. If it encounters 0, it iterates down the list with a new continuation. If the new continuation is sent a list starting with 1, it sends the tail of that list to the current continuation; otherwise, it returns false. The initial continuation tests whether it is sent the empty list.

Let us defunctionalize rec1. Two function abstractions occur: one for the initial continuation and one for intermediate continuations.

We identify the result as implementing a push-down automaton [26]. This automaton has two states and one element in the stack alphabet. The two states are represented by the two functions walk and apply2. The stack is implemented by the data type cont. The transitions are the tail-recursive calls. This automaton accepts an input if processing this input ends with an empty stack.

We also observe that cont implements Peano numbers. Let us replace them with ML integers.

```
(* apply3 : (int * int list) -> bool *)
fun apply3 (0, xs')
   = xs' = nil
   apply3 (k, 1 :: xs'')
   = apply3 (k-1, xs'')
  | apply3 (k, _)
   = false
(* rec3 : int list -> bool
                                    *)
(*
   walk : int list * int -> bool
                                   *)
fun rec3 xs
   = let fun walk (0 :: xs', k)
             = walk (xs', k+1)
            | walk (xs, k)
              = apply3 (k, xs)
      in walk (xs, 0)
      end
```

The result is the usual iterative two-state recognizer with a counter.

In summary, we started from a first-order recursive version and we CPS-transformed it, making it higher-order and thus defunctionalizable. We identified that the defunctionalized program implements a push-down automaton. Noticing that the defunctionalized continuation implements Peano arithmetic, we changed its representation to built-in integers and we identified that the result is the usual iterative two-state recognizer with a counter.

3.2 Continuation-based program transformation strategies, reconsidered

Wand's classical work on continuation-based program transformation [53] suggests one (1) to CPS-transform a program; (2) to design a data-structure representation for the continuation; and (3) to use this representation to improve the initial program. We observe that in each of the examples mentioned in Wand's article, defunctionalization answers the challenge of finding a data structure representing the continuation—which is significant because finding such "data-structure continuations" was one of the motivations of the work. Nevertheless, defunctionalization is not considered in the textbooks and articles that refer to Wand's article.¹

At any rate, Wand's work was seminal in that it showed how detouring via CPS yields iterative programs with accumulators. In addition, Reynolds's work shows how defunctionalizing the continuation of CPS-transformed programs gives rise to traditional, first-order accumulators.

¹The textbooks and articles we are aware of include those found in the Research Index at http://citeseer.nj.nec.com/.

We also observe that defunctionalized continuations account for the call/return patterns of recursively defined functions. Therefore, as pointed out by Dijkstra in the late 1950's [16], they evolve in a stack-like fashion. A corollary of this remark is that before defunctionalization, continuations are also used LIFO when they result from the CPS transformation of a program that does not use control operators [10, 11, 12, 14, 15, 39, 40, 48].

4. A Syntactic Theory in the Light of Defunctionalization

In this section, we present a definitional interpreter for a syntactic theory [19, 56] of arithmetic expressions. We observe that this definitional interpreter corresponds to the output of defunctionalization. We present the corresponding higher-order interpreter, which is in continuation-passing style. Its continuation represents the evaluation context of the syntactic theory.

4.1 A syntactic theory

We consider a simplified language of arithmetic expressions. An arithmetic expression is either a value (a literal) or a computation. A computation is either an addition or a conditional expression testing whether its first argument is zero.

$$e ::= n | e + e |$$
 IFZ $e e e$

A syntactic theory provides a reduction relation on expressions by defining values, evaluation contexts, and redexes [19].

The values are literals, and the evaluation contexts are defined as follows.

Plugging an expression e into a context E, written E[e], is defined as follows.

$$\begin{array}{rcl} ([\])[e] &=& e \\ (E[[\]+e'])[e] &=& E[e+e'] \\ (E[v+[]])[e] &=& E[v+e] \\ (E[\mathrm{IFZ}\ [\]e_1\ e_2])[e] &=& E[\mathrm{IFZ}\ e\ e_1\ e_2] \end{array}$$

The reduction relation is then defined by the following rules, where the expressions plugged into the context on the left-hand side are called redexes.

 $\begin{array}{rcl} E[n_1+n_2] & \rightarrow & E[n_3] & \text{where } n_3 \text{ is the sum of } n_1 \text{ and } n_2 \\ E[\text{IFZ } 0 \ e_1 \ e_2] & \rightarrow & E[e_1] \\ E[\text{IFZ } n \ e_1 \ e_2] & \rightarrow & E[e_2] & \text{if } n \neq 0 \end{array}$

These definitions satisfy a "unique decomposition" lemma [19, 56]: any expression, e, that is not a value can be uniquely decomposed into an evaluation context, E, and a redex, r, such that e = E[r].

4.2 Implementation

Arithmetic expressions are defined with the following data type.

In ae, we distinguish between values (literals) and computations (additions and conditional expressions), as traditional.

Evaluation contexts are defined with the following data type.

```
datatype ec = EMPTY
| ADD1 of ec * ae
| ADD2 of ec * int
| IFZ0 of ec * ae * ae
```

The corresponding plugging function reads as follows.

A computation undergoes a reduction step when (1) it is decomposed into a redex and its context, (2) the redex is contracted, and (3) the result is plugged into the context.

Evaluation is specified by repeatedly performing a reduction until a value is obtained.

4.3 **Refunctionalization**

We observe that the program above precisely corresponds to the output of defunctionalization: plug is the apply function of ec. The corresponding input to defunctionalization thus reads as follows.

```
(* reduce1 : comp * (ae -> 'a) -> 'a *)
fun reduce1 (ADD (V i1, V i2), x)
   = x (V (i1+i2))
  | reduce1 (ADD (V i1, C c2), x)
    = reduce1 (c2, fn e2 => x (C (ADD (V i1, e2))))
  | reduce1 (ADD (C c1, e2), x)
    = reduce1 (c1, fn e1 => x (C (ADD (e1, e2))))
  | reduce1 (IFZ (V 0, e1, e2), x)
    = x e1
  | reduce1 (IFZ (V i, e1, e2), x)
    = x e^2
  | reduce1 (IFZ (C c0, e1, e2), x)
    = reduce1 (c0, fn e0 => x (C (IFZ (e0, e1, e2))))
(* eval : ae -> int *)
fun eval (V i)
   = i
  | eval (C c)
    = eval (reduce1 (c, fn e => e))
```

We observe that reduce1 is written in continuation-passing style. Its continuation therefore represents the evaluation context of the syntactic theory.

4.4 Back to direct style

Since reduce1 uses its continuation canonically, it can be mapped back to direct style [10, 14]. The direct-style version of reduce1 reads as follows.

```
(* reduce1 : comp -> ae *)
fun reduce1 (ADD (V i1, V i2))
    = V (i1+i2)
  | reduce1 (ADD (V i1, C c2))
    = C (ADD (V i1, reduce1 c2))
  | reduce1 (ADD (C c1, e2))
    = C (ADD (reduce1 c1, e^{2}))
  | reduce1 (IFZ (V 0, e1, e2))
     = e1
  | reduce1 (IFZ (V i, e1, e2))
    = e^{2}
  | reduce1 (IFZ (C c0, e1, e2))
    = C (IFZ (reduce1 c0, e1, e2))
(* eval : ae -> int *)
fun eval (V i)
    = i
  eval (C c)
    = eval (reduce1 c)
```

The result is a definitional interpreter with an implicit representation of contexts.

4.5 Summary and conclusion

We have considered a naive definitional interpreter for a syntactic theory, and have observed that the contexts and their plugging function are the defunctionalized counterpart of a continuation. This observation has led us to implement the definitional interpreter in direct style. (In that sense, Sections 3 and 4 are symmetric, since Section 3 starts with a direct-style program and ends with a defunctionalized CPS program.)

One may wonder how the various representations of contexts in a syntactic theory influence reasoning about programs. In the next section, we compare two correctness proofs of a program, before and after defunctionalization.

5. A Comparison between Correctness Proofs before and after Defunctionalization: Matching Regular Expressions

We consider a traditional continuation-based matcher for regular expressions [26], we defunctionalize it, and we compare and contrast its correctness proof before and after defunctionalization. To this end, Section 5.1 briefly reviews regular expressions and the languages they represent; Section 5.2 presents the continuation-based matcher, which is higher-order, and its defunctionalized counterpart; and Section 5.3 compares and contrasts their correctness proofs.

5.1 Regular expressions

r

The grammar for regular expressions, r, over the alphabet Σ and the corresponding language, $\mathcal{L}(r)$, are as follows.

::=	0	$\mathcal{L}(0)$	=	Ø
	1	$\mathcal{L}(1)$	=	$\{\epsilon\}$
	С	$\mathcal{L}(\mathbf{c})$	=	$\{\mathbf{c}\}\$ where $\mathbf{c}\in\Sigma$
	r r	$\mathcal{L}(r_1 \; r_2)$	=	$\mathcal{L}(r_1)\mathcal{L}(r_2)$

$$\begin{array}{rrr} r+r & \mathcal{L}(r_1+r_2) &=& \mathcal{L}(r_1) \cup \mathcal{L}(r_2) \\ r^* & \mathcal{L}(r^*) &=& \mathcal{L}(r)^* = \bigcup_{i \in \omega} (\mathcal{L}(r))^i \end{array}$$

We represent strings as lists of ML characters, and regular expressions as elements of the following ML datatype.

```
datatype regexp = ZERO | ONE | CHAR of char
| CAT of regexp * regexp
| SUM of regexp * regexp
| STAR of regexp
```

We define the corresponding notion of "the language of a regular expression" as follows.

The concatenation of languages is defined as $L_1L_2 = \{x @ y \mid x \in L_1 \land y \in L_2\}$, where we use the append function (noted @ as in ML) to concatenate strings.

5.2 The two matchers

Our reference matcher for regular expressions is higher-order (Figure 1). We then present its defunctionalized counterpart (Figure 2).

5.2.1 The higher-order matcher

Figure 1 displays our reference matcher, which is compositional and continuation-based. Compositional: all recursive calls to accept operate on a proper subpart of the regularexpression under consideration. And continuation-based: the control flow of the matcher is driven by continuations.

The main function is match. It is given a regular expression and a list of characters, and calls accept with the regular expression, the list, and an initial continuation expecting a list of characters and testing whether this list is empty.

The accept function recursively descends its input regular expression, threading the list of characters.

The accept_star function is a lambda-lifted version of a recursive continuation defined locally in the STAR branch. (The situation is exactly the same as in a compositional matcher for an imperative language with while loops. There, one writes an auxiliary recursive function as well.) This recursive continuation checks that matching has progressed in the string.

Recently, Harper has published a similar matcher to illustrate "proof-directed debugging" [25]. Playfully, he considered a non-compositional matcher that does not check progress when matching a Kleene star. His article shows (1) how one stumbles on the non-compositional part when attempting a proof by structural induction; and (2) how one realizes that the matcher diverges for pathological regular expressions such as STAR ONE. Harper then (1) makes his matcher compositional and (2) normalizes regular expressions to exclude pathological regular expressions. Instead, we start from a compositional matcher and we include a progress test in accept_star, which lets us handle pathological regular expressions.

```
: regexp * char list * (char list -> bool) -> bool
   accept
(* accept_star : regexp * char list * (char list -> bool) -> bool
fun accept (r, s, k)
    = (case r of ZERO
                              => false
                             => k s
               ONE
                             => (case s of (c'::s') => c = c' and also k s'
               CHAR c
                                                     => false)
                                          nil
               | CAT (r1, r2) => accept (r1, s, fn s' => accept (r2, s', k))
                SUM (r1, r2) => accept (r1, s, k) orelse accept (r2, s, k)
               STAR r'
                             => accept_star (r', s, k))
and accept_star (r, s, k)
    = k s orelse accept (r, s, fn s' => not (s = s') andalso accept_star (r, s', k))
(* match : regexp * char list -> bool *)
fun match (r, s)
    = accept (r, s, fn s' \Rightarrow s' = nil)
               Figure 1: Higher-order, continuation-based matcher for regular expressions
```

```
datatype regexp_stack = EMPTY | ACCEPT of regexp * regexp_stack | ACCEPT_STAR of char list * regexp * regexp_stack
   accept_def
                    : regexp * char list * regexp_stack -> bool
   accept_star_def : regexp * char list * regexp_stack -> bool
                                                                *)
(*
(* pop_and_accept : regexp_stack * char list
                                                                 *)
fun accept_def (r, s, k)
    = (case r of ZERO
                              => false
               ONE
                              => pop_and_accept (k, s)
                             => (case s of (c'::s') => c = c' and also pop_and_accept (k, s')
               CHAR c
                                                    => false)
                                          nil
               | CAT (r1, r2) => accept_def (r1, s, ACCEPT (r2, k))
                SUM (r1, r2) => accept_def (r1, s, k) orelse accept_def (r2, s, k)
                             => accept_star_def (r', s, k))
               STAR r'
and accept_star_def (r, s, k)
   = pop_and_accept (k, s) orelse accept_def (r, s, ACCEPT_STAR (s, r, k))
and pop_and_accept (EMPTY, s')
    = s' = nil
  | pop_and_accept (ACCEPT (r2, k), s')
    = accept_def (r2, s', k)
  | pop_and_accept (ACCEPT_STAR (s, r, k), s')
    = not (s = s') andalso accept_star_def (r, s', k)
(* match : regexp * char list -> bool *)
fun match (r, s)
    = accept_def (r, s, EMPTY)
                    Figure 2: First-order, stack-based matcher for regular expressions
```

5.2.2 The first-order matcher

Defunctionalizing the matcher of Figure 1 yields a data type representing the continuations and its associated apply function.

The data type represents a stack of regular expressions (possibly with a side condition for the test in Kleene stars). The apply function merely pops the top element off this stack and tries to match it against the rest of the string. We thus name the data type "regexp_stack" and the apply function "pop_and_accept". We also give a meaningful name to the datatype constructors. Figure 2 displays the result.

5.3 The two correctness proofs

We give a correctness proof of both the higher-order version and the first-order version, and we investigate whether each proof can be converted to a proof for the other version.

The correctness criterion we choose is simply that for all regular expressions r and strings s (represented by a list of characters),

 $\left\{\begin{array}{l} \texttt{match (r, s) terminates, and} \\ s \in \mathcal{L}(r) \iff \texttt{match (r, s)} \rightsquigarrow \texttt{true} \end{array}\right.$

When writing match $(r, s) \rightarrow true$, we mean that evaluating match (r, s) terminates and yields the result true. More generally we equate expressions if they evaluate to the same result (and therefore divergent expressions are not equivalent to anything). We also reason about ML programs equationally.

5.3.1 Correctness proof of the higher-order matcher

Since match (r, s) = accept (r, s, fn s' => s' = nil), by definition, it is sufficient to prove that for s and r as above, and for any function from lists of characters to booleans terminating on all suffixes of s, denoted by k,

```
\left\{\begin{array}{ll} \texttt{accept (r, s, k) terminates, and} \\ \texttt{s} \in \mathcal{L}(\texttt{r})\mathcal{L}(\texttt{k}) \iff \texttt{accept (r, s, k)} \rightsquigarrow \texttt{true} \end{array}\right.
```

where we define the language of a "string-acceptor" k as the set $\{s \mid k \ s \rightsquigarrow true\}$.

The proof is by structural induction on the regular expression. In the case where $\mathbf{r} = \mathbf{STAR} \mathbf{r'}$, a subproof shows that the following holds for any string.

$$\left\{\begin{array}{l} \texttt{accept_star} \ (\texttt{r'}, \texttt{ s, k}) \ \texttt{terminates}, \texttt{ and} \\ \texttt{s} \in \mathcal{L}(\texttt{r'})^* \mathcal{L}(\texttt{k}) \ \Leftrightarrow \ \texttt{accept_star} \ (\texttt{r'}, \texttt{ s, k}) \rightsquigarrow \texttt{true} \end{array}\right.$$

The subproof is by well-founded induction on the structure of the string (suffixes are smaller) for the " \Leftarrow " direction, and by mathematical induction on the natural number n such that $\mathbf{s} \in \mathcal{L}(\mathbf{r}')^n \mathcal{L}(\mathbf{k})$ for the " \Rightarrow " direction. Both subproofs use the outer induction hypothesis for accept (r', s, k).

We can transfer this proof to the defunctionalized version. Since k s translates to pop_and_accept (k, s), we define $\mathcal{L}(k)$ to read {s | pop_and_accept (k, s) \rightsquigarrow true}. The proof then goes through in exactly the same format.

5.3.2 Correctness proof of the first-order matcher

Alternatively, if we were to prove the correctness of the firstorder matcher directly, we would be less inclined to recognize the stack k as representing a function. Instead, we could easily end up proving the following three propositions by mutual induction.

$$\begin{array}{rl} P_1(\mathbf{r},\mathbf{s},\mathbf{k}) := & \\ & \texttt{accept} \ (\mathbf{r},\ \mathbf{s},\ \mathbf{k}) \rightsquigarrow \texttt{true} \ \Leftrightarrow \ \mathbf{s} \in \mathcal{L}(\mathbf{r})\mathcal{L}(\mathbf{k}) \\ P_2(\mathbf{k},\mathbf{s}) := & \\ & \texttt{pop-and_accept} \ (\mathbf{k},\ \mathbf{s}) \sim \texttt{true} \ \Leftrightarrow \ \mathbf{s} \in \mathcal{L}(\mathbf{k}) \\ P_3(\mathbf{r},\mathbf{s},\mathbf{k}) := & \\ & \texttt{accept_star} \ (\mathbf{r},\ \mathbf{s},\ \mathbf{k}) \sim \texttt{true} \ \Leftrightarrow \ \mathbf{s} \in \mathcal{L}(\mathbf{r})^* \mathcal{L}(\mathbf{k}) \end{array}$$

where we define the language of a stack of regular expressions as follows.

For brevity we ignore the termination part of the proof and assume that all the functions are total. We prove, by well-founded induction on the propositions themselves, that P_1 , P_2 , and P_3 hold for any choices of \mathbf{s} , \mathbf{r} , and \mathbf{k} . The ordering is an intricate mapping into $\omega \times \omega$, ordered lexicographically so that the proof of a proposition only depends on "smaller" propositions.

This proof is more convoluted than the higher-order one for two reasons:

- 1. it separates the language of the continuation from the function that matches it, so one has to check whether the function really matches the correct language; and
- 2. it combines the two nested inductions of the higherorder proof into one well-founded induction.

Still this proof reveals a property of the continuations in the higher-order version, namely that there are at most three different kinds of continuations in use, something that cannot be seen from the type of the continuation—a full function space.

We could thus define a subset of this function space inductively, so that it only contains the functions that can be generated by the three abstractions. The first-order proof could then be extended to the higher-order program by assuming everywhere that the continuation k lies in this subset and showing that newly generated continuations do too. In effect, the set of continuations is partitioned into disjoint subsets, just as the first-order datatype represents a sum, and then we can prove something about elements in each part.

5.4 Summary and conclusion

We have considered a matcher for regular expressions, both in higher-order form and in first-order form, and we have compared them and their correctness proof. The difference between the function-based and the datatype-based representation of continuations is reminiscent of the concept of 'junk' in algebraic semantics [22]. One representation is a full function space where many elements do not correspond to an actual continuation, and the other representation only contains elements corresponding to actual continuations. This difference finds an echo in the correctness proofs of the two matchers. In the first we cannot know what the function will do, and in the second we can inspect the value. On the other hand, we could make assumptions about the functions by restricting the function space (even if only in the proof) to a smaller one that is still closed under the constructions used.

Another difference between the two proofs is where the language of a continuation is treated. In the first-order case, a continuation can be inspected, so we can prove something for all continuations independently of where each one is defined. In the higher-order case, however, the only place where we know anything about a continuation is where it is constructed, because in the proof, we can look inside the abstraction where this continuation appears textually.

More generally, this section also illustrates that defunctionalizing a functional interpreter for a backtracking language that uses success continuations yields a recursive interpreter with one stack [13, 31, 41]. Similarly, defunctionalizing a functional interpreter that uses success and failure continuations yields an iterative interpreter with two stacks [13, 34].

6. Conclusions and Issues

Reynolds's defunctionalization technique connects the world of higher-order programs and the world of first-order programs. In this article, we have illustrated this connection by considering a variety of situations where defunctionalization proves fruitful in a declarative setting.

Higher-order functions provide a convenient support for specifying and for transforming programs. As we have shown, defunctionalization can lead to more concrete specifications, e.g., that use first-order accumulators. And as we have seen with Wand's continuation-based program-transformation strategies, defunctionalization can automate eureka steps to represent data-structure continuations.

Conversely, defunctionalization also increases one's awareness that some first-order programs naturally correspond to other, higher-order, programs. For example, functional interpreters for backtracking languages are variously specified with one or two control stacks and with one or two continuations, but these specifications are not disconnected, since defunctionalizing the continuation-based interpreters yields the corresponding stack-based ones. On a related note, CPS-transforming an interpreter with one continuation is already known to automatically yield an interpreter with two continuations [12]. We are, however, not aware of a similar transformation for their stack-based counterparts.

We also have compared and contrasted the correctness proofs of a program, before and after defunctionalization. We have found that while the first-order and the higherorder programming methods suggest different proof methods, each of the proofs can be adapted to fit the other version of the program.

Finally, we have pointed out at the type-theoretical foundations of defunctionalization.

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