

Monads, Indexes and Transformations

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Abstract

The specification and derivation of substitution for the de Bruijn representation of λ -terms is used to illustrate programming with a function-sequence monad. The resulting program is improved by interactive program transformation methods into an efficient implementation that uses primitive machine arithmetic. These transformations illustrate new techniques that assist the discovery of the arithmetic structure of the solution.

Introduction

Substitution is one of many problems in computer science that, once understood in one context, is understood in all contexts. Why, then, must a different substitution function be written for every abstract syntax implemented? This paper shows how to define substitution once and use the monadic structure of the definition to instantiate it on different abstract syntax structures. It also shows how to interactively derive an efficient implementation of substitution from this very abstract definition.

Formal methods that support reasoning about free algebras from first principles based on their inductive structure are theoretically attractive because they have simple and expressive

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theories. However, in practice they often lead to inefficient algorithms because they fail to exploit the “algebras” implemented in computer hardware. This paper examines this problem by giving a systematic program development and then describing a series of (potentially) automatic program transformations that may be used to achieve an efficient implementation.

The particular program development style employed is based on the categorical notion of a *monad*. This approach to specification has been advocated by Wadler[11] and is strongly influenced by Moggi’s work on semantics[9]. The substitution algorithm for λ -calculus terms represented with de Bruijn indexes serves as the primary example. The development of the algorithm is a refinement of an example in Hook, Kieburtz and Sheard[7]. It is noteworthy because a non-standard category is used; the earlier work did not identify this category.

The algorithm is transformed into first-order equations using techniques implemented in the partial evaluator Schism[6] and an implementation of Reynolds algorithm for defunctionalization by Bell[2]. It is then refined to an equivalent first-order specification with techniques implemented in the ASTRE program transformation system[3]. Finally the program is transformed to introduce standard arithmetic and boolean operators, thus achieving an efficient algorithm.

1 The Motivating Example: de Bruijn Representation

The de Bruijn representation of terms in the λ -calculus avoids the problems of bound variable names by using indexes to represent variables[4, 5]. The index assigned to an occurrence of a variable is the number of λ ’s in the abstract syntax tree between the occurrence and the λ that binds the variable. For example, the term:

$$\lambda u. (\lambda v. uv(\lambda w. uvw))(\lambda z. zu) \tag{1}$$

is represented:

$$\lambda.(\lambda.10(\lambda.210))(\lambda.01) \tag{2}$$

This representation is most easily visualized by looking at the tree representing the term, which is given in Figure 1.

The de Bruijn representation has the advantage that α -congruent λ -terms have identical representations. There is also no need to calculate sets of free and bound variables when performing substitution. Substitution is still not trivial, however, since indexes require adjustment as terms are moved into different binding contexts. This paper develops and refines a substitution algorithm for terms that use the de Bruijn representation.

Contracting the redex in (1) yields

$$\lambda u. u(\lambda z. zu)(\lambda w. u(\lambda z. zu)w)$$

which is represented:

$$\lambda.0(\lambda.01)(\lambda.1(\lambda.02)0) \tag{3}$$

Figure 2 illustrates this term as a tree. Note that the term that replaced v occurs with two distinct representations, $\lambda.01$ and $\lambda.02$, and the indexes associated with the occurrences of u within the scope of v in (2) are decremented in (3) because the λ binding v was removed in the contraction.

The index adjustments required are described by Abadi and others in terms of two simple operations: lift and shift[1]. Fundamentally, a substitution is a map from indexes to terms. Whenever a substitution enters a new binding context (i.e. a λ), the substitution function must be *shifted* to accommodate the new mapping of indexes to variables. For example, if 0 was mapped to $\lambda x.x$ (technically $\lambda 0$ in de Bruijn form) outside the lambda, then inside the lambda 1 must be mapped to $\lambda x.x$.

The second operation, *lift*, adjusts the indexes representing non-local variables, such as u in the example above. Every time a new binding context is entered, the value of the substitution

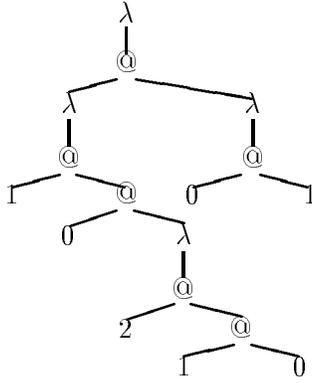


Figure 1: Tree representation of $\lambda u.(\lambda v.uv(\lambda w.uvw))(λz.zu)$.

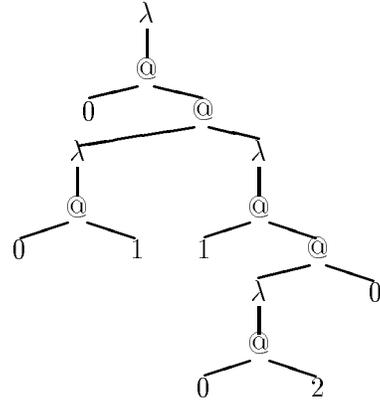


Figure 2: Representation of the contracted term.

function on every point in the domain must be lifted.

In the algorithm developed below an indexed family of functions is defined that gives the appropriately “lifted and shifted” substitution function for each binding context. Continuing the example from above, to do the β -reduction the initial substitution, σ_0 , must map all references to the index 0 to $\lambda.0\ 1$ while decrementing all references to global variables, i.e. $\sigma_0 0 = \lambda.0\ 1$ and $\sigma_0(n + 1) = n$. Note that both right hand sides are terms, not simply integers¹. In the second context σ_0 must be shifted and all terms in the image of σ_0 must be lifted. This gives $\sigma_1 0 = 0$, $\sigma_1 1 = \lambda.0\ 2$ and $\sigma_1(n + 2) = (n + 1)$. In this case, these are the only substitutions needed, but in general any number may be required. The key to this development is to calculate this sequence of functions and then use a generic recursion scheme, such as that provided by the *map* function, that has been specialized to select the function from the family appropriate to the context.

The shifting transformation is easily captured by the approximate recurrence: $\sigma_{i+1} 0 = 0$

¹The coercion of numbers to terms implicit here will become explicit in the programs developed below.

and $\sigma_{i+1}(n+1) \approx \sigma_i n$. To make it exact it is necessary to lift $\sigma_i n$. This is done by another sequence of functions:

$$\begin{aligned}
 f_0 n &= n + 1 \\
 f_1 0 &= 0 \\
 f_1(n+1) &= n + 2 \\
 f_2 0 &= 0 \\
 f_2 1 &= 1 \\
 f_2(n+2) &= n + 3
 \end{aligned}$$

Observe that in the example a single application of f_1 to the body of $\sigma_1 1$ accounts for $\lambda.0 1$ being lifted to $\lambda.0 2$. In general the f_i are generated by $f_{i+1} 0 = 0$ and $f_{i+1}(n+1) = (f_i n) + 1$. So, assuming a *map* that applies a family of functions, the family of substitution functions, $(\sigma_0, \sigma_1, \dots)$, is given by the initial substitution, σ_0 , and the recurrence:

$$\begin{aligned}
 \sigma_{i+1} 0 &= 0 \\
 \sigma_{i+1}(n+1) &= \text{map}(f_0, f_1, \dots)(\sigma_i n)
 \end{aligned}$$

Given the sequence of functions, $(\sigma_0, \sigma_1, \dots)$, mapping indexes to terms, the *map* function for sequences can be used to apply the sequence of substitution functions. This, however, results in terms of terms, since every variable has replaced its index by a term. This is not a problem, however, because the *Term* type constructor developed below is designed to be a monad; monads have a polymorphic function, *mult*, which performs the requisite flattening.

2 Monads

A *monad* is a concept from category theory that has been used to provide structure to semantics[9] and to specifications[11]. In the computer science setting a monad is defined by a parametric data type constructor, T , and three polymorphic functions:

$$\text{map} : (\alpha \rightarrow \beta) \rightarrow T\alpha \rightarrow T\beta$$

$$\begin{aligned} \mathit{unit} & : \alpha \rightarrow T\alpha \\ \mathit{mult} & : TT\alpha \rightarrow T\alpha \end{aligned}$$

The *map* function is required to satisfy:

$$\begin{aligned} \mathit{map} \ \mathit{id}_\alpha & = \ \mathit{id}_{T\alpha} \\ \mathit{map} (f \circ g) & = \ \mathit{map} \ f \circ \mathit{map} \ g \end{aligned}$$

The polymorphic functions *unit* and *mult* must satisfy:

$$\begin{aligned} \mathit{mult}_\alpha \circ \mathit{unit}_{T\alpha} & = \ \mathit{id}_{T\alpha} \\ \mathit{mult}_\alpha \circ (\mathit{map} \ \mathit{unit}_\alpha) & = \ \mathit{id}_{T\alpha} \\ \mathit{mult}_\alpha \circ \mathit{mult}_{T\alpha} & = \ \mathit{mult}_\alpha \circ (\mathit{map} \ \mathit{mult}_\alpha) \end{aligned}$$

A simple example of a monad is *list*. For lists, *map* is the familiar `mapcar` function of Lisp, *unit* is the function that produces a singleton list, and *mult* is the concatenate function that flattens a list of lists into a single list. Other examples of monads are given by Wadler[11].

Several categorical concepts are implicit above. The functional programming category has types as objects and (computable) functions as arrows. (Values are viewed as constant functions—arrows from the one element type.) The requirements on *map* specify that the type constructor *T* and the *map* function together define a *functor*. The polymorphic types of *unit* and *mult* implicitly require them to be *natural transformations*. The three laws given for them are the *monad laws*.

Monads have been used to structure specifications (and semantics) because it is often possible to characterize interesting facets of a specification as a monad. Algorithms to exploit the particular facet may frequently be expressed in terms of the *map*, *unit* and *mult* functions with no explicit details of the type constructors. Finally, the many facets are brought together by composing the type constructors.

3 The Term Monad

3.1 Naive terms

Term structures and substitution are natural candidates for the application of monads. In this section monads are illustrated by terms without binding structure. In the next section the full substitution algorithm for de Bruijn terms is given in a monadic setting.

Consider the very simple term data type:

```
datatype Term'(α) = Var(α)
                  | App(Term'(α) * Term'(α))
```

It is easily verified that $Term'$ is a monad. The map, unit and multiplier are easily calculated from the definition with the techniques of Hook, Kieburtz and Sheard[7]. Taking the viewpoint that a substitution is a function from variables to terms, it is natural to associate the type $\alpha \rightarrow Term'(\beta)$ with a substitution function. It is then meaningful to apply the *map* function of the monad to a substitution, which yields a $Term'(Term'(\beta))$.

This intermediate “term-term” is the least intuitive aspect of the example. Essentially a term over type α has been converted to a term-term over β by replacing the α -values with β -terms, but not the *Var* constructors that had been applied to them. The multiplier function, which has the type $Term'(Term'(\alpha)) \rightarrow Term'(\alpha)$, is exactly what is needed to clean up this situation. In this case it removes the residual applications of the *Var* constructor in the term-term.

In summary, if σ is an appropriately typed substitution function, the action of the substitution on the simple term type above is given by:

$$mult \circ map \sigma$$

This use of the multiplier and the map together to obtain a function of type $T(\alpha) \rightarrow T(\beta)$ from a function f of type $\alpha \rightarrow T(\beta)$ is called *Kleisli star* or the *natural extension* of f . Monads can

be defined in terms of Kleisli star, map and unit.

3.2 Terms with binding

The development in Section 1 suggests that the specification of the substitution operation will be straightforward in a monadic data type with an appropriate *map*. The following type declaration extends the naive type above with λ -abstraction:

$$\begin{aligned} \mathbf{datatype} \text{ Term}(\alpha) &= \text{Var}(\alpha) \\ &| \text{Abs}(\text{Term}(\alpha)) \\ &| \text{App}(\text{Term}(\alpha) * \text{Term}(\alpha)) \end{aligned}$$

As above, it is possible to automatically generate *map*, *mult* and *unit* functions for this type realizing a monadic structure. Unfortunately, the *map* function obtained with those techniques does not work with families of functions.

To accommodate the function sequences a new category, **FUNSEQ**, is used. The objects are data types, as before, but the morphisms are sequences of functions (formally $\mathbf{Hom}(A, B) = (B^A)^\omega$). Identities are constant sequences of identities from the underlying category; composition is pointwise, i.e. $(f_i)_{i \in \omega} \circ (g_i)_{i \in \omega} = (f_i \circ g_i)_{i \in \omega}$.

The *map* function for *Term* exploits the new structure by shifting the series of functions whenever it enters a new context. Its definition is given as a functional program:

$$\begin{aligned} \text{map } (f_0, f_1, \dots) (\text{Var } x) &= \text{Var}((f_0, f_1, \dots) x) \\ \text{map } (f_0, f_1, \dots) (\text{Abs } t) &= \text{Abs}(\text{map } (f_1, f_2, \dots) t) \\ \text{map } (f_0, f_1, \dots) (\text{App}(t, t')) &= \text{App}(\text{map } (f_0, f_1, \dots) t, \text{map } (f_0, f_1, \dots) t') \end{aligned}$$

It is easily verified that $(\text{Term}, \text{map})$ satisfy the categorical definition of a functor.

Looking at these definitions, it is clear how to insert an ordinary function or value into the category, and it is straightforward to insert the families of functions needed for the example by giving the initial element of the sequence and the functional that generates all others. However, it is also necessary to define the mapping that pulls a computation from **FUNSEQ** back into the category of functional programs. This is accomplished by taking the first element of the

function sequence. Thus, one way to realize the *map* function of **FUNSEQ** in a functional programming setting is with the *map_with_policy* function introduced in Hook, Kieburtz and Sheard[7]:

$$\begin{aligned}
\text{map_with_policy } Z \ f \ (\text{Var } x) &= \text{Var}(fx) \\
\text{map_with_policy } Z \ f \ (\text{Abs } t) &= \text{Abs}(\text{map_with_policy } Z \ (Zf) \ t) \\
\text{map_with_policy } Z \ f \ (\text{App}(t, t')) &= \text{App}(\text{map_with_policy } Z \ f \ t, \\
&\quad \text{map_with_policy } Z \ f \ t')
\end{aligned}$$

In this encoding Z is the functional that generates the sequence and f is the seed value. That is,

$$(\text{map } (f, Zf, Z^2 f, \dots))_0 = \text{map_with_policy } Z \ f$$

Note the projection of the first element from the family of functions on the left hand side indicated by the subscript 0.

The name *map_with_policy* refers to the notion of *policy function* introduced by Kieburtz[8, 7]. It refers to a type-specific function, such as Z above, that is embedded into the program for a general polymorphic operator to produce a specialized, monomorphic operator using a similar control scheme.

The *unit* and *mult* functions automatically generated for *Term* can be lifted to **FUNSEQ**. Their definitions are:

$$\begin{aligned}
\text{unit} &= \text{Var} \\
\text{mult } (\text{Var } x) &= x \\
\text{mult } (\text{Abs } t) &= \text{Abs}(\text{mult } t) \\
\text{mult } (\text{App}(t, t')) &= \text{App}(\text{mult } t, \text{mult } t')
\end{aligned}$$

Simple induction proofs show that they satisfy the monad laws.

With these definitions in place the complete definition of substitution is given in Figure 3. Note that the algorithm makes no explicit mention of the data constructors. It only uses the information about the type implicit in the definition of *map_with_policy*, *unit* and *mult*.

```

fun apply_substitution  $\sigma_0$   $M$  =
  let fun succ  $x = x + 1$ 
    fun lift  $f$ 
      =  $\lambda n.$  if  $n = 0$  then  $0$  else  $1 + f(n - 1)$ 
    fun shift  $\sigma$ 
      =  $\lambda n.$  if  $n = 0$  then unit  $0$ 
        else map_with_policy lift succ ( $\sigma(n - 1)$ )
  in mult(map_with_policy shift  $\sigma_0$   $M$ )
end

```

Figure 3: Substitution function

3.3 An alternate formulation of terms

An anonymous referee suggested we consider the following alternate definition of the term data type:

```

datatype Sum( $\alpha$ ) = Local
                  | Global( $\alpha$ )
and      Term( $\alpha$ ) = Var( $\alpha$ )
                  | Abs(Term(Sum( $\alpha$ )))
                  | App(Term( $\alpha$ ) * Term( $\alpha$ ))

```

In this formulation the identity function $\lambda x. x$ is encoded $Abs(Var(Local))$ and would have type $Term(\alpha)$. The K combinator, $\lambda x. \lambda y. x$, is encoded $Abs(Abs(Var(Global(Local))))$. Essentially, instead of using the integer data type to encode the indexes, the recursive structure of $Term$, together with the Sum data type, give an encoding of the natural numbers in which $Local$ is zero and $Global$ is the successor function.

This data type is outside the scope of those considered in our earlier work on generating monadic functions because it is not a “sum-of-products” or “polynomial” data type. The occurrence of a $Term(Sum(\alpha))$ in the definition of $Term(\alpha)$ violates the sum-of-products condition.

It is possible to define a monad based on this construction, and in that monad the Kleisli

star appears to yield the correct substitution function. Unfortunately, the functions defining the *map* and *mult* functions for this monad are not typable in Standard ML, which is the primary implementation language used in this investigation. As above, the problems stem from the occurrence of $Term(Sum(\alpha))$.

The typing problem is illustrated by the natural definition of *map* for this data type:

```

fun  mapSum f Local = Local
      | mapSum f (Global x) = Global (f x)
fun  map f (Var x) = Var (f x)
      | map f (Abs x) = Abs (map (mapSum f) x)
      | map f (App (x, y)) = App (map f x, map f y);

```

Consider the occurrence of *map* on the right hand side of the *Abs* case. If f has type $\alpha \rightarrow \beta$ then this occurrence of *map* has type $(Sum(\alpha) \rightarrow Sum(\beta)) \rightarrow Term(Sum(\alpha)) \rightarrow Term(Sum(\beta))$. The whole right-hand-side then has type $Term(\beta)$, thus the occurrence of *map* on the left hand side of the definition has type $(\alpha \rightarrow \beta) \rightarrow Term(\alpha) \rightarrow Term(\beta)$.

The type generalization rule in Standard ML only allows function definitions that, at the top level, can be typed with a fixed but arbitrary monotype to be generalized to a polytype. Consequently, the type system does not allow the *map* definition since the occurrences in the definition cannot be viewed as instances of the same monotype, even though both occurrences are instances of the same polytype. The same issues arise in type checking the multiplier.

In addition to these technological problems with this, arguably more elegant, alternate data type, we did not find a systematic method to discover and verify the monadic structure.

4 Transformation to a First-Order Set of Equations

To obtain a practical algorithm, the substitution function *apply_substitution* in Figure 3 must be made more efficient. This section shows how this transformation can be done automatically. Program transformation systems operate on systems of first-order equations. To apply them

to the algorithm of substitution the higher-order facets must be translated into first-order structures. A partial evaluation system is used to accomplish this.

The software allowing a complete automatic transformation is not yet written. The transformations below have been performed with the Schism partial evaluator [6], the program called Firstify [2] which performs the Reynolds Algorithm [10] and the Astre program transformation system [3], which are not yet integrated and do not use the same language.

4.1 Transformation of the *map_with_policy* Operator

The first step is to rewrite the program using the *map_with_policy* operator for the type $Term(\alpha)$ as a system of first-order functions. A partial evaluator can be used to specialize higher-order functions decreasing their order level. For example, consider the particular function σ_0 in the example in Section 1, and the call *apply_substitution* σ_0 . A partial evaluator produces a program that does not contain *apply_substitution* in its full generality; it specializes the definition of *apply_substitution* for the particular constant σ_0 . This specialization, called *apply_substitution_* σ_0 , does not have a function as an argument, so it is first-order.

Unfortunately, this technique is insufficient for processing calls of *map_with_policy*, which is called twice in the program in Figure 3. The specialization of *map_with_policy* for a particular policy function K and seed function g_0 gives the following function *Mwp_g*:

$$\begin{aligned} Mwp_g (g, Var(n)) &= Var(g(n)) \\ Mwp_g (g, Abs(t)) &= Abs(Mwp_g(K g, t)) \\ Mwp_g (g, App(t, t')) &= App(Mwp_g(g, t), Mwp_g(g, t')) \end{aligned}$$

The function *Mwp_g* has a function as an argument. But if it is specialized for a particular function g_0 , the partial evaluator has to specialize the internal call *Mwp_g*($K g, t$); it loops on this attempt. Fortunately, the partial evaluator is able to detect this circumstance, allowing it to select another technique. The alternative technique translates the higher-order functions into a system of first-order functions. This standard encoding, which is due to Reynolds [10],

is implemented in a program called Firstify [2]. Let us outline below how it works with the *map_with_policy* operator.

1. The first step constructs a data type that encodes how the higher-order arguments are manipulated and applied. In this case the functions to be encoded are g_0 and $K g$. For the constant function, g_0 , a constant C is introduced as a summand in the data type *Func*. The argument $K g$ cannot be encoded by a simple constant value because it contains g as a free variable. Since g is a higher-order parameter, it will already be represented by a value of type *Func*. Hence the new constructor, F , representing the application of K , must have type $Func \rightarrow Func$. This gives the data type *Func*, defined

$$\mathbf{datatype} \textit{Func} = C \mid F(\textit{Func}).$$

The introduction of this type is a rediscovery of the sequence of functions g_0, g_1, \dots because it encodes each function in the family. The function g_0 is encoded by C , and the function g_3 , for example, is encoded by $F(F(F(C)))$, which is written F^3 .

2. The functions appearing as actual arguments are replaced by their encodings. The argument functions do not exist anymore—they are replaced by first-order data. In the call $Mwp_g(g_0, M)$, g_0 is no longer a function but a first-order value, $[g_0]$, of type *Func*. The definition of Mwp_g leads to the new function Mwp_g' :

$$\begin{aligned} Mwp_g'([g], Var(n)) &= Var([g](n)) \\ Mwp_g'([g], Abs(t)) &= Abs(Mwp_g'(F([g]), t)) \\ Mwp_g'([g], App(t, t')) &= App(Mwp_g'([g], t), Mwp_g'([g], t')) \end{aligned}$$

But since $[g]$ is not a function, the application $[g](n)$ is nonsense.

3. To make sense of the applications of functional parameters in the original programs “application” functions are introduced. Specifically the function *apply_g*, defined below, decodes applications of the form $[g](n)$.

$$\textit{apply_g}(C, n) = g_0(n)$$

$$apply_g(F(\lceil g \rceil), n) = (K \lambda n. apply_g(\lceil g \rceil, n))(n). \quad (4)$$

Note that $apply_g$ is a first-order function because its argument, $\lceil g \rceil$, is an element of the type $Func$. The definition of the policy function K is unfolded to get a first-order expression of $apply_g(F(\lceil g \rceil), n)$. The definition of Mwp_g' can be completed into:

$$\begin{aligned} Mwp_g'(\lceil g \rceil, Var(n)) &= Var(apply_g(\lceil g \rceil, n)) \\ Mwp_g'(\lceil g \rceil, Abs(t)) &= Abs(Mwp_g'(F(\lceil g \rceil), t)) \\ Mwp_g'(\lceil g \rceil, App(t, t')) &= App(Mwp_g'(\lceil g \rceil, t), Mwp_g'(\lceil g \rceil, t')) \end{aligned}$$

This encoding is done with respect to a specific call of $map_with_policy Z g_0 M$. In the program in Figure 3 there are two such calls. The new functions corresponding to Mwp_g and $apply_g$ constitute a first-order program equivalent to the functions generated by map_with_policy .

4.2 Application to $apply_substitution$

Using the preceding techniques, the function $apply_substitution$ is successfully transformed into the first-order program in Figure 4. For a given substitution σ_0 , partial evaluation of an instance $apply_substitution \sigma_0$ specializes the function $apply_substitution$ into a function $apply_substitution_sigma_0$. The data type $Subst$ and the data type $Fseq$ are introduced using the program `Firstify` which implements above techniques for the encodings of $lift$ and $shift$.

$$\begin{array}{ll} \mathbf{datatype} \textit{Subst} = S0 & \mathbf{datatype} \textit{Fseq} = SUCC \\ \quad | SUBST(Subst) & \quad | FSEQ(Fseq) \end{array}$$

These two data types are isomorphic to the data type Nat^2 which is implemented efficiently in the hardware. However, the specialized function Mwp_sigma does not exploit the efficient implementation since it uses the (essentially unary) representation of the data type instead. Thus, the function $apply_sigma$ must peel off all of the data constructors each time Mwp_sigma

²The constructors for the data type Nat are 0 and s , i.e. $\mathbf{datatype} \textit{Nat} = 0 | s(Nat)$.

```

fun apply_substitution_σ0(M) =
  let fun apply_f(SUCC, n)      = s(n)
      | apply_f(FSEQ(f), n)    = if n = 0 then 0
                                      else s(apply_f(f, n - 1))
      fun Mwp_f(f, Var(n))    = Var(apply_f(f, n))
      | Mwp_f(f, Abs(t))      = Abs(Mwp_f(FSEQ(f), t))
      | Mwp_f(f, App(t, t')) = App(Mwp_f(f, t), Mwp_f(f, t'))
      fun apply_σ(S0, n)       = σ0(n)
      | apply_σ(SUBST(σ), n) = if n = 0 then unit(0)
                                      else Mwp_f(SUCC, (apply_σ(σ, n - 1)))
      fun Mwp_σ(σ, Var(n))    = Var(apply_σ(σ, n))
      | Mwp_σ(σ, Abs(t))      = Abs(Mwp_σ(SUBST(σ), t))
      | Mwp_σ(σ, App(t, t')) = App(Mwp_σ(σ, t), Mwp_σ(σ, t'))
  in mult(Mwp_σ(S0, M))
end

```

Figure 4: First-order Program

is applied to $Var(n)$. For example, after three levels of abstraction, σ_3 is represented by $SUBST(SUBST(SUBST(S0)))$. (The same is also true of the function Mwp_f .) To eliminate this inefficiency, which was present in the calling behavior of the original algorithm, the data types $Subst$ and $Fseq$ must be changed to the uniform data type Nat . This transformation can be performed automatically by *Astre*. Ultimately the explicit use of Nat will facilitate the use of primitive arithmetic in the program.

5 Simple Transformations

The following two simple transformations are performed automatically by *Astre* after introducing new function symbols. The first one introduces indexes to count the level of abstractions. The second replaces the composition of Mwp with the function $mult$ by a single function. The order of these transformations does not matter; they can be done simultaneously.

For technical reasons recursive definitions of the form

$$g(n) = \mathbf{if} \ n = 0 \ \mathbf{then} \ e_1 \ \mathbf{else} \ e_2$$

are manipulated more effectively by Astre in the equivalent form:

$$\begin{aligned} g(0) &= e_1[0/n] \\ g(s(n)) &= e_2[s(n)/n] \end{aligned}$$

The notation $e[e'/x]$ denotes the substitution of expression e' for x in e . This restriction of the form of equations ensures the termination of the rewriting used by Astre to unfold the definition of g .

5.1 Introduction of Indexes

The isomorphism between the automatically generated type *Subst* and the natural numbers is made explicit by introducing the function $iso_\sigma : Nat \rightarrow Subst$:

$$\begin{aligned} \mathbf{fun} \quad iso_\sigma(s(i)) &= SUBST(iso_\sigma(i)) \\ | \quad iso_\sigma(0) &= S0 \end{aligned}$$

The functions $apply_\sigma$ and Mwp_σ are replaced by the new functions $\sigma(i, n)$ (for $\sigma_i(n)$) and Mwp_σ' , respectively. These functions satisfy $\sigma(i, n) = apply_\sigma(iso_\sigma(i), n)$ and $Mwp_\sigma'(i, n) = Mwp_\sigma(iso_\sigma(i), n)$. Using these new equations, the Astre system implements the data type *Subst* using the data type *Nat*. New functions to implement the data type *Fseq* using *Nat* are also provided to the Astre system which then gives the program in Figure 5. The program in Figure 5 does not improve the performance of the program in Figure 4. However, its explicit use of numbers is key to the improvements presented in the next section.

5.2 Composition Step

The transformation continues with a simple (automatic) step that replaces the composition of *mult* with Mwp_σ' by a single function.³ This is accomplished automatically by the introduction

³*Ewp* is a mnemonic for extension with policy.

```

fun apply_substitution $\sigma_0(M)$  =
  let fun  $f(0, n)$  =  $s(n)$ 
    |  $f(s(i), 0)$  =  $0$ 
    |  $f(s(i), s(n))$  =  $s(f(i, n))$ 
  fun  $Mwp\_f'(i, Var(n))$  =  $Var(f(i, n))$ 
    |  $Mwp\_f'(i, Abs(t))$  =  $Abs(Mwp\_f'(s(i), t))$ 
    |  $Mwp\_f'(i, App(t, t'))$  =  $App(Mwp\_f'(i, t), Mwp\_f'(i, t'))$ 
  fun  $\sigma(0, n)$  =  $\sigma_0(n)$ 
    |  $\sigma(s(i), n)$  =  $unit(0)$ 
    |  $\sigma(s(i), s(n))$  =  $Mwp\_f'(0, \sigma(i, n))$ 
  fun  $Mwp\_{\sigma}'(i, Var(n))$  =  $Var(\sigma(i, n))$ 
    |  $Mwp\_{\sigma}'(i, Abs(t))$  =  $Abs(Mwp\_{\sigma}'(s(i), t))$ 
    |  $Mwp\_{\sigma}'(i, App(t, t'))$  =  $App(Mwp\_{\sigma}'(i, t), Mwp\_{\sigma}'(i, t'))$ 
in  $mult(Mwp\_{\sigma}'(0, M))$ 
end

```

Figure 5: Program with indexes

of a function symbol, Ewp , which is equated to the composition of $mult$ with Mwp_{σ}' , i.e., $Ewp(0, M) = mult(Mwp_{\sigma}'(0, M))$. Astre gives a program which uses neither $mult$, nor Mwp_{σ}' that includes the following definition of Ewp :

```

fun  $Ewp(i, Var(n))$  =  $\sigma(i, n)$ 
  |  $Ewp(i, Abs(t))$  =  $Abs(Ewp(s(i), t))$ 
  |  $Ewp(i, App(t, t'))$  =  $App(Ewp(i, t), Ewp(i, t'))$ 

```

The main body of the function is then replaced by $Ewp(0, M)$. The functions $mult$ and Mwp_{σ}' , which have become useless, are removed. Since the Mwp_{σ}' has now been eliminated, Mwp_f' is renamed Mwp to simplify the nomenclature below.

6 Transformation of the Sequence of the σ Functions

The transformations in this section exploit the arithmetic arguments introduced above to improve the expensive and redundant recursive calculations in σ and Ewp . Indeed, the transformation aims at discovering conditionals and subtraction from a constructor-based definition of

```

fun apply_substitution_σ0(M) =
  let fun f(0, n)           = s(n)
      | f(s(i), 0)         = 0
      | f(s(i), s(n))     = s(f(i, n))
  fun Mwp(i, Var(n))      = Var(f(i, n))
      | Mwp(i, Abs(t))     = Abs(Mwp(s(i), t))
      | Mwp(i, App(t, t')) = App(Mwp(i, t), Mwp(i, t'))
  fun σ(0, n)              = σ0(n)
      | σ(s(i), n)        = unit(0)
      | σ(s(i), s(n))     = Mwp(0, σ(i, n))
  fun Ewp(i, Var(n))    = σ(i, n)
      | Ewp(i, Abs(t))     = Abs(Ewp(s(i), t))
      | Ewp(i, App(t, t')) = App(Ewp(i, t), Ewp(i, t'))
in   Ewp(0, M)
end

```

Figure 6: Composed Program

a binary arithmetic symbol.

The function $\sigma(i, n)$ of the transformed program is a rediscovery of the series of functions $\sigma_i(n)$ of Section 1. To further refine this program, a specific instance of *apply_substitution* σ_0 must be specified. In what follows, the substitution function σ_0 , needed for the contraction described in Section 1, is used to illustrate the specialization. Recall that σ_0 replaces variables of index 0 with the term $\lambda.0\ 1$, which is represented by $Abs(App(Var(0), Var(1)))$. Thus, $\sigma_0(0) = Abs(App(Var(0), Var(1)))$ and $\sigma_0(s(n)) = unit(n)$. Unfolding these equations yields a complete constructor-based definition of $\sigma(i, n)$:

$$\begin{aligned}
\sigma(0, 0) &= Abs(App(Var(0), Var(1))) \\
\sigma(0, s(n)) &= unit(n) \\
\sigma(s(i), 0) &= unit(0) \\
\sigma(s(i), s(n)) &= Mwp(0, \sigma(i, n))
\end{aligned} \tag{5}$$

Since the equational program is complete with respect to $Nat * Nat$, the computation of any

instance of $\sigma(i, n)$ results in a ground constructor term. For example, $\sigma(4, 2)$ yields:

$$\sigma(s(s(s(s(0)))), s(s(0))) \rightarrow \quad (6)$$

$$Mwp(0, \sigma(s(s(s(0))), s(0))) \rightarrow \quad (7)$$

$$Mwp(0, Mwp(0, \sigma(s(s(0)), 0))) \rightarrow^* Var(s(s(0)))$$

Rewrites (6) and (7) are unfoldings by equation (5). Computation of any instance of $\sigma(i, n)$ by naturals can begin with unfoldings using (5) until a subterm, $\sigma(u, v)$, in which u and/or v are equal to 0 is obtained.

This suggests a target program of the form:

$$\sigma(i, n) = \mathbf{if } i > n \mathbf{ then } e_1 \mathbf{ else if } i = n \mathbf{ then } e_2 \mathbf{ else } e_3$$

where e_1 , e_2 , and e_3 are expressions. The transformation will be beneficial if these expressions are efficient. This step introduces a form of function definition by a conditional (instead of structural induction) that violates the technical restriction on programs used to assure termination of rewriting as required by the Astre system. Presently, Astre does not perform this part of the transformation. Moreover, the transformation does not directly generate the conditional; instead it generates the complete definition: $\sigma(s(i) + k, k) = u_1$, $\sigma(k, k) = u_2$ and $\sigma(k, s(n) + k) = u_3$. This definition, which is no longer constructor-based, is translated directly into a conditional following the pattern above.

6.1 First Transformation Step

The general strategy of the two transformation steps that follow is to discover arithmetic operations implicit in the recursion structure of programs. The goal of the first transformation step is to find the conditional and subtraction from a constructor-based definition of a binary arithmetic symbol which is a simultaneous iterator like σ . Such functions follow the following general pattern for simultaneous iterators:

$$G(0, 0) = t$$

$$\begin{aligned}
G(s(i), 0) &= h(i) \\
G(0, s(n)) &= k(n) \\
G(s(i), s(n)) &= \varphi(G(i, n))
\end{aligned}$$

The first step in this process is a definition that makes the iteration structure of functions explicit. A function G computes $G(6, 2)$ as $\varphi(\varphi(G(4, 0))) = \varphi^2(h(3))$. In the same way, it computes $G(3, 7)$ as $\varphi^3(k(3))$, and $G(4, 4)$ as $\varphi^4(t)$. The results are the same with a function G following the conditional pattern:

$$G(i, n) = \mathbf{if } i > n \mathbf{ then } \varphi^n(h(i - n - 1)) \mathbf{ else if } i = n \mathbf{ then } \varphi^n(t) \mathbf{ else } \varphi^i(k(n - i - 1))$$

The number k of applications of the function φ denoted by φ^k is made explicit by an index k in the following definition:

Definition 1 *Let x be a variable of type α , let y_i be a term of type β_i for each $i = 1, \dots, n$, and let φ be a function of type $\beta_1 * \dots * \alpha * \dots * \beta_n \rightarrow \alpha$. The function $\hat{\varphi}$ of type $\text{Nat} * (\beta_1 * \dots * \alpha * \dots * \beta_n) \rightarrow \alpha$ is defined by:*

$$\begin{aligned}
\hat{\varphi}(s(k), (y_1, \dots, x, \dots, y_n)) &= \varphi(y_1, \dots, \hat{\varphi}(k, (y_1, \dots, x, \dots, y_n)), \dots, y_n) \\
\hat{\varphi}(0, (y_1, \dots, x, \dots, y_n)) &= x
\end{aligned}$$

Proposition 1

$$\hat{\varphi}(k, (y_1, \dots, \varphi(y_1, \dots, y, \dots, y_n), \dots, y_n)) = \varphi(y_1, \dots, \hat{\varphi}(k, (y_1, \dots, y, \dots, y_n)), \dots, y_n)$$

Proof: By induction on k . \square

An immediate consequence of Definition 1 is $\hat{\varphi}(1, x) = \varphi(x)$, where $x : \beta_1 * \dots * \alpha * \dots * \beta_n$.

Having made the iteration structure of functions explicit, the next theorem helps program transformations exploit that structure. To simplify the exposition, consider the case in which $\varphi : \alpha \rightarrow \alpha$. In this case $\hat{\varphi} : \text{Nat} * \alpha \rightarrow \alpha$ and $\hat{\varphi}(k, n) = \varphi^k(x)$, where φ^k denotes k applications of φ . Suppose now that $f : \text{Nat} * \text{Nat} \rightarrow \alpha$ satisfies the equation: $f(s(i), s(n)) = \varphi(f(i, n))$; then $f(4, 7) = \varphi^4(f(0, 3)) = \hat{\varphi}(4, f(0, 3))$. More generally, $f(i + k, n + k) = \hat{\varphi}(k, f(i, n))$. In fact, if

$F : Nat * Nat \rightarrow \alpha$ then F is a simultaneous iterator if and only if $\hat{\varphi}(k, F(x, y)) = F(x+k, y+k)$, which is the result expressed by Theorem 1.

Theorem 1 *Assume f of type $Nat^n \rightarrow \alpha$, let y_i be a term of type β_i for each $i = 1, \dots, n$, and let φ be a function of type $\beta_1 * \dots * \alpha * \dots * \beta_n \rightarrow \alpha$. The following are equivalent:*

1. $f(s(x_1), \dots, s(x_n)) = \varphi(y_1, \dots, f(x_1, \dots, x_n), \dots, y_m)$
2. $\hat{\varphi}(k, (y_1, \dots, f(x_1, \dots, x_n), \dots, y_n)) = f(x_1 + k, \dots, x_n + k)$

Proof: That 1 implies 2 is obvious by instantiating k to 1. The converse is proved by induction on k . \square

To apply this theorem to (5), let $Mwp0(x)$ be $Mwp(0, x)$ and introduce the equation:

$$\widehat{Mwp0}(k, \sigma(i, n)) = \sigma(i + k, n + k)$$

This gives the equational definition of $\sigma(i, n)$:

$$\begin{aligned} \sigma(s(i) + k, k) &= \widehat{Mwp0}(k, unit(0)) \\ \sigma(k, k) &= \widehat{Mwp0}(k, Abs(App(Var(0), Var(1)))) \\ \sigma(k, s(n) + k) &= \widehat{Mwp0}(k, unit(n)) \end{aligned}$$

This definition can be rewritten in the conditional form described at the beginning of the section with

$$\begin{aligned} e_1 &= \widehat{Mwp0}(n, unit(0)) \\ e_2 &= \widehat{Mwp0}(i, Abs(App(Var(0), Var(1)))) \\ e_3 &= \widehat{Mwp0}(i, unit(n - i - 1)) \end{aligned}$$

6.2 Second Transformation Step

The second transformation step transforms the expressions e_1 , e_2 and e_3 . The definition of $\widehat{Mwp0}$ of type $Term \rightarrow Term$, obtained by Definition 1, refers to the (inefficient) function

Mwp0. To get an efficient program an alternative (but equivalent) definition of $\widehat{Mwp0}$ that does not refer to *Mwp0* must be generated. Theorem 2 addresses this issue.

To introduce Theorem 2, consider the function *upto*. Informally, $upto(i, n) = [i, i + 1, \dots, n]$. The function *upto* satisfies $upto(s(i), s(n)) = map\ s\ upto(i, n)$. Let *map_s* be the specialization of the definition of *map* by *s*:

$$\begin{aligned} map_s\ [] &= [] \\ map_s\ (x :: xs) &= s(x) :: (map_s\ xs) \end{aligned}$$

The operators $[]$ and $::$ are the constructors of the data type $List(\alpha)$. By Theorem 1,

$$(\widehat{map_s})(k, upto(i, n)) = (map_s)^k(upto(i, n)) = upto(i + k, n + k)$$

Theorem 2 will yield the following recursive definition of $(map_s)^k$, (that is of $\widehat{map_s}$); it does not refer to *map_s*.

$$\begin{aligned} (map_s)^k\ [] &= [] \\ (map_s)^k\ (x :: xs) &= s^k(x) :: ((map_s)^k\ xs) \end{aligned}$$

Note, in this definition $(map_s)^k$ is the function being defined. It is to be regarded atomically; *map_s* is neither defined nor referred to.

Theorem 2 *Let y_i be a term of type β_i for each $i = 1, \dots, n$, let φ be a function of type $\beta_1 * \dots * \alpha * \dots * \beta_n \rightarrow \alpha$, and let C be a constructor of type α . The following are equivalent:*

1. $\varphi(y_1, \dots, C(x_1, \dots, x_n), \dots, y_n) = C(\varphi_1(x_1), \dots, \varphi_n(x_n))$
2. $\hat{\varphi}(k, (y_1, \dots, C(x_1, \dots, x_n), \dots, y_n)) = C(\hat{\varphi}_1(k, x_1), \dots, \hat{\varphi}_n(k, x_n))$

Proof: That 1 implies 2 is obvious by instantiating *k* to 1. The converse is proved by induction on *k*. \square

If C is a constructor of arity zero, Theorem 2 degenerates to the two equations

$$\begin{aligned}\varphi(y_1, \dots, C, \dots, y_n) &= C \\ \hat{\varphi}(k, (y_1, \dots, C, \dots, y_n)) &= C\end{aligned}$$

To apply this result to $\widehat{Mwp0}$, recall that $Mwp0(x) = Mwp(0, x)$ and that:

$$\begin{aligned}Mwp(i, Var(n)) &= Var(f(i, n)) \\ Mwp(i, Abs(t)) &= Abs(Mwp(s(i), t)) \\ Mwp(i, App(t, t')) &= App(Mwp(i, t), Mwp(i, t')).\end{aligned}$$

Introduction of the specializations $f_0(x) = f(0, x)$, and $Mwp1(x) = Mwp(1, x)$ allows the application of Theorem 2, producing:

$$\begin{aligned}\widehat{Mwp0}(k, Var(n)) &= Var(\widehat{f_0}(k, n)) \\ \widehat{Mwp0}(k, Abs(t)) &= Abs(\widehat{Mwp1}(k, t)) \\ \widehat{Mwp0}(k, App(s, t)) &= App(\widehat{Mwp0}(k, s), \widehat{Mwp0}(k, t)).\end{aligned}$$

It is easy to show that $\widehat{f_0} = \hat{s}$ because $f(0, x) = s(x)$, and that $\hat{s}(k, a) = a + k$ by induction on k . Therefore $\widehat{Mwp0}(k, Var(n)) = Var(\widehat{f_0}(k, n))$, which is equivalent to $Var(\hat{s}(k, n))$, which can be rewritten $Var(n + k)$. Although this appears to have progressed, it is incomplete because $\widehat{Mwp1}$ is still defined in terms of $Mwp1$. Attempts to define $\widehat{Mwp1}$ by this method, however, will require the function $\widehat{Mwp2}$; this would continue forever. Fortunately, there is another way in which Theorem 1 may be applied to (5), yielding the equation $\widehat{Mwp}(k, (0, \sigma(i, n))) = \sigma(i + k, n + k)$. Applying the same transformation as above produces another conditional definition of $\sigma(i, n)$ with $e_1 = unit(n)$, $e_2 = \widehat{Mwp}(i, (0, Abs(App(Var(0), Var(1))))$ and $e_3 = unit(n - 1)$. Application of Theorem 2 produces a recursive definition of \widehat{Mwp} that does not refer to Mwp :

$$\begin{aligned}\widehat{Mwp}(k, (i, Var(n))) &= Var(\widehat{f}(k, (i, n))) \\ \widehat{Mwp}(k, (i, Abs(t))) &= Abs(\widehat{Mwp}(k, (s(i), t))) \\ \widehat{Mwp}(k, (i, App(s, t))) &= App(\widehat{Mwp}(k, (i, s)), \widehat{Mwp}(k, (i, t)))\end{aligned}\tag{8}$$

The transformation is not yet finished. Equation (8) remains to be improved by finding a recursive definition of \widehat{f} that does not refer to the function f .

6.3 Transformation of \hat{f}

Recall the equations for f :

$$f(0, n) = s(n) \quad (9)$$

$$f(s(i), 0) = 0 \quad (10)$$

$$f(s(i), s(n)) = s(f(i, n)) \quad (11)$$

Applying Theorem 2 to (11) yields:

$$\hat{f}(k, (s(i), s(n))) = s(\hat{f}(k, (i, n))). \quad (12)$$

This suggests attempting a conditional definition for \hat{f} . Using equations (9), (10), (11), Theorem 2, Theorem 1, and Definition 1 produces:

$$\hat{f}(k, (0, s(n))) = s(\hat{s}(k, n)) = s(n + k) \quad (13)$$

$$\hat{f}(k, (s(i), 0)) = 0 \quad (14)$$

$$\hat{f}(k, (0, 0)) = k \quad (15)$$

Applying Theorem 1 to (12) gives: $\hat{f}(k, (i + p, n + p)) = \hat{s}(p, \hat{f}(k, (i, n))) = \hat{f}(k, (i, n)) + p$.

Applying that to equations (13), (14), (15) produces

$$\hat{f}(k, (s(i) + p, p)) = p$$

$$\hat{f}(k, (p, s(n) + p)) = n + 1 + k + p$$

$$\hat{f}(k, (p, p)) = k + p$$

This equational definition is equivalent to the program:

$$\hat{f}(k, (i, n)) = \mathbf{if } i > n \mathbf{ then } n \mathbf{ else if } i = n \mathbf{ then } n + k \mathbf{ else } n + k.$$

The program simplifies to: $\hat{f}(k, (i, n)) = \mathbf{if } i > n \mathbf{ then } n \mathbf{ else } n + k$. By unfolding \hat{f} and by a well known property of the conditional, equation (8) becomes:

$$\widehat{Mwp}(k, (i, Var(n))) = \mathbf{if } i > n \mathbf{ then } Var(n) \mathbf{ else } Var(n + k)$$

Including the transformed form of σ , which comes from above, produces the program in Figure 7 which does not perform redundant computations for σ_i and f_i . The transformation involved

```

fun apply_substitution_σ0(M) =
  let fun  $\widehat{Mwp}(k, (i, Var(n)))$  = if i > n then Var(n) else Var(n + k)
    |  $\widehat{Mwp}(k, (i, Abs(t)))$  = Abs( $\widehat{Mwp}(k, (s(i), t))$ )
    |  $\widehat{Mwp}(k, (i, App(t, t')))$  = App( $\widehat{Mwp}(k, (i, t))$ ,  $\widehat{Mwp}(k, (i, t'))$ )
  fun  $\sigma(i, n)$  = if i > n then unit(n)
    else if i = n then
       $\widehat{Mwp}(i, (0, Abs(App(Var(0), Var(1))))$ )
    else unit(n - 1)
  fun Ewp(i, Var(n)) =  $\sigma(i, n)$ 
    | Ewp(i, Abs(t)) = Abs(Ewp(s(i), t))
    | Ewp(i, App(t, t')) = App(Ewp(i, t), Ewp(i, t'))
in Ewp(0, M)
end

```

Figure 7: Final result

in this section has been done manually. However the transformation process is systematic and involves equational reasoning using Theorem 1 and Theorem 2. It shows implicitly how to automatically transform a constructor-based definition of a simultaneous iterator function of type $Nat * Nat \rightarrow Nat$ into a more efficient conditional form.

7 Directions

The paper has presented a clearly motivated and correct specification for a subtle representation of λ -terms, the implementation of which has, in the second authors experience, been prone to “off by one” errors. It has taken this abstract algorithm, with its extensive use of higher-order concepts, reduced it to a first-order program, introduced index arithmetic and produced an efficient algorithm that exploits computer arithmetic.

This development illustrates several new techniques. First, it makes the monadic structure in the development of the algorithm explicit by showing that it is a monad in **FUNSEQ**. It supports this structure with new program transformation techniques that allow the implicit

use of arithmetic to be “rediscovered” formally. Finally, it demonstrates the feasibility of integrating tools for monadic programming and specification, which tend to be higher-order, with relatively standard program transformation technology, which is strictly first-order.

7.1 Technology

Currently our technology is a tower of Babel. Automatic support for monadic programming, including automatic program generation, exists in CRML, a Standard ML derivative developed by Sheard. The partial evaluator, Schism, uses its own (typed) dialect of Scheme as its object language. The program Firstify, which implements Reynolds’ Algorithm, is written in CRML. Astre, Bellegarde’s program transformation system, is written in CAML. It uses a very simple first-order language as its object language. Moreover, a new tool is required to achieve the translation of constructor-based binary simultaneous iterators into conditionals.

In this environment, claims that the development is automatable mean that we have automated the process “piecewise”, translating between the formalisms in a nearly mechanical fashion. However translators interfacing these tools are currently being implemented. It is, of course, our vision that one day these tools will all work in concert, allowing a development to proceed from specification to efficient realization with human intervention only when necessary.

7.2 Reuse

Although this paper has focused on the λ -calculus, the specification can be applied to virtually any abstract syntax with a regular binding structure provided its type can be expressed as a monad and the appropriate definition of *map_with_policy* can be given. For example, adding boolean constants and a conditional has no effect on the definition of substitution and only changes *map_with_policy* by defining it to apply f recursively on the components of the conditional without applying Z . Adding *let* is also trivial; again, no changes need to be made to

the specification of substitution—only to *map_with_policy*. In this case, *map_with_policy* must apply Z to f when it enters the component in which the bound variable has been introduced. This ability to reuse specifications is one of the strongest arguments for the adoption of monads as a tool to structure program development.

But what about the transformations? Can we reuse program improvements? Here we have less experience, however the decisions that are required to improve programs for the different scenarios outlined above are substantially the same. It appears that a transformation system that records its development may be able to replay the development and obtain similar improvements.

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