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 specify substitution once and use the monadic structure of the specification to instantiate it on different abstract syntax structures. It also shows how to interactively derive an efficient implementation of substitution from this very abstract specification.

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 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[8] and is strongly influenced by Moggi's work on semantics[6]. The substitution algorithm for λ -calculus terms represented with de Bruijn indexes serves as the primary example. The development of the specification is a refinement of an example in Hook, Kieburtz and Sheard[5]. It is noteworthy because a non-standard category is used; the earlier work did not identify this category.

The specification is transformed into first-order equations using techniques implemented in the partial evaluator Schism[4]. It is then refined to an equivalent first-

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The first thing to observe about the sequence is that its general shape is $\sigma_{i+1}0 = 0$ and $\sigma_{i+1}(n+1) \approx \sigma_i n$. To make it exact it is necessary to increment all global variables in $\sigma_i n$ without incrementing the local variables. This is done by another sequence of functions:

$$f_0 n = n + 1 \qquad f_1 0 = 0 \qquad f_2 0 = 0 \\f_1(n+1) = n + 2 \qquad f_2 1 = 1 \\f_2(n+2) = n + 3$$

Observe that in the example a single application of f_1 to the body of $\sigma_1 1$ accounts for λ . 0.1 being adjusted to λ . 0.2. In general the f_i are generated by $f_{i+1}0 = 0$ and $f_{i+1}(n+1) = (f_in) + 1$. So, assuming a map that applies a family of functions, the family of substitution functions, $(\sigma_0, \sigma_1, \ldots)$, is given by the initial substitution, σ_0 , and the recurrence $\sigma_{i+1}0 = 0$ and $\sigma_{i+1}(n+1) = map(f_0, f_1, \ldots)(\sigma_i n)$. Given the sequence of functions, $(\sigma_0, \sigma_1, \ldots)$, 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[6] and to specifications[8]. In the computer science setting a monad is defined by a parametric data type constructor, T, and three polymorphic functions: $map: (\alpha \rightarrow \beta) \rightarrow T\alpha \rightarrow T\beta$, $unit: \alpha \rightarrow T\alpha$, and $mult: TT\alpha \rightarrow T\alpha$. The map function is required to satisfy map $id_{\alpha} = id_{T\alpha}$ and $map (f \circ g) = map f \circ map g$. The polymorphic functions unit and mult must satisfy $mult_{\alpha} \circ unit_{T\alpha} = id_{T\alpha}$, $mult_{\alpha} \circ$ $(map unit_{\alpha}) = id_{T\alpha}$ and $mult_{\alpha} \circ mult_{T\alpha} = mult_{\alpha} \circ (map mult_{\alpha})$. 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[8].

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

The development in Sect. 1 suggests that the specification of the substitution operation will be straightforward in a monadic data type with an appropriate map. To be monadic, the data type must be parametric. The following simple type declaration is sufficient²:

datatype
$$Term(\alpha) = Var(\alpha)$$

| $Abs(Term(\alpha))$
| $App(Term(\alpha) * Term(\alpha))$

Using techniques developed in earlier work, it is possible to automatically generate map, mull and unit functions for this type realizing a monadic structure[5]. 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 $\text{Hom}(A, B) = (B^A)^{\omega}$). 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:

$$\begin{array}{ll} map \ (f_0, f_1, \ldots) \ (Var \ x) &= Var((f_0, f_1, \ldots) \ x) \\ map \ (f_0, f_1, \ldots) \ (Abs \ t) &= Abs(map \ (f_1, f_2, \ldots) \ t) \\ map \ (f_0, f_1, \ldots) \ (App(t, t')) &= App(map \ (f_0, f_1, \ldots) \ t, map \ (f_0, f_1, \ldots) \ t') \end{array}$$

It is easily verified that (*Term*, *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[5]:

```
\begin{array}{ll} map\_with\_policy \ Z \ f \ (Var \ x) &= Var(fx) \\ map\_with\_policy \ Z \ f \ (Abs \ t) &= Abs(map\_with\_policy \ Z \ (Zf) \ t) \\ map\_with\_policy \ Z \ f \ (App(t,t')) &= App(map\_with\_policy \ Z \ f \ t, \\ map\_with\_policy \ Z \ f \ t') \end{array}
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In this encoding Z is the functional that generates the sequence and f is the seed value. That is, $(map (f, Zf, Z^2f, ...))_0 = map_with_policy Z f$. Note the projection

² This is a simplified form of the Term data type in Hook, Kieburtz and Sheard[5]. An anonymous referee has pointed out that an alternative structure can be used instead. The argument to *Abs* may be given the type $Term(1 + \alpha)$ (where + is interpreted as a discriminated union). While this structure is very interesting, it is not possible to express the map function for this type in the Standard ML type system. Preliminary results indicate this structure can be used to specify substitution.

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

The unit and mult functions automatically generated for *Term* can be lifted to FUNSEQ. Simple inductions show that they satisfy the monad laws.

With these definitions in place the complete definition of substitution is given in Fig. 1. 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 transform_index f

= \lambda n. if n = 0 then n else 1 + f(n - 1)

fun transform_substitution \sigma

= \lambda n. if n = 0 then unit 0

else map_with_policy transform_index succ (\sigma(n - 1))

in mult(map_with_policy transform_substitution \sigma_0 M)

end
```

Fig. 1. Substitution function

4 Transformation to a First-Order Set of Equations

To obtain a practical algorithm, the substitution function *apply_substitution* in Fig. 1 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 specification 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 [4] and the Astre program transformation system [1], 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 Sect. 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 Fig. 1. The specialization of map_with_policy for a particular policy function K and seed function g_0 gives the following function Mwp_g :

$$\begin{array}{ll} Mwp_{-g} (g, Var(n)) &= Var(g(n)) \\ Mwp_{-g} (g, Abs(t)) &= Abs(Mwp_{-g}(K \ g, t)) \\ Mwp_{-g} (g, App(t, t')) &= App(Mwp_{-g}(g, t), Mwp_{-g}(g, t')) \end{array}$$

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 [7], is outlined below.

- 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 **datatype** *Func* = C | F(Func).. The introduction of this type is a rediscovery of the sequence of functions g_0, g_1, \ldots 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, $\lceil g_0 \rceil$, of type Func. The definition of Mwp_g leads to the new function Mwp_g' :

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

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 $\lceil g \rceil(n)$.

$$apply_g(C, n) = g_0(n)$$

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

Note that $apply_g$ is a first-order function because its argument, [g], is an element of the type *Func*. The partial evaluator unfolds the definition of the policy

function K to get a first-order expression of $apply_g(F(\lceil g \rceil), n)$. The definition of Mwp_g' can be completed into:

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

Recall that this encoding is done with respect to a specific call of *map_with_policy* $Z g_0 M$. In the program in Fig. 1 there are two such calls. If the partial evaluator succeeds in the transformation of (4), then the new functions corresponding to Mwp_g and $apply_g$ will constitute a first-order program equivalent to the functions generated by map_with_policy . This step of the transformation can be automated using a partial evaluator.

4.2 Application to apply_substitution

Using the preceding techniques, the function *apply_substitution* is successfully transformed into the first-order program in Fig. 2. The data type *Subst* and the data type *Fseq* are introduced using the techniques above for the encodings of *transform_index* and *transform_substitution*.

fun apply_substitution_ $\sigma_0(M) =$			
\mathbf{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')) $	==	$App(Mwp_{\tau}f(f,t), Mwp_{\tau}f(f,t'))$
	fun $apply_{\sigma}(S0, n)$	===	$\sigma_0(n)$
	$ apply_{\sigma}(SUBST(\sigma), n)$) ==	if $n = 0$ then $unit(0)$
			else $Mwp_f(Succ, (apply_{\sigma}(\sigma, n-1)))$
	fun $Mwp_\sigma(\sigma, Var(n))$	==	$Var(apply \sigma(\sigma, n))$
	$ Mwp_\sigma(\sigma, Abs(t)) $	=	$Abs(Mwp_\sigma(SUBST(\sigma), t))$
	$Mwp_\sigma(\sigma, App(t, t'))$		$App(Mwp_{\sigma}(\sigma, t), Mwp_{\sigma}(\sigma, t'))$
in	$mult(Mwp_{\sigma}(\sigma)(S0,M))$		
\mathbf{end}			

Fig. 2. First-order Program

These two data types are isomorphic to the data type Nat^3 which is implemented efficiently in the hardware. However, the specialized function $Mwp_{-\sigma}$ does not exploit

³ The constructors for the data type Nat are 0 and s, i.e. datatype Nat = 0 | s(Nat).

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_{σ} 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 specification, 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) = ifn = 0thene₁elsee₂ are manipulated more effectively by Astre in the equivalent form $g(0) = e_1[0/n]$ and $g(s(n)) = e_2[s(n)/n]$. The notation c[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 $iso_{-\sigma} : Nat \rightarrow Subst$:

fun fun
$$iso_{\sigma}(s(i)) = SUBST(iso_{\sigma}(i))$$

| $iso_{\sigma}(0) = S\theta$

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 $\sigma(i, n) = apply_{\sigma}(iso_{\sigma}\sigma(i), n)$ and $Mwp_{\sigma}'(i, n) = Mwp_{\sigma}(iso_{\sigma}\sigma(i), n)$. 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 Fig. 3. The program in Fig. 3 does not improve the performance of the program in Fig. 2. 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.⁴ This is accomplished by introducing a function symbol, Ewp, which is equated to the composition of *mult* with

⁴ This composition is often called the *Kleisli star* or *natural extension*. *Ewp* is a mnemonic for extension with policy.

$$\begin{aligned} & \text{fun } apply_substitution_\sigma_0(M) = \\ & \text{let } \text{fun } f(0,n) = s(n) \\ & | f(s(i),0) = 0 \\ & | f(s(i),s(n)) = s(f(i,n)) \\ & \text{fun } Mwp_f'(i,Var(n)) = Var(f(i,n)) \\ & | Mwp_f'(i,Abs(t)) = Abs(Mwp_f'(s(i),t)) \\ & | Mwp_f'(i,App(t,t')) = App(Mwp_f'(i,t),Mwp_f'(i,t')) \\ & \text{fun } \sigma(0,n) = \sigma_0(n) \\ & | \sigma(s(i),n) = unit(0) \\ & | \sigma(s(i),s(n)) = Mwp_f'(0,\sigma(i,n)) \\ & \text{fun } Mwp_\sigma'(i,Var(n)) = Var(\sigma(i,n)) \\ & | Mwp_\sigma'(i,App(t,t')) = App(Mwp_\sigma'(s(i),t)) \\ & | Mwp_\sigma'(i,App(t,t')) = App(Mwp_\sigma'(i,t),Mwp_\sigma'(i,t')) \\ & \text{in } mult(Mwp_\sigma'(0,M)) \end{aligned}$$

Fig. 3. Program with indexes

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

$$\begin{aligned} & \operatorname{fun} \ Ewp(i, \operatorname{Var}(n)) &= \sigma(i, n) \\ & | \ Ewp(i, \operatorname{Abs}(t)) &= \operatorname{Abs}(Ewp(s(i), t)) \\ & | \ Ewp(i, \operatorname{App}(t, t')) &= \operatorname{App}(Ewp(i, t), Ewp(i, t')) \end{aligned}$$

The main body of the function is then replaced by Ewp(0, M). The functions mult and $Mwp_{\sigma'}$, which have become useless, are removed. Since the $Mwp_{\sigma'}$ 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 replace the expensive and redundant recursive calculations in σ and *Ewp* with index arithmetic.

The function $\sigma(i, n)$ of the transformed program is a rediscovery of the series of functions $\sigma_i(n)$ of Sect. 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 Sect. 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 definition of $\sigma(i, n)$:

$$\sigma(0,0) = Abs(App(Var(0), Var(1)))$$

$$\sigma(0,s(n)) = unit(n)$$

$$\sigma(s(i),0) = unit(0)$$

$$\sigma(s(i),s(n)) = Mwp(0,\sigma(i,n))$$
(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:

$$\sigma(s(s(s(0)))), s(s(0))) \to \tag{6}$$

$$Mwp(0, \sigma(s(s(0))), s(0))) \to$$
(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:

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

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 $\sigma(k, s(n) + k) = u_3$.

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 first step in this process is a definition that makes the iteration structure of functions explicit.

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 $\beta_1 * \dots * \alpha * \dots * \beta_n \to \alpha$. The function $\hat{\varphi}$ of type $Nal * (\beta_1 * \dots * \alpha * \dots * \beta_n) \to \alpha$ is defined by:

$$\hat{arphi}(s(k),(y_1,\cdots,x,\cdots,y_n))=arphi(y_1,\cdots,\hat{arphi}(k,(y_1,\cdots,x,\cdots,y_n)),\cdots,y_n))$$

 $\hat{arphi}(0,(y_1,\cdots,x,\cdots,y_n))=x$

Proposition 2.

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

Proof. By induction on k.

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

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 $\varphi : \alpha \to \alpha$. In this case $\hat{\varphi} : Nat * \alpha \to \alpha$ and $\hat{\varphi}(k, n) = \varphi^k(x)$, where φ^k denotes k applications of φ . Suppose now that $f : Nat * Nat \to \alpha$ 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, $f(i+k, n+k) = \hat{\varphi}(k, f(i, n))$, which is the result expressed by Theorem 3. **Theorem 3.** Assume f of type $Nal^n \to \alpha$, let y_i be a term of type β_i for each $i = 1, \dots, n$, and let φ be a function of type $\beta_1 * \dots * \alpha * \dots * \beta_n \to \alpha$. 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.

To apply this theorem to (5), let $Mwp\theta(x)$ be Mwp(0, x) and introduce the equation: $\widehat{Mwp}\theta(k, \sigma(i, n))) = \sigma(i + k, n + k)$. This gives the equational definition of $\sigma(i, n)$:

$$\sigma(s(i) + k, k) = \widehat{Mwp0}(k, unit(0))$$

$$\sigma(k, k) = \widehat{Mwp0}(k, Abs(App(Var(0), Var(1))))$$

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

This definition can be rewritten in the conditional form described at the beginning of the section with $e_1 = \widehat{Mwp}\theta(n, unit(0)), e_2 = \widehat{Mwp}\theta(i, Abs(App(Var(0), Var(1))))$ and $e_3 = \widehat{Mwp}\theta(i, unit(n-i-1)).$

6.2 Second Transformation Step

The second transformation step transforms the expressions e_1 , e_2 and e_3 . The definition of $\widehat{Mwp}\theta$ of type $Term \rightarrow Term$, obtained by Definition 1, refers to the (inefficient) function $Mwp\theta$. To get an efficient program an alternative (but equivalent) definition of $\widehat{Mwp}\theta$ that does not refer to $Mwp\theta$ must be generated. Theorem 4 addresses this issue.

To introduce Theorem 4, 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:

$$map_{s} [] = []$$

 $map_{s} (x :: xs) = s(x) :: (map_{s} xs)$

The operators [] and :: are the constructors of the data type $List(\alpha)$. By Theorem 3,

$$(map_s)(k, upto(i, n)) = (map_s)^k (upto(i, n)) = upto(i + k, n + k)$$

Theorem 4 will yield the following recursive definition of $(map_s)^k$, (that is of $\widehat{map_s}$); it does not refer to map_s .

$$(map_s)^k$$
 [] = []
 $(map_s)^k$ (x :: xs) = $s^k(x)$:: $((map_s)^k$ xs)

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 4. Let y_i be a term of type β_i for each $i = 1, \dots, n$, let φ be a function of type $\beta_1 * \cdots * \alpha * \cdots * \beta_n \to \alpha$, 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. $\hat{\varphi}(k, (y_1, \dots, C(x_1, \dots, x_n), \dots, y_n)) = C(\widehat{\varphi_1}(k, x_1), \dots, \widehat{\varphi_n}(k, x_n))$

Proof. That 1 implies 2 is obvious by instanciating k to 1. The converse is proved by induction on k.

If C is a constructor of arity zero, Theorem 4 degenerates to the two equations $\varphi(y_1, \dots, C, \dots, y_n) = C$ and $\hat{\varphi}(k, (y_1, \dots, C, \dots, y_n)) = C$.

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

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

Introduction of the specializations $f_0(x) = f(0, x)$, and MwpI(x) = Mwp(1, x) allows the application of Theorem 4, producing:

$$\begin{aligned}
\widehat{Mwp}\theta(k, Var(n)) &= Var(\widehat{f}_0(k, n)) \\
\widehat{Mwp}\theta(k, Abs(t)) &= Abs(\widehat{Mwp}I(k, t)) \\
\widehat{Mwp}\theta(k, App(s, t)) &= App(\widehat{Mwp}\theta(k, s), \widehat{Mwp}\theta(k, t)).
\end{aligned}$$

It is easy to show that $\widehat{f}_0 = \widehat{s}$ because f(0, x) = s(x), and that $\widehat{s}(k, a) = a + k$ by induction on k. Therefore $\widehat{Mwp}\theta(k, \operatorname{Var}(n)) = \operatorname{Var}(\widehat{f}_0(k, n))$, which is equivalent to $\operatorname{Var}(\widehat{s}(k, n))$, which can be rewritten $\operatorname{Var}(n + k)$. Although this appears to have progressed, it is incomplete because $\widehat{Mwp}I$ is still defined in terms of MwpI. Attempts to define \widehat{MwpI} by this method, however, will require the function $\widehat{Mwp2}$; this would continue forever. Fortunately, there is another way in which Theorem 3 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 $e_1 = unit(n), e_2 = \widehat{Mwp}(i, (0, \operatorname{Abs}(\operatorname{App}(\operatorname{Var}(0), \operatorname{Var}(1)))))$ and $e_3 = unit(n-1)$. Application of Theorem 4 produces a recursive definition of \widehat{Mwp} that does not refer to Mwp:

$$\widehat{Mwp}(k, (i, Var(n))) = Var(\widehat{f}(k, (i, n)))$$

$$\widehat{Mwp}(k, (i, App(s, t))) = App(\widehat{Mwp}(k, (i, s)), \widehat{Mwp}(k, (i, t)))$$

$$\widehat{Mwp}(k, (i, Abs(t))) = Abs(\widehat{Mwp}(k, (s(i), t)))$$
(8)

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

6.3 Transformation of f

Recall the equations for f:

$$f(0,n) = s(n) \tag{9}$$

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

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

Applying Theorem 4 to (11) yields:

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

This suggests attempting a conditional definition for \hat{f} . Using equations (9), (10), (11), Theorem 4, Theorem 3, and Definition 1 produces:

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

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

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

Applying Theorem 3 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

$$f(k, (s(i) + p, p)) = p$$

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

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

This equational definition is equivalent to the program:

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

The program simplifies to: $\hat{f}(k, (i, n)) = \text{if } i > n \text{ then } n \text{ else } n + k$. By unfolding \hat{f} and by a well known property of the conditional, equation (8) becomes: $\widehat{Mwp}(k, (i, Var(n))) = \text{if } i > n \text{ then } Var(n) \text{ else } Var(n + k)$. Including the transformed form of σ , which comes from above, produces the program in Fig. 4 which does not perform redundant computations for σ_i and f_i . The transformation involved in this section has been done manually. However the transformation process is systematic and involves equational reasoning using Theorem 3 and Theorem 4. It shows implicitly how to automatically transform a 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 specification, with its extensive use of higher-order concepts, reduced it to a first-order program,

```
fun apply_substitution_\sigma_0(M) =
     let fun Mwp(k, (i, Var(n)))
                                        = if i > n then Var(n) else Var(n+k)
              |Mwp(k, (i, Abs(t)))|
                                        = Abs(Mwp(k, (s(i), t)))
              |\widetilde{Mwp}(k, (i, App(t, t'))) = App(\widetilde{Mwp}(k, (i, t)), \widetilde{Mwp}(k, (i, t')))
                                        = if i > n then unit(n)
          fun \sigma(i, n)
                                           else if i = n then
                                                     Mwp(i, (0, Abs(App(Var(0), Var(1)))))
                                           else unit(n-1)
          fun Ewp(i, Var(n))
                                        = \sigma(i,n)
                                        = Abs(Ewp(s(i), t))
              | Ewp(i, Abs(t)) |
                                        = App(Ewp(i, t), Ewp(i, t'))
              | Ewp(i, App(t, t'))
          Ewp(0, M)
     in
     end
```

Fig. 4. Final result

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 specification explicit by showing that it is a monad in FUNSEQ. It supports this structure with new program transformation techniques which 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. The importance of partial evaluation technology in bridging this gap cannot be overstated.

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. Astre, Bellegarde's program transformation system, is written in CAML. It uses a very simple first-order language as its object language.

In this environment, claims that the development is automatable mean that we have automated the process "piccewise", translating between the formalisms in a nearly mechanical fashion. 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 specification 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 Zto 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 specification and 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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