Reduction Strategies in Lambda Term Normalization and their Effects on Heap Usage\footnote{This article is a modified version of the master’s thesis of Xiaochu Qi}

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February 1, 2008
Abstract

Higher-order representations of objects such as programs, proofs, formulas and types have become important to many symbolic computation tasks. Systems that support such representations usually depend on the implementation of an intensional view of the terms of some variant of the typed $\lambda$-calculus. Various notations have been proposed for $\lambda$-terms to explicitly treat substitutions as basis for realizing such implementations. There are, however, several choices in the actual reduction strategies. The most common strategy utilizes such notations only implicitly via an incremental use of environments. This approach does not allow the smaller substitution steps to be intermingled with other operations of interest on $\lambda$-terms. However, a naive strategy explicitly using such notations can also be costly: each use of the substitution propagation rules causes the creation of a new structure on the heap that is often discarded in the immediately following step. There is thus a tradeoff between these two approaches. This thesis describes the actual realization of the two approaches, discusses their tradeoffs based on this and, finally, offers an amalgamated approach that utilizes recursion in rewrite rule application but also suspends substitution operations where necessary.
Acknowledgments

I take this opportunity to express my gratitude to my advisor Dr. Gopalan Nadathur for his guidance, support, and valuable instruction throughout this entire project. I am grateful to Dr. Chuck C. Liang for his help and interest in this project. Thanks are also due to Dr. Eric Van Wyk and Dr. William Messing for their interest in this project.

I would also like to thank Natalie Linnell, Lijesh Krishnan, and Jimin Gao for their comments on drafts and this thesis.

Work on this thesis has been partially supported by NSF Grant CCR-0096322, a Grant-in-Aid of Research from the University of Minnesota and by funds provided by the Institute of Technology and the Department of Computer Science and Engineering at the University of Minnesota.
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Chapter 1

Introduction

This thesis is concerned with the treatment of λ-terms in a situation where they are used as a means for representing syntactic objects whose structures involve binding. Such a use occurs in a variety of metaprogramming and symbolic computation tasks, such as proof assistants [5, 6, 8, 22], logical frameworks [7, 11] and metalanguages [18, 23]. The usefulness of λ-terms in representing higher-order syntactic objects, i.e. objects involving binding, lies in the following two aspects. First, the binding notions can be encoded by λ-abstractions explicitly. For example, in a theorem proving context, the first-order logic formula \( \forall x \, P(x) \), where \( P(x) \) represents an arbitrary formula in which \( x \) perhaps appears free, can be encoded by the λ-term \( \text{all} (\lambda x \, P(x)) \), where \( P(x) \) denotes, recursively, the representation of \( P(x) \), and the constructor \( \text{all} \) encodes the universal quantifier. The binding scope of the universal quantifier over \( x \) in the above formula is explicitly represented by the λ-abstraction. Second, the important substitution computation on such objects is captured by the attendant β-reduction operation on λ-terms. For example, in the formula above, the instantiation of the quantifier over \( x \) with a term denoted by \( t \) can be simply represented as \( \lambda x \, P(x) \) \( t \). The displayed λ-term can be rewritten to a form in which the occurrences of \( x \) in \( P(x) \) have been replaced by \( t \) using the β-reduction operation, and therefore represents the result of substituting \( t \) properly for \( x \) when we assume a notion of equality on λ-terms based on this operation.

Since λ-terms are used as data structures to represent syntactic objects, these terms may often have to be compared in the course of symbolic computation over such objects. To perform comparisons properly, the equality relation between λ-terms must incorporate variable renaming, i.e. α-conversion. For example, the two λ-terms \( \text{all} (\lambda x \, P(x)) \) and \( \text{all} (\lambda y \, P(y)) \) which represent formulae \( \forall x \, P(x) \) and \( \forall y \, P(y) \) respectively, should be recognized as being equal. Further, as we have noted already, in determining equality, it is necessary to take into account the notion of β-conversion. For instance, in a theorem proving context, we may want to check whether the formula generated from instantiating the quantifier over \( x \) in the formula

\[
\forall x \, (\forall y \, (P(x, y) \land Q(x, y)))
\]

is a universally quantified formula with a conjunction as its top-level connective inside the quantifier. This computation requires matching the λ-term

\[
(\lambda x \, (\text{all} (\lambda y \, (P(x, y), Q(x, y)))))) \, t
\]
with a term of the form \((\text{all } (\lambda z \text{ (and } (R, T))))\), where \(R\) and \(T\) are schema variables that may be instantiated in the course of the matching; we note that we are using the constructor \text{and} here to encode the logical connective \&. An important point to note here is that in order for the matching to be performed, the \(\beta\)-redex in the first term has to be contracted and the top-level structure of the resulting formula has to be exposed. The latter actually means that it is necessary to propagate a substitution into a context embedded within an abstraction. This is an aspect that is novel to the use of \(\lambda\)-terms as representational devices. In the context of functional programming, for instance, it is never necessary to look inside abstraction contexts.

Considering the frequency with which it is used, the efficiency of the implementation of the \(\beta\)-reduction operation has a significant impact on the performance of the system that supports the use of \(\lambda\)-terms as its data structures. Focusing on this issue in the realization of such systems is therefore important. A significant part of the \(\beta\)-reduction operation is substitution. Traditional presentations of \(\beta\)-contraction, the single step rewriting process from which the \(\beta\)-reduction operation is constructed, take a rather simplistic view of substitution. The operation is usually presented via a rule such as

\[(\lambda x \ t_1) \ t_2 \rightarrow t_1[x := t_2],\]

where \(t_1[x := t_2]\) denotes the term obtained by replacing the free occurrences of \(x\) in \(t_1\) by \(t_2\), carrying out the necessary renaming in the process to ensure that binding scopes are properly respected. Unfortunately, from an implementation perspective, the substitution operation is too complex to be performed as an atomic step. In particular, this substitution operation requires going through the structure of \(t_1\), taking care to rename the bound variables where necessary to avoid illegal capture, and eventually replacing free occurrences of \(x\) with \(t_2\). For this reason, in real implementations, the substitution operation is often broken into smaller steps. Each step focuses on one specific substructure of the term. For example, consider the term \((\lambda x \ (t_1 (\lambda y \ t_2))) \ t_3\). When it is observed that this term can be rewritten using the \(\beta\)-contraction rule, the reduction process registers the substitution of \(t_3\) for \(x\) in an environment. Calling this environment \(e\), the task now becomes that of propagating it over \(t_1\) and \(\lambda y \ t_2\). In processing the term with the abstraction, it may become necessary to rename the bound variable and this can be built into the rule for this case, possibly resulting in the addition of the substitution of, say, \(z\) for \(y\) to the environment \(e\). Finally, in traversing \(t_1\) and \(t_2\), a variable may be encountered and the result in this case would be to possibly substitute a term based on the environment.

The use of an environment actually leads to some possible improvements in the implementation of reduction. First, the delaying of substitutions gives us the ability to combine substitutions generated by different \(\beta\)-contractions into the same environment so that they can all be performed in one traversal over the involved term. For
example, consider the term \((\lambda x \ \lambda y \ t_1) \ t_2 \ t_3\). There are two redices that have to be contracted in normalizing this term. If the naive approach to \(\beta\)-contraction is used, it would be necessary to walk through the structure of \(t_1\) twice in effecting the necessary substitutions. With the delaying of substitutions, the two substitutions \([x := t_2]\) and \([y := t_3]\) can be combined into one environment and performed in the same traversal over \(t_1\). The delaying of substitutions also gives us more opportunities to avoid unnecessary term traversals. For example, in the term considered above, the variable \(y\) that is to be substituted for by \(t_3\) can only occur inside \(t_1\). Under the naive approach to \(\beta\)-contraction, we would first substitute \(t_2\) for all the free occurrences of \(x\) in \(t_1\). Then the traversal to substitute \(t_3\) for \(y\) would also examine these (new) occurrences of \(t_2\) to see if there are any free occurrences of \(y\) in them to replace. However, there are no such \(y\)'s in \(t_2\). With the delayed performance of substitution, such substitution traversals can be recognized and avoided. This kind of approach to substitution and reduction has, in fact, been central to the implementation of functional programming languages. In recent years, it has also been given a formal basis by the work on explicit substitution notations (e.g. see [1, 14, 21]) that incorporate the possibility of encoding suspended substitutions in terms. These notations also make it possible to extend this approach to reduction even to situations where we need to look inside abstractions.

The above discussion leads naturally to an implementation of \(\beta\)-reduction that is environment based. In the simplest form, such a procedure would be guided by an explicit substitution notation but would use suspended substitutions only implicitly, i.e. it would not explicitly create terms with suspended substitutions as their (sub)structures, but, instead, it would record those suspended substitutions via local variables and parameters of the reduction procedure. Thus the terms eventually produced by such a procedure would not contain subparts encoding suspended substitutions. More specifically, when the non-reducible head of a term is found, the procedure would need to actually carry out the suspended substitutions on the remaining part of the term structure. The consequence of this is that the ability to delay and combine substitutions is limited to the extent of a single invocation of the reduction procedure, which means the opportunities for sharing the substitution walks that are caused by contracting redices generated dynamically by other kinds of computation steps are missed. For example, consider a formula in the first-order logic that is represented by \((\forall x \ldots(\forall y \ P)\ldots))\), where \(P\) is an arbitrary \(\lambda\)-term. Suppose that we now carry out a computation over this formula that involves recognizing and instantiating all its universal quantifiers. This computation would first recognize the outermost quantifier and instantiate it by generating the term \((\lambda x \ldots(\forall y \ P)\ldots) \ t\). Now the outer redex would be contracted, generating a substitution computation involving the variable \(x\). At a later stage, the inner
quantifier will be noticed, generating another substitution computation, this time involving the variable $y$. Thus, it is necessary in principle to substitute for two different variables in the structure represented by $P$. If we do not have the ability to delay substitutions beyond the extent of one invocation of the reduction procedure, each of these substitutions requires a separate walk over the structure of $P$. This leads to overhead in both processing time and in the creation of term structures.

To overcome this kind of overhead, it becomes meaningful to consider a reduction procedure that uses the ability to suspend substitutions explicitly by sometimes returning terms that have (sub)structures encoding other terms with substitutions yet to be performed on them. Now, explicit substitution notations are usually presented via rules that generate and propagate substitutions. For example, the $\beta$-contraction operation may be expressed via a rule of the form

$$(\lambda x \ t_1) \ t_2 \rightarrow [t_1, (x, t_2) :: nil],$$

where an expression of the form $[t_1, e]$ represents the term $t_1$ with substitutions contained in the environment $e$ to be performed on it, and environments are represented as lists of bindings. Similarly, we may have a rule of the form

$$[(t_1 \ t_2), e] \rightarrow [t_1, e] [t_2, e]$$

that realizes the propagation of substitutions over applications. Assuming such a presentation, the simplest way of realizing the kind of reduction procedure we desire would be to use these kinds of rules directly, explicitly creating structures corresponding to the righthand sides when matching those corresponding to the lefthand sides. In the end, when the top-level structure of the term has been exposed to the extent desired, i.e., the non-reducible head of the term is found, the rewriting process is stopped. Notice that in this process some subterms may be left in the form of $[t, e]$ to be further evaluated as desired at some later stage of computation.

The second strategy that we have described clearly solves the problems noted for the first strategy but it also has problems of its own. In particular, it has the potential drawback for creating too many new structures. This would happen if, for instance, the righthand sides of rules that we create become the lefthand sides of other rules and have to be rewritten immediately. Now, new terms that are created have obviously to be allocated in dynamic space, i.e., in the heap. If a lot of space is unnecessarily allocated in the heap, it will become necessary in an industrial-strength system to reclaim such space using a garbage collector. The running time of the garbage collector becomes a factor in the overall performance of the computational system, and therefore we would like to reduce it as much as possible.

The organization of the first reduction procedure based on environment suggests a way to avoid such a potentially profligate use of heap space. Rather than creating
new terms with embedded substitutions immediately, the suspended substitutions may be represented implicitly by the parameters and local variables of the reduction procedure. However when the non-reducible head of a term is found, rather than performing the substitutions on the remaining term structures right away, new structures that maintain such substitutions in suspended forms can be created explicitly. This approach combines the implicit and explicit treatments of substitutions and can accrue the benefits of both.

In earlier paragraphs, we have outlined three different approaches to realizing reduction and have discussed their potential drawbacks and advantages. In this thesis we lend concreteness to these informal discussions. Our particular contributions are twofold:

1. Using a specific explicit substitution notation [17], we develop the three strategies into reduction procedures that can be embedded in actual systems. The development of the third strategy is new to our work and that of the first extends usual environment based procedures to a situation where it is important to look within abstractions. We also include correctness proofs with our procedures.

2. We quantify the differences between the different strategies through experiments on “real-life” computations. To conduct this study, we have realized our reduction procedures in the C language and have embedded them within the Teyjus implementation [19] of λProlog [18]—a language that provides λ-terms as data structures—and have collected data from a suite of user programs using the resulting versions of the system. We believe this kind of a study to be unique to our work and its encompassing project [20, 15].

The rest of this thesis is organized as follows. In the next chapter we introduce the λ-calculus and describe an explicit substitution calculus called the suspension notation [21]; this notation has already been used in two practical systems [19, 24] and is therefore an appealing basis for our study. Chapters 3, 4 and 5 then present reduction procedures realizing the three different approaches of interest. These procedures are presented using the SML language both for simplicity of exposition and for concreteness, although the same ideas can be deployed in realizations in any other language as well. Chapter 6 contains a quantitative comparison of these approaches using, in fact, a C based realization of each. Chapter 7 concludes the thesis.
Chapter 2

The $\lambda$-Calculus and Explicit Substitutions

This chapter provides technical background needed for our later discussions. In Section 2.1, we give an overview of the $\lambda$-calculus. Section 2.2 introduces the de Bruijn notation. In Section 2.3, we introduce the idea of explicit substitution calculi and describe the suspension notation as a representative.

2.1 An Overview of the $\lambda$-Calculus

Invented by Alonzo Church in 1930’s, the $\lambda$-calculus is designed to capture the most basic aspects of functionality, i.e. what it is means to be a function and what it means to apply a function to arguments under this interpretation. Using $\lambda$-terms to represent syntactic objects naturally requires the ability to perform comparisons between $\lambda$-terms. The usual method is to transform the terms to their $\beta$-normal forms first and then to check the equality between those normal forms, which we will discuss in detail in Section 2.1.3. Thus the normal forms of the terms under comparison should be guaranteed to exist. In the context of using $\lambda$-terms to represent syntactic objects, we are mainly interested in the use of typed $\lambda$-calculi. In these situations, the set of terms is restricted to only those that satisfy certain typeable constraints, and this restriction usually ensures the existence of $\beta$-normal forms. However, since we are not interested in any property associated with the types of $\lambda$-terms other than the guarantee of the existence of $\beta$-normal forms, our discussion in this thesis is still based on the untyped $\lambda$-calculus for generality and simplicity. Section 2.1.1 introduces the terms of the untyped $\lambda$-calculus. Section 2.1.2 presents the substitution operation. Section 2.1.3 describes the important $\alpha$-conversion and $\beta$-conversion operations and the equality notion of $\lambda$-terms based upon them.

2.1.1 Terms in the $\lambda$-Calculus

We begin with the definition of $\lambda$-terms.

Definition 2.1.1.1. We assume in the beginning that we are given a set of constants, a set of abstractable variables and a set of instantiatable variables. The set of $\lambda$-terms is then the smallest set obtained from the combination of these sets using the following operations:
1. abstraction, that produces the term \((\lambda x \ t)\) given an abstractable variable \(x\) and a \(\lambda\)-term \(t\), and

2. application, that produces the term \((t_1 \ t_2)\) given two \(\lambda\)-terms \(t_1\) and \(t_2\).

In an abstraction of the form \((\lambda x \ t)\), we say that the scope of this abstraction is \(t\) and we also refer to \(t\) as the body of this abstraction. In an application of the form \((t_1 \ t_2)\), we refer to \(t_1\) as the function and \(t_2\) as the argument of this application.

The instantiatable variables in this definition are also referred to as logic variables. They differ from the abstractable variables in the sense that they cannot be substituted by \(\beta\)-reductions, which we will discuss later, but possibly be replaced by other operations trying to make two \(\lambda\)-terms equal, i.e., unifications.

For the sake of readability, we often omit parentheses surrounding abstractions and applications when we write terms, assuming that these can be inserted using the following conventions: applications associate to the left and have a higher priority than abstractions.

Intuitively, the abstraction term \((\lambda x \ t)\) is intended to represent the function that when given \(x\) returns \(t\). In this sense, \(x\) is the formal argument and \(t\) is the body of this function. For example, using + as an infix operator, the abstraction \((\lambda x \ x + 1)\) represents a function that when given a value for \(x\) returns \((x + 1)\).

Now consider two \(\lambda\)-terms \((\lambda x \ x + 1)\) and \((\lambda y \ y + 1)\). It can be seen that these two terms both represent the same function: when given the same actual argument, they return the same value, that is, the actual argument plus one. For this reason, we want to recognize these two terms as being equal. The equality relation that we describe for \(\lambda\)-terms in Section 2.1.3 actually encompasses this idea.

The intuitive meaning of an application term is the application of a function to actual arguments. For example, the term \(((\lambda x \ x + 1) \ 2)\) represents the application of the function \((\lambda x \ x + 1)\) to \(2\). Naturally, this application term is equal to \(2 + 1\). For this reason, we expect to generally recognize the term representing the application of a function to a value, and the term representing the result of evaluating this application, to be equal. The notion of equality we formalize in Section 2.1.3 also encompasses this idea.

**Definition 2.1.1.2.** Term \(t\) is said to be an immediate subterm of \(s\) when \(s\) is in the form of \((\lambda x \ t)\), \((t \ t_1)\) or \((t_1 \ t)\). A term \(t\) is a subterm of \(s\) if it is \(s\) or, recursively, a subterm of an immediate subterm of \(s\).

**Definition 2.1.1.3.** Let \(t\) be a \(\lambda\)-term that has a subterm \((\lambda x \ t_1)\). All the occurrences of \(x\) in \((\lambda x \ t_1)\) are said to be bound in \(t\), and \(x\) is called a bound variable of the subterm \((\lambda x \ t_1)\). Any non-bound occurrence of \(x\) is said to be free in \(t\). If \(x\) has at least one
free occurrence in \( t \), then it is called a free variable of \( t \); the set of all the free variables of \( t \) is represented by \( FV(t) \). If \( FV(t) = \emptyset \), we refer to \( t \) as a closed term.

According to this definition, \( x \) is a bound variable of the closed term \( (\lambda x \ x + 1) \). For another example, consider the term \( \lambda y (\lambda x \ x + y) \). The variable \( y \) is free in its subterm \( (\lambda x \ x + y) \), even though it is bound in the top-level term.

2.1.2 Substitutions

To compare two \( \lambda \)-terms \((\lambda x \ t)\) and \((\lambda y \ s)\), it is required to rename their formal arguments to be the same. In particular, we need to rename the variable \( y \) in \( s \) by \( x \) first, then further check whether the resulting function body is the same as the one represented by \( t \). The evaluation of function application \((\lambda x \ t) \ s\) also requires replacing the occurrences of its formal argument \( x \) by \( s \) inside \( t \). In this sense, these two kinds of operations both have substitution as a main component. However, the substitution operation is not always so straightforward and extra attention should be paid to perform it correctly. For example, consider the evaluation of the \( \lambda \)-term \((\lambda y \ ((\lambda x \ yx) \ y))\), which requires substituting the variable \( y \) for the variable \( x \) in its subterm \( (\lambda y \ x) \). Note that the occurrence of the variable \( y \) is bound by the top level abstraction but is free in the abstraction it will be substituted in. If we directly replace \( x \) with \( y \), the evaluation result would be \((\lambda y \ (\lambda y \ y))\), in which \( y \) is incorrectly bound by the inner abstraction instead of the top level one. To preserve the correct binding relation, we need to first rename \( y \) in \((\lambda x \ y)\) to a new abstractable variable \( z \), and then replace \( x \) with \( y \) to obtain the term \((\lambda y \ (\lambda z \ y))\). To present such term replacement operations systematically, we define the substitution of \( \lambda \)-terms as the following:

**Definition 2.1.2.1.** For any \( \lambda \)-terms \( t \), \( s \) and abstractable variable \( x \), \( t[x := s] \) represents the result of substituting \( s \) for every free occurrence of \( x \) in \( t \) simultaneously and is defined recursively on the structure of \( t \) as the following:

1. If \( t \) is an abstractable variable, \( t[x := s] = \begin{cases} s & \text{if } t = x \\ t & \text{if } t \neq x \end{cases} \);

2. If \( t \) is an instantiatable variable, \( t[x := s] = t \);

3. If \( t \) is a constant, \( t[x := s] = t \);

4. If \( t \) is an application \((t_1 \ t_2), \ (t_1 \ t_2)[x := s] = (t_1[x := s]) \ (t_2[x := s])\);
If \( t \) is an abstraction \((\lambda y \ t_1)\),

\[
(\lambda y \ t_1)[x := s] = \begin{cases} 
\lambda y \ t_1 & \text{if } y = x \\
\lambda y \ (t_1[y := s]) & \text{if } y \neq x \text{ and } y \notin FV(s) \\
\lambda z \ (t_1[y := z][x := s]) & \text{if } y \neq x, \ y \in FV(s) \text{ and } z \notin FV(t_1) \cup FV(s).
\end{cases}
\]

Among these substitution rules the last case of rule (5) takes care of renaming bound variables to avoid illegal capture, i.e. name clashes.

### 2.1.3 Rules of \( \lambda \)-Conversions

One component of the equality relation that we want to define on \( \lambda \)-terms is that of recognizing the irrelevance of bound variable names. This is formalized through the notion of \( \alpha \)-conversion defined below.

**Definition 2.1.3.1.** Let \( t \) be a \( \lambda \)-term that has a subterm \((\lambda x \ s)\), and let \( y \) be an abstractable variable such that \( y \notin FV(s) \). The action of replacing this subterm \((\lambda x \ s)\) with \((\lambda y \ (s[x := y]))\) is called an \( \alpha \)-conversion. We say \( t \) \( \alpha \)-converts to \( t' \) if and only if \( t' \) has been obtained from \( t \) by a finite (perhaps empty) series of \( \alpha \)-conversions.

Note that \( \alpha \)-conversion is also used implicitly in the substitution operation.

The evaluation process of a function application represented by term \(((\lambda x \ t) \ s)\) is the operation of replacing the free occurrences of \( x \) inside \( t \) with \( s \), which can be denoted as \( t[x := s] \). This process is captured by the \( \beta \)-contraction operation.

**Definition 2.1.3.2.** Let \( t \) be a \( \lambda \)-term that has a subterm in the form of \(((\lambda x \ t_1) \ t_2)\) which is called a \( \beta \)-redex. The action of replacing this subterm with \((t_1[x := t_2])\) is called a \( \beta \)-contraction. We say \( t \Downarrow_\beta t' \) if and only if \( t' \) has been obtained from \( t \) by a \( \beta \)-contraction. A finite (perhaps empty) series of \( \beta \)-contractions is called a \( \beta \)-reduction.

Clearly, the following property is preserved by \( \beta \)-contraction.

**Lemma 2.1.3.3.** Let \( t \) and \( s \) be \( \lambda \)-terms. If \( t \Downarrow_\beta s \), then \( FV(s) \subseteq FV(t) \).

If there are any \( \beta \)-redices left in terms after the \( \beta \)-reduction, then these terms can intuitively still be evaluated. When we have finished all such evaluations, we may think of having reached a final value, i.e. a \( \beta \)-normal form.

**Definition 2.1.3.4.** A \( \lambda \)-term \( t \) which contains no \( \beta \)-redices is called a \( \beta \)-normal form.
We can define the notion of equality that we desire by using the notions of $\beta$-contraction and $\alpha$-conversion as follows.

**Definition 2.1.3.5.** We say a term $t$ is $\beta$-convertible to a term $s$ if and only if $s$ is obtained from $t$ by a finite (perhaps empty) series of $\beta$-contractions, reversed $\beta$-contractions and $\alpha$-conversions.

To qualify as a satisfactory notion of equality, the $\beta$-convertibility relation between $\lambda$-terms must possess the properties of being symmetric, reflexive and transitive. Thus, it must be an equivalence relation, which is assured by the following theorem.

**Theorem 2.1.3.6.** The relations $\beta$-conversion and $\alpha$-conversion are equivalence relations.

The proof of this theorem can be found in [12].

Now we need a method to determine equality between $\lambda$-terms based on $\beta$-conversions. We could first try to reduce these terms to their $\beta$-normal forms, and then check if these normal forms are identical, allowing for renaming of bound variables. If the $\beta$-normal forms of the terms we are trying to compare exist, this comparison approach is justified by the Church-Rosser Theorem for $\beta$-conversion and its corollary.

**Theorem 2.1.3.7 (Church-Rosser Theorem for $\beta$-conversion).** If a term $p$ is $\beta$-convertible to a term $q$, then there exists a term $t$ such that $p$ and $q$ both $\beta$-reduce to $t$.

This theorem follows from the Church-Rosser Theorem for $\beta$-reduction [12] and its proof can be found in [12].

From the Church-Rosser Theorem for $\beta$-conversion, we can obtain the following corollary.

**Corollary 2.1.3.8.** If normal forms exist for the terms $t$ and $s$, then $t$ and $s$ are $\beta$-convertible if and only if their normal forms are identical up to $\alpha$-conversions.

**Proof.** By the definition of $\beta$-conversion, a term and its normal form are $\beta$-convertible to each other. The necessity of this claim is obvious because two identical (up to $\alpha$-conversion) terms are $\beta$-convertible to each other and $\beta$-conversion is transitive. The sufficiency of this claim is proved as the following: suppose $t'$ and $s'$ are the normal forms of $t$ and $s$ respectively. By the transitivity of $\beta$-conversion, $t'$ is $\beta$-convertible to $s'$. Theorem 2.1.3.7 gives a term $r$ that $t'$ and $s'$ both reduce to. Since $t'$ and $s'$ contain no redices, they must both be $\alpha$-convertible to $r$. 

$\square$
Consider the comparison of two $\lambda$-terms ($(\lambda x \ (x \ t_1)) \ a$) and ($(\lambda x \ (x \ t_2)) \ b$), where $a$ and $b$ are distinct constants. The reductions of the top-level redices generate two terms in the form of $(a \ t_1[x := a])$ and $(b \ t_2[x := b])$. Since the difference between constants $a$ and $b$ already implies that the normal forms of the two terms we are trying to compare cannot be identical modulo $\alpha$-conversion, we are not interested in the reduction results of $t_1[x := a]$ and $t_2[x := b]$ any more and, therefore, the reduction on $t_1[x := a]$ and $t_2[x := b]$ can be ignored. To describe such an improvement of our comparison approach, the idea of a head normal form is useful.

**Definition 2.1.3.9.** We say a $\lambda$-term is in head normal form if it has the structure \((\lambda x_1 \ldots (\lambda x_n (\ldots (h \ t_1) \ldots) \ t_m))\ldots\) where $h$ is a constant, any one of $x_1, \ldots, x_n$ or an instantiatable variable. By a harmless abuse of the notation, we permit $n$ and $m$ to be 0 in this presentation. Given such a form, $t_1, \ldots, t_m$ are called its arguments, $h$ is called its head, $x_1, \ldots, x_n$ are called its binders and $n$ is its binder length.

We can observe that a term has a normal form only if it has a head normal form.

There are certain kinds of reduction sequences that are guaranteed to produce a head normal form of a given term whenever one exists. The following definition identifies a sequence of this kind.

**Definition 2.1.3.10.** The head redex of a $\lambda$-term $t$ that is not a head normal form is identified as follows. If $t$ is a redex, then it is its own head redex. Otherwise $t$ must be of the form $(t_1 \ t_2)$ or $(\lambda x \ t_1)$. In either case, the head redex of $t$ is identical to that of $t_1$.

The head reduction sequence of a term $r_0$ is the sequence $s = r_0, r_1, r_2, \ldots, r_n, \ldots$, where, for $i \geq 0$, there is a term succeeding $r_i$ if $r_i$ is not a head normal form and, in this case, $r_{i+1}$ is obtained from $r_i$ by rewriting the head redex using the $\beta$-contraction rule. Such a sequence is obviously unique and terminates just in case there is an $m \geq 0$ such that $r_m$ is a head normal form.

The following theorem justifies that if a term has a head normal form, then its head reduction sequence will terminate with such a form.

**Theorem 2.1.3.11.** A $\lambda$-term $t$ has a head normal form if and only if the head reduction sequence of $t$ terminates.

The proof of this theorem can be found in [2].

Thus to compare two $\lambda$-terms, we can first try to reduce them into their head normal forms following their head reduction sequences, and then check the identity of the binder lengths and the number of arguments and the identity (up to $\alpha$-conversion) of the heads of these head normal forms. After that, we can proceed to compare their arguments, if this is still relevant.
As we discussed previously, this comparison method is meaningful only if the (head) normal forms of the terms we are trying to compare exist. There is no promise of such an existence in the untyped $\lambda$-calculus. However, in the context of representing syntactic objects, we are interested eventually in typed $\lambda$-calculi in which the set of terms is restricted to contain only the typeable ones of the untyped $\lambda$-calculus. In most useful cases of typed $\lambda$-calculi, head normal forms are known to exist for every term.

2.2 The De Bruijn Notation

In the comparison approach we illustrated previously, after the $\lambda$-terms are reduced to their head normal forms, we need to check the identity of their heads based on $\alpha$-conversions, i.e. renaming the relevant bound variables. From the perspective of real implementations, the ease of $\alpha$-conversions in the identity checking is of special significance. The notation proposed by de Bruijn [4] provides an elegant way of handling this problem by ignoring the bound variable names and thus the need of renaming bound variables during identity checking. In this section, we give an overview of the de Bruijn notation.

2.2.1 Terms in the De Bruijn Notation

The de Bruijn terms are defined as follows.

**Definition 2.2.1.1.** The set of de Bruijn terms are given by the following syntactic rules.

$$\langle DT \rangle ::= \langle C \rangle \mid \langle V \rangle \mid \#\langle I \rangle \mid (\langle DT \rangle \langle DT \rangle) \mid (\lambda \langle DT \rangle)$$

In these rules, $\langle C \rangle$ represents constants, $\langle V \rangle$ represents instantiatable variables and $\langle I \rangle$ represents the category of positive numbers.

In the de Bruijn notation, a bound variable occurrence is denoted by an index which counts the number of abstractions between the occurrence of this variable and the abstraction binding it. Since we are in fact interested in only top-level closed terms, all the abstractable variables can be transformed to their indices in this way. This correspondence is exposed by the transformation function $\zeta$ defined as the following, where we correspondingly assume that the term to be transformed is closed at the top-level.

**Definition 2.2.1.2.** The mapping $\zeta$ from the closed name-carrying terms to the de Bruijn terms is given as $\zeta(t) = \xi(t, \text{nil})$ where $\xi$ is a mapping from the class of name-carrying terms and the class of bound variable name lists to the class of de Bruijn
terms and is defined as follows. (For simplicity, we assume that the bound variable names of the term to be transformed are distinct from each other without loss of generality.)

1. If $t$ is a constant, $\xi(t, l) = t$;
2. If $t$ is an instantiatable variable, $\xi(t, l) = t$;
3. If $t$ is an abstractable variable, $\xi(t, l) = \#i$, where $t = ith(l)$;
4. If $t$ is an application $(t_1 t_2)$, $\xi((t_1 t_2), l) = (\xi(t_1, l) \xi(t_2, l))$;
5. If $t$ is an abstraction $(\lambda x \ t_1)$, $\xi((\lambda x \ t_1), l) = \lambda (\xi(t_1, x :: l))$.

For example, consider two $\alpha$-convertible terms

$$(\lambda x \ (\lambda y \ x \ y) \ x) \text{ and } (\lambda z \ (\lambda w \ z \ w) \ z)$$

in the name-carrying scheme. Their de Bruijn representations obtained from the application of the transformation function $\zeta$ both have the same form as

$$(\lambda (\lambda \#2 \#1) \#1).$$

In general, it can be seen that the need for bound variable renaming is eliminated in determining the identity of the de Bruijn terms.

### 2.2.2 Substitutions in the De Bruijn Notation

Since an index is used to count the number of abstractions between the occurrence of a bound variable and the abstraction binding it, extra attention should be paid when a term is substituted into the bodies of some abstractions. Consider the term

$$(\lambda ((\lambda \lambda ((\#1 \#2) \#3))(\lambda \#2)))$$

The $\beta$-contraction of the redex inside this term requires substituting $\lambda \#2$ for the first free variable of $(\lambda ((\#1 \#2)\#3))$ which is denoted by the index $\#2$. The first thing we need to note is that the variable occurrence represented by index $\#2$ in $(\lambda \#2)$ is in fact bound by the top level abstraction of the entire term. Thus after the substitution, this index should be increased by one to preserve the correct binding relation, because there appears an extra abstraction between this variable occurrence and the abstraction binding it. Second, the variable occurrence represented by the index $\#3$ in the subterm $(\lambda ((\#1 \#2) \#3))$ is also bound by the top-level abstraction of the entire term. After the contraction, its index should be decreased by one to reflect that an abstraction between this variable occurrence and the abstraction binding it disappears. In fact, all the free variable occurrences of this subterm should be affected in this way. For this reason, we are
more interested in a generalized notation of substitutions, that of substituting terms for all the free variables simultaneously, the precise definition of which is given as the following.

**Definition 2.2.2.1.** Let \( t \) be a de Bruijn term and let \( s_1, s_2, s_3, \ldots \) be an infinite sequence of de Bruijn terms. The result of simultaneously substituting \( s_i \) for the \( i \)th free variable of \( t \) is denoted by \( S(t; s_1, s_2, s_3, \ldots) \) and is defined recursively as the following:

1. if \( t \) is a constant, \( S(t; s_1, s_2, s_3, \ldots) = t; \)
2. if \( t \) is an instantiatable variable, \( S(t; s_1, s_2, s_3, \ldots) = t; \)
3. if \( t \) is a variable reference \( \#i \), \( S(t; s_1, s_2, s_3, \ldots) = s_i; \)
4. if \( t \) is an application \( (t_1 \ t_2) \), \( S((t_1 \ t_2); s_1, s_2, s_3, \ldots) = (S(t_1; s_1, s_2, s_3, \ldots)S(t_2; s_1, s_2, s_3, \ldots)); \)
5. if \( t \) is an abstraction \( (\lambda t_1) \), \( S((\lambda t_1); s_1, s_2, s_3, \ldots) = (\lambda S(t_1; \#1, s'_1, s'_2, s'_3, \ldots)), \)
\[ \text{where, for } i \geq 1, \ s'_i = S(s_i; \#2, \#3, \#4, \ldots). \]

The last substitution rule is used to deal with some of the issues we illustrated by the previous example. First, we note that within an abstraction \( (\lambda t) \), the first free variable has an index \#2, the second has an index \#3 and so on. Since \( s_i \) is intended to be substituted for the \( i \)th free variable of \( t \), the variable occurrences with indices less than \#2, which are bound in \( t \), should not be changed by this substitution. Thus, in rule (5), we add \#1 in the front of the infinite substitution sequence to achieve such a protection. Furthermore, since an extra abstraction appears in front of \( s_i \) after the substitution is pushed into the abstraction, the indices of the free variables of \( s_i \) should be increased by one to preserve the correct binding relation. Substitution \( S(s_i; \#2, \#3, \#4, \ldots) \) is used for this renumbering operation. Note that although the implicit use of \( \alpha \)-conversions is eliminated from the substitution operation, extra effort should be made to renumber the indices of the free variables to preserve the correct binding relation.

### 2.2.3 Rule of \( \beta \)-Contraction in the De Bruijn Notation

With the presentation of substitutions in the de Bruijn notation, we can now formally describe the \( \beta \)-contraction schema within this context.

**Definition 2.2.3.1.** The \( \beta \)-contraction rule in the de Bruijn notation is the following.
\((\lambda t_1) t_2) \rightarrow S(t_1; t_2, \#1, \#2, \ldots)\),

where \(t_1\) and \(t_2\) are de Bruijn terms.

Let \(t\) be a de Bruijn term that has a subterm in the form of \((\lambda t_1) t_2)\). If the de Bruijn term \(s\) is obtained from \(t\) by replacing its subterm \((\lambda t_1) t_2)\) with \(S(t_1; t_2, \#1, \#2, \ldots)\), then we say \(t \triangleright^d s\).

The intuitive meaning of this rule is: after the contraction, the occurrences of the first free variable of \(t_1\) should be replaced with the term \(t_2\). At the same time, the indices of all the other free variables of \(t_1\) should be decreased by one to reflect the disappearance of the abstraction in the front.

Now we want to utilize the de Bruijn notation in our comparison approach to eliminate the renaming operation during the identity checking. In particular, we can first translate the name-carrying terms into their de Bruijn representations, and then follow the method we discussed in Section 2.1.3 to compare these de Bruijn terms. This approach is meaningful only if the properties of the name-carrying \(\lambda\)-calculus we discussed in the Section 2.1.3 still hold in the de Bruijn notation. We first adapt Definition 2.1.3.9 and 2.1.3.10 to the de Bruijn notation in the obvious way, and then use Theorem 2.2.3.4 and 2.2.3.5 to exhibit a close correspondence between the contractions in the name-carrying \(\lambda\)-calculus and those in the de Bruijn notation, and hence assure that the properties we are interested in still follow in the context of the de Bruijn notation.

The following two lemmas are used in the proofs of Theorems 2.2.3.4 and 2.2.3.5.

Consider the situation of substituting a name-carrying term \(t\) into a context embedded under \(m\) abstractions. Lemma 2.2.3.2 assures that the result of the transformation of \(t\) is the same no matter whether we transform \(t\) to its de Bruijn representation first, and then increase the indices of its free variables by \(m\), or we perform the substitution in the name-carrying scheme first, and then transform the entire term.

**Lemma 2.2.3.2.** Let \(t\) be a name-carrying term with all the names of its free variables contained in the list \((u_1 :: ... :: u_n :: l)\).

\[
S(\xi(t, u_1 :: ... :: u_n :: l); \#1, \#2, \ldots, \#n, #(m+1+n), #(m+2+n), \ldots) = \xi(t, u_1 :: ... :: u_n :: v_1 :: v_2 :: ... :: v_m :: l),
\]

where each \(v_i\), for \(1 \leq i \leq m\), does not occur amongst \(u_1, \ldots, u_n\), or in \(l\).

This lemma can be proved by straightforward induction on the structure of \(t\).

Consider the situation of substituting a name-carrying term \(t_2\) for the free variable \(x\) in a name-carrying term \(t_1\). Lemma 2.2.3.3 assures that the result of transformation is the same no matter whether we perform the substitution \(t_1[x := t_2]\) first, and then translate the entire term to its de Bruijn representation, or we transform \(t_1\) and \(t_2\) first, and then perform the substitution in the context of de Bruijn notation.
Lemma 2.2.3.3. Let \( t_1 \) be a name-carrying term with all the names of its free variables contained in the list \((v_1 :: v_2 :: ... :: v_m :: x :: l)\).

\[
S(\xi(t_1,v_1 :: v_2 :: ... :: v_m :: x :: l); #1,...,#m,s', #(m+1), #(m+2),...) = \xi(t_1[x := t_2],v_1 :: v_2 :: ... :: v_m :: l),
\]

where \( s' = S(\xi(t_2,l); #(m+1), #(m+2),...) \).

With the aid of Lemma 2.2.3.2, this lemma can be easily proved by induction on the structure of \( t_1 \).

Theorem 2.2.3.4. Let \( t_1 \) be a name-carrying \( \lambda \)-term such that all the names of its free variables are contained in the list \( l \). If \( t_1 \triangleright_{\beta} t_2 \), then \( \xi(t_1,l) \triangleright_{\beta}^{d} \xi(t_2,l) \). Further, if the contracted redex is a head redex in the name-carrying scheme, then the translation to the de Bruijn term is realized by contracting a head redex in the de Bruijn notation.

Proof. The first part of this theorem is proved by induction on the structure of \( t_1 \), and the second part can be easily observed during this process.

Now we consider the cases of the structure of \( t_1 \). Since \( t_1 \) contains a redex, it can only be an abstraction or an application.

Suppose \( t_1 \) is an application \((s_1 s_2)\). There are two subcases: first, \( t_1 \) itself is the redex contracted; second, the redex contracted is a subterm of one of \( s_1 \) or \( s_2 \).

In the first case, as a redex being contracted, \( t_1 \) is in the form of \(((\lambda x \ s'_1) s_2)\), and correspondingly, \( t_2 \) is in the form of \( s'_1[x := s_2] \). According to the definition of function \( \xi \),

\[
\xi(t_1,l) = (\lambda \xi(s'_1, x :: l)) \xi(s_2, l) \text{ and } \xi(t_2,l) = \xi(s'_1[x := s_2], l).
\]

Following the \( \beta \)-contraction rule in the de Bruijn notation,

\[
\xi(t_1,l) \triangleright_{\beta}^{d} S(\xi(s'_1, x :: l); \xi(s_2, l), #1, #2, ...).
\]

As an instance of Lemma 2.2.3.3,

\[
S(\xi(s'_1, x :: l); \xi(s_2, l), #1, #2, ...) = \xi(s'_1[x := s_2], l).
\]

In the second case, without loss of generality, we assume that the redex contracted is a subterm of \( s_1 \). Thus \( t_2 \) must have the form of \((s'_1 s_2)\), where \( s_1 \triangleright_{\beta} s'_1 \). By Lemma 2.1.3.3, we know that \( l \) contains all the free variable names of \( s'_1 \). By the induction hypothesis, \( \xi(s_1,l) \triangleright_{\beta}^{d} \xi(s'_1,l) \). Clearly,

\[
(\xi(s_1,l) \xi(s_2,l)) \triangleright_{\beta}^{d} (\xi(s'_1,l) \xi(s_2,l)).
\]

According to the definition of function \( \xi \),

\[
\xi(t_1,l) = (\xi(s_1,l) \xi(s_2,l)) \text{ and } \xi(t_2,l) = (\xi(s'_1,l) \xi(s_2,l)).
\]
Thus we have proven that $\xi(t_1, l) \not\models^d_\beta \xi(t_2, l)$ in the case that $t_1$ is an application.

Suppose $t_1$ is an abstraction ($\lambda x \ t_1'$). Since $t_1 \not\models^\beta t_2$, $t_2$ must be in the form of $(\lambda x \ t_2')$ where $t_1' \not\models^\beta t_2'$. By Lemma 2.1.3.3, $FV(t_2') \subseteq FV(t_1')$ and therefore, all the free variable names of $t_1$ and $t_2$ are contained in the list $(x :: l)$. Hence, by the induction hypothesis,

$$\xi(t_1', x :: l) \not\models^d_\beta \xi(t_2', x :: l).$$

Hence

$$(\lambda \xi(t_1', x :: l)) \not\models^d_\beta (\lambda \xi(t_2', x :: l)).$$

According to the definition of function $\xi$,

$$\xi(t_1, l) = (\lambda \xi(t_1', x :: l)) \text{ and } \xi(t_2, l) = (\lambda \xi(t_2', x :: l)).$$

Thus we have proven that $\xi(t_1, l) \not\models^d_\beta \xi(t_2, l)$ in this case. $\square$

**Theorem 2.2.3.5.** Let $t_1$ be a name-carrying $\lambda$-term such that all the names of its free variables are contained in the list $l$. If $\xi(t_1, l) \not\models^d_\beta \xi(t_2, l)$, then $t_1 \not\models^\beta t_2$. Further, if the contracted redex is a head redex in the de Bruijn notation, then the corresponding redex before the transformation is a head redex in the name-carrying scheme.

**Proof.** The first part of this theorem is proved by induction on the structure of $t_1$, and the second part can be easily observed during this process.

Now we consider the cases of the structures of $t$. Since $\xi(t_1, l)$ contains a redex, $\xi(t_1, l)$ can only be an application or an abstraction and therefore so can $t_1$.

Suppose $t_1$ is an application ($s_1 \ s_2$). Then

$$\xi(t_1, l) = (\xi(s_1, l)) \xi(s_2, l)).$$

If the redex contracted is $\xi(t_1, l)$ itself, then $\xi(s_1, l)$ must have the form $\lambda x \xi(s'_1, x :: l)$, and $\xi(t_2, l)$ must be in the form

$$S(\xi(s'_1, x :: l); \xi(s_2, l), \#1, \#2, ...).$$

According to the definition of function $\xi$,

$$\lambda x \xi(s'_1, x :: l) = \xi(\lambda x \ s'_1, l).$$

Thus $t_1$ has the form $((\lambda x \ s'_1) \ s_2)$. Following the $\beta$-contraction rule in the name-carrying scheme, this redex should be rewritten to $s'_1[x := s_2]$. As an instance of Lemma 2.2.3.3,

$$S(\xi(s'_1, x :: l); \xi(s_2, l), \#1, \#2, ...) = \xi(s'_1[x := s_2]).$$
Now we consider the case that the redex contracted is not \( \xi(t_1, l) \) itself but is a subterm of one of \( \xi(s_1, l) \) or \( \xi(s_2, l) \). Without loss of generality, we assume the redex contracted is inside \( \xi(s_1, l) \), and \( \xi(s_1, l) \beta \triangleright \xi(s'_1, l) \). Thus \( \xi(t_2, l) \) must be in the form

\[
(\xi(s'_1, l) \xi(s_2, l)),
\]

and therefore \( t_2 = (s'_1 s_2) \). By the induction hypothesis, \( s_1 \beta \triangleright s'_1 \) in the name carrying scheme. Clearly, \( (s_1 s_2) \beta \triangleright (s'_1 s_2) \). Thus we have proven that \( t_1 \beta \triangleright t_2 \) in the case that \( t_1 \) is an application.

Suppose \( t_1 \) is an abstraction \( (\lambda x \ t'_1) \). Then

\[
\xi(t_1, l) = \lambda \xi(t'_1, x :: l).
\]

Since \( \xi(t_1, l) \beta \triangleright \xi(t_2, l) \), \( \xi(t_2, l) \) must have the form \( \lambda \xi(t'_2, x :: l) \), where

\[
\xi(t'_1, x :: l) \beta \triangleright \xi(t'_2, x :: l).
\]

Thus, \( t_2 \) has the form of \( (\lambda x \ t'_2) \). By the induction hypothesis, \( t'_1 \beta \triangleright t'_2 \) in the name-carrying scheme. Clearly, \( (\lambda x \ t'_1) \beta \triangleright (\lambda x \ t'_2) \). Thus we have proven that \( t_1 \beta \triangleright t_2 \) in this case.

Suppose two terms \( t \) and \( s \) are \( \beta \)-convertible to each other in the name-carrying scheme. Then \( \zeta(t) \) and \( \zeta(s) \) are also \( \beta \)-convertible in the context of the de Bruijn notation. By Corollary 2.1.3.8, we know that \( t \) and \( s \) have a common normal form \( p \) (up to \( \alpha \)-conversion), if their normal forms exist. According to Theorem 2.2.3.4 and Theorem 2.2.3.5, the contractions performed on \( t \) and \( s \) will be mapped exactly to those performed on \( \zeta(t) \) and \( \zeta(s) \). Thus \( \zeta(t) \) and \( \zeta(s) \) have a common (head) normal form \( \zeta(p) \), if the normal forms of \( \zeta(t) \) and \( \zeta(s) \) exist. Further, Theorem 2.2.3.4 and Theorem 2.2.3.5 also assure that the contraction steps performed on a name-carrying term \( t \) when following its head reduction sequence will be mapped exactly to those performed on \( \zeta(t) \) when following its head reduction sequence in the context of the de Bruijn notation. Therefore Theorem 2.1.3.11 holds in this context, too. Finally, we are only interested in the terms for which normal forms exist. Thus we can refine our comparison approach to the following: we first transform the name-carrying terms under comparison into their de Bruijn representations, and then try to reduce these de Bruijn terms into their head normal forms. After that, we simply match the binder lengths and the heads of those head normal forms, and proceed to compare their arguments if this is still relevant. It is clear that the main issue of the comparison approach is the head reduction process of the de Bruijn terms under comparison.
2.3 Explicit Substitution Calculi

Hitherto the substitution in the course of $\beta$-reduction has still been viewed as a rather atomic operation in the sense that once generated, it will be performed on the corresponding term structures immediately. However, the performance of substitutions consists of the traversals of the term structures which are not yet, but will be, reduced. Thus, if we can temporarily suspend the substitutions once they are generated and delay their performance so that they can be carried out alone with the reduction steps, the substitution process can gain the ability to interact more with the reduction process. For instance, we can hopefully combine the substitutions generated at different reduction stages and which are to be performed on the same term structures, and carry them out in one term traversal. Thus we can also avoid some redundant effort incurred by the performance of those substitutions which turns out to be unnecessary due to later reduction results.

Explicit substitution calculi extend the de Bruijn notation to record suspended substitutions directly into term structures, thereby offering our desired flexibility in ordering computations. We study the benefits of this flexibility in this thesis based on a particular calculus known as the suspension notation [21]. We outline this notation in this section to facilitate this discussion. Although our empirical study must utilize a particular system, the suspension notation is general enough for our observations to eventually be calculus independent. We make this point below by contrasting this system with the other explicit substitution calculi in existence.

2.3.1 The Suspension Notation

To explicitly record substitutions, the explicit substitution notations involve at least two syntactic categories: those correspond to terms, and to the environment in which the suspended substitutions are recorded. As we noticed in Section 2.2.2, when substitutions are pushed into an abstraction, the free variable indices of terms to be substituted in should be increased by one to reflect the change in their embedding levels. Thus in a notation such as the $\lambda\sigma$-calculus [1] that uses exactly two categories of expressions, such an adjustment should be performed on the entire environment each time that the environment is propagated into an abstraction. The suspension notation instead uses a global mechanism for recording the adjustment to be made on the free variable indices of the terms to be substituted in, so that the adjustment can be made only once at the time that the substitutions are actually performed, rather than in an iterated manner. To support this possibility, the suspension notation includes a third category of expressions called environment terms that encode terms to be substituted in, together with their embedding context.
Definition 2.3.1.1. The syntactical definition of suspension terms is given by the following rules.

\[
\langle \text{STerm} \rangle ::= \langle C \rangle \mid \langle V \rangle \mid \#\langle I \rangle \mid (\langle \text{STerm} \rangle \langle \text{STerm} \rangle) \mid (\lambda \langle \text{STerm} \rangle) \mid [\langle \text{STerm} \rangle, \langle N \rangle, \langle N \rangle, \langle Env \rangle]
\]

\[
\langle \text{Env} \rangle ::= \text{nil} \mid \langle \text{ETerm} \rangle ::= \langle \text{Env} \rangle
\]

\[
\langle \text{ETerm} \rangle ::= @\langle N \rangle \mid (\langle \text{STerm} \rangle, \langle N \rangle)
\]

In these rules, \( \langle C \rangle \) represents constants, \( \langle V \rangle \) represents instantiatable variables, \( \langle I \rangle \) is the category of positive numbers and \( \langle N \rangle \) is the category of nonnegative numbers.

Besides the de Bruijn terms, there is a new type of terms called suspensions, of the form \([t, ol, nl, e]\), corresponding to the temporarily suspended substitutions with the term they should be performed on. The intuitive meaning of a suspension in this form is that the first \( ol \) variables of term \( t \) should be substituted for in a way determined by \( e \) and the other variables of \( t \) should be renumbered to reflect the fact that the embedding level of \( t \) was originally \( ol \) but now is \( nl \). Note that a suspension has the ability to record multiple substitutions generated from the contractions of different redices. This ability is necessary for the realization of substitution combinations.

An environment, corresponding to the category \( \langle \text{Env} \rangle \), is a finite list in which the term to be substituted for the \( i \)th free variable, together with its embedding context, is maintained in the \( i \)th position. Hence in a well-formed suspension term, the length of this environment list must be the same as \( ol \).

Represented by the category \( \langle \text{ETerm} \rangle \), two kinds of environment terms can appear within the environment. They correspond to variables bound by two different types of abstractions in the original term: \( (t, l) \) denotes a term replacement to be made on the variables bound by abstractions which disappear after reductions, while \( @l \) represents the adjustment to be made on the variables bound by abstractions which persist. The natural number \( l \) inside these two kinds of terms encodes the new embedding level at the relevant abstraction, \( i.e. \) for the variables bound by abstractions that persist after the reduction, we intend this to be the new embedding level just within the scope of the abstraction. Consequently, there are also constraints on \( nl \) and \( l \) in a well-formed suspension term: the \( l \) in \( (t, l) \) should be less than or equal to \( nl \), and the \( l \) in \( @l \) should be less than \( nl \).

Along with term representations, there is a collection of rewrite rules to simulate \( \beta \)-reduction. These rules are presented in Figure 2.1. We use \( e[i] \) to refer to the \( i \)th item in the environment list.

Among these rules, \( \beta_s \) and \( \beta'_s \) generate the suspended substitutions corresponding to \( \beta \)-contraction; rules \( (r1) \)-\( (r9) \), referred to as reading rules, are used to actually carry out those substitutions.
(\beta_s) \quad ((\lambda t_1) t_2) \rightarrow [t_1, 1, 0, (t_2, 0) :: nil] \\
(\beta') \quad (\lambda [t_1, ol + 1, nl + 1, @nl :: e]) t_2 \rightarrow [t_1, ol + 1, nl, (t_2, nl) :: e] \\
(r1) \quad [c, ol, nl, e] \rightarrow c \\
\quad \text{provided } c \text{ is a constant} \\
(r2) \quad [x, ol, nl, e] \rightarrow x \\
\quad \text{provided } x \text{ is an instantiatable variable} \\
(r3) \quad [#i, ol, nl, e] \rightarrow #j \\
\quad \text{provided } i > ol \text{ and } j = i - ol + nl. \\
(r4) \quad [#i, ol, nl, e] \rightarrow #j \\
\quad \text{provided } i \leq ol \text{ and } e[i] = @l \text{ and } j = nl - l. \\
(r5) \quad [#i, ol, nl, e] \rightarrow [t, 0, j, nil] \\
\quad \text{provided } i \leq ol \text{ and } e[i] = (t, l) \text{ and } j = nl - l. \\
(r6) \quad [(t_1 t_2), ol, nl, e] \rightarrow ([t_1, ol, nl, e] [t_2, ol, nl, e]). \\
(r7) \quad [\lambda (\lambda [\lambda \lambda]) t, ol, nl, e] \rightarrow (\lambda [t, ol + 1, nl + 1, @nl :: e]). \\
(r8) \quad [t, ol, nl, e], 0, nl', nil] \rightarrow [t, ol, nl + nl', e]. \\
(r9) \quad [t, 0, 0, nil] \rightarrow t \\

Figure 2.1: Rewrite rules for the suspension notation

Now we use a concrete example to illustrate the roles played by the rewrite rules to simulate \(\beta\)-reduction and the way in which the substitutions are combined. Consider the de Bruijn term

\[ ((\lambda (\lambda ((\#1 \#2) \#3)) t_2)) t_3), \]

where \(t_2\) and \(t_3\) are arbitrary de Bruijn terms. Using rule \((\beta_s)\) to contract the outermost redex, the term is rewritten to

\[ [[((\lambda (\lambda ((\#1 \#2) \#3))) t_2), 1, 0, (t_3, 0) :: nil]]. \]

Using rule \((r6)\) to propagate the substitution into the top-level application inside the suspension, the term is rewritten to

\[ [[(\lambda (\lambda ((\#1 \#2) \#3))), 1, 0, (t_3, 0) :: nil] [t_2, 1, 0, (t_3, 0) :: nil]]. \]

Using rule \((r7)\) to propagate the substitution into the top-level abstraction inside the former suspension, the whole term is rewritten to

\[ (\lambda [((\lambda ((\#1 \#2) \#3))), 2, 1, @0 :: (t_3, 0) :: nil]) [t_2, 1, 0, (t_3, 0) :: nil]. \]

Now using rule \((\beta'_s)\) to contract the redex and combine the substitution generated by this contraction with the one already existing in the environment, the term is rewritten to
\[(\lambda ((\#1 \#2 \#3)), 2, 0, ([t_2, 1, 0, (t_3, 0) :: nil], 0) :: (t_3, 0) :: nil)].

Using rule (r7) and (r6) several times to propagate the substitution into applications and abstractions, the term is transformed to

\[(\lambda (([\#1, 1, 3, 1, @0 :: ([t_2, 1, 0, (t_3, 0) :: nil], 0) :: (t_3, 0) :: nil])
\[\#2, 3, 1, @0 :: ([t_2, 1, 0, (t_3, 0) :: nil], 0) :: (t_3, 0) :: nil])
\[\#3, 3, 1, @0 :: ([t_2, 1, 0, (t_3, 0) :: nil], 0) :: (t_3, 0) :: nil])).

At this time, reaching the abstractable variables, substitutions can actually be performed. Using rule (r4) to rewrite the first suspension, the term is rewritten to:

\[(\lambda (([\#1, 1, 3, 1, @0 :: ([t_2, 1, 0, (t_3, 0) :: nil], 0) :: (t_3, 0) :: nil])
\[\#2, 3, 1, @0 :: ([t_2, 1, 0, (t_3, 0) :: nil], 0) :: (t_3, 0) :: nil])
\[\#3, 3, 1, @0 :: ([t_2, 1, 0, (t_3, 0) :: nil], 0) :: (t_3, 0) :: nil])).

Using rule (r5) to rewrite the current first suspension, the term is transformed to

\[(\lambda (([\#1, 1, 3, 1, @0 :: ([t_2, 1, 0, (t_3, 0) :: nil], 0) :: (t_3, 0) :: nil])
\[\#3, 3, 1, @0 :: ([t_2, 1, 0, (t_3, 0) :: nil], 0) :: (t_3, 0) :: nil])).

Using rule (r8) to combine renumbering with the existing substitution, the term is rewritten to

\[(\lambda (([\#1, 1, 3, 1, @0 :: ([t_2, 1, 0, (t_3, 0) :: nil], 0) :: (t_3, 0) :: nil]))
\[\#3, 3, 1, @0 :: ([t_2, 1, 0, (t_3, 0) :: nil], 0) :: (t_3, 0) :: nil])).

Similarly, by the application of rule (r5), the term is transformed to

\[(\lambda (([\#1, 1, 3, 1, @0 :: ([t_2, 1, 0, (t_3, 0) :: nil], 0) :: (t_3, 0) :: nil]))
\[\#2, 3, 1, @0 :: ([t_2, 1, 0, (t_3, 0) :: nil], 0) :: (t_3, 0) :: nil])).

Depending on the particular structures of \(t_2\) and \(t_3\), the rewrite rules can be applied to finally produce a de Bruijn term which is \(\beta\)-reduced from the original term.

\[(r10) \ [\#i, ol, nl, e] \rightarrow t,
\text{provided } i \leq ol, \ e[i] = (t, l) \text{ and } nl = l.
\[(r11) \ [\#i, ol, nl, e] \rightarrow [t, ol', nl' + nl - l, e'],
\text{provided } i \leq ol, \ e[i] = ([t, ol', nl', e'], l), \text{ and } nl \neq l.
\[(r12) \ [\#i, ol, nl, e] \rightarrow [t, 0, nl - l, nil],
\text{provided } i \leq ol, \ e[i] = (t, l), \ t \text{ is not a suspension, and } nl \neq l.

Figure 2.2: The enhanced version of rule (r5)
If our sole purpose is to simulate \( \beta \)-reduction, the rule \( (\beta'_s) \) is redundant: whenever \( (\beta'_s) \) is applied, rule \( (\beta_s) \) is applicable too. However, as illustrated in the previous example, \( (\beta'_s) \) is the rule in our rewriting system that serves to combine the substitutions newly generated by a contraction, with those already recorded in the environment. This rule requires the redex to be contracted to have the form of

\[
((\lambda [t_1, ol + 1, nl + 1, @nl :: e]) t_2),
\]

which means that the suspension as the abstraction body is obtained from pushing the suspension \([\lambda t_1, ol, nl, e]\) into the top-level abstraction inside it. If the reduction process strictly follows the outermost and leftmost order, which fits the reduction order required by head reduction sequences, all substitutions generated during the reduction process can be combined in this way. Similarly, rule \( (r8) \) is redundant, but serves to combine the renumbering needed after a term has been substituted into a new embedding context with the already existing substitutions to be performed on the same term in the environment. It requires the nested suspension to have the form of \([[[t, ol, nl, e], 0, nll', nll]], \[t', ol', nl', e']\] which means that this suspension is generated from the application of the rule \( (r5) \). In fact, the main uses of \( (r9) \) also arise after a use of \( (r5) \). Thus we can further eliminate rules \( (r8) \) and \( (r9) \) in favor of the enhanced versions of \( (r5) \) shown in Figure 2.2.

This course is followed in our reduction procedures.

### 2.3.2 Some Formal Properties

To justify that the comparison approach we discussed before still works in the context of the suspension notation, we need to first show that the suspension notation is capable of simulating reductions in the de Bruijn notation.

Theorem 2.3.2.1 assures that for every well-formed suspension term, there is a unique de Bruijn term underlying it.

**Theorem 2.3.2.1.** Let \( t \) be a well-formed term in the suspension notation. If terms \( t_1 \) and \( t_2 \) are different suspension terms obtained from \( t \) by a series (maybe empty) of applications of the reading rules, then there exists a de Bruijn term \( s \), which can be obtained from \( t \) by a series (maybe empty) of applications of the reading rules, such that \( t_1 \) and \( t_2 \) can be transformed to \( s \) by a series (maybe empty) of applications of reading rules.

Theorem 2.3.2.2 assures that every rewrite sequence from a well-formed suspension term to the de Bruijn term underlying it terminates.

**Theorem 2.3.2.2.** Every well-formed term \( t \) in the suspension notation can be transformed to a de Bruijn term by a finite series (maybe empty) applications of the reading
rules, regardless of the specific choice of a reading rule when there are multiple rules applicable.

The proofs of the above two theorems can be found in [21].

The following theorem, which is proved in [21], establishes the correspondence between the reductions in the de Bruijn notation and the term transformations in the suspension notation which are intended to simulate those reductions.

**Theorem 2.3.2.3.** Let $t$ be a de Bruijn term. Then $t$ $\beta$-reduces to the de Bruijn term $s$ if and only if $t$ can be transformed to $s$ by a series (maybe empty) of applications of rules in Figure 2.1 and 2.2.

Head normal forms are extended to the suspension notation by permitting their arguments to be arbitrary suspension terms. For the convenience of our later discussion, we refer to a term in the suspension notation as being a weak head normal formal form if it is a head normal form or it is of the form of $(\lambda s)$, where $s$ is a suspension term. Following the theorems above, Theorem 2.3.2.4, which is proved in [21], assures that if a de Bruijn term $t$ has a (weak) head normal form $s$ in the context of the de Bruijn notation, then $t$ has one or more (weak) head normal forms in the suspension notation from which $s$ can be calculated out by a finite series (maybe empty) of applications of the reading rules.

**Theorem 2.3.2.4.** Let $t$ be a de Bruijn term and suppose that the rules in Figure 2.1 allow $t$ to be rewritten to a (weak) head normal form in the suspension notation that has $h$ as its head, $n$ as its binder length and $t_1, \ldots, t_m$ as its arguments. Let $|t_i|$ be the de Bruijn term obtained from $t_i$ by a series (maybe empty) of applications of reading rules. Then $t$ has the term

$$(\lambda \ldots (\lambda (\ldots (h |t_1|) \ldots |t_m|) \ldots))$$

with a binder length of $n$ as a (weak) head normal form in the de Bruijn notation.

Comparing with the de Bruijn notation, there is one more possibility for terms and there is also a larger set of rewriting rules in the suspension notation. Taking these aspects into account, we generalize the notions of head redex and head reduction sequence to the suspension notation and also define the notions of weak head redex and weak head reduction sequence as the following.

**Definition 2.3.2.5.** Let $t$ be a suspension term that is not in (weak) head normal form.

1. Suppose that $t$ has the form $(t_1 t_2)$. If $t_1$ is an abstraction, then $t$ is its sole (weak) head redex. Otherwise the (weak) head redices of $t$ are the weak head redices of $t_1$; notice that $t_1$ cannot be a weak head normal form here.
2. If \( t \) is of the form \((\lambda t_1)\), its head redices are identical to those of \( t_1 \). (This case does not arise if \( t \) is not a weak head normal form.)

3. If \( t \) is of the form \([t_1, ol, nl, e]\), then its (weak) head redices are itself and all the (weak) head redices of \( t_1 \).

Let two subterms of a term be considered non-overlapping just in case neither is contained in the other. Then a (weak) head reduction sequence of a suspension term \( t \) is a sequence \( t = r_0, r_1, r_2, \ldots, r_n, \ldots \), in which, for \( i \geq 0 \), there is a term succeeding \( r_i \) if \( r_i \) is not in (weak) head normal form and, in this case, \( r_{i+1} \) is obtained from \( r_i \) by simultaneously rewriting a finite set of non-overlapping subterms that includes a (weak) head redex using the rule schemata in Figure 2.1 or 2.2. Obviously, such a sequence terminates if for some \( m \geq 0 \) it is the case that \( r_m \) is in (weak) head normal form.

The following theorem, which is proved in [21], assures that if a term in the de Bruijn notation has a (weak) head normal form then its (weak) head reduction sequences terminate.

**Theorem 2.3.2.6.** A term \( t \) in the suspension notation has a (weak) head normal form if and only if every (weak) head reduction sequence of \( t \) terminates.

Thus we show that the comparison approach we illustrated before still works in the context of the suspension notation. Further, the extension of head normal forms to the suspension notation permits the performance of those substitutions over the arguments to be delayed until we actually need to compare the arguments.

### 2.3.3 Other Explicit Substitution Calculi

According to their combination ability, explicit substitution calculi can be classified into two categories. The calculi in the first category do not have the ability to combine substitutions at all. Their purposes are only to delay substitutions in the course of simulating the \( \beta \)-reduction. The \( \lambda \nu \)-calculus [3] and the \( \lambda s_e \)-calculus [14] are two representative calculi in this category. On the other hand, the calculi in the second category have the ability to combine substitutions during the reduction process. The suspension notation we presented previously and the \( \lambda \sigma \)-calculus [1] both belong to this category.

Without the ability to combine substitutions, the terms used to record explicit substitutions in the first kind of calculi have the characteristic that they can each record the substitutions generated by only one contraction. Certainly, this kind of information can be covered by a subset of the suspension terms with a certain pattern.
For example, the two kinds of terms used to record substitutions in the $\lambda s_r$-calculus can be represented by suspension terms of the form

$$[[t, j, j - 1, \@ (j - 2) :: \@ (j - 3) :: \ldots \@ 0 :: (t', 0)]]$$

for renumbering after a term is substituted into a new embedding context, and of the form

$$[[t, k, (i - 1) + k, \@ (i - 2 + k) :: \@ (i - 3 + k) :: \ldots :: \@ (i - 1) :: \text{nil}]]$$

for the term replacement and renumbering caused by one contraction. Correspondingly, the effects of the rewrite rules in such calculi can also be achieved by a subset of the rewrite rules of the suspension notation. In particular, since the rewrite rules in those calculi are used to purely simulate the $\beta$-contractions, the same effect can be achieved by the rewrite rules in the suspension notation without ($\beta'_s$) and (r8).

The other explicit substitution calculus $\lambda \sigma$ also has the ability to combine substitutions to be performed on the same term structures. While the $\lambda \sigma$-calculus has the ability to combine arbitrarily nested suspended substitutions, in the suspension notation we presented previously, the substitution combination rules ($\beta'_s$) and (r8) have certain requirements on the substitutions to be combined. Although we know that if strictly following the leftmost and outermost reduction order, all the substitutions can be combined by these two rules, the permission to share the reduction results and the binding of instantiatable variables caused by unification could sometimes violate this reduction order and may cause the failure of the combination of the suspended substitutions. For example, the binding of the instantiatable variable $F$ to a suspension $[[t, 1, 0, (s, 0) :: \text{nil}]]$ in the term $((\lambda F) t_1)$ generates the term $((\lambda [t, 1, 0, (s, 0) :: \text{nil}]) t_1)$. To contract this redex, the only applicable rule is ($\beta_3$). This contraction results in a suspension term in the form of $[[[t, 1, 0, (s, 0) :: \text{nil}], 1, 0, (t_1, 0) :: \text{nil}]]$. In this nested suspension, the combination of the common substitution walks over $t_1$ is lost. In fact, the suspension notation we represented in this thesis is a restricted version of the calculus presented in [19]. In particular, the full calculus allows for the transformation from an arbitrarily nested suspension in the form of $[[[t, ol1, nl1, e1], ol2, nl2, e2]]$ to a single suspension $[[t, ol, nl, e]]$. The main task in this transformation is the computation of the effect of the substitutions embodied in the environment $e2$ on each of the terms in $e1$. The richer calculus includes expression forms and rules that allow for this computation to be carried out through genuinely atomic steps. However, from the perspective of implementations, it is desired that substitution combination be realized in a simple step, as opposed to a series of operations. Secondly, in reality, following head reduction sequences, a situation where the application of ($\beta'_s$) fails when substitution combination is needed, occurs relatively rarely. Thus we sacrifice some of the ability to combine substitutions
in order to simplify the combination process by using \((\beta'_s)\) and \((r8)\) to “over-look” some steps of combinations and directly generate the combination result. As the full calculus of the suspension notation does, the \(\lambda\sigma\)-calculus uses a set of merging rules to combine arbitrarily nested substitutions. Thus the problem with the sophisticated suspension notation we discussed above also exists in this context: the complex set of merging rules is not suitable for real implementations. Requiring the reduction process to follow head reduction sequences, the merging rules in \(\lambda\sigma\)-calculus can also be simplified to a rule which can recognize redices in the form of \((\lambda t_1) t_2\), where \(t_1\) is an explicit substitution term with a certain pattern, and directly rewrite it into the combination of the substitutions generated from these two contractions by losing some of the ability to combine substitutions.

The main difference between the \(\lambda\sigma\)-calculus and the suspension notation is the way they record the adjustment to be made on indices corresponding to term replacement or renumbering. In the suspension notation, this adjustment is not explicitly maintained, but is computed from \(nl\) and the natural number \(l\) associated with the environment terms. For example, consider a suspension term \([s, 1, nl, (t, l) :: nil]\). When the substitution is to be carried out, the indices of the free variables of \(t\) should be increased by \((nl - l)\). In \(\lambda\sigma\)-calculus, this increment information is maintained explicitly within the environment term as \((t, (nl - l))\). Thus when a substitution is pushed into an abstraction, this number also needs to be increased by one, which means all the items in the environment list should be adjusted. For example, to push a delayed substitution into an abstraction, \([\lambda s, 1, nl, (t, l) :: nil]\), in the suspension notation the only work on the environment list is to add a dummy environment term: \(\lambda [s, 2, nl + 1, @nl :: (t, l) :: nil]\). On the other hand, in the \(\lambda\sigma\)-calculus, the already existing environment terms also need to be walked through to perform the increment: \(\lambda [s, 2, nl + 1, @1 :: (t, nl - l + 1) :: nil]\).

In summary, we believe that the suspension notation provides a concrete yet sufficiently general basis for examining the use of explicit substitution systems and the effect of the various choices afforded by them on actual implementations.
Chapter 3

Environment Based Reduction

As we discussed previously, the head normalization process which reduces the de Bruijn terms under comparison to their head normal forms when following head reduction sequences is the main issue of the comparison approach we want to realize for the systems using \(\lambda\)-terms to represent syntactic objects. Guided by the suspension notation, there is still flexibility to choose a specific strategy to realize the head normalization procedure, and these choices have different impacts on the heap usage of the computation systems. Now we discuss these possible reduction strategies and their impact on heap usage by using SML procedures for simplicity of exposition and for concreteness, although the same ideas can be deployed in realizations in any other language as well. Here we assume a basic familiarity with SML which one can obtain from [10]. All the procedures we present are graph-based, i.e. \(\lambda\)-terms are encoded as directed graphs and destructive changes are used to register, and thus to share the reduction steps.

3.1 An Environment Based Head Normalization Procedure

According to the suspension notation, it is natural to consider a reduction procedure based on an environment to achieve the delaying and combination of substitutions. The most straightforward way to realize the environment is to use the local variables and parameters of this reduction procedure. This idea is encompassed by the first head normalization procedure we present. In particular, suspensions are realized mainly through the structure of recursive calls to the normalization routine; they are not explicitly embedded into terms built on the heap, and thus the input and output terms of this procedure are pure de Bruijn terms. In this sense, the suspension notation is used only implicitly in this reduction strategy.

Figure 3.1 provides the datatype declarations in SML that serve to represent the structures needed in this reduction procedure.

SML expressions of types `rawterm` and `term` can be viewed as directed graphs, which are used to support a graph-based approach to reduction. We refer to such expressions as being acyclic if the graphs they correspond to in this sense are acyclic. An important assumption for our later discussion is that all the SML expressions
datatype rawterm = const of string  
| bv of int  
| fv of string  
| ptr of (rawterm ref)  
| app of (rawterm ref * rawterm ref)  
| lam of (rawterm ref)

type term = (rawterm ref)

datatype eitem = dum of int  
| bndg of clos * int  
and clos = cl of term * int * int * (eitem list)

type env = (eitem list)

Figure 3.1: Type declarations for an environment based head normalization procedure

we deal with are acyclic. In particular, we expect the input terms of our reduction procedures to hold this property, and we will show that our reduction procedures preserve this property.

Among these declarations, the de Bruijn terms are realized as references to appropriate SML expressions of the type rawterm. Correspondingly, the declaration of the type rawterm reflects, for the most part, the possible structures of de Bruijn terms. The constructor ptr in the declaration of rawterm serves to aid the sharing of reduction results which means that at certain points in our reduction process, we want to identify (the representations of) terms in a way that makes the subsequent rewriting of one of them correspond to the rewriting of the others. Such an identification is usually realized by representing both expressions as pointers to a common location whose contents can be changed to effect shared rewritings. In SML it is possible to update only references and so the common location itself must be a pointer. The constructor ptr is used to encode indirections of this kind when they are needed.

The declaration of the type eitem reflects the possible structures of the environment terms. SML expressions of type clos are used to record the term paired with an environment, which are referred to as closures in the usual leftmost and outermost reduction control regime. Guided by the suspension notation, we encode closures in the form of suspensions. This is the only explicit use of suspensions in this reduction procedure. The possible appearances of these closures are only at the top level of the implicit suspensions which are represented by the explicit terms on the heap together
with their environment, *i.e.* they will not be embedded into the structures of other explicit terms, and will not persist after the termination of the head normalization procedure.

There are some auxiliary functions that help with manipulation of the SML expressions of the types in Figure 3.1. Under the requirement of indirections, functions `deref` and `assign` are used to look up the value of a term, and to assign one term to another respectively. Their definitions are given as the following:

```plaintext
fun deref(term as ref(ptr(t))) = deref(t)
   | deref(term) = term

fun assign(t1,ref(ptr(t))) = assign(t1,t)
   | assign(t1,t2) = t1 := ptr(t2)
```

Invocations of these two functions on acyclic SML expressions will obviously terminate and do not introduce cycles if the input structures are acyclic.

In the course of reduction, we often need to look up a value in the environment list. The function `nth` serves this purpose.

```plaintext
fun nth(x::l,1) = x
   | nth(x::l,n) = nth(l,n-1)
```

The environment based head normalization procedure we currently present essentially has two phases. In the first phase, it traces a head reduction sequence to produce a head normal form. Once such a term is exposed, the second phase is entered to compute the effect of all the substitutions suspended by the first phase. Procedures `hn_eb` and `subst` in Figure 3.2 and Figure 3.3 serve to implement these two phases respectively. The procedures in Figure 3.4 are used to update or build terms on the heap depending on whether the reduction results can be shared or not.

The procedure `hn_eb` follows head reduction sequences in the following way. Its last parameter, which has a boolean type, is used to indicate whether the current term under manipulation is the function of an application term (when it is set to `true`) or not (when it is set to `false`). Consider the case that the input term of `hn_eb` is an abstraction and its last parameter has the value `true`. This indicates that a head redex, which is required to be contracted first following head reduction sequences, is exposed. Thus the recursive call(s) of `hn_eb` returns this abstraction together with the environment around it. Then `hn_eb` proceeds to contract this head redex by using rule $(\beta_s)$ or $(\beta'_s)$, depending on whether the environment around this abstraction is empty or not. In other words, when the last parameter of `eb_hn` is set to `true`, a weak head normal form of the incoming implicit suspension is computed, instead of a head normal form, when it is set to `false`. However, at this time, if the environment
fun hn_eb(term as ref(bv(i)),0,0,nil,_) = (term,0,0,nil)
| hn_eb(term as ref(bv(i)),ol,nl,env,whnf) = 
  if (i > ol) then (ref(bv(i-ol+nl)),0,0,nil)
  else (fn dum(l) => (ref(bv(nl - l)),0,0,nil)
    | bndg(cl(t',ol',nl',env'),l) =>
      if (l = nl) then hn_eb(t',ol',nl',env',whnf)
      else hn_eb(t,ol',nl+nl'-l,env',whnf)) (nth(env, i))
| hn_eb(term as ref(lam(t)),ol,nl,env,true) = (term,ol,nl,env)
| hn_eb(term as ref(lam(t)),ol,nl,env,false) =
  let val (t',ol',nl',env') =
    if (ol = 0) andalso (nl = 0) then hn_eb(t,0,0,nil,false)
    else hn_eb(t,ol+1,nl+1,dum(nl)::env,false)
  in build_lam(term,t',ol,nl)
  end
| hn_eb(term as ref(app(t1,t2)),ol,nl,e,whnf) =
  let val (f,fo,fl,ef) = hn_eb(t1,ol,nl,e,true)
  in (fn ref(lam(t)) =>
    let val s=hn_eb(t,fo+1,fl,bndg(cl(t2,ol,nl,e),nl)::ef,whnf)
    in update_app(term,s,ol,nl)
    end
    | t => build_app(term,t,t2,ol,nl,e)) (deref(f))
| hn_eb(ref(ptr(t1)),ol,nl,env,whnf)=hn_eb(deref(t1),ol,nl,env,whnf)
| hn_eb(term,_,_,_,_)=(term,0,0,nil)

Figure 3.2: Head normalization with implicit use of suspensions

around the abstraction is not empty, i.e. the implicit suspension is not trivial, \textit{hn\_eb} does not actually push this implicit suspension into the abstraction as required by the rewrite rule (r7), and the quadruple returned by \textit{hn\_eb} does not actually represent a weak head normal form of the incoming implicit suspension, but a “pre-step” of it. The reason for this is that implicit suspensions are local to the reduction procedure, and thus cannot be shared with or interact with other computation processes. It is unnecessary to explicitly carry out this propagation, i.e. increasing \textit{ol}, \textit{nl}, and building a dummy environment term, and therefore the effort spent on it can be saved. For this reason, we are using the (\(\beta'_s\)) rule in favor of the following form:

\[([\lambda t_1, ol, nl, env]) t_2) \rightarrow [t_1, ol + 1, nl, (t_2, nl) :: env].\]

For convenience, we also refer to this “pre-step” weak head normal form as a weak
fun subst(ref(app(t1,t2)),ol,nl,env) = ref(app(subst(t1,ol,nl,env),subst(t2,ol,nl,env)))
| subst(ref(lam(t)),ol,nl,env) = ref(lam(subst(t,ol+1,nl+1,dum(nl)::env)))
| subst(ref(bv(i)), ol, nl, env) = if i > ol then ref(bv(i+ol-nl))
  else (fn dum(l) => ref(bv(nl - l))
  | bndg(cl(t,ol',nl',e'),l) =>
      if (ol'=0) andalso (nl+nl'-l=0) then t
      else subst(t,ol',nl+nl'-l,e')(nth(env, i))
| subst(ref(ptr(t)),ol,nl,env) = subst(deref(t),ol,nl,env)
| subst(term,_,_,_) = term

Figure 3.3: Calculating out suspensions

fun build_lam(term,body,0,0) = (term,0,0,nil)
| build_lam(term,body,ol,nl) = (ref(lam(body)),0,0,nil)

fun update_app(term,(t,0,0,nil),0,0) = (assign(term,t);
  (t,0,0,nil))
| update_app(term,s,ol,nl) = s

fun build_app(term,f,arg,0,0,nil) = (assign(term,ref(app(f,arg)));
  (term,0,0,nil))
| build_app(term,f,arg,ol,nl,env) = (ref(app(f,subst(arg,ol,nl,env))),0,0,nil)

Figure 3.4: Construction functions

head normal form. Another thing to be noted here is that, in reality, the returned implicit suspension will be trivial in all cases other than this one.

Any given term $t$ may be transformed into a head normal form by invoking the procedure $head\_norm1$ that is defined as follows:

fun head_norm1(t) = hn_eb(t,0,0,nil,false)

At the end of such a call, $t$ is intended to be a reference to a head normal form of
its original value as might be expected in a graph-based reduction scheme. That \texttt{head\_norm1} correctly realizes this purpose is the content of the following theorems.

**Theorem 3.1.1.** Let $t$ be a de Bruijn term and let $[t, ol, nl, env]$ be a well-formed suspension. Let $t'$ be a reference to the SML expression representing $t$, and $env'$ be an SML list representing $env$. Then $\text{subst}(t', ol, nl, env')$ terminates, preserving the property of acyclicity and returning a reference to the SML expression representing a de Bruijn term $r$ that is transformed from $[t, ol, nl, env]$ by applying a series of the reading rules in Figures 2.1 and 2.2.

**Proof.** In the proof of this theorem, we refer to a rewrite sequence of a suspension $r_0$ as a sequence $s = r_0, r_1, r_2, ..., r_n$, where $r_n$ is a de Bruijn term; for $i \geq 0$, there is a suspension term succeeding $r_i$ if $r_i$ is not a de Bruijn term and, in this case $r_{i+1}$ is obtained from $r_i$ by the application of one of the reading rules in Figures 2.1 and 2.2. Theorem 2.3.2.1 and 2.3.2.2 assure that every rewrite sequence of a well-formed suspension terminates at the de Bruijn term underlying that suspension.

This theorem is proved by induction first on the length of the longest rewrite sequence of $[t, ol, nl, env]$ and then on the structure of $t'$. Note that in the latter induction, we say that an SML expression $t'$ is simpler than $s'$ if and only if the number of value constructors appearing in the structure of $t'$ is less than that of $s'$. Thus, the latter induction requires our SML expressions to be acyclic. The preservation of acyclicity follows easily from the fact that there are no assignments in the definition of $\text{subst}$. For the rest, we consider the cases for the structure of $t'$.

The theorem follows obviously if $t'$ is in the form of $\text{ref}(\text{const}(c))$ or $\text{ref}(\text{fv}(f))$.

Suppose that $t'$ is in the form of $\text{ptr}(s')$. If $s'$ is acyclic, we know that $\text{deref}(s')$ terminates and returns a reference to the SML expression representing $t$. Since the structure of $s'$ is simpler than that of $t'$, by the property of acyclicity, $\text{subst}(s', ol, nl, env')$ terminates and returns the SML expression referring to the representation of the de Bruijn term underlying $[t, ol, nl, env]$.

Suppose $t'$ is in the form of $\text{ref}(\text{bv}(i))$. Then the suspension to be rewritten is $[#i, ol, nl, env]$. There are three subcases: first, $i > ol$; second, $i \leq ol$ and $\text{nth}(env',i)$ returns $\text{dum}(l)$; third, $i \leq ol$ and $\text{nth}(env',i)$ returns $\text{bndg}((\text{cl}(s_1', ol', nl', e'), l))$. The theorem holds straightforwardly in the first two cases. In the third case, suppose $s_1$ is the de Bruijn term represented by the SML expression referred by $s_1'$ and $e$ is the environment represented by the SML list $e'$. Then we have

$$env[i] = ([s_1, ol', nl', e], l).$$
Note that $[s_1, ol', nl', e]$ could be a trivial suspension here. Following reading rule (r11), there is a rewrite step from $[#i, ol, nl, env]$ to $[s_1, ol', nl' + nl - l, e']$. Now, if $ol' = 0$ and $nl' + nl - l = 0$, then

$$[s_1, ol', nl' + nl - l, e'] = s_1,$$

and $s_1$ is the de Bruijn term underlying the original suspension $[#i, ol, nl, env]$. If $ol'$ and $nl' + nl - l$ are not both equal to zero, by the argument already outlined, the length of the longest rewrite sequence of

$$[s_1, ol', nl' + nl - l, e']$$

must be less than that of $[#i, ol, nl, env]$ by at least 1. By the induction hypothesis,$$
subst(s'_1, ol' + nl - l, e')$$

terminates and returns a reference to the SML expression representing the de Bruijn term $r$ underlying $[s_1, ol', nl' + nl - l, e]$. Further, $r$ is also the de Bruijn term underlying $[#i, ol, nl, env]$. The theorem follows from these observations and an inspection of the definition of $subst$.

The cases in which $t'$ is in the form of $ref(lam(t'_1))$ and $ref(app(t'_1, t'_2))$ both involve the use of a rewrite rule and hence the proof in these cases invokes the induction hypothesis based on the length of the longest rewrite sequence of $[t, ol, nl, env]$. We consider in detail the case of $ref(lam(t'_1))$; the other case is similar.

Suppose that $t'$ is in the form of $ref(lam(t'_1))$. The suspension to be rewritten is in the form of $[\lambda t_1, ol, nl, env]$, where the SML expression representing $t_1$ is referred to by $t'_1$. Following reading rule (r7), there is a rewrite step from $[\lambda t_1, ol, nl, env]$ to

$$\lambda [t_1, ol + 1, nl + 1, @nl :: env].$$

Thus the longest rewrite sequence of suspension

$$[t_1, ol + 1, nl + 1, @nl :: env]$$

is shorter than that of $[\lambda t_1, ol, nl, env]$ by at least one. By the induction hypothesis, $$subst(t'_1, ol + 1, nl + 1, dum(nl) :: env')$$

terminates, and returns a reference to the SML representation of the term $r$ which is the de Bruijn term underlying

$$[t_1, ol + 1, nl + 1, @nl :: env].$$

Moreover, $(\lambda r)$ is the de Bruijn term that $[\lambda t_1, ol, nl, env]$ should be rewritten to. From these observations and an inspection of the code, the theorem follows in this case too.
Theorem 3.1.2. Let $t'$ be a reference to the SML expression representing a de Bruijn term $t$ that has a head normal form. Then head_norm1($t'$) terminates and, when it does, $t'$ is a reference to the SML expression representing a head normal form of the original term $t$.

Proof. Since $t$ has a head normal form, Theorem 2.3.2.6 assures that every (weak) head reduction sequence of $t$ terminates. Hence we claim the following. If every head reduction sequence (weak head reduction sequence) of $t$ terminates, then

$$hn_{eb}(t',ol,nl,env',whnf)$$

terminates, preserving the acyclicity property and returning a quadruple

$$(r',rol,rnl,renv')$$

representing a head normal form (when $whnf$ is set to $false$) or a weak head normal form (when $whnf$ is set to $true$), of $[t, ol, nl, env]$, where $env$ is represented by the SML list $env'$. Further, the returned quadruple is in the form of $(r',0,0,nil)$ in all the cases other than that where the term that is computed is a weak head normal form of a non-trivial suspension with an abstraction as its term skeleton; if $ol = 0$, $nl = 0$, $env' = nil$ and $whnf = false$, $t'$ is set to $r'$ at the termination of the procedure call. The theorem is an immediate consequence of this claim.

The claim is proved by induction first on the length of the longest (weak) head reduction sequence of $t$ and then on the structure of $t'$. By the arguments we mentioned in the previous theorem, the latter induction requires our SML expressions to be acyclic. The preservation of acyclicity follows easily from Theorem 3.1.1 and by observing that the assignments in functions $build_lam$, $update_app$ and $build_app$ won’t introduce cycles where these did not exist already. For the rest, we consider the cases for the structure of $t'$.

The claim follows obviously if $t'$ is in the form of $ref(const(c))$ or $ref(fv(f))$.

Suppose that $t'$ is of the form $ref(ptr(s'))$. If $s'$ is acyclic, we know that $deref(s')$ terminates and returns a reference to the SML expression representing $t$. Since the structure of $s'$ is simpler than that of $t'$, by the property of acyclicity,

$$hn_{eb}(s',ol,nl,env',whnf)$$

terminates and returns a quadruple preserving the properties in our claim. Thus the claim follows in this case.

Suppose $t'$ is in the form of $ref(bv(i))$. If $ol = 0$, $nl = 0$ and $env' = nil$, the claim holds obviously. Otherwise, the term to be (weak) head normalized is in fact a non-trivial suspension in the form of $[#i, ol, nl, env]$. The claim follows obviously in the case $i > ol$ and the case $i \leq ol$ and $nth(env',i)$ returns $dum(j)$. Consider the case that $i \leq ol$, and $nth(env',i)$ returns $bdng(cl(s',ol,nl,env1'),l)$. Let $s$ be the de Bruijn
term represented by the SML expression referred by $s'$ and $env1$ be the environment represented by the SML list $env1'$. Then we have

$$env[i] = ([s, ol1, nl1, env1], l).$$

Following reading rule (r10), (r11) or (r12), a head reduction step occurs from the term $[[#i, ol, nl, env]]$ to

$$[s, ol1, nl1, env1]$$

or

$$[s, ol1, nl1 + nl - l, env1].$$

Hence the the longest (weak) head reduction sequence of $[[#i, ol, nl, env]]$ is longer than that of

$$[s, ol1, nl1, env1]$$

or

$$[s, ol1, nl1 + nl - l, env1]$$

by at least one. By the induction hypothesis,

$$hn_{eb}(s', ol1, nl1, env1', whnf)$$

or

$$hn_{eb}(s', ol1, nl1 + nl - l, env1', whnf)$$

terminates and returns the quadruple representing a (weak) head normal form of

$$[s, ol1, nl1, env1]$$

or

$$[s, ol1, nl1 + nl - l, env1],$$

which is also a (weak) head normal form of the term $[[#i, ol, nl, env]]$. The claim follows from these observations and an inspection of the definition of $hn_{eb}$ in this case.

Suppose $t'$ has the form of $ref(lam(s'))$. Let $s$ be the de Bruijn term represented by the SML expression referred by $s'$. Then $t$ is in the form of $\lambda s$. Clearly, the quadruple $(t', ol, nl, env')$ itself is a weak head normal form of $[[\lambda s, ol, nl, env]]$. Further, if $[[\lambda s, ol, nl, env]]$ is a trivial suspension, $(t', ol, nl, env')$ is in the form of $(t', 0, 0, nil)$. Now consider the case that a head normal form is computed. Suppose that $ol = 0$, $nl = 0$ and $env' = nil$. Then

$$[[\lambda s, ol, nl, env]] = \lambda s.$$

Since the longest head reduction sequence of $s$ is at most as long as that of $t$ and the structure of $s'$ is simpler than that of $t'$, by the induction hypothesis, $hn_{eb}(s', 0, 0, nil, false)$ terminates and returns a quadruple in the form of $(r', 0, 0, nil)$ where $r'$ refers to the SML expression representing a head normal form $r$ of $s$, and further, $s'$ is updated to a reference to $r'$. It can be seen that $\lambda r$ is a head normal form of $t$, and correspondingly, $t'$ is a reference to the representation of $\lambda r$ at the point $hn_{eb}(s', 0, 0, nil, false)$ terminates. Suppose that $ol$, $nl$ and $env'$ represent a non-empty environment. There is a head normalization step from the original suspension

$$[[\lambda s, ol, nl, env]]$$

to

$$(\lambda [s, ol + 1, nl + 1, @nl :: env]).$$
Hence the longest head reduction sequence of
\[ [s, ol + 1, nl + 1, @nl :: env] \]

is shorter than that of \([\lambda s, ol, nl, env]\) by at least one. By the induction hypothesis,
\[ \text{hn}_e(b(s', ol + 1, nl + 1, dum(nl) :: env', false) \]

terminates and returns a quadruple in the form of \((r', 0, 0, nil)\), representing a head normal form \(r\) of \([s, ol + 1, nl + 1, @nl :: env]\). According to reading rule \((r7)\), \(\lambda r\) is a head normal form of the original suspension. With these observations and an inspection of the definition of \(\text{hn}_e\), the claim holds in this case.

Suppose \(t'\) is in the form of \(\text{ref}(\text{app}(s'_1, s'_2))\). Let \(s^1_1\) and \(s^1_2\) be the de Bruijn terms represented by \(s'_1\) and \(s'_2\) respectively.

First, consider the case that \(ol = 0, nl = 0\) and \(env' = nil\). Let \(s^1_1, ..., s^k_1, ...\) be a weak head reduction sequence of \(s^1_1\), and for \(i \leq 1, s^{i+1}_2\) is obtained from \(s^1_2\) by rewriting some of its subterms that are identical to the weak head redex of \(s^1_1\). Then
\[ (s^1_1 s^1_2), (s^2_1 s^2_2), ..., (s^k_1 s^k_2), ... \]
is an initial segment of (weak) head reduction sequence of \(t\). Thus, the longest weak head reduction sequence of \(s^1_1\) is at most as long as the longest (weak) head reduction sequence of \(s\). Since the structure of \(s'_1\) is simpler than that of \(t'\), by the induction hypothesis, \(\text{hn}_e(b(s'_1, 0, 0, nil, true)\) terminates and returns the quadruple which is in the form of \((r'_1, 0, 0, nil)\) and represents a weak head normal form of \(s^1_1\). Let \(r_1\) be the de Bruijn term represented by the SML expression referred by \(r'_1\) and let \(r_2\) be the term represented by \(s^1_2\) at the point \(\text{hn}_e(b(s'_1, 0, 0, nil, true)\) terminates. Then there is a (weak) head reduction step from \(t\) to \((r_1 r_2)\). Now, if \(r_1\) is not in the form of \(\lambda x\), then \((r_1 r_2)\) is already a head normal form of the term \(t\). Correspondingly, in the definition of \(\text{hn}_e\), \(t'\) is set to refer to the SML expression representing \((r_1 r_2)\) via the function \(\text{build}_\text{app}\), and the quadruple to be returned is set to \((t', 0, 0, nil)\). If \(r_1\) is in the form of \(\lambda x\), then \((r_1 r_2)\) itself is a (weak) head redex. Following the \((\beta_\alpha)\) rule, there is a head reduction step from the term \((r_1 r_2)\) to \([r_1, 1, 0, (r_2, 0) :: nil]\). Hence, the length of the longest head reduction sequence of \([r_1, 1, 0, (r_2, 0) :: nil]\) is at least smaller than that of \(t\) by one. By the induction hypothesis,
\[ \text{hn}_e(b(r'_1, 1, 0, bndg(cl(s_2, 0, 0, nil, 0)), 0) :: nil, \text{whnf}) \]

terminates and returns a quadruple \((r', rol, rnl, renv')\) which represents a (weak) head normal form of \([r_1, 1, 0, (r_2, 0) :: nil]\) and is also a (weak) head normal form of \(t\). Further, if \(\text{whnf}\) is set to \(false\), this quadruple must have the form of \((r', 0, 0, nil)\).

In the definition of \(\text{hn}_e\), \(t'\) is correspondingly set to refer to \(r'\) via the function \(\text{update}_\text{app}\). From these observations and an inspection of the definition of \(\text{hn}_e\), the claim follows.
Now consider the case that \( ol, nl \) and \( env' \) represents a non-empty environment.

The term to be head normalized is in fact the non-trivial suspension
\[
[(s_1^1, s_2^2), ol, nl, env].
\]

Following the rewriting rules, there is a head reduction step from that term to
\[
([s_1^1, ol, nl, env] [s_2^1, ol, nl, env]).
\]

Thus the longest weak head reduction sequence of \([s_1^1, ol, nl, env]\) is shorter than the (weak) head reduction sequence of
\[
[(s_1^1, s_2^2), ol, nl, env]
\]
by at least one. Then by the induction hypothesis, \( \text{hn}_\text{eb}(s_1^1, ol, nl, env, true) \) terminates and returns a quadruple \((r_1', ol + 1, nl + 1, env')\) representing a weak head normal form of \( s_1^1 \). Note that if \( r_1' \) is not in the form of \( \text{ref}((\lambda x')) \), then \( ol = 0, nl = 0 \) and \( env' = nil \). Let \([r_1, ol + 1, nl + 1, env1]\) be this weak head normal form, and \( r_2 \) be the term represented by what \( s_2^2 \) refers to at this time. Then there is a (weak) head reduction step from \([t, ol, nl, env]\) to
\[
([r_1, ol + 1, nl + 1, env1] [r_2, ol, nl, env]).
\]

Now suppose \( r_1 \) is not in the form of \( \lambda x \). Then \([r_1, ol + 1, nl + 1, env1] = r_1 \). From Theorem 3.1.1, we know that \( \text{subst}(r_2, ol, nl, env) \) terminates and returns a reference to a de Bruijn term, say \( r_3 \), which is the de Bruijn term underlying \([r_2, ol, nl, env]\). Thus the term \((r_1 r_3)\) is a (weak) head normal form of \([t, ol, nl, env]\). Correspondingly, in the definition of \( \text{hn}_\text{eb} \), the quadruple to be returned is set to \((\text{ref}(\text{app}(r_1', s_2^2)), 0, 0, nil)\) via the function \( \text{build}_{app} \). On the other hand, if \( r_1 \) is in the form of \( \lambda x \), following rule \((\beta')\), there is a reduction step from term
\[
([r_1, ol + 1, nl + 1, env1] [r_2, ol, nl, env])
\]
to term
\[
([r_1, ol + 1, nl1, ([r_2, ol, nl, env], nl1) :: env1]).
\]

Hence the length of the longest head reduction sequence of
\[
([r_1, ol + 1, nl1, ([r_2, ol, nl, env], nl1) :: env1])
\]
is less than that of \([t, ol, nl, env]\) by at least one. By the induction hypothesis, \( \text{hn}_\text{eb}(r_1', ol + 1, nl1, (cl(r_2', ol, nl, env'), 0) :: env1', whnf) \) terminates and returns the representation of a (weak) head normal form of
\[
[r_1, ol + 1, nl1, ([r_2, ol, nl, env], nl1) :: env1],
\]
which is also the representation of a (weak) head normal form of $[t, ol, nl, env]$. From these observations and the inspection of the code, we can see the claim follows in this case.

\[ \]

### 3.2 Discussion on Heap Usage

In the reduction process of this strategy, substitutions generated by contractions of the head redices of term are delayed and performed along with the head reduction steps. In particular, if the (sub)structures of a term have been normalized, then the substitutions involving them are combined and carried out in one term traversal. Consequently, the new structures corresponding to such terms are created on the heap only once. However, in a head normalization process, once the head of a head normal form is exposed, the reduction process terminates without further normalizing of its arguments. Since all delayed substitutions are maintained locally to this head normalization procedure, those delayed substitutions to be performed on the arguments have to be carried out before the termination of the reduction process and therefore before the normalization of those arguments. This is not yet the necessary point at which those substitutions have to be carried out, and performing substitutions at this point potentially has the drawback of missing opportunities to combine substitution walks in the following two situations. First, new redices involving those arguments could be generated by other computation processes dynamically, such as the binding of instantiatable variables after unification which is used in pattern matching. For example, consider a quantified formula such as $\forall x \forall y P(x, y)$, where $P(x, y)$ itself represents a possibly complex formula containing occurrences of $x$ and $y$. The encoding of this formula using $\lambda$-terms would take the form $(all \lambda x (all \lambda y P(x, y)))$, where $all$ is a constructor chosen to represent the universal quantifier and $P(x, y)$ represents the encoding of $P(x, y)$. In a theorem-proving context in which a universal quantifier is processed by substitution with an instantiatable variable, this calculation would be effected by first recognizing a formula that fits the pattern (all $F$) and then applying the instantiation of $F$ to a new variable. In particular, when the term $(all \lambda x (all \lambda y P(x, y)))$ is recognized as fitting the pattern (all $F$), its subterm $(\lambda x (all \lambda y P(x, y)))$ is applied to an instantiatable variable, say $X$, and hence a head redex is generated. Then the newly formed application term is head normalized and the head normal form (all $\lambda y P(X, y)$) is created. Note that, using this environment based reduction strategy, the substitution $[x := X]$ has already been carried out over $P(x, y)$. After that, the pattern matching process is invoked on this head normal form again, recognizing that the incoming term fits the pattern (all $F$), generating a new application in the form of $(\lambda y P(X, y)) Y$. The head normalization of this term
generates the substitution \([y := Y]\) and carries it out over \(P(X, y)\). Although the two substitutions \([x := X]\) and \([y := Y]\) are performed on the same term structure \(P(x, y)\), they are not combined but are carried out in distinct term traversals. In this situation, the two redices are generated dynamically and are not revealed to the same invocation of the head normalization procedure. Thus from the view of the whole computation process, the performance of the delayed substitutions over \(P(x, y)\) each time before the head normalization procedure terminates is too eager. The second reason that this reduction strategy misses opportunities to combine substitution walks over the same term structures because of the eagerness of the performance of substitutions, is that there can be redices embedded inside these arguments on which substitutions are performed, and later computations could require them to be (head) normalized. For example, consider the head normalization of the term \((\lambda t_1) t_2\). When this reduction strategy is used, the external substitution would be percolated over this term, resulting in a walk over the structure of \(t_1\). At a later point, the embedded redex may be contracted, producing another substitution traversal over \(t_1\). If the substitutions can be delayed until they are needed, these two distinct walks can actually be combined into one.
Chapter 4

Explicit Use of Suspensions

A way to overcome the potential shortcomings of the reduction procedure we presented in the previous chapter is to explicitly build suspensions on the heap. Thus after the termination of one invocation of the reduction procedure, the suspended substitutions will persist and therefore can be delayed to the point when it is actually necessary for them to be carried out. Guided by the suspension notation, the simplest way to realize such a head normalization procedure is to build all the suspensions appearing in the reduction process on the heap. In particular, by matching the input term structures to the those on the lefthand sides of rewrite rules, this reduction procedure can choose a proper rewrite rule to apply, and then explicitly create the term structures appearing on the righthand side of that rule on the heap. In this sense, suspensions are used explicitly. In this chapter, we present a head normalization procedure explicitly using suspensions in this fashion.

4.1 A Head Normalization Procedure with Explicit Suspensions

The datatype declarations used in this head normalization procedure are presented in Figure 4.1. They differ from those in Figure 3.1 in the following two aspects: first, suspensions are explicitly accepted as a possible term structure of the type rawterm and denoted by the constructor susp; second, the structures appearing in the environment can be an arbitrary term as opposed to only closures in the environment based head normalization procedure in Chapter 3.

The auxiliary functions deref, assign, and nth are still available to this procedure.

This reduction approach involves the creation of representations on the heap for all the new structures that appear on the righthand side of a rule immediately on the application of that rule. Thus, suppose that at a certain point in computation, we use the rule

$$\left[[t_1, t_2], ol, nl, e\right] \rightarrow \left[[t_1, ol, nl, e] \ [t_2, ol, nl, e]\right]$$

for propagating substitutions over applications. In the mode that we are presently considering, we will create the new structures $[[t_1, ol, nl, e]]$ and $[[t_2, ol, nl, e]]$ and destructively update the term on the lefthand side with an application formed out of
datatype rawterm = const of string
    | fv of string
    | bv of int
    | ptr of (rawterm ref)
    | lam of (rawterm ref)
    | app of (rawterm ref) * (rawterm ref)
    | susp of (rawterm ref)*int*int*(eitem list)
and eitem = dum of int
    | bndg of (rawterm ref) * int

type env = (eitem list)

type term = (rawterm ref)

Figure 4.1: Type declarations for suspension terms

these two pieces before proceeding to the next step in reduction. Thus once a head
normal form is exposed, this procedure has no problem in terminating immediately
without accessory operations to carry out the suspended substitutions. A consequence
of this approach is that it should include mechanisms for incrementally ‘unravelling’
the suspensions met during the reduction processing.

Procedure lazy_read in Figure 4.2 is used to incrementally expose the top-level
non-suspension structure from a suspension when such a term is met during the
normalizing process. Procedure beta_contract in Figure 4.3 serves to determine which
of the ($\beta_1$) and ($\beta_1'$) rules is appropriate to use when a $\beta$-redex has been discovered
and to effect the corresponding rewriting step. Procedure hn_ex in Figure 4.3 realizes
the overall control of the reduction process. Similar to the procedure hn_exb, hn_ex can
also be invoked in two modes according to its last parameter with true to generate
a weak head normal form and false to generate a head normal form, and follows
the head reduction sequences in the same way that hn_ex does. Note that in this
procedure, first, all the term structures are created explicitly on the heap and thus
can be shared by other computation processes, and second, once a suspension is met,
the non-suspension structure resulting from the application of one of the reading
rules must be created on the heap for the reduction procedure to progress; therefore,
the propagation of a suspension in the form of $[\lambda t, ol, nl, env]$ over the abstraction
inside can not be avoided. Thus the weak head normal forms of suspensions with
abstractions as their term skeletons in this reduction procedure are their actual weak
head normal forms in the form of $\lambda [t, ol + 1, nl + 1, @nl :: env]$, as opposed to the
fun lazy_read(term as ref(susp(t,ol,nl,env))) =  
  lazy_read_aux(term,deref(t),ol,nl,env)  
| lazy_read(_) = ()  

and lazy_read_aux(t1,ref(bv(i)),ol,nl,env) =  
  if i > ol then t1 := bv(i + nl - ol)  
  else ((fn dum(l) => t1 := bv(nl - l)  
    | bndg(t2,l) =>  
      (if (nl = l) then assign(t1,t2)  
      else ((fn ref(susp(t3,ol',nl',e')) =>  
        t1 := susp(t3,ol',nl'+ nl - l,e')  
      | t => t1 := susp(t,0,nl - l,nil)  
      ) (deref t2));  
    (lazy_read t1))) (nth (env,i)))  
| lazy_read_aux(t1,ref(app(t2,t3)),ol,nl,env) =  
  t1 := app(ref(susp(t2,ol,nl,env)),ref(susp(t3,ol,nl,env))))  
| lazy_read_aux(t1,ref(lam(t2)),ol,nl,env) =  
  t1 := lam(ref(susp(t2,ol+1,nl+1,dum(nl)::env)))  
| lazy_read_aux(t1,t,ol,nl,env) =  
  (lazy_read(t) ; lazy_read_aux(t1,deref(t),ol,nl,env))  
| lazy_read_aux(t1,t2,_,_,_) = t1 := !t2

Figure 4.2: Auxiliary procedure for exposing term structures under suspensions

“pre-steps” of them in the form of \[ \lambda t, ol, nl, env \].

Any given term \( t \) may be transformed into a head normal form by invoking the procedure \( \text{head\_norm2} \) that is defined as follows:

fun head_norm2(t) = hn_ex(t,false)

At the end of such a call, \( t \) is intended to be a reference to a head normal form of its original value as might be expected in a graph-based reduction scheme. That \( \text{head\_norm2} \) correctly realizes this purpose is the content of the following theorem.

**Theorem 4.1.1.** Let \( t \) be a reference to the representation of a suspension term that translates via the reading rules to a de Bruijn term with a head normal form. Then \( \text{head\_norm2}(t) \) terminates and, when it does, \( t \) is a reference to the representation of a generalized head normal form of the original term.

*Proof.* See [17].
fun beta_contract(term, t1 as ref(susp(t3, ol, nl, dum(n1)::e)), t2) = 
    if nl = n1 + 1 then term := susp(t3, ol, n1, bndg(t2, n1)::e) 
    else term := susp(t1, 1, 0, [bndg(t2, 0)]) 
| beta_contract(term, t1, t2) = term := susp(t1, 1, 0, [bndg(t2, 0)])

fun hn_ex(term as ref(app(t1, t2)), whnf) = 
    (hn_ex(t1, true); 
    (fn ref(lam(t)) => (beta_contract(term, t, t2); 
        hn_ex(term, whnf)) 
    | _ => ()) (deref t1)) 
| hn_ex(ref(lam(t)), false) = hn_ex(t, false) 
| hn_ex(term as ref(susp(_, _, _, _)), whnf) = 
    (lazy_read(term); hn_ex(term, whnf)) 
| hn_ex(term as ref(ptr(t)), whnf) = 
    (hn_ex(t, whnf); assign(term, t)) 
| hn_ex(_, _) = ()

Figure 4.3: Head normalization using suspensions and immediate rewriting

### 4.2 Discussion on Heap Usage

With the ability to record suspensions on the heap, this head normalization procedure need not carry out the delayed substitutions on the arguments of a head normal form before its termination. Consequently, this head normalization procedure has the ability to combine the substitutions caused by contractions of redices dynamically generated across computation steps and by contractions of redices nested inside the arguments. However, there is still a significant drawback in its heap usage: in the course of reduction, many term structures resulting from the application of the rewrite rules are only intermediate to the reduction process, because once created, they are immediately rewritten by the next application of a rewrite rule. In this sense, these kinds of terms are in fact only local to the reduction procedure. The creation of such local terms on the heap is certainly unnecessary. For example, consider the rule for propagating substitutions over applications:

\[ ([t_1, t_2], ol, nl, e] \rightarrow ([t_1, ol, nl, e] \; [t_2, ol, nl, e]) \]

An eager creation of the structures \([t_1, ol, nl, e]\), \([t_2, ol, nl, e]\) and the application on the righthand side has the potential for using heap space unnecessarily: the very next steps may require the first of these suspensions to be rewritten and, a few steps later, the outer application itself may be recognized as a \(\beta\)-redex. This problem is avoided
by the reduction procedure we describe in Chapter 3, because it utilizes the recursion stack to record the intermediate terms and only commits structures on the heap when these are known to be necessary.
Chapter 5
Combining Implicit and Explicit Uses of Suspensions

The two head reduction procedures we presented in the previous chapters have complementary benefits and drawbacks. The environment based head normalization procedure in Chapter 3 effectively utilizes local variables and parameters to avoid the creation of intermediate term structures in the head reduction process, but fails to delay the substitutions to be performed on the arguments of the head normal forms out of one invocation of the reduction procedure. The procedure in Chapter 4 delays the substitutions to be performed on the arguments of the head normal forms out of one invocation of the reduction procedure in the form of explicit suspensions on the heap, but builds all the intermediate term structures of the head reduction process on the heap too. Now we present a synthesis of those two reduction procedures, and then combine the benefits of both. The essential idea is to follow the basic regime of the environment based reduction process in Chapter 3, but once a head normal form is found, to explicitly build suspensions on the heap to delay the substitutions further out of the current invocation of the reduction procedure.

In order to achieve the ability to explicitly build suspensions over arguments of the head normal forms, it is necessary to use the richer representation of terms that includes an encoding of suspensions. Assuming the datatype declarations in Figure 4.1 and the accessory function deref, assign, and nth, a collection of SML functions that utilize the proposed idea is presented in Figures 5.1 and 5.2.

Among these functions, hn.co actually performs the main work in the reduction. Functions build_lam, update_app and build_app serve to update or create new term structures on the heap according to whether the reduction results can be shared or not. It can be observed that these functions are in most respects identical to the environment based procedures we presented in Chapter 3. However, there are two significant differences. First, once a non-reducible head of an application is exposed, as opposed to carrying out the delayed substitutions on its argument as hn.eb does by calling subst, this reduction procedure directly builds a non-trivial suspension over the argument and constructs a new application term having this suspension as its argument. Second, suspensions should also be considered as a possible term category the reduction procedure could encounter. It is interesting to note that, in this case,
fun build_lam(term, body, ol, nl) = (ref(lam(body)), ol, nl, nil)

fun update_app(term, (t, 0, 0, nil), 0, 0) =
  (assign(term, t);
   (t, 0, 0, nil))

fun build_app(term, f, arg, ol, nl, env) =
  (assign(term, ref(app(f, arg)));
   (term, 0, 0, nil))

fun mk_explicit(term, (t, 0, 0, nil), _, _) =
  (assign(term, t); (t, 0, 0, nil))

fun mk_explicit(term, (t, ol, nl, env), 0, 0) =
  (assign(term, ref(susp(t, ol, nl, env))); (t, ol, nl, env))

fun mk_explicit(term, (ref(lam(t)), ol, nl, env), ol', nl') =
  (assign(term, ref(lam(ref(susp(t, ol+1, nl+1, dum(nl)::env)))));
   (term, 0, 0, nil))

fun arg(t, 0, 0, nil) = t

if the incoming suspension is under a non-empty environment, in order to preserve the ability to commit structures to the heap only when necessary, the embedded suspension needs to be processed first. This reduction order is different from the one used by the reduction procedure in Chapter 4, which commits structures to the heap eagerly, and actually is not leftmost and outermost. However, the progression of reduction steps is still encompassed by the notion of a (weak) head reduction sequence in Definition 2.3.2.5. Function mk_explicit serves to update the explicit suspension to its (weak) head normal form. Consider the situation in which a weak head normal form of an explicit suspension is computed, and this weak head normal form has an abstraction as its term skeleton. For the reason we discussed in Chapter 3, the quadruple returned by hn_co does not actually represent a weak head normal form.
fun hn_co(term as ref(bv(i)),0,0,[],_) = (term,0,0,[])
| hn_co(term as ref(bv(i)),ol,nl,env,w) =
  if (i > ol) then (ref(bv(i+ol-nl))),0,0,nil)
  else (fn dum(l) => (ref(bv(nl-l)),0,0,nil)
    | bndg(t,l) => if (nl = l) then hn_co(t,0,0,nil,w)
      else (fn ref(susp(t2,o,n,e))=>hn_co(t2,o,n+nl-l,e,w)
        | t=>hn_co(t,0,nl-l,[],w))(deref(t)))(nth(env,i))
| hn_co(term as ref(lam(t)),ol,nl,env,true) = (term,ol,nl,env)
| hn_co(term as ref(lam(t)),ol,nl,env,w) =
  let val (t’,o,n,e)=if (ol=0) andalso (nl=0) then hn_co(t,0,0,[],w)
    else hn_co(t,ol+1,nl+1,dum(nl)::env,w)
in build_lam(term,t’,ol,nl) end
| hn_co(term as ref(app(t1,t2)),ol,nl,env,w) =
  let val (f,fo,fl,fe) = hn_co(t1,ol,nl,env,true)
in (fn ref(lam(t))=>
    let val s=hn_co(t,fo+1,fl,bndg(arg(t2,ol,nl,env),nl)::fe,w)
in update_app(term,s,ol,nl) end
    | t => build_app(term,t,t2,ol,nl,env))(deref(f)) end
| hn_co(term as ref(susp(t,ol,nl,env)),ol’,nl’,env’,whnf) =
  let val s = mk_explicit(term,hn_co(t,ol,nl,env,whnf),ol’,nl’) in
    if (ol’=0) andalso (nl’=0) then s
    else hn_co(term,ol’,nl’,env’) end
| hn_co(ref(ptr(t)),ol,nl,env,whnf) = hn_co(deref(t),ol,nl,env,whnf)
| hn_co(term,_,_,_,_) = (term,0,0,nil)

Figure 5.2: Head normalization using suspensions implicitly and explicitly

of this suspension in the form of $\lambda \left[ t, ol + 1, nl + 1, @nl :: env \right]$, but a “pre-step” of it in the form of $\left[ \lambda t, ol, nl, env \right]$. However, if the environment around this suspension is not empty, i.e., the explicit suspension is embedded in an implicit one, in order to make the reduction procedure progress, we have to actually propagate the suspension into the abstraction, and update the explicit suspension to its actual weak head normal form: $\lambda \left[ t, ol + 1, nl + 1, @nl :: env \right]$. This situation is also taken cared of by the function $mk_explicit$.

Any given term $t$ may be transformed into head normal form by invoking the procedure $head_norm3$ that is defined as follows:

fun head_norm3(t) = hn_co(t,0,0,nil,false)

At the end of such a call, $t$ is intended to be a reference to a head normal form
of its original value as might be expected in a graph-based reduction scheme. The correctness of head_norm3 is the content of the following theorem whose proof is similar to that of Theorem 3.1.2.

**Theorem 5.1.** Let \( t' \) be a reference to the representation of a suspension term \( t \) that translates via the reading rules to a de Bruijn term with a head normal form. Then head_norm3(t') terminates and, when it does, \( t' \) is a reference to the representation of a generalized head normal form of the original term.

**Proof.** Since \( t \) has a head normal form, Theorem 2.3.2.6 assures that every (weak) head reduction sequence of \( t \) terminates. As in the proof of Theorem 3.1.2, we therefore claim the following. If every head reduction sequence (weak head reduction sequence) of \( t \) terminates, then

\[
\text{hn_co}(t',\text{ol, nl, env'},\text{whnf})
\]

terminates, preserving the acyclicity property and returning a quadruple

\[(r',\text{ol},\text{nl},\text{env'})\]

representing a head normal form (when whnf is set to false) or a weak head normal form (when whnf is set to true) of \([t, \text{ol, nl, env}]\), where env is represented by the SML list env'. Further, the returned quadruple is in the form of \((r',0,0,nil)\) in all the cases other than that where a weak head normal form of \([t, \text{ol, nl, env}]\) is computed and this weak head normal form is a non-trivial suspension with an abstraction as its term skeleton; if \( \text{ol} = 0, \text{nl} = 0, \text{env}' = \text{nil} \) and \( \text{whnf} = \text{false} \), \( t' \) is set to \( r' \) at the termination of the procedure call. The theorem is an immediate consequence of this claim.

The claim is proved by induction first on the length of the longest (weak) head reduction sequence of \( t \) and then on the structure of \( t' \). The preservation of acyclicity follows easily by observing that the assignments in \( \text{hn_co}, \text{make_explicit}, \text{build_app}, \text{build_lam} \) and \( \text{update_app} \) do not introduce cycles if these did not exist already. For the rest, we consider the cases for the structure of \( t' \).

When \( t' \) is in the form of \( \text{ref(const(c))}, \text{ref(fv(c))}, \text{ref(ptr}(t'_1))\), \( \text{ref(bv}(i))\), or \( \text{ref(lam}(s'))\), the proof of this claim is exactly the same as that of Theorem 3.1.2 in such cases.

Now suppose \( t' \) is in the form of \( \text{ref(app}(s'_1,s'_2))\). The proof of this claim is the same as that of Theorem 3.1.2 in all the cases other than the following: the environment represented by \( \text{ol}, \text{nl} \) and \( \text{env}' \) is not empty, and \( \text{hn_co}(s'_1,\text{ol, nl, env'},\text{true}) \) returns the quadruple \((r'_1,\text{ol1},\text{nl1},\text{env1}')\), where \( r'_1 \) is not in the form of \( \text{ref(lam}(x'))\). Note that in this case, \( \text{ol1} = 0, \text{nl1} = 0 \) and \( \text{env1}' = \text{nil} \) and a head of the (weak) head normal form of \([t, \text{ol, nl, env}]\) is exposed. Let \( r_1 \) be the term represented by the SML
expression referred to by \( r'_1 \) and let \( r_2 \) be the term represented by the SML expression referred to by \( s'_2 \) at the point that \( \text{hn\_co}(s'_1, ol, nl, env', true) \) terminates. Then the term 
\[
(r_1 \left[ r_2, ol, nl, env \right])
\]
is a (weak) head normal form of \([t, ol, nl, env] \). Correspondingly, in the definition of \( \text{hn\_co} \), the quadruple to be returned is set to
\[
(\text{ref(app}(r'_1, \text{ref(susp}(s'_2, ol, nl, env)))), 0, 0, nil)
\]
via the function \( \text{build\_app} \). Therefore, the claim holds in this case.

Now consider the case that \( t' \) is in the form of \( \text{ref(susp}(s', ol_1, nl_1, env_1')) \) which is a reference to the SML expression representing the term \([s, ol_1, nl_1, env_1] \). Since the structure of the term \( s' \) is simpler than that of \( \text{ref(susp}(s', ol_1, nl_1, env_1')) \), by the induction hypothesis, \( \text{hn\_co}(s', ol_1, nl_1, env_1, \text{whnf}) \) terminates and returns a quadruple \((r', rol, rnl, renv')\) representing a (weak) head normal form of \([s, ol_1, nl_1, env_1] \).

If \( ol=0, nl=0, env'=nil \), then \([t, ol, nl, env] = t \), and clearly the suspension represented by \((r', rol, rnl, renv')\) is already a (weak) head normal form of \( t \). Further, if \( \text{whnf} \) is \emph{false}, by the induction hypothesis, \((r', rol, rnl, renv')\) must have the form of \((r', 0, 0, nil)\). Correspondingly, in the definition of \( \text{hn\_co} \), via the function \( \text{mk\_explicit} \), \( t' \) is updated to a reference to \( r' \) if \((r', rol, rnl, renv')\) is in the form of \((r', 0, 0, nil)\), and is updated to a reference to \( \text{ref(susp}(r', rol, rnl, renv')) \) otherwise.

On the other hand, if the environment represented by \( ol, nl \) and \( env' \) is not empty, the term to be (weak) head normalized is in fact in the form of
\[
[[[s, ol_1, nl_1, env_1], ol, nl, env]].
\]
Suppose \( r \) is the term represented by the SML expression referred to by \( r' \) and \( renv \) is the environment represented by the SML list \( renv' \). Then the (weak) head reduction sequence of
\[
[[[s, ol_1, nl_1, env_1], ol, nl, env]]
\]
must have the form
\[
[[[s, ol_1, nl_1, env_1], ol, nl, env]], ..., [[[r, rol, rnl, renv]], ol, nl, env], ....
\]
Now if \( r \) is in the form of \((\lambda x)\), and \([r, rol, rnl, renv] \) is not a trivial suspension, then the term
\[
[\lambda \left[ x, rol + 1, rnl + 1, @rnl :: renv \right], ol, nl, env]
\]
must occur somewhere in the reduction sequence of
\[
[[[r, rol, rnl, renv]], ol, nl, env],
\]
and therefore in the reduction sequence of
\[
[[[s, ol_1, nl_1, env_1], ol, nl, env]].
\]
Thus the longest (weak) head reduction sequence of

\[[[s, ol1, nl1, env1], ol, nl, env]\]

is longer than that of

\[[\lambda [x, rol + 1, rnl + 1, @rnl :: renv], ol, nl, env].

Let \(x'\) be the reference to the SML expression representing \(x\). By the induction hypothesis,

\[hn_{co}(\text{ref}(\text{lam}(\text{ref}(\text{susp}(x', rol + 1, rnl + 1, \text{dum}(\text{rnl})::\text{renv}')))), ol, nl, env', \text{whnf})\]

terminates and returns a quadruple representing a (weak) head normal form of

\[[[s, ol1, nl1, env1], ol, nl, env]\].

Now suppose \([r, rol, rnl, renv]\) is trivial (note that if \(r\) is not an abstraction, then this suspension must be a trivial one by our induction hypothesis), then

\[[[r, rol, rnl, renv], ol, nl, env]\]

is in fact \([r, ol, nl, env]\). Thus the longest (weak) head reduction sequence of

\[[[s, ol1, nl1, env1], ol, nl, env]\]

is longer than that of

\([r, ol, nl, env]\).

By the induction hypothesis,

\[hn_{co}(r', ol, nl, env', \text{whnf})\]

terminates and returns a quadruple representing a (weak) head normal form of

\[[[s, ol1, nl1, env1], ol, nl, env]\].

The claim follows from these observations and an inspection of the definition of \(hn_{co}\). □
Chapter 6

Comparisons of Different Head Reduction Strategies

In this chapter, we consider a quantification of the relevance in practice of the intuitions underlying the various reduction procedures discussed in the earlier chapters.

Our experiment is based on the higher-order logic programming language $\lambda$Prolog. This language employs $\lambda$-terms as a means for realizing higher-order approaches to the processing of syntactic structure. Thus, within it, $\lambda$-terms are available for use in representing objects whose understanding embodies binding notions, and operations such as higher-order unification and reduction can be utilized for manipulating such representations in logically meaningful ways. By running a variety of actual $\lambda$Prolog programs and collecting suitable data over these, we can therefore obtain an understanding of the impact of the different approaches to reduction. At the computation level, the use $\lambda$Prolog makes of $\lambda$-terms is quite similar to what is done in logical frameworks, proof assistants and metalanguages such as Twelf, Isabelle and Coq. The observations we make relative to this language therefore carry over naturally to all these other contexts.

We have carried out the described idea by taking advantage of a compiler and abstract machine based implementation of $\lambda$Prolog called Teyjus. This system, implemented in the C language, supports a low-level encoding of $\lambda$-terms based on the suspension notation. Reduction computations within it are isolated in a head normalization procedure. Thus we can easily vary the reduction strategies used in this procedure and measure the effects of these variations. As a basis for our study, we have implemented three different head normalization procedures following the lines of discussion in this thesis, and we have metered these to collect information about the number of heap cells created over the entire duration of any given user program.

6.1 Experiment Examples

The data that we provide have been obtained by running the following representative user programs:

- [Compiler] This is a compiler for a small imperative language with object-oriented features. This program includes a bottom-up parser, a continuation
passing-style intermediate language, and generation of native byte code. Significant parts of the computation in this program do not in fact involve \( \lambda \)-terms. However, there are also major parts that do and our study reveals that choices in reduction strategies here can have a significant impact on behavior.

- \([\text{Typeinf}]\) This is a program that infers principal type schemes for ML-like programs. The representation of types treats quantification explicitly within this program and abstraction in the metalanguage is used to capture the binding effect. Given the treatment of type variables, unification over types is explicitly programmed. Thus, many of the typical features of a metalanguage are exercised by this program.

- \([\text{Hilbert}]\) This is an encoding in \( \lambda \)Prolog of the process of solving diophantine equations through higher-order unification. Solutions are not generated completely by this program in many instances. Rather, solvability is often determined, the exact identity of solutions being dependent on the unifiers for ‘flexible-flexible’ disagreement pairs left behind at the end of the computation.

- \([\text{Funtrans}]\) This is an collection of transformations on functional programs, such as through partial evaluation.

- \([\text{SKI}]\) This program realizes an object-level head normalization on arbitrary compositions of the well-known combinators \( S, K \) and \( I \). The data that is collected is based on the application of this procedure to a collection of five hundred combinator compositions that were created with help from a random number generator.

- \([\text{Church}]\) This program involves arithmetic calculations based on Church’s encoding of numerals and the combinators for addition and multiplication. The largest ‘number’ used in this program is around twenty thousand.

The first two programs exemplify what might be called the L\( \lambda \) style of programming [16]. As an programming idiom, this is a popular one amongst \( \lambda \)Prolog, Elf and Isabelle users and, in fact, arguably the most important case to consider in performance assessments. Computations in this class proceed by first dispensing with all abstractions in \( \lambda \)-terms using new constants, then carrying out a first-order style analysis over the remaining structures and eventually abstracting out the new constants. The process of abstraction elimination is realized in the following way: once an abstraction is recognized by the pattern matching process, it is applied to a new constant and thus a redex is generated. After that, the head normalization process is invoked on the newly formed application. In this sense, the generation of redices
is interleaved with the head reduction process and thus most redices are not revealed
to one invocation of the head normalization procedure. The unification operation in
such a language subset is known to be deterministic, and most of the redices have
the characteristic that the arguments of them are all constants.

Programs Hilbert and Funtrans include cases of genuine higher-order unification
calculations. Unlike the unification process in the $\lambda$ class that always terminates
and returns the unique unifier, there may be branching in unification. In particular,
in these cases, different $\lambda$-terms may have to be posited as bindings for instantiable
variables and reductions and other computations would have to be carried out, and
possibly backtracked over, using such terms.

Programs SKI and Church represent a situation in which $\lambda$-terms are used mainly
in reduction, the unification computation is largely first-order in nature.

### 6.2 Experiment Results

|                  | implicit suspensions | explicit suspensions | combination approach |
|------------------|----------------------|----------------------|----------------------|
| [Compiler]       | 2,640,909            | 635,851              | 134,316              |
|                  | 19,703,580           | 6,372,836            | 1,764,172            |
| [Typeinf]        | 7,142,880            | 7,691,000            | 1,722,696            |
|                  | 61,045,064           | 80,893,824           | 22,012,896           |
| [Hilbert]        | 170,123              | 18,894               | 5,642                |
|                  | 1,387,192            | 196,596              | 75,020               |
| [Funtrans]       | 28,027               | 62,277               | 24,404               |
|                  | 319,740              | 620,632              | 313,744              |
| [SKI]            | 98,319               | 180,777              | 76,779               |
|                  | 1,164,656            | 1,800,160            | 939,104              |
| [church]         | 44,797               | 137,936              | 37,162               |
|                  | 610,528              | 1,342,076            | 531,892              |

Figure 6.1: Heap usage for different reduction approaches

Figure 6.1 tabulates information that we have gathered using the different implementa-
tions of head normalization over the collection of examples illustrated in the
previous section. The two rows corresponding to each $\lambda$Prolog program indicate, re-
spectively, the number of internal term nodes created and the number of bytes those
terms occupied in the course of executing the program; these figures are distinct
because the number of bytes needed for a given term node varies in the Teyjus imple-
mentation depending on the type of the node. The columns are to be understood as
follows: \textit{implicit suspensions} corresponds to the reduction scheme where suspensions are recorded only in the structure of recursive procedure calls, \textit{explicit suspensions} corresponds to the approach that explicitly realizes each rewrite rule in Figure 2.1 and the \textit{combination approach} represents the amalgamation of the other two.

The data in Figure 6.1 show that the combination reduction approach has significant superiority, especially in the cases of the first four programs. Comparing the performance of the first reduction strategy, which performs substitutions eagerly, with that of the combination reduction strategy, which follows the same control regime of the former one but performs the substitution lazily, the advantage of the delayed substitution strategy is significant. In the case of \textit{compiler} and \textit{hilbert}, the structure creation using the combination reduction strategy is less than 5% of that using the eager substitution reduction strategy.

The better performance of the lazy substitution strategy is attributable, ultimately, to the fact that delaying creates substantially more opportunities for sharing in the structure traversal required for substitution and reduction. As we discussed in Section 3.2, the eager substitution strategy has potential drawbacks in the following two situations: first, redices are generated dynamically across the computation steps, which occurs frequently in the $\text{L}_\lambda$ programs; second, redices are embedded in the term into which the substitutions have to be performed. These drawbacks are avoided by the lazy substitution strategies.

Towards understanding the enormous performance differences between the first and the third reduction strategies in Figure 6.1, we observe that structures having significant quantities of embedded redices can be produced whenever the programs embody an intrinsic use of higher-order unification. A central part of this computation is that of positing substitutions towards reconciling the differences between what are known as \textit{flexible-rigid} disagreement pairs, \textit{i.e.} a pair of terms of the form

$$\langle \lambda x_1 \ldots \lambda x_l (F \, t_1 \ldots \, t_n), \lambda x_1 \ldots \lambda x_l (c \, s_1 \ldots \, s_m) \rangle$$

where $F$ is an instantiatable variable, $c$ is a constant or an abstractable variable occurrence which is bound by one of $x_1, \ldots, x_l$ and $t_1, \ldots, t_n, s_1, \ldots, s_m$ are arbitrary terms; we assume here that the binder lengths of the two terms are identical, something that can be arranged based on typing considerations under $\beta$-conversion. Using the procedure due to Huet [13], a collection of substitutions known as the imitation and projection substitutions would be posited for $F$ in this situation. These substitutions all have the structure

$$\{ \langle F, \lambda w_1 \ldots \lambda w_n (h \, (H_1 \, w_1 \ldots \, w_n) \ldots \, (H_o \, w_1 \ldots \, w_n)) \rangle \}$$

where $h$ is either a constant or one of $w_1, \ldots, w_n$ and $H_1, \ldots, H_o$ are new instantiatable variables. Now, in subsequent steps of the computation, these new variables may
themselves become instantiated in a similar way yielding embedded redices at all the places where $F$ appears. Moreover, the instantiations for the variables $H_1, \ldots, H_n$ may themselves contain embedded redices, resulting in further embedded redices in the binding for $F$. Thus, after several invocations of the unification computations, there are several embedded uncontracted redices left in the binding determined for $F$. An interesting point to note is that these embedded redices all appear at the argument position of the term serving as the binding of $F$. Thus, each of these redices will be left in place by the head normalization procedure whenever it is invoked to manifest the top-level structure of a subterm in which the redices are embedded. If the entire computation ends once a binding for $F$ is determined, then the embedded redices are a harmless artifact and do not have significantly influence performance characteristics. However, in most cases, it is expected that the bindings found for variables such as $F$ are used in further computations. In these situations, the terms on which the substitutions are performed have to be eventually (head) normalized. The performance differences noted relative to our test suite owe significantly to manifestations of this kind of phenomenon.

Theoretically, the eager substitution strategy has certain benefits when the computation system involves backtracking. However, in real executions, the benefits gained is not significant enough to outweigh its other disadvantages we discussed before. Backtracking is used to implement nondeterminism and is realized in the following way. When there are multiple branches the computation process can proceed to, the current computation status and term structures under manipulation are recorded, and then the computation process proceeds to one of the possible branches; if failure is encountered on the chosen branch, the computation procedure backtracks to the nearest choice point by resetting the computation status and relevant term structures, and then proceeds to the next possible branch. Since the first reduction strategy tends to perform substitutions eagerly, it has more opportunities to create new structures generated from the substitutions on the heap before choice points. After backtracking, these structures persist and certainly do not need to be reset. If these term structures do not have redices embedded inside, i.e. they are in their normal forms, they will not be affected by the subsequent reductions, and their (head) normalization will not create new terms on the heap. On the other hand, if the lazy reduction strategies are used, the term structures created before choice point may involve delayed substitutions. Thus, each time after backtracking to this choice point, the unreduced terms will be restored, and their (head) normal forms will be rebuilt on the heap by later reductions. However, if there are redices embedded inside the structures on which substitutions will be performed, the terms created by the eager substitution strategy are not normal forms either, and later reductions will still build new terms. In this situation, the eager substitution strategy gains no benefits, and
further the advantages of using lazy reduction strategies to combine the substitution walks are significant. As we discussed before, in most cases, there are complex reductions embedded inside the structures on which substitutions are performed. Thus, the disadvantages of this eager substitution strategy we discussed previously outweigh its benefit in a large degree. This is the reason that although the two genuine unification programs require frequent backtracking, their heap usage with the eager substitution strategy is far worse than that with the combination one.

The disadvantage of the eager substitution strategy is more obvious when the structures of the arguments of the head normal forms are complicated. As we discussed above, in general situations, the arguments of a head normal form created by the eager substitution strategy are overwritten by the following invocations of the head normalization process, thereby being redundant. It is apparent that the more complex these structures are, the more heap cells are unnecessarily consumed by the head normalization process using the eager substitution strategy. This explains the difference of the improvements from the combination strategy to the eager substitution one in different test cases appears in Figure 6.1. Specifically, the ratios between the heap usage of the combination approach and the implicit one are 19.66 in the compiler case, while this number in the typeinf case is 4.15, although the two programs both belong to the $L_\lambda$ subset. A similar fact can be observed from the two programs of the genuine higher-order class: the ratio is 30.15 in the hilbert case, but only 1.15 in funtrans. Such a difference of ratios is mainly caused by the different sizes of the terms under manipulation of these programs, which are reflected by the number of nodes of the input terms. For instance, in the compiler case, by controlling the number of nodes of the input term, we obtain the heap usage of the implicit and combination approaches shown in Figure 6.2.

| the number of nodes in the input term | implicit suspensions | combination approach | ratio |
|---------------------------------------|----------------------|----------------------|-------|
| 31                                    | 2,683                | 625                  | 4.29  |
| 49                                    | 7,670                | 1,278                | 6.00  |
| 103                                   | 30,056               | 3,222                | 9.34  |
| 202                                   | 101,204              | 6,786                | 14.91 |

Figure 6.2: The effect of the term size

It can be observe from Figure 6.2 that when the size of the input term is small, the ratio is around 4, which is similar to that in the typeinf case. However, when the size of the input term increases, the disadvantage of the eager substitution approach is exaggerated, and therefore the ratio increases rapidly.
Chapter 7

Conclusions

We have examined different approaches to using explicit substitutions in reduction computations in the thesis. The computation contexts we are interested in are computation systems of common metalanguages, logical frameworks and proof assistants. In these situations, many substitutions may have to be performed into the same subcomponent of a given object in the course of a larger calculation, and these substitutions are effected by creating and contracting at different points of time $\beta$-redices that span over the relevant structure. We have shown that the explicit substitution notation is useful in these situations to combine such substitutions and avoid redundant structure creation. In fact, most simplifiers for $\lambda$-calculus actually take advantage of the explicit substitution notation in spirit, as is manifest in their use of environments and closures.

However, in the situations in which the term is known at the beginning and is going to be eventually fully normalized, it is beneficial to fully normalize the term using the explicit notation only implicitly instead of normalizing the term in a demand-driven manner as the head normalization strategies do, because heap space used to record suspensions during the reduction process can be avoided. Further, if the computation system involves non-deterministic search situations implemented using backtracking, following the discussion in Chapter 6, the eagerness in creating normal forms on the heap has potential benefits. The benefits of the eager substitution strategy are not obvious because in most cases, the structures on which substitutions are performed have redices embedded inside. Taking into account this factor together with the possible benefits of using explicit substitution only implicitly, it is natural to consider a reduction strategy which reduces the term eagerly. Following the control regime of the eager substitution strategy, at the point where the head of a head normal form is exposed and there are delayed substitutions to be performed on the arguments of that head normal form, instead of actually carrying out the substitutions or explicitly building suspensions over those arguments, the reduction procedure recursively calls itself to normalize the arguments under the delayed substitutions. In this sense, the (sub)term is fully normalized if there are suspended substitutions involving it. It is obvious that this reduction strategy has more opportunities to create normal forms before choice points than the eager substitution and lazy reduction ones. However, if the subsequent computation on the term do not require its normal form to be fully
exposed, for example, the failure of comparison between two unequal terms can be
detected before their normal forms are fully revealed, the effort spent on normalizing
the unneeded parts of the terms is redundant. This is in fact a tradeoff: if a term
remains fixed till a successful path is found or until its full normal form is needed,
it is beneficial to reduce it completely before a backtracking point is encountered
so that rollbacks in computation do not cause such reductions to be undone and
subsequently redone; on the other hand, if only part of the term is needed possibly
because its structure is never fully examined in a successful computation or because
failure occurs after only part of it is examined, the lazy substitution strategies have a
better chance to avoid traversing the term completely and normalizing its unneeded
parts. While a detailed analysis of this problem is beyond this thesis, we mention that
studies have been conducted subsequent to the work in this thesis towards the precise
manner in which these two factors impact behavior in practice [15]. The experiment
results show that the heap usage of the eager reduction strategy is comparable to
that of the combined one, and in some test cases is even slightly better, which implies
that in real programs the first situation occurs more frequently.

To further improve the heap usage of our reduction strategies, we observe the fact
that if a term $t$ is closed, it will not be affected by the substitutions generated from
the reductions of the structures enclosing it. In particular, in this case, a suspension
of form $[t, ol, nl, env]$ can be simplified to $t$. If we can recognize such a closed term
before traversing it, then the effort spent on the traversal over this term for substitu-
ction performance can be saved. In fact, there is a variation of the suspension notation
which associates annotations with terms to denote their closedness [17]. Annotations
have different impacts on the heap usage of the different reduction strategies accord-
ing to their ability to combine substitutions. We conducted experiments comparing
the heap usage of these reduction strategies with annotations and the experimental
data show that with annotations, the heap usage of the eager substitution strategy is
improved significantly in most test cases, while the improvements of the lazy substi-
tution and lazy reduction strategies are relatively less. The reason for this difference
is the following. As we discussed in Chapter 6, the structures produced by higher-
order unification often have significant quantities of embedded redices. Such a redex
is generated from the binding of a free variable, say $F$, in an environment such as
$\lambda x_1\ldots\lambda x_l(\ldots(F\ t_1\ldots t_n)\ldots)$, to a term of form $\lambda w_1\ldots\lambda w_m\ s$. It can be observed that
the redex formed after this substitution is closed, i.e., it would not be affected by
the delayed substitutions over it. Thus annotations can help the eager substitution
strategy avoid the redundant term traversals purely for substitution performance,
over such redices. Note that the reduction walk over such term structures cannot
be avoided, since there are redices embedded inside them. However, the lazy substi-
tution strategies avoid separate substitution and reduction walks by delaying those
substitutions to be performed along with the reduction steps, while the eager reduction strategy avoids such separate walks by eagerly performing reductions along with the substitution traversals. Since these reductions have to eventually be normalized, the improvements gained by adding annotations to these reduction strategies are not as much as that of the eager substitution one. While a detailed analysis of this problem is beyond this thesis, we conducted the subsequent studies towards the precise manner in which the annotations impact behavior in practice in [15].

Our focus in this work has been mainly on a comparison of space usage and the elimination of redundant structure creation. Another important factor to consider is the time efficiency of each of the reduction approaches. The procedure based on the naive view of rewriting is the simplest to realize and the Teyjus system, in fact, embodies an iterative rendition of this procedure using a term stack. Adapting such an optimized implementation to the other reduction strategies, and including a way in which garbage collection costs are taken into account, it is meaningful to obtain and compare the time measurements of these reduction strategies. A different aspect that is relevant to study concerns the compiled realization of reduction. Recent work relative to the Coq system has shown how to use compilation assuming eager reduction and substitution strategies to obtain substantial speedups in comparison with the existing interpretive approach [9]. The examples considered in this study seem to be ones where the terms to be normalized are available in complete form at the beginning of the computation. As we have argued, this situation is different from what is encountered in metalanguages such as λProlog and Elf. It is, therefore, of interest to see if explicit substitutions can be built into a compilation model towards harnessing the benefits of laziness in substitution over and above those of compilation in these contexts.
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