A Comparison of Formalizations of the Meta-Theory of a Language with Variable Bindings in Isabelle

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Abstract. Theorem provers can be used to reason formally about programming languages and there are various general methods for the formalization of variable binding operators. Hence there are choices for the style of formalization of such languages, even within a single theorem prover. The choice of formalization can affect how easy or difficult it is to do automated reasoning. The aim of this paper is to compare and contrast three formalizations (termed de Bruijn, weak HOAS and full HOAS) of a typical functional programming language. Our contribution is a detailed report on our formalizations, a survey of related work, and a final comparative summary, in which we mention a novel approach to a hybrid de Bruijn/HOAS syntax.

1 Introduction

Theorem provers can be used to reason about programming languages. For example, Ambler and Crole have used Isabelle to prove results about a small functional language PL [2], by formalizing it within Isabelle/HOL. A key feature of PL is that variable binding is pervasive. Further, there are a number of methods which form the theoretical basis for the formalization of variable binding operators, whatever setting they occur in; in particular, there are choices for a formalization of PL. The choice of method can have a big effect on how easy or difficult it is to do automated reasoning about PL. In more detail we might hope that automated proofs mirror informal mathematical proofs, that we can minimize the difficulty of proofs and the level of infrastructure (such as "book-keeping" lemmas), and maximize genericity and scalability. The aim of this paper is to compare and contrast three formalizations of PL, by examining such requirements in each case. It is clearly extremely difficult to objectively compare such requirements between different formalizations of one object level language. Our contribution is to report our experiences as clearly as possible, and we hope our findings will be useful to those working in related areas who wish to make informed choices about the pros and cons of formalizing variable binding.

We give three formalizations in Isabelle [27] of the (meta)theory of a small core functional programming language. The types and terms are given respectively by

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A ::= \mathbf{Nat} \mid A_1 \to A_2
M ::= x \mid \mathbf{lam} \ x . \ M \mid M @ M' \mid \mathbf{z} \mid \mathbf{s} \ M \mid (\mathbf{case} \ M \ \mathbf{of} \ \mathbf{z} \Rightarrow M_1 \mid \mathbf{s} \ x \Rightarrow M_2) \mid \mathbf{rec} \ x . \ M
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and the language has type assignments $\Gamma \vdash M : A$, big step evaluation $M \Downarrow V$ where V is a value, and small step transitions $M \leadsto M'$. The operational semantics is call-by-name; we omit the standard definitions (see for example [35]). We formalize type assignment,

evaluation (natural/big-step) and transition (single step) operational semantics, and prove some basic results, such as the determinacy of operational semantics; subject reduction (run-time type preservation); the progress lemma (well-typed closed non-values do not get stuck at run-time); and the equivalence of big and small step evaluation. These properties are standard, and quite elementary. However, they can be regarded as a benchmark for such core languages as ours (see for example [28, 20, 17]).

We refer to our three methods as de Bruijn, weak HOAS and full HOAS. The de Bruijn method for describing binding operators is very well known [4]. It is exemplified in the Isabelle library by Nipkow's Church-Rosser's proofs [25] (see also for example [34, 2]). The method tackles some of the standard problems (such as α -renaming) associated with name-handling over concrete syntax. However, de Bruijn systems incur costs of additional programming infrastructure and the notation itself is unreadable. Higher Order Abstract Syntax (HOAS) attempts to deal with some of these problems. It is perhaps less well known, so we give some details—however, we assume readers are broadly familiar with the ideas. Note that HOAS is not a precisely defined system; a number of "systems" fit the title which seems to appear first in [29].

The ideas underlying HOAS go back to Church and also appear in Martin-Löf's theory of arities [26]. The basic idea is that the meta-language into which an object language (such as **PL**) is translated will typically have a single variable binding construct (usually given by function abstraction) and a single definition of infrastructure such as capture-avoiding substitution, along with notions of variable-renaming and freshness of names. This is used to represent the various binding operations found in the object language. In particular, if the object language is altered, one does not need to substantially re-code the infrastructure for binding operations. We introduce some non-standard terminology. A meta-language for HOAS is *full* if

- Object-level bound variables are encoded as meta-level bound variables.
- Object level contexts are encoded as meta-level contexts.
- Object-level substitution is encoded as meta-level β -conversion.

It is called *weak* if the third condition does not hold. In such a case substitution is typically defined as an inductive relation at the object level.

We have carried out our study with Isabelle and Isabelle/HOL because they are systems which seem to offer most automation, but many of our observations may apply to other tactics-based systems such as Coq [8]. The paper is organized as follows. In section 2 we report on de Bruijn formalizations in Isabelle/HOL. In Section 3 we move to weak HOAS, by following Despeyroux et al's approach in the Calculus of Inductive Constructions. This too is in Isabelle/HOL. In Section 4 we restrict to the primitive Isabelle language to give a full HOAS encoding in the spirit of LF [14]; this has to be understood more as a simulation of what is achievable in systems such as Twelf [30], rather than as a full-fledge proposal to implement full HOAS in Isabelle, since a comparison with Twelf itself is complicated by the fact the latter is not biased towards interactive theorem-proving. In Section 5 we review work related to ours. In Section 6 we summarize the results of our comparisons, and mention a novel approach to a hybrid de Bruijn/HOAS syntax.

2 The de Bruijn Method

The use of de Bruijn notation is a standard technology in the implementation of theorem provers and other systems which represent and manipulate syntax with variable

binding [4]. The same technology can be used within a theorem prover to represent and reason about an object language with variable binding. This approach has been used successfully by a number of authors (see for example [25]). In the pure form of de Bruijn notation, all variables within an expression, whether free or bound, are represented by natural number indices. The work reported in [2] used a pure form of de Bruijn notation to represent the functional programming language fragment PL in Isabelle/HOL and reason about its operational semantics. Examining the Isabelle theories produced for PL reveals both the strengths and the weaknesses of the de Bruijn approach. A clear strength is that the technology is available off-the-shelf: expressions are represented by the elements of an inductive datatype exp, operations such as substitution are given by primitive recursive functions, and judgements are given by (co)inductively defined sets. These features are all well supported by packages within Isabelle/HOL. On the other hand, it is a weakness of this approach that the de Bruijn notation differs considerably from that used in informal mathematical exposition. It is difficult, even with experience, to read such expressions. A greater problem is that the index assigned to a variable is given by its position relative to the corresponding binder (in the case of bound variables) or relative to a corresponding occurrence of that variable in an environment (in the case of free variables). The consequence is that any operation which alters the relative position of variables, for example, swapping the position of two variables in the typing environment or substituting one expression into another, necessitates the relabelling of indices. The de Bruijn encoding of **PL**, in common with other theories of this sort, is dominated by a large number of lemmas dealing with the relabelling of indices. These lemmas are more a book-keeping aspect of the representation rather than anything to do with the object language being formalized.

An alternative to the pure form of de Bruijn notation is a mixed form in which bound variables are represented by indices but free variables have explicit names. It is a variant of this form which is used in the implementation of Isabelle itself. For our language we define a datatype of expressions by

```
datatype exp = Var var | Bnd bnd | Abs exp | App exp exp | Fix exp
Zero | Succ exp | Case exp exp exp
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The type var of free variables and the type bnd of bound variable indices are both declared to be the type of natural numbers. Taking var as the naturals is *simply* a way to ensure that we have a countably infinite supply of distinct free variables—there are no index computations.

Proofs involving the mixed form of de Bruijn notation are less dependent on lemmas about relabelling of indices. However, the work is transfered elsewhere. As free and bound variables are explicitly distinguished, we require functions to transform a free variable to a bound variable, and to instantiate a bound variable as a free variable or possibly some other expression. These functions are defined by primitive recursion on the structure of expressions, and have types given by

```
bind :: var \Rightarrow bnd \Rightarrow exp \Rightarrow exp
inst :: bnd \Rightarrow exp \Rightarrow exp
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The standard presentation of the typing judgement uses an explicit type environment coded as a list. This is not a requirement or a feature specific to the de Bruijn approach, but a choice. This presentation has the advantage that it is easy to code using the tools already available in Isabelle-HOL. Typing judgements $env \vdash e ::: a$ are given as an

inductive definition. In particular, the introduction rule for the type of an abstraction takes the form

$$\frac{\texttt{newIn} \ n \ env}{env \vdash (Abs \ s) ::: a \to b} \frac{\texttt{Cons}(n,a) \ env \vdash (\texttt{inst} \ 0 \ (\texttt{Var} \ n) \ s) ::: b}{env \vdash (Abs \ s) ::: a \to b} dbtype_abs$$

The predicates newIn and newFor are used to check that the nth free variable does not occur in the typing environment or the expression s, that is, n is the name of a fresh free variable. The task of reasoning about the typing judgement is quickly dominated by quite routine lemmas about the freshness of names.

In the proof of the subject reduction lemma for 'big-step' evaluation we first have to relate typing and substitution of an expression for a free variable:

$$\frac{Cons(n,a)\ env \vdash s ::: b}{env \vdash s || t || ma} SubLemma$$

The proof is by induction on the derivation of the typing of s and uses a second result, which states that weakening is admissible for the typing judgement:

$$\frac{env \vdash s ::: a \quad \texttt{newIn} \ i \ env \quad \texttt{newFor} \ i \ s}{Cons(i,b) \ env \vdash s ::: a} TWeak$$

A straightforward proof of this by induction on the derivation of the typing of s runs into problems in choosing suitably fresh names for the variables introduced in the abstraction case. A proof technique which overcomes these difficulties is given by McKinna and Pollack [21]. The trick is to define a second version of the typing judgement in which the introduction rule for an abstraction has a universal quantifier

$$\frac{\forall n \,.\, \mathsf{newIn} \,\, n \,\, env \,\rightarrow \, \mathsf{newFor} \,\, n \,\, s \,\rightarrow \, Cons(n,a) \,\, env \,\vdash \, \mathsf{inst} \,\, 0 \,\, (\mathtt{Var} \,\, n) \,\, s \, ... \,\, b}{env \,\vdash \, (Abs \,\, s) \,\, ... \,\, a \,\rightarrow \, b} \,\, dbtype_abs' \,\, dbtype_abs'$$

and the reader should compare this rule to the rule $typeof_abs$ in Section 3 and rule ofLam in Section 4 which addresses a similar issue in HOAS. Thus the premise states that s instantiated with Var n has type b for all choices of fresh variable n, rather than some specific choice. One develops a theory of relabelling for the free variables within an expression and uses this to show that the two versions of the typing judgement coincide. The key idea is to show that these typing judgements are preserved by a bijective relabelling of free variables and so, in particular, they are preserved when the names of two free variables are swapped. The cost in terms of programming infrastructure is quite high but the mathematics is relatively straightforward.

It is worth stressing that the approaches described in this section are entirely compatible with classical higher order logic and are purely definitional. It is one of the main tenets of the philosophy amongst users of HOL and Isabelle/HOL that new concepts should, wherever possible, be defined via some representation involving the concepts that are already given. Properties of the new concept can then be derived from the properties of its underlying representation, rather than postulated axiomatically. This ensures the consistency of each extension relative to a small core of the logic. The work needed to achieve this is all done within the theorem prover. An axiomatic approach dispenses with the need to prove derived properties, but must rely on an external mathematical justification for its consistency (see Section 4).

3 The Weak HOAS Method

In this section we explore Despeyroux et al.'s approach [5] to HOAS, which leads us to a formalization of a weak form of HOAS in Isabelle/HOL. Variable binders should be represented as functions in the meta-logic. This "requires" an inductive datatype definition involving function types, such as datatype $\exp = Abs (\exp \Rightarrow \exp) | App \exp \exp \dots$ which is not allowed because the source \exp occurs negatively (the associated operator would not be monotone). Thus we introduce a separate type for variables, with an explicit coercion for variables into expressions, and say that the datatype has been positivized. This yields the following HOL data-type:

It is standard to define a translation function $\lceil - \rceil$ from the object language to expressions in the meta-logic, with object level binding captured by function abstraction; for example $\lceil \operatorname{lam} x \cdot x \rceil = \operatorname{Abs}(\lambda x : \operatorname{var}.(\operatorname{Var} x))$. Operations involving variable binding (i.e. α -renaming etc) are delegated to the meta-level. Further, no lemmas concerning de Bruijn index manipulation are required.

In an inductive framework, the choice of representation of the set of bound variables is crucial. Despeyroux [5] took this to be any set isomorphic to the natural numbers, to realize a possibly infinite number of bound variables. However, taking var to be an inductive set will create so-called *exotic* terms. These are terms of type exp which do not represent any object-level functional program and hence the translation function can not yield an adequate representation. In fact not only are exotic terms given by case-analysis possible, but there are terms representing "free" variables, such as Var(Succ Zero), which we do not need. However, as pointed out in [18], if the set of variables is *not* inductive, no *closed* exotic term is produced. In fact, in the Calculus of Construction it is possible to leave the set of variables completely unspecified ("parametric" in Coq terminology).

For the formalization of the semantics of our programming language, differently from other systems such as the π -calculus [18], we do not need to have an infinite supply of names for bound variables. On the contrary we do not need to name them at all. The only requirement is to test them for distinctness. In Isabelle/HOL, types need to be non-empty and in fact we identify var with a set containing at least two elements and we add the axiom

$$\frac{}{\forall y \!:\! \mathtt{var.}\, \lambda x \!:\! (\mathtt{Var}\; x) \neq \lambda x \!:\! (\mathtt{Var}\; y)} Var_neq$$

which is clearly validated by our representation. This ensures that both kinds of closed exotic terms present in Despeyroux et al.'s approach are excluded. However, the primitive language of HOL contains the description operator which creates closed exotic terms such as

$$\operatorname{Abs}(\lambda x.(\operatorname{if}\ x=(\epsilon w.True)\ \operatorname{then}\ (\operatorname{Var}\ x)\ \operatorname{else}\ (\operatorname{App}\ (\operatorname{Var}\ x)))$$

Note however that no exotic terms can be *constructively* created: in an intuitionistic version of HOL, all exotic terms would be ruled out. Yet, Isabelle/HOL is a classical set-theory, so we do introduce in Figure 1 an object-level predicate (traditionally called 'valido') which identifies the class of meta-level terms representing programs (we write

upper and lower case characters, i.e. E and e, for second and first order terms respectively). The identification is modulo extensionality—built-in in Isabelle/HOL, although not in Coq. Moreover, validity can be useful in so far as it provides an induction principle over second-order terms: we can prove, for example, that substitution is a total relation (which otherwise would be, in general, unprovable). In [31] validity is used to prove the theory of contexts.

$$\frac{valid_1 \; (\lambda x \, . \, (\text{Var} \; v))}{valid_1 \; (\lambda x \, . \, (\text{Var} \; x))} v_1 \text{-} ref } \\ \frac{valid_1 \; E \qquad valid_1 \; E'}{valid_1 \; (\lambda x \, . \, (\text{App} \; (E \; x) \; (E' \; x)))} v_1 \text{-} app } \\ \frac{(\forall \, u. \, valid_1 \; (\lambda x \, . \, (\text{App} \; (E \; x) \; (E' \; x)))}{valid_1 \; (\lambda x \, . \, (\text{Abs} \; (E \; x)))} v_1 \text{-} abs } \\ \frac{(\forall \, u. \, valid_1 \; (\lambda x \, . \, (\text{Abs} \; (E \; x)))}{valid_1 \; (\lambda x \, . \, (\text{Abs} \; (E \; x)))} \\ \frac{valid_0 \; (\text{Var} \; v)}{valid_0 \; (\text{Var} \; v)} v_0 \text{-} app \qquad \frac{valid_1 \; E}{valid_0 \; (\text{Abs} \; E)} v_0 \text{-} abs }$$

Fig. 1. Validity predicates

Weak HOAS does not obviously extend beyond second-order binding. Consider a third-order operator such as callcc, which in full HOAS would have the type $((exp \Rightarrow exp) \Rightarrow exp) \Rightarrow exp$. It is not clear how this might be positivized. On the other hand, we can formalize several other binding operators such as logical quantifiers or operators in process-calculi. For instance, in the polymorphic λ -calculus, type abstraction can be given the type $(tp\Rightarrow exp)\Rightarrow exp$, while the polymorphic quantifier should be positivized into $(var\Rightarrow tp)\Rightarrow tp$.

Substitutions In Weak HOAS, meta-level functions have source type $var \Rightarrow exp$; thus substitution of expression for expression cannot be rendered by meta-level β -conversion. Ideally we seek a primitive recursive definition which would be directly applicable to a substitution-based evaluation semantics. It is well known that this is not possible in the traditional setting of inductive definitions [7, 10]. Substitution must be implemented, in the spirit of [24], as an inductive relation with rules such as

In fact establishing the functionality of the relation in Isabelle/HOL turns out to be quite tricky. Getting an appropriate elimination rule is far from immediate, partly because the simplifier (which refines the general elimination rule stemming from the fixed

point definition via some free equality rewriting) does not simplify at higher types. Since simply adding extensionality to the reasoner is not practical, we have to establish freeness of constructors manually. While injectivity of constructors is fairly immediate, distinctness needs to rely on the Var_neq axiom. Once established and temporarily added to the simplifier, the correct elimination rules are obtained.

The proof of functionality of substitution is a simple structural induction. Instead, the proof that substitution is a total relation requires the *validity* condition for functions, and also the ϵ -operator, although a different proof by induction the rank of second-order expression is possible. We comment on this point further in Section 6.

Typing A key feature of the (Weak) HOAS approach is that an object-level context $\Gamma \equiv x_1:A_1...x_n:A_n$ is represented as a meta-level context. This provides benefits which we illustrate by examining typing judgements. We can represent typing without explicitly mentioning the typing context as follows. First consider these rules

$$\begin{array}{c} ::: :: (\texttt{exp} * \texttt{tp}) \; set \\ tpv :: \texttt{var} \Rightarrow \texttt{tp} \Rightarrow \texttt{bool} \\ \\ \hline \frac{tpv \; x \; t}{(\texttt{Var} \; x) \; ::: \; t} typeof_var & \frac{e ::: \; (t' \rightarrow t) \qquad e' ::: \; t'}{(\texttt{App} \; e \; e') \; ::: \; t} typeof_app \\ \hline \frac{(\forall x \, . \, tpv \; x \; t \rightarrow (E \; x) \; ::: \; t')}{(\texttt{Abs} \; E) \; ::: \; (t \rightarrow t')} typeof_abs \\ \hline \end{array}$$

We extend the representation function by defining $\lceil \Gamma \rceil$ to be the *set* of Isabelle assumptions $tpv \ x_1 \lceil A_1 \rceil \dots tpv \ x_n \lceil A_n \rceil$. Clearly $\lceil \Gamma, x : A \rceil = \lceil \Gamma \rceil, \lceil x : A \rceil$. Again, note that we have a positivized encoding, achieved by introducing an auxiliary predicate tpv. As tpv is *not* an inductive predicate, we need to axiomatize its behavior so that it faithfully encodes object-level contexts. In particular, the latter are functional. This is enforced by the axiom tpv_unique . Moreover, we need to ensure (axiom tpv_ex) that there exists at least one variable for every type:

$$\frac{tpv \ x \ t}{t = t'} tpv_unique \qquad \frac{tpv \ x \ t'}{\forall t \ . \ \exists \ x \ . \ tpv \ x \ t} tpv_ex$$

Since the object-level context Γ is represented as a meta-level context, weakening, contraction and exchange come for free. It is essential that the notion of provability is constructive. This will force a proof of $\phi \to \psi$ to a be a proof of ϕ from the assumption ψ , rather than, say the tautology $\neg \phi \lor \psi$. For example, there is a classical proof of $\exists y . \mathsf{Abs}(\lambda x . (\mathsf{Var}\ y)) ::: s \to s$, although the expression does not correspond to any object-level term.

Even though inversion is provided by the elimination rule(s) of the inductive definition, we do need to prove that substitution preserves typing. Our formalization is directly inherited from [5]:

$$\frac{subst \ E \ p \ n \qquad \exists x \, . \, (\mathtt{Var} \ x) \, \ldots \ t' \wedge p \ \ldots \ t' \wedge (E \ x) \, \ldots \ t}{n \ \ldots \ t} SubLemma$$

The mechanized proof mirrors the informal one (induction on substitution and inversion on typing), but with an appeal to the tpv_unique axioms in the base case.

An issue which did not manifest itself in Despeyroux et al [5] is that sometimes the induction principle generated by ::: is not appropriate, because it will always contain a base case for (free) variables. This turns out to be a problem, for example, when formalizing the progress lemma. Indeed, the lemma holds only for closed expressions which must have empty typing contexts. But contexts in the encoding of ::: are implicit and therefore cannot be explicitly manipulated. Thus we need to introduce another version of typing with an additional argument, to be read as a boolean flag which signals whether the context is empty or not. These typing rules (given below) will update the flag from its initial default value false, to true.

$$\begin{array}{cccc} typf :: (\texttt{exp} * \texttt{tp} * \texttt{bool}) \; set \\ \\ \underline{tpv \; x \; t & f = True} \\ typf \; (\texttt{Var} \; x) \; t \; f & typf \; e \; (t' \to t) \; f & typf \; e' \; t' \; f \\ \hline typf \; (\texttt{App} \; e \; e') \; t \; f & typf _app \\ \\ \underline{(\forall \; x. \; tpv \; x \; t \to typf \; (E \; x) \; t' \; (\lambda y \; . \; True) \; f)} \\ typf \; (\texttt{Abs} \; E) \; (t \to t') \; f & typf _abs \\ \end{array}$$

We have proven the two typing judgements equivalent with a straightforward derivation.

Evaluation The encoding of operational semantics as inductive relations does not bring in any new ideas. However, note the role of substitution, for example in:

$$>> :: (\texttt{exp} * \texttt{exp}) \; set$$

$$\xrightarrow{1} :: (\texttt{exp} * \texttt{exp}) \; set$$

$$\underbrace{e_1 \; >> \; (\texttt{Abs} \; E) \quad subst \; E \; e_2 \; e_3 \quad e_3 \; >> \; v_1}_{ \left(\texttt{App} \; e_1 \; e_2\right) \; >> \; v_1} eval_app}_{ \left(\texttt{App} \; (\texttt{Abs} \; E) \; e_2 \; \right) \xrightarrow{1} \; e_3} step_app}$$

It is clear that properties of substitution are central in every proof involving evaluation, and moreover no other infrastructure is required in the Weak HOAS setting:

- Determinacy of operational semantics: for evaluation there is a fully automatic proof
 which uses as expected functionality of substitution plus distinctness of numerals.
 Similarly for SOS, which also uses the facts that there are no steps possible from
 values and specialized elimination rules for the latter.
- Subject reduction for evaluation. The proof (by induction on the evaluation judgement) uses as expected introduction and elimination rules for typing and the substitution lemma, but it also requires the tpv_ex axiom every time a dynamic typing assumption is needed. The same applies to small step reduction.
- The Progress lemma requires the flagged type judgement, so that we can get rid of the variable case. Further, since we need totality of substitution to fire the β rules, we need to add the *validity* condition.

$$\frac{typf \ e \ t \ f \qquad (f = False) \qquad valid_0 \ e}{value \ e \lor \exists e'. \ e^{\frac{1}{\longrightarrow}}e} \ Progress$$

¹ A more elegant treatment would use a linear context for the same aim.

4 Full HOAS

The final approach we consider is a way to address full HOAS in a system such as Isabelle. In the LF style, expressions are declared by simply introducing an appropriate signature and *not* a data-type: exp and tp have kind term, and lambda abstraction, for example, receives the second-order type (exp⇒exp)⇒exp. We thus give the following declaration.

App :: $\exp \Rightarrow \exp \Rightarrow \exp$ Abs :: $(\exp \Rightarrow \exp) \Rightarrow \exp$ Fix :: $(\exp \Rightarrow \exp) \Rightarrow \exp$ Zero :: \exp

Succ :: exp⇒exp

 $\mathtt{Case} :: \mathtt{exp} {\Rightarrow} \mathtt{exp} {\Rightarrow} (\mathtt{exp} {\Rightarrow} \mathtt{exp}) {\Rightarrow} \mathtt{exp}$

This has the crucial feature that we can easily prove that every α -equivalent object-term is uniquely represented by a *canonical* (that is η -long β -normal) term built out of App, Abs, Zero, Succ, Case, Fix. In particular, there is no construct for bound variables and no exotic term may arise. It is of course vital that its expressive power is essentially the one of the simply-typed λ -calculus and its derivability strictly intuitionistic. We thus step back to Isabelle's *IFOL* (intuitionistic first-order logic).

Relations such as typing or evaluation are not inductively defined. The benefits of "left-recursiveness" show themselves for example in the typing relation (given below), where note how the variable case is left entirely implicit. To stress that we are not in HOL anymore, we use IFOL first-order syntax:

$$\begin{array}{c} of :: \mathtt{exp} \Rightarrow \mathtt{tp} \Rightarrow \mathtt{bool} \\ eval :: \mathtt{exp} \Rightarrow \mathtt{exp} \Rightarrow \mathtt{bool} \\ \\ \underline{of(e_1, t' \to t) \quad of(e_2, t')} \\ of(\mathtt{App}(e_1, e_2), t) \quad ofApp \quad \frac{\forall x . of(x, t_1) \to of(E(x), t_2)}{of(\mathtt{Abs}(\lambda x . E(x)), t_1 \to t_2)} \\ \underline{of(e_1, \mathbf{Nat}) \quad of(e_2, t) \quad (\forall x . of(x, Num) \to of(E_3(x), t))} \\ \underline{of(\mathtt{Case}(e_1, e_2, E_3), t)} \\ ofCase \end{array}$$

It is the eigenvariable condition in the meta-level which replaces the tpv_unique axiom in Weak HOAS to guarantee functionality of contexts. The use of meta-level substitution is apparent in the encoding of evaluation:

$$\frac{eval(e_1, \mathtt{Abs}(\lambda x \,.\, E(x)))}{eval(\mathtt{App}(e_1, e_2), v)} \frac{eval(E(e_2), v)}{eval(\mathtt{App}} \frac{eval(E(\mathtt{Fix}(E)), v)}{eval(\mathtt{Fix}(E), v)} \frac{eval(\mathtt{Fix}(E), v)}{eval(\mathtt{Fix}(E), v)} evalFix$$

Note how in the case for application E_1 returns a function $Abs(\lambda x. E(x))$ and the object-level reduction is encoded by application in the logical framework, that is $E(e_2)$.

This is very elegant and well-known as far as object-level reasoning, such as typing or evaluation, but it is clearly not enough for meta-reasoning, which needs at least some form of case analysis and induction. One way to provide the former is to view a relation such as typing as a *Partial Inductive Definition* [13], a generalization of inductive definitions [1] to definiens containing parametric and hypothetical judgements.

If $b \Leftarrow G$ is an introduction rule for the predicate a and $\mathcal{D}(a)$ is the collection of the former, then the rule of *Definitional Reflection*

$$\frac{\{\sigma\Gamma, \sigmaG \vdash_{\mathcal{D}} A \mid \sigma = mgu(a, b), b \Leftarrow G \in \mathcal{D}(a)\}}{\Gamma, a \vdash_{\mathcal{D}} A} \mathcal{D} - L$$

is a proof-theoretic device that allows theories to be considered as "closed" (in the sense of logic programming closed worlds) and thus provides a convenient way to perform case-analysis on judgements. Indeed, it can be seen as the 'mother' of every elimination rule, since, once we endow the meta-logic (i.e. IFOL) with such a rule, the elimination rules (as well as freeness equality of the data-type) of an inductive definition can be *derived*, thus freeing the user from stating and asserting them in the theory.

As well-known, induction in this setting can cause problems. For example, paradoxes such as non-termination of the logical framework [11] arise when the higher-order encoding of a relation is seen as an inductive type, with corresponding strong elimination rule. It is the latter rule that allows a definition of the offending terms. Other less dramatic problems, such as the loss of the adequacy of the representation via creation of exotic terms, can come from a naive combination of higher-order induction principles in impredicative systems with the axiom of unique choice [16].

The main challenge is to-reintroduce some form of induction. Some recent research [30, 20] has shown that one way to make sense of this is to separate a meta-logic where we formalize our object logic from a meta-meta-logic where we inductively reason about the meta-logic. Miller & McDowell [20] introduce a meta-meta logic, $FO\lambda^{\Delta N}$, that is based on intuitionistic logic augmented with definitional reflection and induction on natural numbers. Other inductive principles are derived via the use of appropriate measures. At the meta-meta level, they reason about object-level judgements formulated in second-order logic. They prove the consistency of the method by showing that $FO\lambda^{\Delta N}$ enjoys cut-elimination [19].

Our approach is somewhat more naive than Miller's, in that we blur the distinction between meta-meta and meta-logic and we do not formalize an explicit logic of judgements, which we represent directly in an Isabelle. This entails considering judgements directly as *definitions*, which is not allowed in Miller's approach due to the restriction on the cut-elimination proof. Another difference is that we assert structural induction as an *axiom* on any class of judgements. For example, we assert the structural induction principle for typing (restricting here for the sake of space to the Abs, App fragment):

$$\begin{aligned} of(b,a) & \quad of(e,(t'\to t)) \wedge P(e,(t'\to t) \wedge of(e',t') \wedge P(e',t') \to P(\texttt{App}(e,e'),t)) \\ & \quad \underbrace{(\forall v \,.\, of(v,t) \to of(E(v),t') \wedge P(E(v),t') \to P(\texttt{Abs} \ \lambda x \,.\, E(x),t \to t'))}_{P(b,a)} \\ & \quad ofIne(b,a) \end{aligned}$$

(Note that the size of v is not limited, so that this does not present a straightforward induction on the size of terms, and must be justified some other way.) A consequence of this is that the cut-elimination result does not apply directly and thus consistency is not automatically established. Those axioms, as far as a simple language such as \mathbf{PL} is concerned, can be shown to be consistent via a semantics [16]. A similar axiomatic approach is proposed in [17], as we remark in the next Section.

In a robust implementation, there must be some support to automatically infer such principles from the defined judgements. Indeed, it is possible to modify the ML code which produces induction rules for HOL inductive definitions; in fact, the above axioms

are simple manual modifications of the principles generated in Weak HOAS. Once this is in place, the proof-scripts tend to shrink dramatically: the structure of the top-level theorems does not alter much, but the required infra-structure disappears. In fact, they are comparable to *Twelf's* proofs. We find that

- Subject reduction can be proven with no preliminaries.
- Determinism of operational semantics does not need functionality of substitution.
- Progress Lemma uses the standard typing judgement is sufficient and does not need totality of substitution.

5 Related Work

In the literature, there are several large-scale machine-assisted proofs of properties of languages with variable binding using first-order encodings, see for example [34, 15, 21, 3]. Here we review papers that try to overcome the problems of first-order encodings by using some form of HOAS; there are other intermediate approaches aimed at reducing the aforementioned issue [33, 12], which we do not have the space here to mention.

We can distinguish two main (and not unrelated) approaches to the integration of HOAS and induction: one "functional" and the other "logical". In the "functional" approach, the emphasis is on trying to allow (primitive) recursive definitions on functions of higher type (cf our substitution function introduced in Subsection 3). The aim is to preserve adequacy of representations, while still allowing "functional programming with higher-order terms". This was first suggested for a fragment of ML by Miller in [23] and was realized for the simply-typed case in [7] and more recently for the dependentlytyped case in [6]. Here the idea is to separate at the type-theoretic level, via an S4 modal operator, the primitive recursive space (which encompasses functions defined via case distinction and iteration) from the parametric function space (whose members are those convertible to terms built only via the constructors). An interpretation of the modal operator in terms of functor categories has been given in [16], providing an alternative proof of adequacy. Such categorical semantics can also be used to give a sensible interpretation to higher-order induction principles. Recently, in [10] Gabbay and Pitts have introduced a novel approach to this issue, based on a set-theory with an internal notion of permutation of variables. This yields a primitive notion of freshness and of name-abstraction, so that it can adequately encode object-level syntax modulo α -conversion. This work takes an alternative route to HOAS, with the intention of manipulating names of bound variables explicitly, something that HOAS falls short (but see [17] reviewed later on). Such a set-theory yields a natural notion of structural induction and recursion over α -equivalence classes of expressions. On the other hand, the approach shies away from the other two focal points in logical frameworks, namely delegating to the latter object-level substitutions and environment maintainance. An ML-like programming language, FreshML is under construction geared towards metaprogramming applications. The fertility of such an approach is still to be tested.

On the "logical" side, the Twelf project [30] is built on the idea of devising an explicit (meta-)meta-logic, for reasoning (inductively) about logical frameworks, in a fully automated way. \mathcal{M}_2 is a constructive first-order logic, whose quantifiers range over possibly open LF object over a signature. In the meta-logic it is possible to express and inductively prove meta-logical properties of an object logic. By the adequacy of the encoding, the proof of the existence of the appropriate LF object(s) guarantees the proof of the corresponding object-level property. Twelf is to date the only implementation of a theorem-prover which successfully marries HOAS and induction, as the

fully automated proofs of non-trivial results such as Church-Rosser or cut-elimination testify. In particular, all the results mentioned here are proven in a fully automated way with no infrastructure. Thus, it represents a benchmark for any other system which aims to use HOAS, although it must be remarked that Twelf is explicitly built as a non-interactive system (i.e. not programmable by tactics). $FO\lambda^{\Delta N}$ approach [20] is interactive, and briefly over-viewed in Section 4. While all the derivations mentioned in [20] have been proof-checked via the Pi editor [9], an automated tool, code-named Iris, is under development.

An even more recent development is Honsell et al.'s Ψ framework [17], which explicitly embraces an axiomatic approach to meta-reasoning with HOAS. It consists of classical higher-order logic extended with a set of axioms, called the theory of contexts, parametric to a HOAS signature. Those axioms include the reification of some properties of bound variables such as unsat: $\forall M. \exists x. x \notin M$, which asserts the existence of fresh names. More crucially, higher-order induction and recursion schemata are also assumed, such as the principle of induction on terms of type var ⇒exp. The consistency of such axioms w.r.t. functor categories is left to a forthcoming paper. Two main applications have been investigated so far. One is the development of the formal theory of strong late bisimilarity in the π -calculus [18]. The other [22] is an implementation for the simply-typed λ -calculus which studies the same properties we have considered. In particular, the proof of totality of substitution relies essentially on the axiom of induction on second-order expressions, while the axiom unsat is required in the proof of determinacy of substitution (playing the role of our Var_neq) Further, extensionality axioms are also needed in the binding cases. After that the script follows ours, confirming the crucial interaction of substitution and bound variables.

In [31] the authors present a Weak HOAS formalization of the π -calculus in Isabelle/HOL. Binding operators are represented as functions from names to processes into processes. Because both channels and messages are names, there is no need for object-level substitution. Variables are isomorphic to the natural numbers, hence exotic terms are excluded via well-formedness inductive predicates analogous to our validity predicates, the former also providing the only structural induction principle. The paper shows how Honsell's theory of contexts, namely the principles of monotonicity, extensionality and expansion can be proven, rather than axiomatized, provided there is an inductive characterisation of the set of variables. Nevertheless, the proof of the last property is quite intricate and requires an embedding into a first-order encoding. Due to the limited scope of the paper, the authors do not employ hypothetical judgements, so none of the above mentioned problems with classical logic arise.

6 Conclusions

It is now generally accepted that HOAS is a promising tool in meta-reasoning over syntax with binders. Representing bound variables in expressions as meta-level bound variables makes the statement of theorems far closer to established mathematical practice than in de Bruijn notation, and representing object-level environments as meta-level assumptions can lead to elegant proofs. Unfortunately, there is currently no off-the-shelf system which supports HOAS with all of the features that one would like for the formal verification of languages with variable bindings. Such features include structural induction and primitive recursion; co-induction and co-recursion; interactive proofs combined with powerful automatic provers and re-writers; and various kinds of meta-logics. We

conclude by summarizing the benefits (B) and costs (C) of each of the three methodologies.

The de Bruijn Method

- **B** The encodings are purely definitional.
- **B** The logic can be classical.
- **B** Utilises and is well supported by (co)inductive datatype packages and (co)recursion.
- C Plain de Bruijn notation is unreadable.
- C Proofs do not resemble informal mathematical practice.
- C Any operation requiring variable transposition requires tedious index relabelling via significant book-keeping infrastructure.
- C Mixed de Bruijn is more readable, with a reduction in relabelling infrastructure, but requires coercion functions between free and bound variables which leads to new infrastructure to establish freshness of names.
- C Weakening for the typing judgement needs to be proved explicitly, for example in the case of mixed de Bruijn by the method of Pollack and McKinna. The same would apply to any other judgement involving environments.
- C Infrastructure must be redone on a case-by-case basis for each object level language.

Following the definitional spirit, we have developed a novel hybrid approach to syntax which bridges the gap between the concrete de Bruijn notation and HOAS notation. This introduces a binding operation Abs :: (exp => exp) => exp so that λ -abstractions can be written in the form $Abs(\lambda x \cdot E \cdot x)$. However, the meaning of such expressions is reduced to an underlying de Bruijn representation. The use of HOAS is thus a form of syntactic sugar. An expression can be translated freely back and forth between its sugared version and its underlying representation. We have derived some basic properties of expressions written in this HOAS form, for example, the following induction principle over the structure of expressions is derived.

```
\begin{array}{l} proper\ u\\ \forall n.\ P\ (\text{Var}\ n)\\ \forall s.\ \forall t.\ (P\ s \land P\ t) \rightarrow P\ (\text{App}\ s\ t)\\ \hline \frac{\forall E.\ (abstr\ E \land \forall t.\ proper\ t \rightarrow P\ t \rightarrow P\ (E\ t)) \rightarrow P\ (\text{Abs}\ (\lambda x\,.\, E\ x))}{P\ u}\ expInd \end{array}
```

The predicates *proper* and *abstr* are used to rule out exotic terms and can be seen as analogues of Despeyroux's predicates $valid_0$ and $valid_1$.

The state of this work is not sufficiently advanced to be able to prove all of the results discussed in this paper. This is the focus of ongoing research. However, some results have been proved (e.g. determinacy of evaluation and single step reduction). We intend to give a full account of this idea in a forthcoming paper.

The Weak HOAS Method

- $\, {\bf B} \,$ Utilises the inductive data type package.
- **B** Bound variables handled at the meta-level.
- **B** Provides a limited form of implicit contexts.

- **C** The logic must be intuitionistic.
- C One may have to deal with exotic terms and associated validity predicates.
- C The only infrastructure required concerns object-level substitution—this must be defined as an inductive relation.
- C For some applications, substitution needs to be proven to be a function (Progress lemma), yet a quick proof of totality requires the choice operator, which is problematic (see below), or the postulation of a induction principle on second-order expressions.

Hoffman [16] in fact has shown how the principle of unique choice (AC!) is troublesome w.r.t. HOAS. While this is avoided in a system such as Coq where AC! is not provable and hence second-order induction on expressions can be assumed, the same cannot be said for HOL. The description axiom entails AC!; more generally, classical typed set-theories do not match very well with the much weaker intuitionistic derivability that HOAS requires. This applies also to the issue of implicit management of contexts; to begin with the forced positivization of hypothetical judgements in an inductive framework makes them sometimes ineffective, compared to full HOAS, since the auxiliary new predicates which are introduced in place need to be axiomatized in order to be useful in meta-reasoning. For example, the very concise proof of subject reduction in Full HOAS, which relies on the representation of $\Gamma, x:A \vdash e:B$ with $\forall x : exp. \ of(x,A) \to of(E(x),B)$ can only be awkwardly simulated by the Weak HOAS encoding $\forall x : var.tpv \ x \ A \to (E \ x) ::: B \land tpv_ex$. In this sense, we agree with [20]: "These approaches also lessen the power of the meta-level cut rule as a reasoning tool [...]" Moreover, adequacy of the representation of such a judgement holds only constructively. On the other hand, as pointed out by John Harrison (personal communication), it is certainly possible to realize an intuitionistic version of HOL, which would erase those problems. Alas, such a system is not immediately attainable, since the inductive package is heavily based on classical set-theory.

The Full HOAS Method

- **B** Substitution is captured by meta-level application and beta conversion.
- B Embedded implication can be used to full effect.
- C The logic must be intuitionistic.
- C Induction and case analysis should be moved to an additional meta-level to ensure consistency. A straightforward two-level approach such the one in Section 4 is meta-theoretically uncertain.
- C It is difficult to allow (primitive) recursion on higher-order syntax and especially to combine it with induction over open terms [32].
- C No support for co-induction at this time.

The simulation of Full HOAS in Isabelle's IFOL seems successful. Indeed, the proofs of subject reduction, determinism of operational semantics, and the progress lemma resemble informal mathematical practice very closely. However, much of the hard work has been moved elsewhere, namely to the justification of the inductive principles (of course this is a one-time-only effort).

In summary, the practitioner who wishes to verify significant properties of a language with variable binding using machine assistance is faced with some uncomfortable choices: either rely on trusted but labour-intense first-order technology such as variants of de Bruijn, or adopt an HOAS approach. In this case there is no single framework which is endowed with all the reasoning tools we may require.

The Isabelle code described in this paper can be found at

http://www.mcs.le.ac.uk/~amomigliano/isabelle/compar.html

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