

GENERAL BINDINGS AND ALPHA-EQUIVALENCE IN NOMINAL ISABELLE*

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ABSTRACT. Nominal Isabelle is a definitional extension of the Isabelle/HOL theorem prover. It provides a proving infrastructure for reasoning about programming language calculi involving named bound variables (as opposed to de-Brujin indices). In this paper we present an extension of Nominal Isabelle for dealing with general bindings, that means term-constructors where multiple variables are bound at once. Such general bindings are ubiquitous in programming language research and only very poorly supported with single binders, such as lambda-abstractions. Our extension includes new definitions of alpha-equivalence and establishes automatically the reasoning infrastructure for alpha-equated terms. We also prove strong induction principles that have the usual variable convention already built in.

1. INTRODUCTION

So far, Nominal Isabelle provided a mechanism for constructing alpha-equated terms, for example lambda-terms

$$t ::= x \mid t t \mid \lambda x. t$$

where free and bound variables have names. For such alpha-equated terms, Nominal Isabelle derives automatically a reasoning infrastructure that has been used successfully in formalisations of an equivalence checking algorithm for LF [26], Typed Scheme [24], several calculi for concurrency [3] and a strong normalisation result for cut-elimination in classical logic [29]. It has also been used by Pollack for formalisations in the locally-nameless approach to binding [20].

However, Nominal Isabelle has fared less well in a formalisation of the algorithm W [28], where types and type-schemes are, respectively, of the form

$$T ::= x \mid T \rightarrow T \quad S ::= \forall \{x_1, \dots, x_n\}. T \quad (1.1)$$

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* This is a revised and expanded version of [27].

and the \forall -quantification binds a finite (possibly empty) set of type-variables. While it is possible to implement this kind of more general binders by iterating single binders, this leads to a rather clumsy formalisation of W . The need of iterating single binders is also one reason why Nominal Isabelle and similar theorem provers that only provide mechanisms for binding single variables have not fared extremely well with the more advanced tasks in the POPLmark challenge [2], because also there one would like to bind multiple variables at once.

Binding multiple variables has interesting properties that cannot be captured easily by iterating single binders. For example in the case of type-schemes we do not want to make a distinction about the order of the bound variables. Therefore we would like to regard in (1.2) below the first pair of type-schemes as alpha-equivalent, but assuming that x , y and z are distinct variables, the second pair should *not* be alpha-equivalent:

$$\forall \{x, y\}. x \rightarrow y \approx_{\alpha} \forall \{y, x\}. y \rightarrow x \quad \forall \{x, y\}. x \rightarrow y \not\approx_{\alpha} \forall \{z\}. z \rightarrow z \quad (1.2)$$

Moreover, we like to regard type-schemes as alpha-equivalent, if they differ only on *vacuous* binders, such as

$$\forall \{x\}. x \rightarrow y \approx_{\alpha} \forall \{x, z\}. x \rightarrow y \quad (1.3)$$

where z does not occur freely in the type. In this paper we will give a general binding mechanism and associated notion of alpha-equivalence that can be used to faithfully represent this kind of binding in Nominal Isabelle. The difficulty of finding the right notion for alpha-equivalence can be appreciated in this case by considering that the definition given for type-schemes by Leroy in [13, Page 18–19] is incorrect (it omits a side-condition).

However, the notion of alpha-equivalence that is preserved by vacuous binders is not always wanted. For example in terms like

$$\text{let } x = 3 \text{ and } y = 2 \text{ in } x - y \text{ end} \quad (1.4)$$

we might not care in which order the assignments $x = 3$ and $y = 2$ are given, but it would be often unusual (particularly in strict languages) to regard (1.4) as alpha-equivalent with

$$\text{let } x = 3 \text{ and } y = 2 \text{ and } z = \text{foo} \text{ in } x - y \text{ end}$$

Therefore we will also provide a separate binding mechanism for cases in which the order of binders does not matter, but the ‘cardinality’ of the binders has to agree.

However, we found that this is still not sufficient for dealing with language constructs frequently occurring in programming language research. For example in lets containing patterns like

$$\text{let } (x, y) = (3, 2) \text{ in } x - y \text{ end} \quad (1.5)$$

we want to bind all variables from the pattern inside the body of the `let`, but we also care about the order of these variables, since we do not want to regard (1.5) as alpha-equivalent with

$$\text{let } (y, x) = (3, 2) \text{ in } x - y \text{ end}$$

As a result, we provide three general binding mechanisms each of which binds multiple variables at once, and let the user chose which one is intended when formalising a term-calculus.

By providing these general binding mechanisms, however, we have to work around a problem that has been pointed out by Pottier [19] and Cheney [7]: in `let`-constructs of the form

$$\text{let } x_1 = t_1 \text{ and } \dots \text{ and } x_n = t_n \text{ in } s \text{ end}$$

we care about the information that there are as many bound variables x_i as there are t_i . We lose this information if we represent the `let`-constructor by something like

$$\text{let } (\lambda x_1 \dots x_n . s) [t_1, \dots, t_n]$$

where the notation $\lambda _ . _$ indicates that the list of x_i becomes bound in s . In this representation the term `let` $(\lambda x . s) [t_1, t_2]$ is a perfectly legal instance, but the lengths of the two lists do not agree. To exclude such terms, additional predicates about well-formed terms are needed in order to ensure that the two lists are of equal length. This can result in very messy reasoning (see for example [3]). To avoid this, we will allow type specifications for lets as follows

$$\begin{aligned} \text{trm} &::= \dots \\ &| \text{let } \text{as}::\text{assn } s::\text{trm} \text{ binds } \text{bn}(\text{as}) \text{ in } s \\ \text{assn} &::= \text{anil} \\ &| \text{acons } \text{name } \text{trm } \text{assn} \end{aligned}$$

where *assn* is an auxiliary type representing a list of assignments and *bn* an auxiliary function identifying the variables to be bound by the `let`. This function can be defined by recursion over *assn* as follows

$$\text{bn}(\text{anil}) = \emptyset \quad \text{bn}(\text{acons } x \ t \ \text{as}) = \{x\} \cup \text{bn}(\text{as})$$

The scope of the binding is indicated by labels given to the types, for example $s::\text{trm}$, and a binding clause, in this case **binds** $\text{bn}(\text{as})$ **in** s . This binding clause states that all the names the function $\text{bn}(\text{as})$ returns should be bound in s . This style of specifying terms and bindings is heavily inspired by the syntax of the Ott-tool [22]. Our work extends Ott in several aspects: one is that we support three binding modes—Ott has only one, namely the one where the order of binders matters. Another is that our reasoning infrastructure, like strong induction principles and the notion of free variables, is derived from first principles within the Isabelle/HOL theorem prover.

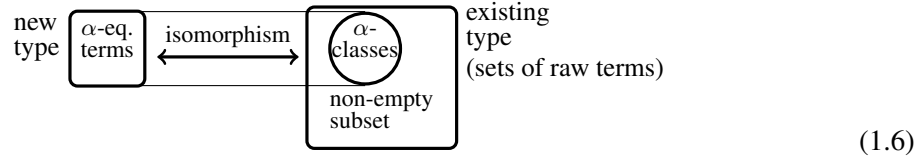
However, we will not be able to cope with all specifications that are allowed by Ott. One reason is that Ott lets the user specify ‘empty’ types like $t ::= t \mid \lambda x. t$ where no clause for variables is given. Arguably, such specifications make some sense in the context of Coq’s type theory (which Ott supports), but not at all in a HOL-based environment where every datatype must have a non-empty set-theoretic model [4]. Another reason is that we establish the reasoning infrastructure for alpha-equated terms. In contrast, Ott produces a reasoning infrastructure in Isabelle/HOL for non-alpha-equated, or ‘raw’, terms. While our alpha-equated terms and the ‘raw’ terms produced by Ott use names for bound variables, there is a key difference: working with alpha-equated terms means, for example, that the two type-schemes

$$\forall \{x\}. x \rightarrow y = \forall \{x, z\}. x \rightarrow y$$

are not just alpha-equal, but actually *equal*! As a result, we can only support specifications that make sense on the level of alpha-equated terms (offending specifications, which for example bind a variable according to a variable bound somewhere else, are not excluded by Ott, but we have to).

Our insistence on reasoning with alpha-equated terms comes from the wealth of experience we gained with the older version of Nominal Isabelle: for non-trivial properties, reasoning with alpha-equated terms is much easier than reasoning with ‘raw’ terms. The fundamental reason for this is that the HOL-logic underlying Nominal Isabelle allows us to replace ‘equals-by-equals’. In contrast, replacing ‘alpha-equals-by-alpha-equals’ in a representation based on ‘raw’ terms requires a lot of extra reasoning work.

Although in informal settings a reasoning infrastructure for alpha-equated terms is nearly always taken for granted, establishing it automatically in Isabelle/HOL is a rather non-trivial task. For every specification we will need to construct type(s) containing as elements the alpha-equated terms. To do so, we use the standard HOL-technique of defining a new type by identifying a non-empty subset of an existing type. The construction we perform in Isabelle/HOL can be illustrated by the following picture:



We take as the starting point a definition of raw terms (defined as a datatype in Isabelle/HOL); then identify the alpha-equivalence classes in the type of sets of raw terms according to our alpha-equivalence relation, and finally define the new type as these alpha-equivalence classes (the non-emptiness requirement is always satisfied whenever the raw terms are definable as datatype in Isabelle/HOL and our relation for alpha-equivalence is an equivalence relation).

The fact that we obtain an isomorphism between the new type and the non-empty subset shows that the new type is a faithful representation of alpha-equated terms. That is not the case for example for terms using the locally nameless representation of binders [14]: in this representation there are ‘junk’ terms that need to be excluded by reasoning about a well-formedness predicate.

The problem with introducing a new type in Isabelle/HOL is that in order to be useful, a reasoning infrastructure needs to be ‘lifted’ from the underlying subset to the new type. This is usually a tricky and arduous task. To ease it, we re-implemented in Isabelle/HOL [10] the quotient package described by Homeier [8] for the HOL4 system. This package allows us to lift definitions and theorems involving raw terms to definitions and theorems involving alpha-equated terms. For example if we define the free-variable function over raw lambda-terms as follows

$$\begin{aligned} fv(x) &\stackrel{def}{=} \{x\} \\ fv(t_1 t_2) &\stackrel{def}{=} fv(t_1) \cup fv(t_2) \\ fv(\lambda x.t) &\stackrel{def}{=} fv(t) - \{x\} \end{aligned}$$

then with the help of the quotient package we can obtain a function fv^α operating on quotients, that is alpha-equivalence classes of lambda-terms. This lifted function is characterised by the equations

$$\begin{aligned}
fv^\alpha(x) &= \{x\} \\
fv^\alpha(t_1 t_2) &= fv^\alpha(t_1) \cup fv^\alpha(t_2) \\
fv^\alpha(\lambda x.t) &= fv^\alpha(t) - \{x\}
\end{aligned}$$

(Note that this means also the term-constructors for variables, applications and lambda are lifted to the quotient level.) This construction, of course, only works if alpha-equivalence is indeed an equivalence relation, and the ‘raw’ definitions and theorems are respectful w.r.t. alpha-equivalence. For example, we will not be able to lift a bound-variable function. Although this function can be defined for raw terms, it does not respect alpha-equivalence and therefore cannot be lifted. To sum up, every lifting of theorems to the quotient level needs proofs of some respectfulness properties (see [8]). In the paper we show that we are able to automate these proofs and as a result can automatically establish a reasoning infrastructure for alpha-equated terms.

The examples we have in mind where our reasoning infrastructure will be helpful include the term language of Core-Haskell (see Figure 1). This term language involves patterns that have lists of type-, coercion- and term-variables, all of which are bound in case-expressions. In these patterns we do not know in advance how many variables need to be bound. Another example is the algorithm W, which includes multiple binders in type-schemes.

Contributions: We provide three new definitions for when terms involving general binders are alpha-equivalent. These definitions are inspired by earlier work of Pitts [17]. By means of automatic proofs, we establish a reasoning infrastructure for alpha-equated terms, including properties about support, freshness and equality conditions for alpha-equated terms. We are also able to automatically derive strong induction principles that have the variable convention already built in. For this we simplify the earlier automated proofs by using the proving tools from the function package [11] of Isabelle/HOL. The method behind our specification of general binders is taken from the Ott-tool, but we introduce crucial restrictions, and also extensions, so that our specifications make sense for reasoning about alpha-equated terms. The main improvement over Ott is that we introduce three binding modes (only one is present in Ott), provide formalised definitions for alpha-equivalence and for free variables of our terms, and also derive a reasoning infrastructure for our specifications from ‘first principles’ inside a theorem prover.

2. A SHORT REVIEW OF THE NOMINAL LOGIC WORK

At its core, Nominal Isabelle is an adaption of the nominal logic work by Pitts [18]. This adaptation for Isabelle/HOL is described in [9] (including proofs). We shall briefly review this work to aid the description of what follows.

Two central notions in the nominal logic work are sorted atoms and sort-respecting permutations of atoms. We will use the letters a, b, c, \dots to stand for atoms and π, π_1, \dots to stand for permutations, which in Nominal Isabelle have type *perm*. The purpose of atoms is to represent variables, be they bound or free. The sorts of atoms can be used to represent different kinds of variables, such as the term-, coercion- and type-variables in Core-Haskell. It is assumed that there is an infinite supply of atoms for each sort. In the interest of brevity, we shall restrict ourselves in what follows to only one sort of atoms.

Permutations are bijective functions from atoms to atoms that are the identity everywhere except on a finite number of atoms. There is a two-place permutation operation written $_ \bullet _ :: perm \Rightarrow \beta \Rightarrow \beta$ where the generic type β is the type of the object over which the permutation acts. In Nominal Isabelle, the identity permutation is written as θ , the composition of two permutations π_1

Type Kinds	$\kappa ::= \star \mid \kappa_1 \rightarrow \kappa_2$
Coercion Kinds	$\iota ::= \sigma_1 \sim \sigma_2$
Types	$\sigma ::= a \mid T \mid \sigma_1 \sigma_2 \mid S_n \bar{\sigma}^n \mid \forall a:\kappa. \sigma \mid \iota \Rightarrow \sigma$
Coercion Types	$\gamma ::= c \mid C \mid \gamma_1 \gamma_2 \mid S_n \bar{\gamma}^n \mid \forall c:\iota. \gamma \mid \iota \Rightarrow \gamma \mid \text{refl } \sigma \mid \text{sym } \gamma \mid \gamma_1 \circ \gamma_2$ $\mid \gamma @ \sigma \mid \text{left } \gamma \mid \text{right } \gamma \mid \gamma_1 \sim \gamma_2 \mid \text{rightc } \gamma \mid \text{leftc } \gamma \mid \gamma_1 \triangleright \gamma_2$
Terms	$e ::= x \mid K \mid \Lambda a:\kappa. e \mid \Lambda c:\iota. e \mid e \sigma \mid e \gamma \mid \lambda x:\sigma. e \mid e_1 e_2$ $\mid \text{let } x:\sigma = e_1 \text{ in } e_2 \mid \text{case } e_1 \text{ of } \bar{p} \rightarrow \bar{e}_2 \mid e \triangleright \gamma$
Patterns	$p ::= K \bar{a}:\bar{\kappa} \bar{c}:\bar{\iota} \bar{x}:\bar{\sigma}$
Constants	C coercion constants T value type constructors S_n n-ary type functions (which need to be fully applied) K data constructors
Variables	a type variables c coercion variables x term variables

Figure 1: The System F_C [23], also often referred to as *Core-Haskell*. In this version of F_C we made a modification by separating the grammars for type kinds and coercion kinds, as well as for types and coercion types. For this paper the interesting term-constructor is `case`, which binds multiple type-, coercion- and term-variables (the overlines stand for lists).

and π_2 as $\pi_1 + \pi_2$, and the inverse permutation of π as $-\pi$. The permutation operation is defined over Isabelle/HOL's type-hierarchy [9]; for example permutations acting on atoms, products, lists, permutations, sets, functions and booleans are given by:

$$\begin{aligned}
\pi \cdot a &\stackrel{\text{def}}{=} \pi a & \pi \cdot \pi' &\stackrel{\text{def}}{=} \pi + \pi' - \pi \\
\pi \cdot (x, y) &\stackrel{\text{def}}{=} (\pi \cdot x, \pi \cdot y) & \pi \cdot X &\stackrel{\text{def}}{=} \{\pi \cdot x \mid x \in X\} \\
\pi \cdot [] &\stackrel{\text{def}}{=} [] & \pi \cdot f &\stackrel{\text{def}}{=} \lambda x. \pi \cdot (f (-\pi \cdot x)) \\
\pi \cdot (x::xs) &\stackrel{\text{def}}{=} (\pi \cdot x)::(\pi \cdot xs) & \pi \cdot b &\stackrel{\text{def}}{=} b
\end{aligned} \tag{2.1}$$

Concrete permutations in Nominal Isabelle are built up from swappings, written as $(a b)$, which are permutations that behave as follows:

$$(a b) = \lambda c. \text{if } a = c \text{ then } b \text{ else if } b = c \text{ then } a \text{ else } c$$

The most original aspect of the nominal logic work of Pitts is a general definition for the notion of the ‘set of free variables of an object x ’. This notion, written $\text{supp } x$, is general in the sense that it applies not only to lambda-terms (alpha-equated or not), but also to lists, products, sets and even functions. Its definition depends only on the permutation operation and on the notion of equality defined for the type of x , namely:

$$\text{supp } x \stackrel{\text{def}}{=} \{a \mid \text{infinite } \{b \mid (a \ b) \cdot x \neq x\}\} \quad (2.2)$$

There is also the derived notion for when an atom a is *fresh* for an x , defined as

$$a \# x \stackrel{\text{def}}{=} a \notin \text{supp } x$$

We use for sets of atoms the abbreviation $as \#^* x$, defined as $\forall a \in as. a \# x$. A striking consequence of these definitions is that we can prove without knowing anything about the structure of x that swapping two fresh atoms, say a and b , leaves x unchanged, namely

Proposition 2.1. *If $a \# x$ and $b \# x$ then $(a \ b) \cdot x = x$.*

While often the support of an object can be relatively easily described, for example for atoms, products, lists, function applications, booleans and permutations as follows

$$\begin{array}{ll} \text{supp } a & = \{a\} \\ \text{supp } (x, y) & = \text{supp } x \cup \text{supp } y \\ \text{supp } [] & = \emptyset \\ \text{supp } (x::xs) & = \text{supp } x \cup \text{supp } xs \end{array} \quad \begin{array}{ll} \text{supp } (fx) & \subseteq \text{supp } f \cup \text{supp } x \\ \text{supp } b & = \emptyset \\ \text{supp } \pi & = \{a \mid \pi \cdot a \neq a\} \end{array} \quad (2.3)$$

in some cases it can be difficult to characterise the support precisely, and only an approximation can be established (as for function applications above). Reasoning about such approximations can be simplified with the notion *supports*, defined as follows:

Definition 2.2. A set S *supports* x , if for all atoms a and b not in S we have $(a \ b) \cdot x = x$.

The main point of *supports* is that we can establish the following two properties.

Proposition 2.3. *Given a set as of atoms.*

(i) *If as supports x and finite as then $\text{supp } x \subseteq as$.*

(ii) *$(\text{supp } x)$ supports x .*

Another important notion in the nominal logic work is *equivariance*. For a function f , say of type $\alpha \Rightarrow \beta$, to be equivariant it is required that every permutation leaves f unchanged, that is

$$\forall \pi. \pi \cdot f = f \quad (2.4)$$

or equivalently that a permutation applied to the application $f x$ can be moved to the argument x . That means for equivariant functions f , we have for all permutations π :

$$\pi \cdot f = f \quad \text{if and only if} \quad \forall x. \pi \cdot (fx) = f (\pi \cdot x) \quad (2.5)$$

From property (2.4) and the definition of *supp*, we can easily deduce that equivariant functions have empty support. There is also a similar notion for equivariant relations, say R , namely the property that

$$x R y \text{ implies } (\pi \cdot x) R (\pi \cdot y)$$

Using freshness, the nominal logic work provides us with general means for renaming binders. While in the older version of Nominal Isabelle, we used extensively Property 2.1 to rename single binders, this property proved too unwieldy for dealing with multiple binders. For such binders the following generalisations turned out to be easier to use.

Proposition 2.4. *If $\text{supp } x \#^* \pi$ then $\pi \cdot x = x$.*

Proposition 2.5. *For a finite set as and a finitely supported x with $as \#^* x$ and also a finitely supported c , there exists a permutation π such that $\pi \cdot as \#^* c$ and $\text{supp } x \#^* \pi$.*

The idea behind the second property is that given a finite set as of binders (being bound, or fresh, in x is ensured by the assumption $as \#^* x$), then there exists a permutation π such that the renamed binders $\pi \cdot as$ avoid c (which can be arbitrarily chosen as long as it is finitely supported) and also π does not affect anything in the support of x (that is $\text{supp } x \#^* \pi$). The last fact and Property 2.4 allow us to ‘rename’ just the binders as in x , because $\pi \cdot x = x$.

Note that $\text{supp } x \#^* \pi$ is equivalent with $\text{supp } \pi \#^* x$, which means we could also formulate Propositions 2.4 and 2.5 in the other ‘direction’; however the reasoning infrastructure of Nominal Isabelle is set up so that it provides more automation for the formulation given above.

Most properties given in this section are described in detail in [9] and all are formalised in Isabelle/HOL. In the next sections we will make use of these properties in order to define alpha-equivalence in the presence of multiple binders.

3. ABSTRACTIONS

In Nominal Isabelle, the user is expected to write down a specification of a term-calculus and then a reasoning infrastructure is automatically derived from this specification (remember that Nominal Isabelle is a definitional extension of Isabelle/HOL, which does not introduce any new axioms).

In order to keep our work with deriving the reasoning infrastructure manageable, we will wherever possible state definitions and perform proofs on the ‘user-level’ of Isabelle/HOL, as opposed to writing custom ML-code that generates them anew for each specification. To that end, we will consider first pairs (as, x) of type $(atom\ set) \times \beta$. These pairs are intended to represent the abstraction, or binding, of the set of atoms as in the body x .

The first question we have to answer is when two pairs (as, x) and (bs, y) are alpha-equivalent? (For the moment we are interested in the notion of alpha-equivalence that is *not* preserved by adding vacuous binders.) To answer this question, we identify four conditions: (i) given a free-atom function fa of type $\beta \Rightarrow atom\ set$, then x and y need to have the same set of free atoms; moreover there must be a permutation π such that (ii) π leaves the free atoms of x and y unchanged, but (iii) ‘moves’ their bound names so that we obtain modulo a relation, say $_ R _$, two equivalent terms. We also require that (iv) π makes the sets of abstracted atoms as and bs equal. The requirements (i) to (iv) can be stated formally as:

Definition 3.1 (Alpha-Equivalence for Set-Bindings).

$$(as, x) \approx_{set}^{R, fa} (bs, y) \stackrel{def}{=} \text{if there exists a } \pi \text{ such that:}$$

- (i) $fa\ x - as = fa\ y - bs$
- (ii) $fa\ x - as \#^* \pi$
- (iii) $(\pi \cdot x)\ R\ y$
- (iv) $\pi \cdot as = bs$

Note that the relation is dependent on a free-atom function fa and a relation R . The reason for this extra generality is that we will use $\approx_{set}^{R, fa}$ for both raw terms and alpha-equated terms. In the latter case, R will be replaced by equality $=$ and we will prove that fa is equal to $supp$.

Definition 3.1 does not make any distinction between the order of abstracted atoms. If we want this, then we can define alpha-equivalence for pairs of the form (as, x) with type $(atom\ list) \times \beta$ as follows

Definition 3.2 (Alpha-Equivalence for List-Bindings).

$$(as, x) \approx_{list}^{R, fa} (bs, y) \stackrel{def}{=} \text{if there exists a } \pi \text{ such that:}$$

- (i) $fa\ x - set\ as = fa\ y - set\ bs$
- (ii) $fa\ x - set\ as \#^* \pi$
- (iii) $(\pi \cdot x)\ R\ y$
- (iv) $\pi \cdot as = bs$

where set is the function that coerces a list of atoms into a set of atoms. Now the last clause ensures that the order of the binders matters (since as and bs are lists of atoms).

If we do not want to make any difference between the order of binders *and* also allow vacuous binders, that means according to Pitts [17] *restrict* atoms, then we keep sets of binders, but drop condition (iv) in Definition 3.1:

Definition 3.3 (Alpha-Equivalence for Set+-Bindings).

$$(as, x) \approx_{set+}^{R, fa} (bs, y) \stackrel{def}{=} \text{if there exists a } \pi \text{ such that:}$$

- (i) $fa\ x - as = fa\ y - bs$
- (ii) $fa\ x - as \#^* \pi$
- (iii) $(\pi \cdot x)\ R\ y$

It might be useful to consider first some examples how these definitions of alpha-equivalence pan out in practice. For this consider the case of abstracting a set of atoms over types (as in type-schemes). We set R to be the usual equality $=$ and for $fa(T)$ we define

$$fa(x) \stackrel{def}{=} \{x\} \quad fa(T_1 \rightarrow T_2) \stackrel{def}{=} fa(T_1) \cup fa(T_2)$$

Now recall the examples shown in (1.2) and (1.3). It can be easily checked that $(\{x, y\}, x \rightarrow y)$ and $(\{y, x\}, y \rightarrow x)$ are alpha-equivalent according to \approx_{set} and \approx_{set+} by taking π to be the swapping $(x\ y)$. In case of $x \neq y$, then $([x, y], x \rightarrow y) \not\approx_{list} ([y, x], x \rightarrow y)$ since there is no permutation that makes the lists $[x, y]$ and $[y, x]$ equal, and also leaves the type $x \rightarrow y$ unchanged. Another example is $(\{x\}, x) \approx_{set+} (\{x, y\}, x)$ which holds by taking π to be the identity permutation. However, if $x \neq y$, then $(\{x\}, x) \not\approx_{set} (\{x, y\}, x)$ since there is no permutation that makes the sets $\{x\}$ and $\{x, y\}$ equal (similarly for \approx_{list}). It can also relatively easily be shown that all three notions of alpha-equivalence coincide, if we only abstract a single atom. In this case they also agree with the alpha-equivalence used in older versions of Nominal Isabelle [25].¹

¹We omit a proof of this fact since the details are hairy and not really important for the purpose of this paper.

In the rest of this section we are going to show that the alpha-equivalences really lead to abstractions where some atoms are bound (or more precisely removed from the support). For this we will consider three abstraction types that are quotients of the relations

$$\begin{aligned} (as, x) &\approx_{\overline{set}}^{\text{supp}} (bs, y) \\ (as, x) &\approx_{\overline{set+}}^{\text{supp}} (bs, y) \\ (as, x) &\approx_{\overline{list}}^{\text{supp}} (bs, y) \end{aligned} \quad (3.1)$$

Note that in these relation we replaced the free-atom function fa with $supp$ and the relation R with equality. We can show the following two properties:

Lemma 3.4. *The relations $\approx_{\overline{set}}^{\text{supp}}$, $\approx_{\overline{set+}}^{\text{supp}}$ and $\approx_{\overline{list}}^{\text{supp}}$ are equivalence relations and equivariant.*

Proof. Reflexivity is by taking π to be 0 . For symmetry we have a permutation π and for the proof obligation take $-\pi$. In case of transitivity, we have two permutations π_1 and π_2 , and for the proof obligation use $\pi_1 + \pi_2$. Equivariance means $(\pi \cdot as, \pi \cdot x) \approx_{\overline{set}}^{\text{supp}} (\pi \cdot bs, \pi \cdot y)$ holds provided $(as, x) \approx_{\overline{set}}^{\text{supp}} (bs, y)$ holds. From the assumption we have a permutation π' and for the proof obligation use $\pi \cdot \pi'$. To show equivariance, we need to ‘pull out’ the permutations, which is possible since all operators, namely $\#^*$, $-$, $=$, \cdot , set and $supp$, are equivariant (see [9]). Finally, we apply the permutation operation on booleans. \square

Recall the picture shown in (1.6) about new types in HOL. The lemma above allows us to use our quotient package for introducing new types $\beta \text{ abs}_{set}$, $\beta \text{ abs}_{set+}$ and $\beta \text{ abs}_{list}$ representing alpha-equivalence classes of pairs of type $(atom \ set) \times \beta$ (in the first two cases) and of type $(atom \ list) \times \beta$ (in the third case). The elements in these types will be, respectively, written as

$$[as]_{set.x} \quad [as]_{set+.x} \quad [as]_{list.x}$$

indicating that a set (or list) of atoms as is abstracted in x . We will call the types *abstraction types* and their elements *abstractions*. The important property we need to derive is the support of abstractions, namely:

Theorem 3.5 (Support of Abstractions). *Assuming x has finite support, then*

$$\begin{aligned} \text{supp } [as]_{set.x} &= \text{supp } x - as \\ \text{supp } [as]_{set+.x} &= \text{supp } x - as \\ \text{supp } [as]_{list.x} &= \text{supp } x - set \ as \end{aligned}$$

In effect, this theorem states that the atoms as are bound in the abstraction. As stated earlier, this can be seen as a litmus test that our Definitions 3.1, 3.2 and 3.3 capture the idea of alpha-equivalence relations. Below we will give the proof for the first equation of Theorem 3.5. The others follow by similar arguments. By definition of the abstraction type abs_{set} we have

$$[as]_{set.x} = [bs]_{set.y} \quad \text{if and only if} \quad (as, x) \approx_{\overline{set}}^{\text{supp}} (bs, y) \quad (3.2)$$

and also

$$\pi \cdot [as]_{set.x} = [\pi \cdot as]_{set.(\pi \cdot x)} \quad (3.3)$$

The second fact derives from the definition of permutations acting on pairs (2.1) and alpha-equivalence being equivariant (see Lemma 3.4). With these two facts at our disposal, we can show the following lemma about swapping two atoms in an abstraction.

Lemma 3.6. *If $a \notin \text{supp } x - as$ and $b \notin \text{supp } x - as$ then $[as]_{\text{set}.x} = [(a\ b) \cdot as]_{\text{set}.((a\ b) \cdot x)}$*

Proof. If $a = b$ the lemma is immediate, since $(a\ b)$ is then the identity permutation. Also in the other case the lemma is straightforward using (3.2) and observing that the assumptions give us $(a\ b) \cdot (\text{supp } x - as) = \text{supp } x - as$. We therefore can use the swapping $(a\ b)$ as the permutation for the proof obligation. \square

Assuming that x has finite support, this lemma together with (3.3) allows us to show

$$(\text{supp } x - as) \text{ supports } [as]_{\text{set}.x} \quad (3.4)$$

which by Property 2.3 gives us ‘one half’ of Theorem 3.5. The ‘other half’ is a bit more involved. To establish it, we use a trick from [17] and first define an auxiliary function aux , taking an abstraction as argument

$$aux ([as]_{\text{set}.x}) \stackrel{\text{def}}{=} \text{supp } x - as$$

Using the second equation in (2.5), we can show that aux is equivariant (since $\pi \cdot (\text{supp } x - as) = \text{supp } (\pi \cdot x) - \pi \cdot as$) and therefore has empty support. This in turn means

$$\text{supp } (aux ([as]_{\text{set}.x})) \subseteq \text{supp } [as]_{\text{set}.x}$$

using the fact about the support of function applications in (2.3). Assuming $\text{supp } x - as$ is a finite set, we further obtain

$$\text{supp } x - as \subseteq \text{supp } [as]_{\text{set}.x} \quad (3.5)$$

This is because for every finite set of atoms, say bs , we have $\text{supp } bs = bs$. Finally, taking (3.4) and (3.5) together establishes the first equation of Theorem 3.5. The others are similar.

Recall the definition of support given in (2.2), and note the difference between the support of a raw pair and an abstraction

$$\text{supp } (as, x) = \text{supp } as \cup \text{supp } x \quad \text{supp } [as]_{\text{set}.x} = \text{supp } x - as$$

While the permutation operations behave in both cases the same (a permutation is just moved to the arguments), the notion of equality is different for pairs and abstractions. Therefore we have different supports. In case of abstractions, we have established in Theorem 3.5 that bound atoms are removed from the support of the abstractions’ bodies.

The method of first considering abstractions of the form $[as]_{\text{set}.x}$ etc is motivated by the fact that we can conveniently establish at the Isabelle/HOL level properties about them. It would be extremely laborious to write custom ML-code that derives automatically such properties for every term-constructor that binds some atoms. Also the generality of the definitions for alpha-equivalence will help us in the next sections.

4. SPECIFYING GENERAL BINDINGS

Our choice of syntax for specifications is influenced by the existing datatype package of Isabelle/HOL [4] and by the syntax of the Ott-tool [22]. For us a specification of a term-calculus is a collection of (possibly mutual recursive) type declarations, say $ty_1^\alpha, \dots, ty_n^\alpha$, and an associated collection of binding functions, say $bn_1^\alpha, \dots, bn_m^\alpha$. The syntax in Nominal Isabelle for such specifications is schematically as follows:

$$\begin{array}{l}
 \text{type} \\
 \text{declaration part} \\
 \\
 \text{binding} \\
 \text{function part}
 \end{array}
 \left\{ \begin{array}{l}
 \mathbf{nominal_datatype} \ ty_1^\alpha = \dots \\
 \mathbf{and} \ ty_2^\alpha = \dots \\
 \dots \\
 \mathbf{and} \ ty_n^\alpha = \dots \\
 \\
 \mathbf{binder} \ bn_1^\alpha \mathbf{and} \dots \mathbf{and} \ bn_m^\alpha \\
 \mathbf{where} \\
 \dots
 \end{array} \right. \quad (4.1)$$

Every type declaration $ty_{1..n}^\alpha$ consists of a collection of term-constructors, each of which comes with a list of labelled types that stand for the types of the arguments of the term-constructor. For example a term-constructor C^α might be specified with

$$C^\alpha \ label_1::ty'_1 \dots label_l::ty'_l \quad \text{binding_clauses}$$

whereby some of the $ty'_{1..l}$ (or their components) can be contained in the collection of $ty_{1..n}^\alpha$ declared in (4.1). In this case we will call the corresponding argument a *recursive argument* of C^α . The types of such recursive arguments need to satisfy a ‘positivity’ restriction, which ensures that the type has a set-theoretic semantics (see [4]). The labels annotated on the types are optional. Their purpose is to be used in the (possibly empty) list of *binding clauses*, which indicate the binders and their scope in a term-constructor. They come in three *modes*:

binds *binders in bodies*
binds (set) *binders in bodies*
binds (set+) *binders in bodies*

The first mode is for binding lists of atoms (the order of bound atoms matters); the second is for sets of binders (the order does not matter, but the cardinality does) and the last is for sets of binders (with vacuous binders preserving alpha-equivalence). As indicated, the labels in the ‘**in**-part’ of a binding clause will be called *bodies*; the ‘**binds**-part’ will be called *binders*. In contrast to Ott, we allow multiple labels in binders and bodies. For example we allow binding clauses of the form:

$$\begin{array}{l}
 Foo_1 \ x::name \ y::name \ t::trm \ s::trm \quad \mathbf{binds} \ x \ y \ \mathbf{in} \ t \ s \\
 Foo_2 \ x::name \ y::name \ t::trm \ s::trm \quad \mathbf{binds} \ x \ y \ \mathbf{in} \ t, \ \mathbf{binds} \ x \ y \ \mathbf{in} \ s
 \end{array}$$

Similarly for the other binding modes. Interestingly, in case of **binds (set)** and **binds (set+)** the binding clauses above will make a difference to the semantics of the specifications (the corresponding alpha-equivalence will differ). We will show this later with an example.

There are also some restrictions we need to impose on our binding clauses in comparison to Ott. The main idea behind these restrictions is that we obtain a notion of alpha-equivalence where it is ensured that within a given scope an atom occurrence cannot be both bound and free at the same

time. The first restriction is that a body can only occur in *one* binding clause of a term constructor. So for example

$$\text{Foo } x::\text{name } y::\text{name } t::\text{trm } \mathbf{binds } x \text{ in } t, \mathbf{binds } y \text{ in } t$$

is not allowed. This ensures that the bound atoms of a body cannot be free at the same time by specifying an alternative binder for the same body.

For binders we distinguish between *shallow* and *deep* binders. Shallow binders are just labels. The restriction we need to impose on them is that in case of **binds (set)** and **binds (set+)** the labels must either refer to atom types or to sets of atom types; in case of **binds** the labels must refer to atom types or to lists of atom types. Two examples for the use of shallow binders are the specification of lambda-terms, where a single name is bound, and type-schemes, where a finite set of names is bound:

<p>nominal_datatype <i>lam</i> =</p> <ul style="list-style-type: none"> <i>Var name</i> <i>App lam lam</i> <i>Lam x::name t::lam binds x in t</i> 	<p>nominal_datatype <i>ty</i> =</p> <ul style="list-style-type: none"> <i>TVar name</i> <i>TFun ty ty</i> and <i>tsc</i> = <i>TAll xs::(name fset) T::ty binds (set+) xs in T</i>
---	---

In these specifications *name* refers to a (concrete) atom type, and *fset* to the type of finite sets. Note that for *Lam* it does not matter which binding mode we use. The reason is that we bind only a single *name*, in which case all three binding modes coincide. However, having **binds (set)** or just **binds** in the second case makes a difference to the semantics of the specification (which we will define in the next section).

A *deep* binder uses an auxiliary binding function that ‘picks’ out the atoms in one argument of the term-constructor, which can be bound in other arguments and also in the same argument (we will call such binders *recursive*, see below). The binding functions are expected to return either a set of atoms (for **binds (set)** and **binds (set+)**) or a list of atoms (for **binds**). They need to be defined by recursion over the corresponding type; the equations must be given in the binding function part of the scheme shown in (4.1). For example a term-calculus containing *Lets* with tuple patterns may be specified as:

$$\begin{aligned}
 &\mathbf{nominal_datatype} \text{ } trm = \\
 &\quad Var \text{ } name \\
 &\quad | \text{ } App \text{ } trm \text{ } trm \\
 &\quad | \text{ } Lam \text{ } x::name \text{ } t::trm \quad \mathbf{binds } x \text{ in } t \\
 &\quad | \text{ } Let_pat \text{ } p::pat \text{ } trm \text{ } t::trm \quad \mathbf{binds } bn(p) \text{ in } t \\
 &\mathbf{and} \text{ } pat = \\
 &\quad PVar \text{ } name \\
 &\quad | \text{ } PTup \text{ } pat \text{ } pat \\
 &\mathbf{binder} \text{ } bn::pat \Rightarrow atom \text{ } list \\
 &\mathbf{where} \text{ } bn(PVar \text{ } x) = [atom \text{ } x] \\
 &\quad | \text{ } bn(PTup \text{ } p_1 \text{ } p_2) = bn(p_1) @ bn(p_2)
 \end{aligned} \tag{4.2}$$

In this specification the function *bn* determines which atoms of the pattern *p* (fifth line) are bound in the argument *t*. Note that in the second-last *bn*-clause the function *atom* coerces a name into the

generic atom type of Nominal Isabelle [9]. This allows us to treat binders of different atom type uniformly.

For deep binders we allow binding clauses such as

$$\text{Bar } p::\text{pat } t::\text{trm} \quad \mathbf{binds } bn(p) \mathbf{ in } p \ t$$

where the argument of the deep binder also occurs in the body. We call such binders *recursive*. To see the purpose of such recursive binders, compare ‘plain’ *Lets* and *Let_recs* in the following specification:

$$\begin{aligned} & \mathbf{nominal_datatype } trm = \dots \\ & \quad | \text{Let } as::\text{assn } t::\text{trm} \quad \mathbf{binds } bn(as) \mathbf{ in } t \\ & \quad | \text{Let_rec } as::\text{assn } t::\text{trm} \quad \mathbf{binds } bn(as) \mathbf{ in } as \ t \\ & \mathbf{and } assn = \\ & \quad \text{ANil} \\ & \quad | \text{ACons } name \ trm \ assn \\ & \mathbf{binder } bn::\text{assn} \Rightarrow \text{atom list} \\ & \mathbf{where } bn(\text{ANil}) = [] \\ & \quad | bn(\text{ACons } a \ t \ as) = [\text{atom } a] @ bn(as) \end{aligned} \tag{4.3}$$

The difference is that with *Let* we only want to bind the atoms $bn(as)$ in the term t , but with *Let_rec* we also want to bind the atoms inside the assignment. This difference has consequences for the associated notions of free-atoms and alpha-equivalence.

To make sure that atoms bound by deep binders cannot be free at the same time, we cannot have more than one binding function for a deep binder. Consequently we exclude specifications such as

$$\begin{aligned} & \text{Baz}_1 \ p::\text{pat } t::\text{trm} \quad \mathbf{binds } bn_1(p) \ bn_2(p) \mathbf{ in } t \\ & \text{Baz}_2 \ p::\text{pat } t_1::\text{trm } t_2::\text{trm} \quad \mathbf{binds } bn_1(p) \mathbf{ in } t_1, \mathbf{ binds } bn_2(p) \mathbf{ in } t_2 \end{aligned}$$

Otherwise it is possible that bn_1 and bn_2 pick out different atoms to become bound, respectively be free, in p . (Since the Ott-tool does not derive a reasoning infrastructure for alpha-equated terms with deep binders, it can permit such specifications.)

We also need to restrict the form of the binding functions in order to ensure the bn -functions can be defined for alpha-equated terms. The main restriction is that we cannot return an atom in a binding function that is also bound in the corresponding term-constructor. Consider again the specification for trm and a contrived version for assignments $assn$:

$$\begin{aligned} & \mathbf{nominal_datatype } trm = \dots \\ & \mathbf{and } assn = \\ & \quad \text{ANil}' \\ & \quad | \text{ACons}' \ x::\text{name } y::\text{name } t::\text{trm } assn \quad \mathbf{binds } y \mathbf{ in } t \\ & \mathbf{binder } bn::\text{assn} \Rightarrow \text{atom list} \\ & \mathbf{where } bn(\text{ANil}') = [] \\ & \quad | bn(\text{ACons}' \ x \ y \ t \ as) = [\text{atom } x] @ bn(as) \end{aligned} \tag{4.4}$$

In this example the term constructor ACons' has four arguments with a binding clause involving two of them. This constructor is also used in the definition of the binding function. The restriction we have to impose is that the binding function can only return free atoms, that is the ones that are *not* mentioned in a binding clause. Therefore y cannot be used in the binding function bn (since

it is bound in $ACons'$ by the binding clause), but x can (since it is a free atom). This restriction is sufficient for lifting the binding function to alpha-equated terms. If we would permit bn to return y , then it would not be respectful and therefore cannot be lifted to alpha-equated lambda-terms.

In the version of Nominal Isabelle described here, we also adopted the restriction from the Ott-tool that binding functions can only return: the empty set or empty list (as in case $ANil'$), a singleton set or singleton list containing an atom (case $PVar$ in (4.2)), or unions of atom sets or appended atom lists (case $ACons'$). This restriction will simplify some automatic definitions and proofs later on.

In order to simplify our definitions of free atoms and alpha-equivalence, we shall assume specifications of term-calculi are implicitly *completed*. By this we mean that for every argument of a term-constructor that is *not* already part of a binding clause given by the user, we add implicitly a special *empty* binding clause, written **binds** \emptyset **in** *labels*. In case of the lambda-terms, the completion produces

```
nominal.datatype lam =
  Var x::name binds  $\emptyset$  in x
| App t1::lam t2::lam binds  $\emptyset$  in t1 t2
| Lam x::name t::lam binds x in t
```

The point of completion is that we can make definitions over the binding clauses and be sure to have captured all arguments of a term constructor.

5. ALPHA-EQUIVALENCE AND FREE ATOMS

Having dealt with all syntax matters, the problem now is how we can turn specifications into actual type definitions in Isabelle/HOL and then establish a reasoning infrastructure for them. As Pottier and Cheney pointed out [7, 19], just re-arranging the arguments of term-constructors so that binders and their bodies are next to each other will result in inadequate representations in cases like $Let\ x_1 = t_1 \dots x_n = t_n\ in\ s$. Therefore we will first extract ‘raw’ datatype definitions from the specification and then define explicitly an alpha-equivalence relation over them. We subsequently construct the quotient of the datatypes according to our alpha-equivalence.

The ‘raw’ datatype definition can be obtained by stripping off the binding clauses and the labels from the types given by the user. We also have to invent new names for the types ty^α and the term-constructors C^α . In our implementation we just use the affix “*_raw*”. But for the purpose of this paper, we use the superscript $^\alpha$ to indicate that a notion is given for alpha-equivalence classes and leave it out for the corresponding notion given on the raw level. So for example we have ty^α / ty and C^α / C where ty is the type used in the quotient construction for ty^α and C is the term-constructor of the raw type ty , respectively C^α is the corresponding term-constructor of ty^α .

The resulting datatype definition is legal in Isabelle/HOL provided the datatypes are non-empty and the types in the constructors only occur in positive position (see [4] for an in-depth description of the datatype package in Isabelle/HOL). We subsequently define each of the user-specified binding functions $bn_{1..m}$ by recursion over the corresponding raw datatype. We also define permutation operations by recursion so that for each term constructor C we have that

$$\pi \cdot (C\ z_1 \dots z_n) = C\ (\pi \cdot z_1) \dots (\pi \cdot z_n) \quad (5.1)$$

We will need this operation later when we define the notion of alpha-equivalence.

The first non-trivial step we have to perform is the generation of *free-atom functions* from the specifications.² For the *raw* types $ty_{1..n}$ we define the free-atom functions

$$fa_{ty_{1..n}} \tag{5.2}$$

by recursion. We define these functions together with auxiliary free-atom functions for the binding functions. Given raw binding functions $bn_{1..m}$ we define

$$fa_{bn_{1..m}}.$$

The reason for this setup is that in a deep binder not all atoms have to be bound, as we saw in (4.3) with the example of ‘plain’ *Lets*. We need therefore functions that calculate those free atoms in deep binders.

While the idea behind these free-atom functions is simple (they just collect all atoms that are not bound), because of our rather complicated binding mechanisms their definitions are somewhat involved. Given a raw term-constructor C of type ty and some associated binding clauses $bc_1 \dots bc_k$, the result of $fa_{ty}(C z_1 \dots z_n)$ will be the union $fa(bc_1) \cup \dots \cup fa(bc_k)$ where we will define below what fa for a binding clause means. We only show the details for the mode **binds (set)** (the other modes are similar). Suppose the binding clause bc_i is of the form

$$\mathbf{binds (set)} \ b_1 \dots b_p \ \mathbf{in} \ d_1 \dots d_q$$

in which the body-labels $d_{1..q}$ refer to types $ty_{1..q}$, and the binders $b_{1..p}$ either refer to labels of atom types (in case of shallow binders) or to binding functions taking a single label as argument (in case of deep binders). Assuming D stands for the set of free atoms of the bodies, B for the set of binding atoms in the binders and B' for the set of free atoms in non-recursive deep binders, then the free atoms of the binding clause bc_i are

$$fa(bc_i) \stackrel{def}{=} (D - B) \cup B'. \tag{5.3}$$

The set D is formally defined as

$$D \stackrel{def}{=} fa_{ty_1} d_1 \cup \dots \cup fa_{ty_q} d_q$$

where in case d_i refers to one of the raw types $ty_{1..n}$ from the specification, the function fa_{ty_i} is the corresponding free-atom function we are defining by recursion; otherwise we set $fa_{ty_i} \stackrel{def}{=} supp$. The reason for the latter is that ty_i is not a type that is part of the specification, and we assume $supp$ is the generic function that characterises the free variables of a type (in fact in the next section we will show that the free-variable functions we define here, are equal to the support once lifted to alpha-equivalence classes).

In order to formally define the set B we use the following auxiliary *bn*-functions for atom types to which shallow binders may refer

²Admittedly, the details of our definitions will be somewhat involved. However they are still conceptually simple in comparison with the ‘positional’ approach taken in Ott [22, Pages 88–95], which uses the notions of *occurrences* and *partial equivalence relations* over sets of occurrences.

$$\begin{aligned}
bn_{atom} a &\stackrel{def}{=} \{atom\ a\} \\
bn_{atom_set} as &\stackrel{def}{=} atoms\ as \\
bn_{atom_list} as &\stackrel{def}{=} atoms\ (set\ as)
\end{aligned}
\tag{5.4}$$

Like the function *atom*, the function *atoms* coerces a set of atoms to a set of the generic atom type. It is defined as $atoms\ as \stackrel{def}{=} \{atom\ a \mid a \in as\}$. The set B in (5.3) is then formally defined as

$$B \stackrel{def}{=} bn_{ty_1} b_1 \cup \dots \cup bn_{ty_p} b_p \tag{5.5}$$

where we use the auxiliary binding functions from (5.4) for shallow binders (that means when ty_i is of type *atom*, *atom set* or *atom list*).

The set B' in (5.3) collects all free atoms in non-recursive deep binders. Let us assume these binders in the binding clause bc_i are

$$bn_1\ l_1, \dots, bn_r\ l_r$$

with $l_{1..r} \subseteq b_{1..p}$ and none of the $l_{1..r}$ being among the bodies $d_{1..q}$. The set B' is defined as

$$B' \stackrel{def}{=} fa_{bn_1} l_1 \cup \dots \cup fa_{bn_r} l_r \tag{5.6}$$

This completes all clauses for the free-atom functions $fa_{ty_{1..n}}$.

Note that for non-recursive deep binders, we have to add in (5.3) the set of atoms that are left unbound by the binding functions $bn_{1..m}$. We used for the definition of this set the functions $fa_{bn_{1..m}}$. The definition for those functions needs to be extracted from the clauses the user provided for $bn_{1..m}$. Assume the user specified a *bn*-clause of the form

$$bn\ (C\ z_1 \dots z_s) = rhs$$

where the $z_{1..s}$ are of types $ty_{1..s}$. For each of the arguments we calculate the free atoms as follows:

- $fa_{ty_i} z_i$ provided z_i does not occur in *rhs*
(that means nothing is bound in z_i by the binding function),
- $fa_{bn_i} z_i$ provided z_i occurs in *rhs* with the recursive call $bn_i z_i$
(that means whatever is ‘left over’ from the *bn*-function is free)
- \emptyset provided z_i occurs in *rhs*, but without a recursive call
(that means z_i is supposed to become bound by the binding function)

For defining $fa_{bn}\ (C\ z_1 \dots z_n)$ we just union up all these sets.

To see how these definitions work in practice, let us reconsider the term-constructors *Let* and *Let_rec* shown in (4.3) together with the term-constructors for assignments *ANil* and *ACons*. Since there is a binding function defined for assignments, we have three free-atom functions, namely fa_{trm} , fa_{assn} and fa_{bn} as follows:

$$\begin{aligned}
fa_{trm} (Let\ as\ t) &\stackrel{def}{=} (fa_{trm}\ t - set\ (bn\ as)) \cup fa_{bn}\ as \\
fa_{trm} (Let_rec\ as\ t) &\stackrel{def}{=} (fa_{assn}\ as \cup fa_{trm}\ t) - set\ (bn\ as) \\
fa_{assn} (ANil) &\stackrel{def}{=} \emptyset \\
fa_{assn} (ACons\ a\ t\ as) &\stackrel{def}{=} (supp\ a) \cup (fa_{trm}\ t) \cup (fa_{assn}\ as) \\
fa_{bn} (ANil) &\stackrel{def}{=} \emptyset \\
fa_{bn} (ACons\ a\ t\ as) &\stackrel{def}{=} (fa_{trm}\ t) \cup (fa_{bn}\ as)
\end{aligned}$$

Recall that *ANil* and *ACons* have no binding clause in the specification. The corresponding free-atom function fa_{assn} therefore returns all free atoms of an assignment (in case of *ACons*, they are given in terms of $supp$, fa_{trm} and fa_{assn}). The binding only takes place in *Let* and *Let_rec*. In case of *Let*, the binding clause specifies that all atoms given by $set\ (bn\ as)$ have to be bound in t . Therefore we have to subtract $set\ (bn\ as)$ from $fa_{trm}\ t$. However, we also need to add all atoms that are free in as . This is in contrast with *Let_rec* where we have a recursive binder to bind all occurrences of the atoms in $set\ (bn\ as)$ also inside as . Therefore we have to subtract $set\ (bn\ as)$ from both $fa_{trm}\ t$ and $fa_{assn}\ as$. Like the function bn , the function fa_{bn} traverses the list of assignments, but instead returns the free atoms, which means in this example the free atoms in the argument t .

An interesting point in this example is that a ‘naked’ assignment (*ANil* or *ACons*) does not bind any atoms, even if the binding function is specified over assignments. Only in the context of a *Let* or *Let_rec*, where the binding clauses are given, will some atoms actually become bound. This is a phenomenon that has also been pointed out in [22]. For us this observation is crucial, because we would not be able to lift the bn -functions to alpha-equated terms if they act on atoms that are bound. In that case, these functions would *not* respect alpha-equivalence.

Having the free-atom functions at our disposal, we can next define the alpha-equivalence relations for the raw types $ty_{1..n}$. We write them as

$$\approx ty_{1..n}.$$

Like with the free-atom functions, we also need to define auxiliary alpha-equivalence relations

$$\approx bn_{1..m}$$

for the binding functions $bn_{1..m}$. To simplify our definitions we will use the following abbreviations for *compound equivalence relations* and *compound free-atom functions* acting on tuples.

$$\begin{aligned}
(x_1, \dots, x_n) (R_1, \dots, R_n) (y_1, \dots, y_n) &\stackrel{def}{=} x_1 R_1 y_1 \wedge \dots \wedge x_n R_n y_n \\
(fa_1, \dots, fa_n) (x_1, \dots, x_n) &\stackrel{def}{=} fa_1 x_1 \cup \dots \cup fa_n x_n
\end{aligned}$$

The alpha-equivalence relations are defined as inductive predicates having a single clause for each term-constructor. Assuming a term-constructor C is of type ty and has the binding clauses $bc_{1..k}$, then the alpha-equivalence clause has the form

$$\frac{prems(bc_1) \dots prems(bc_k)}{C\ z_1 \dots z_n \approx ty\ C\ z'_1 \dots z'_n}$$

The task below is to specify what the premises corresponding to a binding clause are. To understand better what the general pattern is, let us first treat the special instance where bc_i is the empty binding clause of the form

$$\mathbf{binds (set) } \emptyset \mathbf{ in } d_1 \dots d_q.$$

In this binding clause no atom is bound and we only have to ‘alpha-relate’ the bodies. For this we build first the tuples $D \stackrel{def}{=} (d_1, \dots, d_q)$ and $D' \stackrel{def}{=} (d'_1, \dots, d'_q)$ whereby the labels $d_{1..q}$ refer to some of the arguments $z_{1..n}$ and respectively $d'_{1..q}$ to some of $z'_{1..n}$ of the term-constructor. In order to relate two such tuples we define the compound alpha-equivalence relation R as follows

$$R \stackrel{def}{=} (R_1, \dots, R_q) \quad (5.7)$$

with R_i being $\approx ty_i$ if the corresponding labels d_i and d'_i refer to a recursive argument of C and have type ty_i ; otherwise we take R_i to be the equality $=$. Again the latter is because ty_i is not part of the specified types and alpha-equivalence of any previously defined type is supposed to coincide with equality. This lets us now define the premise for an empty binding clause succinctly as $prems(bc_i) \stackrel{def}{=} D R D'$, which can be unfolded to the series of premises

$$d_1 R_1 d'_1 \dots d_q R_q d'_q.$$

We will use the unfolded version in the examples below.

Now suppose the binding clause bc_i is of the general form

$$\mathbf{binds (set) } b_1 \dots b_p \mathbf{ in } d_1 \dots d_q. \quad (5.8)$$

In this case we define a premise P using the relation $\approx_{set}^{R,fa}$ given in Section 3 (similarly $\approx_{set+}^{R,fa}$ and $\approx_{list}^{R,fa}$ for the other binding modes). As above, we first build the tuples D and D' for the bodies $d_{1..q}$, and the corresponding compound alpha-relation R (shown in (5.7)). For $\approx_{set}^{R,fa}$ we also need a compound free-atom function for the bodies defined as

$$fa \stackrel{def}{=} (fa_{ty_1}, \dots, fa_{ty_q})$$

with the assumption that the $d_{1..q}$ refer to arguments of types $ty_{1..q}$. The last ingredient we need are the sets of atoms bound in the bodies. For this we take

$$B \stackrel{def}{=} bn_{ty_1} b_1 \cup \dots \cup bn_{ty_p} b_p.$$

Similarly for B' using the labels $b'_{1..p}$. This lets us formally define the premise P for a non-empty binding clause as:

$$P \stackrel{def}{=} (B, D) \approx_{set}^{R,fa} (B', D').$$

This premise accounts for alpha-equivalence of the bodies of the binding clause. However, in case the binders have non-recursive deep binders, this premise is not enough: we also have to ‘propagate’ alpha-equivalence inside the structure of these binders. An example is *Let* where we have to make sure the right-hand sides of assignments are alpha-equivalent. For this we use relations $\approx_{bn_{1..m}}$ (which we will define shortly). Let us assume the non-recursive deep binders in bc_i are

$$bn_1 l_1, \dots, bn_r l_r.$$

The tuple L consists then of all these binders (l_1, \dots, l_r) (similarly L') and the compound equivalence relation R' is $(\approx_{bn_1}, \dots, \approx_{bn_r})$. All premises for bc_i are then given by

$$prems(bc_i) \stackrel{def}{=} P \wedge L R' L'$$

The auxiliary alpha-equivalence relations $\approx_{bn_{1..m}}$ in R' are defined as follows: assuming a bn -clause is of the form

$$bn (C z_1 \dots z_s) = rhs$$

where the $z_{1..s}$ are of types $ty_{1..s}$, then the corresponding alpha-equivalence clause for \approx_{bn} has the form

$$\frac{z_1 R_1 z'_1 \dots z_s R_s z'_s}{C z_1 \dots z_s \approx_{bn} C z'_1 \dots z'_s}$$

In this clause the relations $R_{1..s}$ are given by

- $z_i \approx_{ty} z'_i$ provided z_i does not occur in rhs and is a recursive argument of C ,
- $z_i = z'_i$ provided z_i does not occur in rhs and is a non-recursive argument of C ,
- $z_i \approx_{bn_i} z'_i$ provided z_i occurs in rhs with the recursive call $bn_i x_i$ and
- *True* provided z_i occurs in rhs but without a recursive call.

This completes the definition of alpha-equivalence. As a sanity check, we can show that the premises of empty binding clauses are a special case of the clauses for non-empty ones (we just have to unfold the definition of $\approx_{set}^{R,fa}$ and take \emptyset for the existentially quantified permutation).

Again let us take a look at a concrete example for these definitions. For the specification shown in (4.3) we have three relations \approx_{trm} , \approx_{assn} and \approx_{bn} with the following rules:

$$\begin{array}{c}
\frac{(bn\ as, t) \approx_{list}^{\approx_{trm}, fa_{trm}} (bn\ as', t') \quad as \approx_{bn} as'}{Let\ as\ t \approx_{trm} Let\ as'\ t'} \\
\\
\frac{(bn\ as, (as, t)) \approx_{list}^{(\approx_{assn}, \approx_{trm}), (fa_{assn}, fa_{trm})} (bn\ as', (as, t'))}{Let_rec\ as\ t \approx_{trm} Let_rec\ as'\ t'} \\
\\
\frac{}{ANil \approx_{assn} ANil} \quad \frac{a = a' \quad t \approx_{trm} t' \quad as \approx_{assn} as'}{ACons\ a\ t\ as \approx_{assn} ACons\ a'\ t'\ as} \\
\\
\frac{}{ANil \approx_{bn} ANil} \quad \frac{t \approx_{trm} t' \quad as \approx_{bn} as'}{ACons\ a\ t\ as \approx_{bn} ACons\ a'\ t'\ as}
\end{array} \tag{5.9}$$

Notice the difference between \approx_{assn} and \approx_{bn} : the latter only ‘tracks’ alpha-equivalence of the components in an assignment that are *not* bound. This is needed in the clause for *Let* (which has a non-recursive binder). The underlying reason is that the terms inside an assignment are not meant to be ‘under’ the binder. Such a premise is *not* needed in *Let_rec*, because there all components of an assignment are ‘under’ the binder. Note also that in case of more than one body (that is in the *Let_rec*-case above) we need to parametrise the relation \approx_{list} with a compound equivalence relation and a compound free-atom function. This is because the corresponding binding clause specifies a binder with two bodies, namely *as* and *t*.

6. ESTABLISHING THE REASONING INFRASTRUCTURE

Having made all necessary definitions for raw terms, we can start with establishing the reasoning infrastructure for the alpha-equated types $ty_{1..n}^\alpha$, that is the types the user originally specified. We give in this section and the next the proofs we need for establishing this infrastructure. One point of our work is that we have completely automated these proofs in Isabelle/HOL.

First we establish that the free-variable functions, the binding functions and the alpha-equivalences are equivariant.

Lemma 6.1.

- (i) The functions $fa_ty_{1..n}$, $fa_bn_{1..m}$ and $bn_{1..m}$ are equivariant.
- (ii) The relations $\approx_{ty_{1..n}}$ and $\approx_{bn_{1..m}}$ are equivariant.

Proof. The function package of Isabelle/HOL allows us to prove the first part by mutual induction over the definitions of the functions.³ The second is by a straightforward induction over the rules of $\approx_{ty_{1..n}}$ and $\approx_{bn_{1..m}}$ using the first part. \square

Next we establish that the alpha-equivalence relations defined in the previous section are indeed equivalence relations.

Lemma 6.2. The relations $\approx_{ty_{1..n}}$ and $\approx_{bn_{1..m}}$ are equivalence relations.

Proof. The proofs are by induction. The non-trivial cases involve premises built up by \approx_{set} , \approx_{set+} and \approx_{list} . They can be dealt with as in Lemma 3.4. However, the transitivity case needs in addition the fact that the relations are equivariant. \square

³We have that the free-atom functions are terminating. From this the function package derives an induction principle [11].

We can feed the last lemma into our quotient package and obtain new types $ty_{1..n}^\alpha$ representing alpha-equated terms of types $ty_{1..n}$. We also obtain definitions for the term-constructors $C_{1..k}^\alpha$ from the raw term-constructors $C_{1..k}$, and similar definitions for the free-atom functions $fa_ty_{1..n}^\alpha$ and $fa_bn_{1..m}^\alpha$ as well as the binding functions $bn_{1..m}^\alpha$. However, these definitions are not really useful to the user, since they are given in terms of the isomorphisms we obtained by creating new types in Isabelle/HOL (recall the picture shown in the Introduction).

The first useful property for the user is the fact that distinct term-constructors are not equal, that is the property

$$C^\alpha x_1 \dots x_r \neq D^\alpha y_1 \dots y_s \quad (6.1)$$

whenever $C^\alpha \neq D^\alpha$. In order to derive this property, we use the definition of alpha-equivalence and establish that

$$C x_1 \dots x_r \not\approx_{ty} D y_1 \dots y_s \quad (6.2)$$

holds for the corresponding raw term-constructors. In order to deduce (6.1) from (6.2), our quotient package needs to know that the raw term-constructors C and D are *respectful* w.r.t. the alpha-equivalence relations (see [8]). Given, for example, C is of type ty with argument types $ty_{1..r}$, respectfulness amounts to showing that

$$C x_1 \dots x_r \approx_{ty} C x'_1 \dots x'_r$$

holds under the assumptions $x_i \approx_{ty_i} x'_i$ whenever x_i and x'_i are recursive arguments of C , and $x_i = x'_i$ whenever they are non-recursive arguments (similarly for D). For this we have to show by induction over the definitions of alpha-equivalences the following auxiliary implications

$$\begin{aligned} x \approx_{ty_i} x' &\text{ implies } fa_ty_i x = fa_ty_i x' \\ x \approx_{ty_l} x' &\text{ implies } fa_bn_j x = fa_bn_j x' \\ x \approx_{ty_l} x' &\text{ implies } bn_j x = bn_j x' \\ x \approx_{ty_l} x' &\text{ implies } x \approx_{bn_j} x' \end{aligned} \quad (6.3)$$

whereby ty_l is the type over which bn_j is defined. Whereas the first, second and last implication are true by how we stated our definitions, the third *only* holds because of our restriction imposed on the form of the binding functions—namely *not* to return any bound atoms. In Ott, in contrast, the user may define $bn_{1..m}$ so that they return bound atoms and in this case the third implication is *not* true. A result is that in general the lifting of the corresponding binding functions in Ott to alpha-equated terms is impossible. Having established respectfulness for the raw term-constructors, the quotient package is able to automatically deduce (6.1) from (6.2).

Next we can lift the permutation operations defined in (5.1). In order to make this lifting to go through, we have to show that the permutation operations are respectful. This amounts to showing that the alpha-equivalence relations are equivariant, which we already established in Lemma 6.2. As a result we can add the equations

$$\pi \cdot (C^\alpha x_1 \dots x_r) = C^\alpha (\pi \cdot x_1) \dots (\pi \cdot x_r) \quad (6.4)$$

to our infrastructure. In a similar fashion we can lift the defining equations of the free-atom functions $fa_ty_{1..n}^\alpha$ and $fa_bn_{1..m}^\alpha$ as well as of the binding functions $bn_{1..m}^\alpha$ and size functions $size_ty_{1..n}^\alpha$. The latter are defined automatically for the raw types $ty_{1..n}$ by the datatype package of Isabelle/HOL.

We also need to lift the properties that characterise when two raw terms of the form

$$C x_1 \dots x_r \approx_{ty} C x'_1 \dots x'_r$$

are alpha-equivalent. This gives us conditions when the corresponding alpha-equated terms are *equal*, namely

$$C^\alpha x_1 \dots x_r = C^\alpha x'_1 \dots x'_r.$$

We call these conditions as *quasi-injectivity*. They correspond to the premises in our alpha-equivalence relations, except that the relations $\approx_{ty_{1..n}}$ are all replaced by equality (and similarly the free-atom and binding functions are replaced by their lifted counterparts). Recall the alpha-equivalence rules for *Let* and *Let_rec* shown in (5.9). For Let^α and Let_rec^α we have

$$\frac{(bn^\alpha as, t) \approx_{list}^{fa_{irm}^\alpha} (bn as', t') \quad as \approx_{bn}^\alpha as'}{Let^\alpha as t = Let^\alpha as' t'} \quad (6.5)$$

$$\frac{(bn^\alpha as, (as, t)) \approx_{list}^{(=, =), (fa_{assn}^\alpha, fa_{irm}^\alpha)} (bn^\alpha as', (as, t'))}{Let_rec^\alpha as t = Let_rec^\alpha as' t'}$$

We can also add to our infrastructure cases lemmas and a (mutual) induction principle for the types $ty_{1..n}^\alpha$. The cases lemmas allow the user to deduce a property P by exhaustively analysing how an element of a type, say ty_i^α , can be constructed (that means one case for each of the term-constructors in ty_i^α). The lifted cases lemma for the type ty_i^α looks as follows

$$\frac{\begin{array}{l} \forall x_1 \dots x_k. y = C_1^\alpha x_1 \dots x_k \Rightarrow P \\ \vdots \\ \forall x_1 \dots x_l. y = C_m^\alpha x_1 \dots x_l \Rightarrow P \end{array}}{P} \quad (6.6)$$

where y is a variable of type ty_i^α and P is the property that is established by the case analysis. Similarly, we have a (mutual) induction principle for the types $ty_{1..n}^\alpha$, which is of the form

$$\frac{\begin{array}{l} \forall x_1 \dots x_k. P_i x_i \wedge \dots \wedge P_j x_j \Rightarrow P (C_1^\alpha x_1 \dots x_k) \\ \vdots \\ \forall x_1 \dots x_l. P_r x_r \wedge \dots \wedge P_s x_s \Rightarrow P (C_m^\alpha x_1 \dots x_l) \end{array}}{P_1 y_1 \wedge \dots \wedge P_n y_n} \quad (6.7)$$

whereby the $P_{1..n}$ are the properties established by the induction, and the $y_{1..n}$ are of type $ty_{1..n}^\alpha$. Note that for the term constructors C_1^α the induction principle has a hypothesis of the form

$$\forall x_1 \dots x_k. P_i x_i \wedge \dots \wedge P_j x_j \Rightarrow P (C_1^\alpha x_1 \dots x_k)$$

in which the $x_{i..j} \subseteq x_{1..k}$ are the recursive arguments of this term constructor (similarly for the other term-constructors).

Recall the lambda-calculus with *Let*-patterns shown in (4.2). The cases lemmas and the induction principle shown in (6.6) and (6.7) boil down in that example to the following three inference rules:

cases lemmas:

$$\frac{\begin{array}{l} \forall x. y = \text{Var}^\alpha x \Rightarrow P_{trm} \\ \forall x_1 x_2. y = \text{App}^\alpha x_1 x_2 \Rightarrow P_{trm} \\ \forall x_1 x_2. y = \text{Lam}^\alpha x_1 x_2 \Rightarrow P_{trm} \\ \forall x_1 x_2 x_3. y = \text{Let_pat}^\alpha x_1 x_2 x_3 \Rightarrow P_{trm} \end{array}}{P_{trm}} \quad \frac{\begin{array}{l} \forall x. y = \text{PVar}^\alpha x \Rightarrow P_{pat} \\ \forall x_1 x_2. y = \text{PTup}^\alpha x_1 x_2 \Rightarrow P_{pat} \end{array}}{P_{pat}}$$

induction principle:

$$\frac{\begin{array}{l} \forall x. P_{trm} (\text{Var}^\alpha x) \\ \forall x_1 x_2. P_{trm} x_1 \wedge P_{trm} x_2 \Rightarrow P_{trm} (\text{App}^\alpha x_1 x_2) \\ \forall x_1 x_2. P_{trm} x_2 \Rightarrow P_{trm} (\text{Lam}^\alpha x_1 x_2) \\ \forall x_1 x_2 x_3. P_{pat} x_1 \wedge P_{trm} x_2 \wedge P_{trm} x_3 \Rightarrow P_{trm} (\text{Let_pat}^\alpha x_1 x_2 x_3) \\ \forall x. P_{pat} (\text{PVar}^\alpha x) \\ \forall x_1 x_2. P_{pat} x_1 \wedge P_{pat} x_2 \Rightarrow P_{pat} (\text{PTup}^\alpha x_1 x_2) \end{array}}{P_{trm} y_1 \wedge P_{pat} y_2} \quad (6.8)$$

By working now completely on the alpha-equated level, we can first show using (6.4) and Property 2.1 that the support of each term constructor is included in the support of its arguments, namely

$$(\text{supp } x_1 \cup \dots \cup \text{supp } x_r) \text{ supports } (C^\alpha x_1 \dots x_r)$$

This allows us to prove using the induction principle for $ty_{1..n}^\alpha$ that every element of type $ty_{1..n}^\alpha$ is finitely supported (using Proposition 2.3(i)). Similarly, we can establish by induction that the free-atom functions and binding functions are equivariant, namely

$$\begin{aligned} \pi \cdot (\text{fa_ty}_i^\alpha x) &= \text{fa_ty}_i^\alpha (\pi \cdot x) \\ \pi \cdot (\text{fa_bn}_j^\alpha x) &= \text{fa_bn}_j^\alpha (\pi \cdot x) \\ \pi \cdot (\text{bn}_j^\alpha x) &= \text{bn}_j^\alpha (\pi \cdot x) \end{aligned}$$

Lastly, we can show that the support of elements in $ty_{1..n}^\alpha$ is the same as the free-atom functions $\text{fa_ty}_{1..n}^\alpha$. This fact is important in the nominal setting where the general theory is formulated in terms of support and freshness, but also provides evidence that our notions of free-atoms and alpha-equivalence ‘match up’ correctly.

Theorem 6.3. *For $x_{1..n}$ with type $ty_{1..n}^\alpha$, we have $\text{supp } x_i = \text{fa_ty}_i^\alpha x_i$.*

Proof. The proof is by induction on $x_{1..n}$. In each case we unfold the definition of *supp*, move the swapping inside the term-constructors and then use the quasi-injectivity lemmas in order to complete the proof. For the abstraction cases we use then the facts derived in Theorem 3.5, for which we have to know that every body of an abstraction is finitely supported. This, we have proved earlier. \square

Consequently, we can replace the free-atom functions by *supp* in our quasi-injection lemmas. In the examples shown in (6.5), for instance, we obtain for Let^α and Let_rec^α

$$\frac{(bn^\alpha as, t) \approx_{list}^{\overline{=}, supp} (bn^\alpha as', t') \quad as \approx_{bn}^\alpha as'}{Let^\alpha as t = Let^\alpha as' t'}$$

$$\frac{(bn^\alpha as, (as, t)) \approx_{list}^{\overline{=}, =}, (supp, supp)}{(bn^\alpha as', (as, t'))}{Let_rec^\alpha as t = Let_rec^\alpha as' t'}$$

Taking into account that the compound equivalence relation $(=, =)$ and the compound free-atom function $(supp, supp)$ are by definition equal to $=$ and *supp*, respectively, the above rules simplify further to

$$\frac{[bn^\alpha as]_{list}.t = [bn^\alpha as']_{list}.t' \quad as \approx_{bn}^\alpha as'}{Let^\alpha as t = Let^\alpha as' t'}$$

$$\frac{[bn^\alpha as]_{list}.(as, t) = [bn^\alpha as']_{list}.(as, t')}{Let_rec^\alpha as t = Let_rec^\alpha as' t'}$$

which means we can characterise equality between term-constructors (on the alpha-equated level) in terms of equality between the abstractions defined in Section 3. From this we can deduce the support for Let^α and Let_rec^α , namely

$$\begin{aligned} supp (Let^\alpha as t) &= (supp t - set (bn^\alpha as)) \cup fa_{bn}^\alpha as \\ supp (Let_rec^\alpha as t) &= (supp t \cup supp as) - set (bn^\alpha as) \end{aligned}$$

using the support of abstractions derived in Theorem 3.5.

To sum up this section, we have established a reasoning infrastructure for the types $ty_{1..n}^\alpha$ by first lifting definitions from the ‘raw’ level to the quotient level and then by proving facts about these lifted definitions. All necessary proofs are generated automatically by custom ML-code.

7. STRONG INDUCTION PRINCIPLES

In the previous section we derived induction principles for alpha-equated terms (see (6.7) for the general form and (6.8) for an example). This was done by lifting the corresponding induction principles for ‘raw’ terms. We already employed these induction principles for deriving several facts about alpha-equated terms, including the property that the free-atom functions and the notion of support coincide. Still, we call these induction principles *weak*, because for a term-constructor, say $C^\alpha x_1 \dots x_r$, the induction hypothesis requires us to establish (under some assumptions) a property $P (C^\alpha x_1 \dots x_r)$ for *all* $x_{1..r}$. The problem with this is that in the presence of binders we cannot make any assumptions about the atoms that are bound—for example assuming the variable convention. One obvious way around this problem is to rename bound atoms. Unfortunately, this leads to very clunky proofs and makes formalisations grievous experiences (especially in the context of multiple bound atoms).

For the older versions of Nominal Isabelle we described in [25] a method for automatically strengthening weak induction principles. These stronger induction principles allow the user to make additional assumptions about bound atoms. The advantage of these assumptions is that they make in most cases any renaming of bound atoms unnecessary. To explain how the strengthening works, we

use as running example the lambda-calculus with *Let*-patterns shown in (4.2). Its weak induction principle is given in (6.8). The stronger induction principle is as follows:

$$\begin{array}{l}
\forall x c. P_{trm} c (Var^\alpha x) \\
\forall x_1 x_2 c. (\forall d. P_{trm} d x_1) \wedge (\forall d. P_{trm} d x_2) \Rightarrow P_{trm} c (App^\alpha x_1 x_2) \\
\forall x_1 x_2 c. atom x_1 \# c \wedge (\forall d. P_{trm} d x_2) \Rightarrow P_{trm} c (Lam^\alpha x_1 x_2) \\
\forall x_1 x_2 x_3 c. (set (bn^\alpha x_1)) \#^* c \wedge \\
\quad (\forall d. P_{pat} d x_1) \wedge (\forall d. P_{trm} d x_2) \wedge (\forall d. P_{trm} d x_3) \Rightarrow P_{trm} c (Let_pat^\alpha x_1 x_2 x_3) \\
\forall x c. P_{pat} c (PVar^\alpha x) \\
\forall x_1 x_2 c. (\forall d. P_{pat} d x_1) \wedge (\forall d. P_{pat} d x_2) \Rightarrow P_{pat} c (PTup^\alpha x_1 x_2) \\
\hline
P_{trm} c y_1 \wedge P_{pat} c y_2
\end{array} \tag{7.1}$$

Notice that instead of establishing two properties of the form $P_{trm} y_1 \wedge P_{pat} y_2$, as the weak one does, the stronger induction principle establishes the properties of the form $P_{trm} c y_1 \wedge P_{pat} c y_2$ in which the additional parameter c is assumed to be of finite support. The purpose of c is to ‘control’ which freshness assumptions the binders should satisfy in the Lam^α and Let_pat^α cases: for Lam^α we can assume the bound atom x_1 is fresh for c (third line); for Let_pat^α we can assume all bound atoms from an assignment are fresh for c (fourth line). In order to see how an instantiation for c in the conclusion ‘controls’ the premises, one has to take into account that Isabelle/HOL is a typed logic. That means if c is instantiated with, for example, a pair, then this type-constraint will be propagated to the premises. The main point is that if c is instantiated appropriately, then the user can mimic the usual ‘pencil-and-paper’ reasoning employing the variable convention about bound and free variables being distinct [25].

In what follows we will show that the weak induction principle in (6.8) implies the strong one (7.1). This fact was established for single binders in [25] by some quite involved, nevertheless automated, induction proof. In this paper we simplify the proof by leveraging the automated proving tools from the function package of Isabelle/HOL [11]. The reasoning principle behind these tools is well-founded induction. To use them in our setting, we have to discharge two proof obligations: one is that we have well-founded measures (one for each type $ty_{1..n}^\alpha$) that decrease in every induction step and the other is that we have covered all cases in the induction principle. Once these two proof obligations are discharged, the reasoning infrastructure of the function package will automatically derive the stronger induction principle. This way of establishing the stronger induction principle is considerably simpler than the earlier work presented in [25].

As measures we can use the size functions $size_ty_{1..n}^\alpha$, which we lifted in the previous section and which are all well-founded. It is straightforward to establish that the sizes decrease in every induction step. What is left to show is that we covered all cases. To do so, we have to derive stronger cases lemmas, which look in our running example are as follows:

$$\begin{array}{l}
\forall x. y = Var^\alpha x \Rightarrow P_{trm} \\
\forall x_1 x_2. y = App^\alpha x_1 x_2 \Rightarrow P_{trm} \\
\forall x_1 x_2. atom x_1 \# c \wedge y = Lam^\alpha x_1 x_2 \Rightarrow P_{trm} \\
\forall x_1 x_2 x_3. set (bn^\alpha x_1) \#^* c \wedge y = Let_pat^\alpha x_1 x_2 x_3 \Rightarrow P_{trm} \\
\hline
P_{trm}
\end{array}
\quad
\begin{array}{l}
\forall x. y = PVar^\alpha x \Rightarrow P_{pat} \\
\forall x_1 x_2. y = PTup^\alpha x_1 x_2 \Rightarrow P_{pat} \\
\hline
P_{pat}
\end{array}$$

They are stronger in the sense that they allow us to assume in the Lam^α and Let_pat^α cases that the bound atoms avoid, or being fresh for, a context c (which is assumed to be finitely supported).

These stronger cases lemmas can be derived from the ‘weak’ cases lemmas given in (6.8). This is trivial in case of patterns (the one on the right-hand side) since the weak and strong cases lemma coincide (there is no binding in patterns). Interesting are only the cases for Lam^α and Let_pat^α , where we have some binders and therefore have an additional assumption about avoiding c . Let us first establish the case for Lam^α . By the weak cases lemma (6.8) we can assume that

$$y = Lam^\alpha x_1 x_2 \quad (7.2)$$

holds, and need to establish P_{trm} . The stronger cases lemma has the corresponding implication

$$\forall x_1 x_2. atom x_1 \# c \wedge y = Lam^\alpha x_1 x_2 \Rightarrow P_{trm} \quad (7.3)$$

which we must use in order to infer P_{trm} . Clearly, we cannot use this implication directly, because we have no information whether or not x_1 is fresh for c . However, we can use Properties 2.4 and 2.5 to rename x_1 . We know by Theorem 6.3 that $\{atom x_1\} \#^* Lam^\alpha x_1 x_2$ (since its support is $supp x_2 - \{atom x_1\}$). Property 2.5 provides us then with a permutation π , such that $\{atom(\pi \cdot x_1)\} \#^* c$ and $supp(Lam^\alpha x_1 x_2) \#^* \pi$ hold. By using Property 2.4, we can infer from the latter that

$$Lam^\alpha(\pi \cdot x_1)(\pi \cdot x_2) = Lam^\alpha x_1 x_2$$

holds. We can use this equation in the assumption (7.2), and hence use the implication (7.3) with the renamed $\pi \cdot x_1$ and $\pi \cdot x_2$ for concluding this case.

The Let_pat^α -case involving a deep binder is slightly more complicated. We have the assumption

$$y = Let_pat^\alpha x_1 x_2 x_3 \quad (7.4)$$

and the implication from the stronger cases lemma

$$\forall x_1 x_2 x_3. set(bn^\alpha x_1) \#^* c \wedge y = Let_pat^\alpha x_1 x_2 x_3 \Rightarrow P_{trm} \quad (7.5)$$

The reason that this case is more complicated is that we cannot directly apply Property 2.5 for obtaining a renaming permutation. Property 2.5 requires that the binders are fresh for the term in which we want to perform the renaming. But this is not true in terms such as (using an informal notation)

$$Let(x, y) := (x, y) \text{ in } (x, y)$$

where x and y are bound in the term, but are also free in the right-hand side of the assignment. We can, however, obtain such a renaming permutation, say π , for the abstraction $[bn^\alpha x_1]_{list}.x_3$. As a result we have $set(bn^\alpha(\pi \cdot x_1)) \#^* c$ and $[bn^\alpha(\pi \cdot x_1)]_{list}.(\pi \cdot x_3) = [bn^\alpha x_1]_{list}.x_3$ (remember set and bn^α are equivariant). Now the quasi-injective property for Let_pat^α states that

$$\frac{[bn^\alpha p]_{list}.t_2 = [bn^\alpha p']_{list}.t'_2 \quad p \approx_{bn}^g p' \quad t_1 = t'_1}{Let_pat^\alpha p t_1 t_2 = Let_pat^\alpha p' t'_1 t'_2}$$

Since all atoms in a pattern are bound by Let_pat^α , we can infer that $(\pi \cdot x_1) \approx_{bn}^\alpha x_1$ holds for every π . Therefore we have that

$$Let_pat^\alpha (\pi \cdot x_1) x_2 (\pi \cdot x_3) = Let_pat^\alpha x_1 x_2 x_3$$

Taking the left-hand side in the assumption shown in (7.4), we can use the implication (7.5) from the stronger cases lemma to infer P_{term} , as needed.

The remaining difficulty is when a deep binder contains some atoms that are bound and some that are free. An example is Let^α in (4.3). In such cases $(\pi \cdot x_1) \approx_{bn}^\alpha x_1$ does not hold in general. The idea however is that π only renames atoms that become bound. In this way π does not affect \approx_{bn}^α (which only tracks alpha-equivalence of terms that are not under the binder). However, the problem is that the permutation operation $\pi \cdot x_1$ applies to all atoms in x_1 . To avoid this we introduce an auxiliary permutation operations, written $_ \bullet_{bn} _$, for deep binders that only permutes bound atoms (or more precisely the atoms specified by the bn -functions) and leaves the other atoms unchanged. Like the functions $fa_bn_{1..m}$, we can define these permutation operations over raw terms analysing how the functions $bn_{1..m}$ are defined. Assuming the user specified a clause

$$bn (C x_1 \dots x_r) = rhs$$

we define $\pi \bullet_{bn} (C x_1 \dots x_r) \stackrel{def}{=} C y_1 \dots y_r$ with y_i determined as follows:

- $y_i \stackrel{def}{=} x_i$ provided x_i does not occur in rhs
- $y_i \stackrel{def}{=} \pi \bullet_{bn} x_i$ provided $bn x_i$ is in rhs
- $y_i \stackrel{def}{=} \pi \cdot x_i$ otherwise

Using again the quotient package we can lift the auxiliary permutation operations $_ \bullet_{bn} _$ to alpha-equated terms. Moreover we can prove the following two properties:

Lemma 7.1. *Given a binding function bn^α and auxiliary equivalence \approx_{bn}^α then for all π*

(i) $\pi \bullet (bn^\alpha x) = bn^\alpha (\pi \bullet_{bn}^\alpha x)$ and

(ii) $(\pi \bullet_{bn}^\alpha x) \approx_{bn}^\alpha x$.

Proof. By induction on x . The properties follow by unfolding of the definitions. \square

The first property states that a permutation applied to a binding function is equivalent to first permuting the binders and then calculating the bound atoms. The second states that $_ \bullet_{bn} _$ preserves \approx_{bn}^α . The main point of the auxiliary permutation functions is that they allow us to rename just the bound atoms in a term, without changing anything else.

Having the auxiliary permutation function in place, we can now solve all remaining cases. For the Let^α term-constructor, for example, we can by Property 2.5 obtain a π such that

$$(\pi \bullet (set (bn^\alpha x_1))) \#^* c \quad \pi \bullet [bn^\alpha x_1]_{list} \cdot x_2 = [bn^\alpha x_1]_{list} \cdot x_2$$

hold. Using the first part of Lemma 7.1, we can simplify this to $set (bn^\alpha (\pi \bullet_{bn}^\alpha x_1)) \#^* c$ and $[bn^\alpha (\pi \bullet_{bn}^\alpha x_1)]_{list} \cdot (\pi \cdot x_2) = [bn^\alpha x_1]_{list} \cdot x_2$. Since $(\pi \bullet_{bn}^\alpha x_1) \approx_{bn}^\alpha x_1$ holds by the second part, we can infer that

$$\text{Let}^\alpha (\pi \bullet_{bn}^\alpha x_1) (\pi \bullet x_2) = \text{Let}^\alpha x_1 x_2$$

holds. This allows us to use the implication from the strong cases lemma, and we are done.

Consequently, we can discharge all proof-obligations about having covered all cases. This completes the proof establishing that the weak induction principles imply the strong induction principles. These strong induction principles have already proved being very useful in practice, particularly for proving properties about capture-avoiding substitution [25].

8. RELATED WORK

To our knowledge the earliest usage of general binders in a theorem prover is described by Naraschewski and Nipkow [15] with a formalisation of the algorithm W. This formalisation implements binding in type-schemes using a de-Brujin indices representation. Since type-schemes in W contain only a single place where variables are bound, different indices do not refer to different binders (as in the usual de-Brujin representation), but to different bound variables. A similar idea has been recently explored for general binders by Charguéraud [5] in the locally nameless approach to binding. There, de-Brujin indices consist of two numbers, one referring to the place where a variable is bound, and the other to which variable is bound. The reasoning infrastructure for both representations of bindings comes for free in theorem provers like Isabelle/HOL and Coq, since the corresponding term-calculi can be implemented as ‘normal’ datatypes. However, in both approaches it seems difficult to achieve our fine-grained control over the ‘semantics’ of bindings (i.e. whether the order of binders should matter, or vacuous binders should be taken into account). To do so, one would require additional predicates that filter out unwanted terms. Our guess is that such predicates result in rather intricate formal reasoning. We are not aware of any formalisation of a non-trivial language that uses Charguéraud’s idea.

Another technique for representing binding is higher-order abstract syntax (HOAS), which for example is implemented in the Twelf system [16]. This representation technique supports very elegantly many aspects of *single* binding, and impressive work by Lee et al [12] has been done that uses HOAS for mechanising the metatheory of SML. We are, however, not aware how multiple binders of SML are represented in this work. Judging from the submitted Twelf-solution for the POPLmark challenge, HOAS cannot easily deal with binding constructs where the number of bound variables is not fixed. For example, in the second part of this challenge, *Lets* involve patterns that bind multiple variables at once. In such situations, HOAS seems to have to resort to the iterated-single-binders-approach with all the unwanted consequences when reasoning about the resulting terms.

Two formalisations involving general binders have been performed in older versions of Nominal Isabelle (one about Psi-calculi and one about algorithm W [3, 28]). Both use the approach based on iterated single binders. Our experience with the latter formalisation has been disappointing. The major pain arose from the need to ‘unbind’ variables. This can be done in one step with our general binders described in this paper, but needs a cumbersome iteration with single binders. The resulting formal reasoning turned out to be rather unpleasant.

The most closely related work to the one presented here is the Ott-tool by Sewell et al [22] and the $\text{C}\alpha\text{ml}$ language by Pottier [19]. Ott is a nifty front-end for creating \LaTeX documents from specifications of term-calculi involving general binders. For a subset of the specifications Ott can also generate theorem prover code using a ‘raw’ representation of terms, and in Coq also a locally nameless representation. The developers of this tool have also put forward (on paper) a definition

for alpha-equivalence and free variables for terms that can be specified in Ott. This definition is rather different from ours, not using any nominal techniques. To our knowledge there is no concrete mathematical result concerning this notion of alpha-equivalence and free variables. We have proved that our definitions lead to alpha-equated terms, whose support is as expected (that means bound atoms are removed from the support). We also showed that our specifications lift from ‘raw’ types to types of alpha-equivalence classes. For this we have established (automatically) that every term-constructor and function defined for ‘raw’ types is respectful w.r.t. alpha-equivalence.

Although we were heavily inspired by the syntax of Ott, its definition of alpha-equivalence is unsuitable for our extension of Nominal Isabelle. First, it is far too complicated to be a basis for automated proofs implemented on the ML-level of Isabelle/HOL. Second, it covers cases of binders depending on other binders, which just do not make sense for our alpha-equated terms. Third, it allows empty types that have no meaning in a HOL-based theorem prover. We also had to generalise slightly Ott’s binding clauses. In Ott one specifies binding clauses with a single body; we allow more than one. We have to do this, because this makes a difference for our notion of alpha-equivalence in case of **binds (set)** and **binds (set+)**. Consider the examples

$$\begin{aligned} & Foo_1 \text{ xs::name fset t::trm s::trm } \mathbf{binds (set)} \text{ xs in } t \text{ s} \\ & Foo_2 \text{ xs::name fset t::trm s::trm } \mathbf{binds (set)} \text{ xs in } t, \mathbf{binds (set)} \text{ xs in } s \end{aligned}$$

In the first term-constructor we have a single body that happens to be ‘spread’ over two arguments; in the second term-constructor we have two independent bodies in which the same variables are bound. As a result we have⁴

$$Foo_1 \{a, b\} (a, b) (a, b) \neq Foo_1 \{a, b\} (a, b) (b, a)$$

but

$$Foo_2 \{a, b\} (a, b) (a, b) = Foo_2 \{a, b\} (a, b) (b, a)$$

and therefore need the extra generality to be able to distinguish between both specifications. Because of how we set up our definitions, we also had to impose some restrictions (like a single binding function for a deep binder) that are not present in Ott. Our expectation is that we can still cover many interesting term-calculi from programming language research, for example the Core-Haskell language from the Introduction. With the work presented in this paper we can define it formally as shown in Figure 2 and then Nominal Isabelle derives automatically a corresponding reasoning infrastructure.

Pottier presents a programming language, called C_oaml, for representing terms with general binders inside OCaml [19]. This language is implemented as a front-end that can be translated to OCaml with the help of a library. He presents a type-system in which the scope of general binders can be specified using special markers, written *inner* and *outer*. It seems our and his specifications can be inter-translated as long as ours use the binding mode **binds** only. However, we have not proved this. Pottier gives a definition for alpha-equivalence, which also uses a permutation operation (like ours). Still, this definition is rather different from ours and he only proves that it defines an equivalence relation. A complete reasoning infrastructure is well beyond the purposes of his

⁴Assuming $a \neq b$, there is no permutation that can make (a, b) equal with both (a, b) and (b, a) , but there are two permutations so that we can make (a, b) and (a, b) equal with one permutation, and (a, b) and (b, a) with the other.

```

atom_decl var cvar tvar
nominal_datatype tkind = KStar | KFun tkind tkind
and ckind = CKSim ty ty
and ty = TVar tvar | T string | TApp ty ty
| TFun string ty_list | TAll tv::tvar tkind ty::ty binds tv in ty
| TArr ckind ty
and ty_list = TNil | TCons ty ty_list
and cty = CVar cvar | C string | CApp cty cty | CFun string co_list
| CALL cv::cvar ckind cty::cty binds cv in cty
| CArr ckind cty | CRefl ty | CSym cty | CCirc cty cty
| CAt cty ty | CLeft cty | CRight cty | CSim cty cty
| CRightc cty | CLeftc cty | Coerce cty cty
and co_list = CNil | CCons cty co_list
and trm = Var var | K string
| LAM_ty tv::tvar tkind t::trm binds tv in t
| LAM_cty cv::cvar ckind t::trm binds cv in t
| App_ty trm ty | App_cty trm cty | App trm trm
| Lam v::var ty t::trm binds v in t
| Let x::var ty trm t::trm binds x in t
| Case trm assoc_list | Cast trm co
and assoc_list = ANil | ACons p::pat t::trm assoc_list binds bv p in t
and pat = Kpat string tvk_list tvck_list vt_list
and vt_list = VTNil | VTCons var ty vt_list
and tvk_list = TVTKNil | TVTKCons tvar tkind tvk_list
and tvck_list = TVCKNil | TVCKCons cvar ckind tvck_list
binder
bv :: pat ⇒ atom list and
bv1 :: vt_list ⇒ atom list and
bv2 :: tvk_list ⇒ atom list and
bv3 :: tvck_list ⇒ atom list
where
  bv (K s tvts tvcs vs) = (bv3 tvts) @ (bv2 tvcs) @ (bv1 vs)
| bv1 VTNil = []
| bv1 (VTCons x ty tl) = (atom x)::(bv1 tl)
| bv2 TVTKNil = []
| bv2 (TVTKCons a ty tl) = (atom a)::(bv2 tl)
| bv3 TVCKNil = []
| bv3 (TVCKCons c cty tl) = (atom c)::(bv3 tl)

```

Figure 2: A definition for Core-Haskell in Nominal Isabelle. For the moment we do not support nested types; therefore we explicitly have to unfold the lists *co_list*, *assoc_list* and so on. Apart from that limitation, the definition follows closely the original shown in Figure 1. The point of our work is that having made such a definition in Nominal Isabelle, one obtains automatically a reasoning infrastructure for Core-Haskell.

language. Similar work for Haskell with similar results was reported by Cheney [6] and more recently by Weirich et al [30].

In a slightly different domain (programming with dependent types), Altenkirch et al [1] present a calculus with a notion of alpha-equivalence related to our binding mode **binds (set+)**. Their definition is similar to the one by Pottier, except that it has a more operational flavour and calculates a partial (renaming) map. In this way, the definition can deal with vacuous binders. However, to our best knowledge, no concrete mathematical result concerning this definition of alpha-equivalence has been proved.

9. CONCLUSION

We have presented an extension of Nominal Isabelle for dealing with general binders, that is where term-constructors have multiple bound atoms. For this extension we introduced new definitions of alpha-equivalence and automated all necessary proofs in Isabelle/HOL. To specify general binders we used the syntax from Ott, but extended it in some places and restricted it in others so that the definitions make sense in the context of alpha-equated terms. We also introduced two binding modes (set and set+) that do not exist in Ott. We have tried out the extension with calculi such as Core-Haskell, type-schemes and approximately a dozen of other typical examples from programming language research [21]. The code will eventually become part of the Isabelle distribution.⁵

We have left out a discussion about how functions can be defined over alpha-equated terms involving general binders. In earlier versions of Nominal Isabelle this turned out to be a thorny issue. We hope to do better this time by using the function package [11] that has recently been implemented in Isabelle/HOL and also by restricting function definitions to equivariant functions (for them we can provide more automation).

There are some restrictions we imposed in this paper that we would like to lift in future work. One is the exclusion of nested datatype definitions. Nested datatype definitions would allow one to specify, for instance, the function kinds in Core-Haskell as *TFun string (ty list)* instead of the unfolded version *TFun string ty_list* (see Figure 2). To achieve this, we need more clever implementation than we have at the moment. However, really lifting this restriction will involve major work on the underlying datatype package of Isabelle/HOL.

A more interesting line of investigation is whether we can go beyond the simple-minded form of binding functions that we adopted from Ott. At the moment, binding functions can only return the empty set, a singleton atom set or unions of atom sets (similarly for lists). It remains to be seen whether properties like

$$fa_ty\ x = bn\ x \cup fa_bn\ x$$

allow us to support more interesting binding functions.

We have also not yet played with other binding modes. For example we can imagine that there is need for a binding mode where instead of usual lists, we abstract lists of distinct elements (the corresponding type *dlist* already exists in the library of Isabelle/HOL). We expect the presented work can be extended to accommodate such binding modes.

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⁵It can be downloaded already from <http://isabelle.in.tum.de/nominal/download>.

the subgrammars of kinds and types in our Core-Haskell example. Ramana Kumar and Andrei Popescu helped us with comments about an earlier version of this paper.

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