Mechanizing the Metatheory of LF

CHRISTIAN URBAN
TU Munich

and

JAMES CHENEY
University of Edinburgh

and

STEFAN BERGHOFER
TU Munich

LF is a dependent type theory in which many other formal systems can be conveniently embedded. However, correct use of LF relies on nontrivial metatheoretic developments such as proofs of correctness of decision procedures for LF’s judgments. Although detailed informal proofs of these properties have been published, they have not been formally verified in a theorem prover. We have formalized these properties within Isabelle/HOL using the Nominal Datatype Package, closely following a recent article by Harper and Pfenning. In the process, we identified and resolved a gap in one of the proofs and a small number of minor lacunae in others. We also formally derive a version of the type checking algorithm from which Isabelle/HOL can generate executable code. Besides its intrinsic interest, our formalization provides a foundation for studying the adequacy of LF encodings, the correctness of Twelf-style metatheoretic reasoning, and the metatheory of extensions to LF.

Categories and Subject Descriptors: F.4.1 [Mathematical Logic and Formal Language]: Mathematical Logic—Lambda calculus and related systems
General Terms: Languages, theorem provers
Additional Key Words and Phrases: Logical frameworks, Nominal Isabelle

1. INTRODUCTION

The (Edinburgh) Logical Framework (LF) is a dependent type theory introduced by Harper, Honsell and Plotkin [1993] as a framework for specifying and reasoning about formal systems. It has found many applications, including proof-carrying...
code [Necula 1997]. The Twelf system [Pfenning and Schürrmann 1999] has been used to mechanize reasoning about LF specifications.

The cornerstone of LF is the idea of encoding judgments-as-types and proofs-as-terms whereby judgments of a specified formal system are represented as LF-types and the LF-terms inhabiting these LF-types correspond to valid deductions for these judgments. Hence, the validity of a deduction in a specified system is equivalent to a type checking problem in LF. Therefore correct use of LF to encode other logics depends on the proofs of correctness of type checking algorithms for LF.

Type checking in LF is decidable, but proving decidability is nontrivial because types may contain expressions with computational behavior. This means that type-checking depends on equality-tests for LF-terms and LF-types. Several algorithms for such equality-tests have been proposed in the literature [Coquand 1991; Goguen 2005b; Harper and Pfenning 2005]. Harper and Pfenning [2005] present a type-driven algorithm that is practical and also has been extended to a variety of richer languages. The correctness of this algorithm is proved by establishing soundness and completeness with respect to the definitional equality rules of LF. These proofs are involved: Harper and Pfenning’s detailed pencil-and-paper proof spans more than 30 pages, yet still omits many cases and lemmas.

We present a formalization of the main results of Harper and Pfenning’s article. To our knowledge this is the first formalization of these or comparable results. While most of the formal proofs go through as described by Harper and Pfenning [2005], we found a few do not go through as described, and there is a gap in the proof of soundness. Although the problem can be avoided easily by adding to or changing the rules of Harper and Pfenning [2005], we found that it was still possible to prove the original results, though the argument was nontrivial. Our formalization was essential not only to find this gap in Harper and Pfenning’s argument, but also to find and validate the possible repairs relatively quickly.

We used Isabelle/HOL [Nipkow et al. 2002] and the Nominal Datatype Package [Urban et al. 2007; Urban and Tasson 2005; Urban 2008] for our formalization. The latter provides an infrastructure for reasoning conveniently about datatypes with a built-in notion of alpha-equivalence: it allows to specify such datatypes, provides appropriate recursion combinators and derives strong induction principles that have the usual variable convention already built-in. The Nominal Datatype Package has already been used to formalize logical relation arguments similar to (but much simpler than) those in Harper and Pfenning’s completeness proof [Narboux and Urban 2007]; it is worth noting that logical relations proofs are currently not easy to formalize in Twelf itself, despite the recent breakthrough by Schürrmann and Sarnat [2008].

Besides proving the correctness of their equivalence algorithm, Harper and Pfenning also sketched a proof of decidability. Unfortunately, since Isabelle/HOL is based on classical logic, proving decidability results of this kind is not straightforward. We have formalized the essential parts of the decidability proof by providing inductive definitions of the complements of the relations we wish to decide. It is clear by inspection that these relations define recursively enumerable sets, which implies decidability, but we have not formalized this part of the proof. A complete proof of decidability would require first developing a substantial amount of com-
Mechanizing the Metatheory of LF

putability theory within Isabelle/HOL, a problem of independent interest we leave for future work.

We followed the arguments in Harper and Pfenning’s article very closely using the Nominal Datatype Package for our formalisation, but the current system does not allow us to generate executable code directly from definitions involving nominal datatypes. We therefore also implemented a type-checking algorithm based on the locally nameless approach for representing binders [McKinna and Pollack 1999; Aydemir et al. 2008]. We proved that the nominal datatype formalization of Harper and Pfenning’s algorithm is equivalent to the locally nameless formulation. Moreover, by making the choice of fresh names explicit, we can generate a working ML implementation directly from the verified formalization.

Outline. We first briefly review LF and its representation in the Nominal Datatype Package (Sec. 2). In Sec. 3, we report on our formalization. To ease comparison, Sec. 3 follows the structure of Harper and Pfenning [2005] closely, although this article is self-contained. Sections 3.1–3.5 summarize our formalization of the basic syntactic properties of LF and soundness and completeness of the equivalence and typechecking algorithms. We discuss additional lemmas, proof details, and other complications arising during the formalization, and discuss the gap in the soundness proof and its solutions in detail. The remainder of Sec. 3 reports upon formalizations of additional results whose proofs were only sketched by Harper and Pfenning [2005]. These include

1. the admissibility of strengthening and strong extensionality rules (Sec. 3.6),
2. a partial formalization of decidability of algorithmic typechecking for LF, and a discussion of the current limitations of Isabelle/HOL in formalizing proofs about decidability (Sec. 3.7),
3. the existence and uniqueness of quasicanonical forms (Sec. 3.8), and
4. a partial formalization of an example proof of adequacy (Sec. 3.9), and a discussion of complications in the proof sketched in [Harper and Pfenning 2005].

In Sec. 4 we define and verify the correctness of a type checking algorithm based on the locally nameless representation of binders, from which Isabelle/HOL can generate executable code. This amounts to a verified typechecker for LF, an original contribution of this article. Sec. 5 summarizes the authors’ experience with the formalization, Sec. 6 discusses related and future work and Sec. 7 concludes.

Contributions. The metatheory of LF is well-understood: it had been studied for many years before the definitive presentation in Harper and Pfenning [2005]. Their main results were not in serious doubt, and formalizing such work might strike some readers as perverse or pedantic. Nevertheless, our formalization is an original and significant contribution to the study of logical frameworks and mechanized metatheory, because:

1. it tests the capabilities of the Nominal Datatype Package for formalizing a large and complex metatheoretical development,
2. it provides high confidence in algorithms that are widely trusted but have never been mechanically verified,
3. it elucidates a few subtle issues in the basic metatheory of LF, and
4. it constitutes a re-usable library of formalized results about LF, providing a
foundation for verification of Twelf-style meta-reasoning about LF specifications, extensions to LF, or related type theories that are not as well-understood.

This article is a revised and extended version of a previous conference paper presenting our initial formalization of the metatheory of LF [Urban et al. 2008]. The formal development described by this article can be obtained by request from the authors, and is available at http://isabelle.in.tum.de/nominal/LF/.

2. BACKGROUND

This article assumes some familiarity with formalization in Isabelle/HOL and its ML-like notation for functions and definitions. We used the Nominal Datatype Package in Isabelle/HOL [Urban et al. 2007; Urban and Tasson 2005; Urban 2008] to formalize the syntax and judgments of LF. The key features we rely upon are

(1) support for nominal datatypes with a built-in notion of binding (i.e. $\alpha$-equivalence classes),

(2) facilities for defining functions over nominal datatypes (such as substitution) by (nominal) primitive recursion, and

(3) strong induction principles for datatypes and inductive definitions that build in Barendregt-style renaming conventions.

Together, these features make it possible to formalize most of the definitions and proofs following their paper versions closely. We will not review the features of this system in this article, but will discuss details of the formalization only when they introduce complications. The interested reader is referred to previous work on nominal techniques and the Nominal Datatype Package for further details [Gabbay and Pitts 2002; Pitts 2006; Urban et al. 2007; Urban and Tasson 2005; Urban 2008].

2.1 Syntax of LF

The logical framework LF [Harper et al. 1993] is a dependently-typed lambda-calculus. We present it here following closely the article by Harper and Pfenning [2005], to which we refer from now on as HP05 for brevity. The syntax of LF includes kinds, type families and objects defined by the grammar:

\[
\begin{align*}
\text{Kinds} & \quad K, L ::= \text{type} \mid \Pi x: A. K \\
\text{Type families} & \quad A, B ::= a \mid \Pi x: A_1. A_2 \mid A M \\
\text{Objects} & \quad M, N ::= c \mid x \mid \lambda x: A. M \mid M_1 M_2
\end{align*}
\]

where variables $x$ and constants $c$ and $a$ are drawn from countably infinite, disjoint sets $\text{Var}$ and $\text{Id}$ of variables and identifiers, respectively. Traditionally, LF has included $\lambda$-abstraction at the level of both types and objects. However, Geuvers and Barendsen [1999] established that type-level $\lambda$-abstraction is superfluous in LF. Accordingly, HP05 omits type-level $\lambda$-abstraction, and so do we.

We formalize the syntax of LF using nominal datatypes since the constructors $\lambda$ and $\Pi$ bind variables. Substitutions are represented as lists of variable-term pairs and we define capture avoiding substitution in the standard way as
\[
x[\sigma] = \text{lookup } \sigma \ x \\
c[\sigma] = c \\
(M \ N)[\sigma] = M[\sigma] \ N[\sigma] \\
(\lambda y : A. \ M)[\sigma] = \lambda y : A[\sigma]. \ M[\sigma] \quad \text{provided } y \not\in \sigma \\
a[\sigma] = a \\
(A \ M)[\sigma] = A[\sigma] \ M[\sigma] \\
(\Pi y : A. \ B)[\sigma] = \Pi y : A[\sigma]. \ B[\sigma] \quad \text{provided } y \not\in \sigma \\
type[\sigma] = \text{type} \\
(\Pi y : A. \ K)[\sigma] = \Pi y : A[\sigma]. \ K[\sigma] \quad \text{provided } y \not\in \sigma
\]

where the variable case is defined in terms of the auxiliary function \(\text{lookup}\):

\[
\text{lookup } [] = x = x \\
\text{lookup } ((y, M) :: \sigma) x = (\text{if } x = y \text{ then } M \text{ else } \text{lookup } \sigma \ x)
\]

The side-conditions \(y \not\in \sigma\) in the above definition are freshness constraints provided automatically by the Nominal Datatype Package and stand for \(y\) not occurring freely in the substitution \(\sigma\). Substitution for a single variable is defined as a special case:

\[
(\lambda x : \sigma. \ M) \& (x := M) \& (\lambda x : \sigma. \ M) = (\lambda x : \sigma. \ M).
\]

We use ML-like notation \([\ ]\) for the empty list and \((x, M) : L\) for list construction. LF includes signatures \(\Sigma\) and contexts \(\Gamma\), both of which we represent as lists of pairs. The former consist of pairs of the form \((c, A)\) or \((a, K)\) associating the constant \(c\) with type \(A\) and the constant \(a\) with kind \(K\) respectively, and the latter consists of pairs \((x, A)\) associating the variable \(x\) with type \(A\). Accordingly, we write \((x, A) : \Gamma\) for context construction (rather than \(\Gamma, x : A\)), \(\Gamma \& \Gamma'\) for context concatenation and \((x, A) \in \Gamma\) for context membership (similarly for \(\Sigma\)). Context inclusion is defined as follows:

\[
\Gamma_1 \subseteq \Gamma_2 \overset{\text{def}}{=} \forall x. \ (x, A) \in \Gamma_1 \text{ implies } (x, A) \in \Gamma_2
\]

2.2 Validity and Definitional Equivalence

HP05 defines two judgments for identifying valid signatures and contexts, which we formalize in Fig. 1. In contrast with HP05, we make explicit that the new bindings do not occur previously in \(\Sigma\) or \(\Gamma\), using freshness constraints such as \(x \not\in \Gamma\). We also make the dependence of all judgments on \(\Sigma\) explicit.

Central in HP05 are the definitions of the validity and definitional equivalence judgments for LF, and of algorithmic judgments for checking equivalence. The validity and definitional equivalence rules are shown in Fig. 2 and 3. There are three judgments for validity and three for equivalence corresponding to objects, type families and kinds respectively:

<table>
<thead>
<tr>
<th>Objects</th>
<th>Type families</th>
<th>Kinds</th>
</tr>
</thead>
<tbody>
<tr>
<td>Validity</td>
<td>(\Gamma \vdash_{\Sigma} \ M : A)</td>
<td>(\Gamma \vdash_{\Sigma} A : K)</td>
</tr>
<tr>
<td>Equivalence</td>
<td>(\Gamma \vdash_{\Sigma} M = N : A)</td>
<td>(\Gamma \vdash_{\Sigma} A = B : K)</td>
</tr>
</tbody>
</table>

These six judgments are defined simultaneously with signature validity (\(\vdash_{\Sigma} \text{ sig}\)) and context validity (\(\vdash_{\Sigma} \text{ ctx}\)) by induction. We added explicit validity hypotheses to some of the rules; these are left implicit in HP05. We also added some (redundant) freshness constraints to some rules in order to be able to use strong induction principles [Urban et al. 2007].
\[ \vdash \Sigma \text{ sig} \]
\[ \vdash \| \text{ sig} \]
\[ \vdash \Sigma \text{ ctx} \]
\[ \vdash \Sigma \text{ type} \]

Fig. 1. Validity rules for signatures and contexts

\[ \vdash \Sigma \text{ ctx} \]
\[ \vdash \Sigma \text{ type} \]
\[ \vdash \Sigma \text{ type} \]
\[ \vdash \Sigma \text{ type} \]
\[ \vdash \Sigma \text{ type} \]
\[ \vdash \Sigma \text{ type} \]
\[ \vdash \Sigma \text{ type} \]
\[ \vdash \Sigma \text{ type} \]

Fig. 2. Validity rules for kinds, type families and objects.
\[
\Gamma \vdash \Sigma M = N : A
\]

\[
\Gamma, (x, A) \in \Sigma \quad \Gamma, c \in \Sigma, \Gamma, (c, A) \in \Sigma
\]

\[
\Gamma \vdash \Sigma M_1 = N_1 : \Pi x : A_2, A_1 \quad \Gamma \vdash \Sigma M_2 = N_2 : A_2 \quad x \# \Gamma
\]

\[
\Gamma \vdash \Sigma M_1 M_2 = N_1 N_2 : A_1[x := M_2]
\]

\[
\Gamma \vdash \Sigma \Gamma A_1 = A_1 : \text{type}
\]

\[
\Gamma \vdash \Sigma A_1'' = A_1 : \text{type} \quad \Gamma \vdash \Sigma A_1 : \text{type} \quad (x, A_1):\Gamma \vdash \Sigma M_2 = N_2 : A_2 \quad x \# \Gamma
\]

\[
\Gamma \vdash \Sigma \lambda x : A_1', M_2 = \lambda x : A_1'', N_2 : \Pi x : A_1, A_2
\]

\[
\Gamma \vdash \Sigma N : \Pi x : A_1, A_2 \quad \Gamma \vdash \Sigma A_1 : \text{type} \quad (x, A_1):\Gamma \vdash \Sigma M x = N x : A_2 \quad x \# \Gamma
\]

\[
\Gamma \vdash \Sigma M = N : \Pi x : A_1, A_2
\]

\[
\Gamma \vdash \Sigma (\lambda x : A_1, M_2) M_1 = N_2[x := N_1] : A_2[x := M_1]
\]

\[
\Gamma \vdash \Sigma M = N : A \quad \Gamma \vdash \Sigma M = N : A \quad \Gamma \vdash \Sigma N = P : A
\]

\[
\Gamma \vdash \Sigma M = P : A
\]

\[
\Gamma \vdash \Sigma A = B : K
\]

\[
\Gamma, (a, K) \in \Sigma
\]

\[
\Gamma \vdash \Sigma a = a : K
\]

\[
\Gamma \vdash \Sigma A = B : \Pi x : C, K \quad \Gamma \vdash \Sigma M = N : C \quad x \# \Gamma
\]

\[
\Gamma \vdash \Sigma A M = B N : K[x := M]
\]

\[
\Gamma \vdash \Sigma A_1 = B_1 : \text{type} \quad \Gamma \vdash \Sigma A_1 : \text{type} \quad (x, A_1):\Gamma \vdash \Sigma A_2 = B_2 : \text{type} \quad x \# \Gamma
\]

\[
\Gamma \vdash \Sigma \Pi x : A_1, A_2 = \Pi x : B_1, B_2 : \text{type}
\]

\[
\Gamma \vdash \Sigma A = B : K \quad \Gamma \vdash \Sigma A = B : K \quad \Gamma \vdash \Sigma B = C : K
\]

\[
\Gamma \vdash \Sigma A = C : K
\]

\[
\Gamma \vdash \Sigma A = B : K \quad \Gamma \vdash \Sigma K = L : \text{kind}
\]

\[
\Gamma \vdash \Sigma A = B : L
\]

\[
\Gamma \vdash \Sigma K = L : \text{kind}
\]

\[
\Gamma \vdash \Sigma \text{type} = \text{type} : \text{kind}
\]

\[
\Gamma \vdash \Sigma A = B : \text{type} \quad \Gamma \vdash \Sigma A : \text{type} \quad (x, A):\Gamma \vdash \Sigma K = L : \text{kind} \quad x \# \Gamma
\]

\[
\Gamma \vdash \Sigma \Pi x : A, K = \Pi x : B, L : \text{kind}
\]

\[
\Gamma \vdash \Sigma K = L : \text{kind} \quad \Gamma \vdash \Sigma L = L' : \text{kind}
\]

\[
\Gamma \vdash \Sigma K = L' : \text{kind}
\]

Fig. 3. Definitional equivalence rules for kinds, type families and objects.
2.3 Algorithmic Equivalence

The definitional equivalence judgment captures equivalence between LF terms, types and kinds declaratively, but it is highly nondeterministic due to the symmetry, transitivity and conversion rules. Accordingly, HP05 introduces algorithmic equivalence judgments that are type- and syntax-directed, and the main contribution of that article is the proof that the algorithmic and declarative systems coincide.

A crucial point of the algorithm in HP05 is that it does not analyze the precise types of objects or kinds of types during equivalence checking; rather it only uses approximate simple types $\tau$ and simple kinds $\kappa$ defined as follows:

$$
\tau ::= a^- | \tau \to \tau' \quad \kappa ::= \text{type}^- | \tau \to \kappa
$$

This simplification is sufficient for obtaining a sound and complete equivalence checking algorithm, and also simplifies the proof development in a number of places.

Similarly, simple contexts $\Delta, \Theta$ consist of lists of pairs $(x, \tau)$ of variables and simple types. We write $\vdash \Delta \text{ setx}$ to indicate that $\Delta$ is valid, i.e. has no repeated variables, and write $\Delta \geq \Delta'$ to indicate that $\Delta$ contains all of the bindings of $\Delta'$ and $\Delta$ is a valid simple context.

Finally, we also introduce simple signatures, also written $\Sigma$, consisting of lists of pairs $(c, \tau)$ or $(a, \kappa)$ of constants and simple kinds or types. We write $\vdash \Sigma \text{ ssig}$ to indicate that $\Sigma$ is a well-formed simple signature with no repeated type or kind assignments.

The erasure function translates families and kinds to simple types and simple kinds:

$$
(a)^- = a^- \\
(A M)^- = A^- \\
(\Pi x:A_1. A_2)^- = A_1^- \to A_2^- \\
(\Pi x:A. K)^- = A^- \to K^- \\
$$

Similarly, we write $\Gamma^-$ for the simple context resulting from replacing each binding $(x, A)$ in $\Gamma$ with $(x, A^-)$. Likewise, we extend the erasure function to map signatures $\Sigma$ to simple signatures $\Sigma^-$ in the natural way.

The rules for the algorithm also employ a weak head reduction relation $(-) \overset{\text{whr}}{\to} (-)$ which performs beta-reductions only at the head of the top-level application of a term. It is defined as

$$
\frac{x \# (A_1, M_1)}{(\lambda x:A_1. M_2) M_1 \overset{\text{whr}}{\to} M_2[x:=M_1]} \quad 
\frac{M_1 \overset{\text{whr}}{\to} M_1'}{M_1 \overset{\text{whr}}{\to} M_1'M_2}
$$

The rules for the equivalence checking algorithm are given in Fig. 4. There are five algorithmic equivalence judgments:

<table>
<thead>
<tr>
<th>Objects</th>
<th>Type families</th>
<th>Kinds</th>
</tr>
</thead>
<tbody>
<tr>
<td>Algorithmic $\Delta \vdash_{\Sigma} M \Leftrightarrow N : \tau$</td>
<td>$\Delta \vdash_{\Sigma} A \Leftrightarrow B : \kappa$</td>
<td>$\Delta \vdash_{\Sigma} K \Leftrightarrow L : \text{kind}^-$</td>
</tr>
<tr>
<td>Structural $\Delta \vdash_{\Sigma} M \leftrightarrow N : \tau$</td>
<td>$\Delta \vdash_{\Sigma} A \leftrightarrow B : \kappa$</td>
<td></td>
</tr>
</tbody>
</table>

Note that the algorithmic rules are type- (or kind-) directed while the structural rules are syntax-directed.

The main results of HP05 are soundness and completeness of the algorithmic judgments relative to the equivalence judgments:

ACM Transactions on Computational Logic, Vol. V, No. N, Month 20YY.
Mechanizing the Metatheory of LF

\[ \Delta \vdash_{\Sigma} M \leftrightarrow N : \tau \]

\[
\begin{align*}
M & \quad \text{whr} \quad \Delta \vdash_{\Sigma} M \leftrightarrow N : a^{-} \\
N & \quad \text{whr} \quad \Delta \vdash_{\Sigma} M \leftrightarrow N' : a^{-}
\end{align*}
\]

\[
\begin{align*}
\Delta & \vdash_{\Sigma} M \leftrightarrow N : a^{-} \\
\Delta & \vdash_{\Sigma} M \rightarrow N : a^{-} \\
\Delta & \vdash_{\Sigma} M \leftrightarrow N : a^{-}
\end{align*}
\]

\[
(x, \tau) : \Delta \vdash_{\Sigma} M x \leftrightarrow N x : \tau_2 \quad x \# (\Delta, M, N)
\]

\[
\Delta \vdash_{\Sigma} M \leftrightarrow N : \tau_1 \rightarrow \tau_2
\]

\[
\begin{align*}
\Delta & \vdash_{\Sigma} M \leftrightarrow N : \tau \\
(x, \tau) & \in \Delta \vdash_{\Sigma} \text{sctx} + \Sigma \text{ssig} \\
\Delta & \vdash_{\Sigma} x \leftrightarrow x : \tau \\
(c, \tau) & \in \Sigma \vdash_{\Sigma} \text{sctx} + \Sigma \text{ssig} \\
\Delta & \vdash_{\Sigma} c \leftrightarrow c : \tau
\end{align*}
\]

\[
\begin{align*}
\Delta & \vdash_{\Sigma} M_1 \leftrightarrow N_1 : \tau_2 \rightarrow \tau_1 \\
\Delta & \vdash_{\Sigma} M_2 \leftrightarrow N_2 : \tau_2 \\
\Delta & \vdash_{\Sigma} M_1 M_2 \leftrightarrow N_1 N_2 : \tau_1
\end{align*}
\]

\[
\begin{align*}
\Delta & \vdash_{\Sigma} A \leftrightarrow B : \kappa \\
\Delta \vdash_{\Sigma} A \leftrightarrow B : \text{type}^{-} \\
\Delta \vdash_{\Sigma} A \leftrightarrow B : \text{type}^{-} \\
(x, \tau) : \Delta \vdash_{\Sigma} A x \leftrightarrow B x : \kappa \quad x \# (\Delta, A, B)
\end{align*}
\]

\[
\begin{align*}
\Delta & \vdash_{\Sigma} A \leftrightarrow B : \tau \rightarrow \kappa \\
\Delta \vdash_{\Sigma} A \leftrightarrow B_1 : \text{type}^{-} \\
(x, \tau) : \Delta \vdash_{\Sigma} A \leftrightarrow B_2 : \text{type}^{-} \\
\Delta \vdash_{\Sigma} A_1 \leftrightarrow B_2 : \text{type}^{-} \\
\Delta \vdash_{\Sigma} A_1 \leftrightarrow B_2 : \text{type}^{-}
\end{align*}
\]

\[
\begin{align*}
\Delta & \vdash_{\Sigma} A \leftrightarrow B : \kappa \\
(a, \kappa) & \in \Sigma \vdash_{\Sigma} \text{sctx} + \Sigma \text{ssig} \\
\Delta & \vdash_{\Sigma} a \leftrightarrow a : \kappa \\
\Delta & \vdash_{\Sigma} A \leftrightarrow B : \tau \rightarrow \kappa \\
\Delta & \vdash_{\Sigma} M \leftrightarrow N : \tau \\
\Delta & \vdash_{\Sigma} A M \leftrightarrow B N : \kappa
\end{align*}
\]

\[
\begin{align*}
\Delta & \vdash_{\Sigma} K \leftrightarrow L : \text{kind}^{-} \\
\vdash_{\Sigma} \text{sctx} + \Sigma \text{ssig} \\
\Delta & \vdash_{\Sigma} \text{type} \leftrightarrow \text{type} : \text{kind}^{-} \\
\Delta & \vdash_{\Sigma} A \leftrightarrow B : \text{type}^{-} \\
(x, \tau) : \Delta \vdash_{\Sigma} K \leftrightarrow L : \text{kind}^{-} \\
\Delta \vdash_{\Sigma} \Pi x : A. K \leftrightarrow \Pi x : B. L : \text{kind}^{-}
\end{align*}
\]

**Fig. 4.** Algorithmic equivalence rules

ACM Transactions on Computational Logic, Vol. V, No. N, Month 20YY.
Similarly if $x$ are needed frequently, explicitly in our formalization, $io$th are straightforward by induction, and both to do with the implicit freshness and validity assumptions that must be handled of the syntactic properties can be found in the electronic appendix, object-level judgments. We will list the main properties however, to aid readability we will only show the statements of most of these properties for the object-level judgments, and we omit symmetric cases. The full formal statements of the syntactic properties can be found in the electronic appendix.

In what follows, we outline the proofs of these results and discuss how we have formalized them, paying particular attention to places where additional lemmas or different proof techniques were needed. We also discuss the gap in the soundness proof of HP05, along with several solutions.

3. THE FORMALIZATION

3.1 Syntactic properties

The proof in HP05 starts by developing a number of useful metatheoretic properties for the validity and equality judgments (shown in Fig. 2), such as weakening, substitution, generalizations of the conversion rules and inversion principles. Most of these properties have multiple parts corresponding to the eight different judgments in the definitional theory of LF. We will list the main properties; however, to aid readability we will only show the statements of most of these properties for the object-level judgments, and we omit symmetric cases. The full formal statements of the syntactic properties can be found in the electronic appendix.

To prove the main syntactic properties we needed two technical lemmas having to do with the implicit freshness and validity assumptions that must be handled explicitly in our formalization. Both are straightforward by induction, and both are needed frequently.

**Lemma 1 (Freshness).** If $x \not\in \Gamma$ and $\Gamma \vdash \Sigma M : A$ then $x \not\in M$ and $x \not\in A$. Similarly, if $x \not\in \Gamma$ and $\Gamma \vdash \Sigma M = N : A$ then $x \not\in M$ and $x \not\in N$ and $x \not\in A$.

**Lemma 2 (Implicit Validity).** If $\Gamma \vdash \Sigma M : A$ or $\Gamma \vdash \Sigma M = N : A$ then $\vdash \Sigma \text{sig}$ and $\vdash \Sigma \text{ctx}$.

**Lemma 3 (Weakening).** Suppose $\vdash \Sigma \Gamma_2 \text{ctx}$ and $\Gamma_1 \subseteq \Gamma_2$.

1. If $\Gamma_1 \vdash \Sigma M : A$ then $\Gamma_2 \vdash \Sigma M : A$.
2. If $\Gamma_1 \vdash \Sigma M = N : A$ then $\Gamma_2 \vdash \Sigma M = N : A$.

**Lemma 4 (Substitution).** Suppose $\Gamma_2 \vdash \Sigma P : C$ and let $\Gamma = \Gamma_1 \emptyset [\{y, C\}] \emptyset \Gamma_2$.

1. If $\vdash \Sigma \Gamma \text{ctx}$ then $\vdash \Sigma \Gamma_1[y := P] \emptyset \Gamma_2 \text{ctx}$.
2. If $\Gamma \vdash \Sigma M : B$ then $\Gamma_1[y := P] \emptyset \Gamma_2 \vdash \Sigma M[y := P] : B[y := P]$.
3. If $\Gamma \vdash \Sigma M = N : A$ then $\Gamma_1[y := P] \emptyset \Gamma_2 \vdash \Sigma M[y := P] = N[y := P] : A[y := P]$.

**Lemma 5 (Context Conversion).** Assume that $\Gamma \vdash \Sigma B : \text{type}$ and $\Gamma \vdash \Sigma A = B : \text{type}$. Then:
LEMMA 6 (FUNCTIONALITY FOR TYPING). Assume that $\Gamma \vdash_{\Sigma} M : C$ and $\Gamma \vdash_{\Sigma} N : C$ and $\Gamma \vdash_{\Sigma} M = N : C$. Then if $\Gamma' = \Gamma \cup \{(y, C)\}$ then $\Gamma' \vdash_{\Sigma} P : B$ then


Since our judgements contain explicit validity hypotheses for contexts, the proof of Lem. 6 relies on the fact that functionality holds also for contexts, namely

LEMMA 7 (FUNCTIONALITY FOR CONTEXTS). If $\vdash_{\Sigma} \Gamma' = \{\!(x, C)\!\} \@ \Gamma \mathbin{ctx}$ and $\Gamma \vdash_{\Sigma} M : C$ then $\vdash_{\Sigma} \Gamma'[x := M] \@ \Gamma \mathbin{ctx}$.

This fact can be established by induction on $\Gamma'$.

LEMMA 8 (VALIDITY). Objects, types and kinds appearing in derivable judgments are valid, that is

(1) If $\Gamma \vdash_{\Sigma} M : A$ then $\Gamma \vdash_{\Sigma} A : \text{type}$.
(2) If $\Gamma \vdash_{\Sigma} M = N : B$ then $\Gamma \vdash_{\Sigma} M : B$ and $\Gamma \vdash_{\Sigma} N : B$ and $\Gamma \vdash_{\Sigma} B : \text{type}$.

LEMMA 9 (TYPING INVERSION). The validity rules are invertible, up to conversion of types and kinds,

(1) If $\Gamma \vdash_{\Sigma} x : A$ then $\exists B. (x, B) \in \Gamma$ and $\Gamma \vdash_{\Sigma} A = B : \text{type}$.
(2) If $\Gamma \vdash_{\Sigma} c : A$ then $\exists B. (c, B) \in \Gamma$ and $\Gamma \vdash_{\Sigma} A = B : \text{type}$.
(3) If $\Gamma \vdash_{\Sigma} M_1 M_2 : A$ then $\exists x A_1 A_2. \Gamma \vdash_{\Sigma} M_1 : \Pi x: A_2. A_1$ and $\Gamma \vdash_{\Sigma} M_2 : A_2 \text{ and } \Gamma \vdash_{\Sigma} A = A_1[x := M_2] : \text{type}$.
(4) If $\Gamma \vdash_{\Sigma} \lambda x : A. M : B$ and $x \notin \Gamma$ then $\exists A'. \Gamma \vdash_{\Sigma} B = \Pi x : A. A' : \text{type and } \Gamma \vdash_{\Sigma} A : \text{type and } (x, A) : \Gamma \vdash_{\Sigma} M : A'$.

Next HP05 established some inversion and invertibility properties for definitional equality:

LEMMA 10 (EQUALITY INVERSION).

(1) If $\Gamma \vdash_{\Sigma} \text{type} = L : \text{kind}$ then $L = \text{type}$.
(2) If $\Gamma \vdash_{\Sigma} A = \Pi x : B_1. B_2 : \text{type and } x \notin \Gamma$ then $\exists A_1 A_2. A = \Pi x : A_1. A_2 \text{ and } \Gamma \vdash_{\Sigma} A_1 = B_1 : \text{type and } (x, A_1) : \Gamma \vdash_{\Sigma} A_2 = B_2 : \text{type}$.
(3) If $\Gamma \vdash_{\Sigma} K = \Pi x : B_1. L_2 : \text{kind and } x \notin \Gamma$ then $\exists K_1 K_2. K = \Pi x : A_1. K_2 \text{ and } \Gamma \vdash_{\Sigma} A_1 = B_1 : \text{type and } (x, A_1) : \Gamma \vdash_{\Sigma} K_2 = L_2 : \text{kind}$.

Finally, we can prove that the product type constructor is injective up to definitional equality, which is needed for soundness:

LEMMA 11 (PRODUCT INJECTIVITY). Suppose $x \notin \Gamma$.

(1) If $\Gamma \vdash_{\Sigma} \Pi x : A_1. A_2 = \Pi x : B_1. B_2 : \text{type then } \exists A_1 A_2. A_1 = B_1 : \text{type and } (x, A_1) : \Gamma \vdash_{\Sigma} A_2 = B_2 : \text{type}$.
(2) If $\Gamma \vdash_{\Sigma} \Pi x : A. K = \Pi x : B. L : \text{kind then } \Gamma \vdash_{\Sigma} A = B : \text{type and } (x, A) : \Gamma \vdash_{\Sigma} K = L : \text{kind}$.

All the metatheoretic properties given above can be proved as stated in HP05 (appealing to Lem. 1 and 2 as necessary); however, since all of the definitional judgments of LF are interdependent, each inductive proof must consider all 35 cases, making each proof nontrivial as a practical matter (it is one of the biggest parts of our formalization).
HP05 organize the proofs of these metatheoretic properties very neatly. For example, as shown in Lem. 8 the validity judgment of terms implies the validity of the type. However, in order to establish this a number of auxiliary facts have to be proved first which depend on this property. In order to get the proof through, some of HP05’s rules given in Fig. 2 are formulated to explicitly include validity constraints such as $\Gamma \vdash_{\Sigma} A : type$ and $\Gamma \vdash_{\Sigma} K : kind$. After proving the above properties, however, we can show that these extra hypotheses are not needed, by establishing stronger forms of the rules.

**Lemma 12 (Strong versions of rules).** The following rules are admissible:

1. $\Gamma \vdash_{\Sigma} M_1 : \Pi x : A_2, A_1 \quad \Gamma \vdash_{\Sigma} M_2 : A_2$

   $\frac{\quad \Gamma \vdash_{\Sigma} M_1 M_2 : A_1[x:=M_2]}{\Gamma \vdash_{\Sigma} M_1 : M_2 : A_1[x:=M_2]}$

2. $\Gamma \vdash_{\Sigma} A : \Pi x : B, K \quad \Gamma \vdash_{\Sigma} M : B$

   $\frac{\quad \Gamma \vdash_{\Sigma} A M : K[x:=M]}{\Gamma \vdash_{\Sigma} (\lambda x : A_1, M_2) M_1 = N_2[x:=N_1] : A_2[x:=M_1]}$

3. 2

**3.2 Algorithmic equivalence**

The main metatheoretic properties of algorithmic equivalence proved in Sec. 3 of HP05 are symmetry and transitivity. Several properties of weak head reduction and erasure needed later in HP05 are also proved. Most of the proofs were straightforward to formalize, given the details in HP05 (where provided). However, there were a few missing lemmas and other complications. The algorithmic system is less well-behaved than the definitional system because derivable judgments may have ill-formed arguments; for example, the judgment $\Gamma \vdash_{\Sigma} (\lambda x : a, c) y \Rightarrow c : b^-$ is derivable, for any object term $y$, provided that $(c, b) \in \Sigma$ since $(\lambda x : a, c) y \Rightarrow_{\text{whr}} c$. Thus, analogues of Lem. 1 and 2 do not hold for the algorithmic system, and in rules involving binding we need to impose additional freshness constraints. Moreover, proof search in the algorithmic system is not necessarily terminating because $(\_) \Rightarrow_{\text{whr}} (\_)$ may diverge if called on ill-formed terms such as $(\lambda x : a, x) (\lambda x : a, x)$.

The erasure preservation lemma establishes basic properties of erasure which are frequently needed in HP05:

**Lemma 13 (Erasure preservation).**

1. If $\Gamma \vdash_{\Sigma} A = B : K$ then $A^- = B^-.$

2. If $\Gamma \vdash_{\Sigma} K = L : \text{kind}$ then $K^- = L^-.$

3. If $(x, A) :: \Gamma \vdash_{\Sigma} B : \text{type}$ then $B^- = B[x:=M]^-$

4. If $(x, A) :: \Gamma \vdash_{\Sigma} K : \text{kind}$ then $K^- = K[x:=M]^-.$

However, we found that the hypotheses of parts 3 and 4 are unnecessary. Indeed, we can easily prove:

**Lemma 14 (Erasure cancels substitution).** For any type family $A$, kind $K$, and substitution $\sigma$, we have

1. $A[\sigma]^-= A^-$

2. $K[\sigma]^-= K^-.$
In the proofs of symmetry and transitivity of the algorithmic judgments (Thm. 3 and Thm. 4), we also needed the following algorithmic erasure preservation lemma (it is omitted from HP05, but straightforward by induction):

**Lemma 15 (Algorithmic Erasure Preservation).**
(1) If $\Delta \vdash_{\Sigma} A \leftrightarrow B : \kappa$ then $A^- = B^-$.  
(2) If $\Delta \vdash_{\Sigma} A \leftrightarrow B : \kappa$ then $A^- = B^-$.  
(3) If $\Delta \vdash_{\Sigma} K \leftrightarrow L : \text{kind}^-$ then $K^- = L^-$.  

The determinacy lemma establishes several important properties of weak head reduction and algorithmic equivalence.

**Lemma 16 (Determinacy).** Suppose that $\vdash \Sigma \text{ sig}$ and $\vdash \Delta$ setx.
(1) If $M \xrightarrow{\text{ whr}} M'$ and $M \xrightarrow{\text{ whr}} M''$ then $M' = M''$.  
(2) If $\Delta \vdash_{\Sigma} M \leftrightarrow N : \tau$ then $\not\exists M'$.  
(3) If $\Delta \vdash_{\Sigma} M \leftrightarrow N : \tau$ then $\not\exists N'$.  
(4) If $\Delta \vdash_{\Sigma} M \leftrightarrow N : \tau$ and $\Delta \vdash_{\Sigma} M \leftrightarrow N : \tau'$ then $\tau = \tau'$.  
(5) If $\Delta \vdash_{\Sigma} A \leftrightarrow B : \kappa$ and $\Delta \vdash_{\Sigma} A \leftrightarrow B : \kappa'$ then $\kappa = \kappa'$.  

However, we needed generalized forms of parts 4 and 5 in the proof of transitivity (Thm. 4). These properties are also later used in Thm. 13 in proving decidability of the algorithmic rules.

**Lemma 17 (Generalized Determinacy).** Suppose that $\vdash \Sigma \text{ sig}$ and $\vdash \Delta$ setx.
(1) If $\Delta \vdash_{\Sigma} M \leftrightarrow N : \tau$ then $\Delta \vdash_{\Sigma} N \leftrightarrow M : \tau$.  
(2) If $\Delta \vdash_{\Sigma} A \leftrightarrow B : \kappa$ then $\Delta \vdash_{\Sigma} B \leftrightarrow A : \kappa$.

Verifying symmetry of the algorithmic judgments is then straightforward, using properties established so far.

**Theorem 3 (Symmetry of Algorithmic Equivalence).**  
1. If $\Delta \vdash_{\Sigma} M \leftrightarrow N : \tau$ then $\Delta \vdash_{\Sigma} N \leftrightarrow M : \tau$.  
2. If $\Delta \vdash_{\Sigma} M \leftrightarrow N : \tau$ then $\Delta \vdash_{\Sigma} N \leftrightarrow M : \tau$.  
3. If $\Delta \vdash_{\Sigma} A \leftrightarrow B : \kappa$ then $\Delta \vdash_{\Sigma} B \leftrightarrow A : \kappa$.  
4. If $\Delta \vdash_{\Sigma} A \leftrightarrow B : \kappa$ then $\Delta \vdash_{\Sigma} A \leftrightarrow B : \kappa'$.  
5. If $\Delta \vdash_{\Sigma} K \leftrightarrow L : \text{kind}^-$ then $\Delta \vdash_{\Sigma} L \leftrightarrow K : \text{kind}^-$.  

However, verifying transitivity required more work.

**Theorem 4 (Transitivity of Algorithmic Equivalence).** Suppose that $\vdash \Sigma \text{ sig}$ and $\vdash \Delta$ setx.
(1) If $\Delta \vdash_{\Sigma} M \leftrightarrow N : \tau$ and $\Delta \vdash_{\Sigma} N \leftrightarrow P : \tau$ then $\Delta \vdash_{\Sigma} M \leftrightarrow P : \tau$.  
(2) If $\Delta \vdash_{\Sigma} M \leftrightarrow N : \tau$ and $\Delta \vdash_{\Sigma} N \leftrightarrow P : \tau$ then $\Delta \vdash_{\Sigma} M \leftrightarrow P : \tau$.  
(3) If $\Delta \vdash_{\Sigma} A \leftrightarrow B : \kappa$ and $\Delta \vdash_{\Sigma} B \leftrightarrow C : \kappa$ then $\Delta \vdash_{\Sigma} A \leftrightarrow C : \kappa$.  
(4) If $\Delta \vdash_{\Sigma} A \leftrightarrow B : \kappa$ and $\Delta \vdash_{\Sigma} B \leftrightarrow C : \kappa$ then $\Delta \vdash_{\Sigma} A \leftrightarrow C : \kappa$.  
(5) If $\Delta \vdash_{\Sigma} K \leftrightarrow L : \text{kind}^-$ and $\Delta \vdash_{\Sigma} L \leftrightarrow L' : \text{kind}^-$ then $\Delta \vdash_{\Sigma} K \leftrightarrow L' : \text{kind}^-$.  

**Proof.** As described in HP05, the proof is by simultaneous induction on the two derivations. For types and kinds, this simultaneous induction can be avoided by performing induction over one derivation and using inversion principles. For the object-level judgments (cases 1 and 2), we formalize this argument in Isabelle by
defining object-level algorithmic judgments instrumented with a height argument, and prove parts 1 and 2 by well-founded induction on the sum of the heights of the derivations.

Because we use induction over the height of the instrumented derivation, we cannot take advantage of the “strong” induction principles for algorithmic derivations [Urban et al., 2007]. As a result, there are several cases where we need to perform some explicit α-conversion and renaming steps; these are places in an informal proof where one usually appeals to renaming principles “without loss of generality”. In the current version of the nominal datatype package offers strong inversion principles that ameliorate this difficulty [Bergbhofer and Urban 2008].

The generalized determinacy property (Lem. 17) is needed here in the case of structural equivalence of applications. □

**Strengthening.** At this point in the development, we can also prove that the algorithmic judgments satisfy strengthening; that is, unused variables can be removed from the context without harming derivability of a conclusion. Strengthening is not discussed in HP05 until later in the article, but we found it helpful in the proof of soundness. We first need an (easily established) freshness-preservation property of weak head reduction.

**Lemma 18 (Weak head reduction preserves freshness).**

*If* \( M \xrightarrow{\text{whr}} N \) *and* \( x \not\in M \) *then* \( x \not\in N \).

With this property in hand, strengthening for algorithmic and structural equivalence can be established by induction on the structure of judgments, making use of basic properties of freshness, valid contexts, and the previous lemma as necessary.

**Lemma 19 (Strengthening of algorithmic equivalence).** *Suppose that* \( x \not\in (\Delta', M, N) \). *Then:*

1. If \( \Delta' \circ ([x, \tau]) \circ \Delta \vdash_{\Sigma} M \leftrightarrow N : \tau \) *then* \( \Delta' \circ \Delta \vdash_{\Sigma} M \leftrightarrow N : \tau \).
2. If \( \Delta' \circ ([x, \tau]) \circ \Delta \vdash_{\Sigma} M \leftrightarrow N : \tau \) *then* \( \Delta' \circ \Delta \vdash_{\Sigma} M \leftrightarrow N : \tau \).

**Proof.** Straightforward induction on derivations, using properties of freshness. Lem. 18 is needed in the cases involving weak head reduction to maintain the freshness constraints needed for the induction hypothesis. □
3.3 Completeness

The proof of completeness involves a Kripke-style logical relations argument. We can define the logical relation for objects, types, and substitutions, by induction on the structure of simple types $\tau$ and kinds $\kappa$ and simple contexts $\Theta$, respectively, as shown in Fig. 5. This kind of logical relation is called Kripke-style because the case for function types is modeled on Kripke’s possible-worlds semantics for intuitionistic logic: it is indexed by a variable context $\Delta$ and in the case for function types and kinds, we quantify over all valid extensions to $\Delta$ when considering the argument terms $M'$, $N'$.

The key steps in proving completeness are showing that logically related terms are algorithmically equivalent (Thm. 5) and that definitionally equivalent terms are logically related (Thm. 6). Many properties can be established by an induction on the structure of types, appealing to the properties of the algorithmic judgments established in section 3 of HP95 and the definition of the logical relation.

**Lemma 20 (Logical relation weakening).** Suppose $\Delta' \geq \Delta$.

1. If $\Delta \vdash_\Sigma M = N \in [\tau]$ then $\Delta' \vdash_\Sigma M = N \in [\tau]$.
2. If $\Delta \vdash_\Sigma A = B \in [\kappa]$ then $\Delta' \vdash_\Sigma A = B \in [\kappa]$.
3. If $\Delta \vdash_\Sigma \sigma = \theta \in [\Theta]$ then $\Delta' \vdash_\Sigma \sigma = \theta \in [\Theta]$.

**Theorem 5 (Logically related terms are algorithmically equivalent).**

Suppose $\vdash \Delta \text{ setx}$.

1. If $\Delta \vdash_\Sigma M = N \in [\tau]$ then $\Delta \vdash_\Sigma M \leftrightarrow N : \tau$.
2. If $\Delta \vdash_\Sigma A \leftrightarrow B : \kappa$ then $\Delta \vdash_\Sigma A = B \in [\kappa]$.

**Lemma 21 (Closure under head expansion).

1. If $M \vdash N'$ and $\Delta \vdash_\Sigma M' = N \in [\tau]$ then $\Delta \vdash_\Sigma M = N \in [\tau]$.
2. If $N \vdash M'$ and $\Delta \vdash_\Sigma M = N' \in [\tau]$ then $\Delta \vdash_\Sigma M = N \in [\tau]$.

**Lemma 22 (Logical relation symmetry).

1. If $\Delta \vdash_\Sigma M = N \in [\tau]$ then $\Delta \vdash_\Sigma N = M \in [\tau]$.
2. If $\Delta \vdash_\Sigma A = B \in [\kappa]$ then $\Delta \vdash_\Sigma B = A \in [\kappa]$.
3. If $\Delta \vdash_\Sigma \sigma = \theta \in [\Theta]$ then $\Delta \vdash_\Sigma \theta = \sigma \in [\Theta]$.

**Lemma 23 (Logical relation transitivity).

Suppose that $\vdash \Sigma \text{ sig}$ and $\vdash \Delta \text{ setx}$.

1. If $\Delta \vdash_\Sigma M = N \in [\tau]$ and $\Delta \vdash_\Sigma N = P \in [\tau]$ then $\Delta \vdash_\Sigma M = P \in [\tau]$.
2. If $\Delta \vdash_\Sigma A = B \in [\kappa]$ and $\Delta \vdash_\Sigma B = C \in [\kappa]$ then $\Delta \vdash_\Sigma A = C \in [\kappa]$.
3. If $\Delta \vdash_\Sigma \sigma = \theta \in [\Theta]$ and $\Delta \vdash_\Sigma \theta = \delta \in [\Theta]$ then $\Delta \vdash_\Sigma \sigma = \delta \in [\Theta]$.

The proof that definitionally equal terms are logically related required some care to formalize. The key step is showing that applying logically related substitutions to definitionally equal terms yields logically related terms. Establishing this (via the following lemma) required identifying and proving a number of standard properties of simultaneous substitutions. In contrast, reasoning about single substitutions sufficed almost everywhere else in the formalization.

**Lemma 24.** Suppose $\vdash \Delta \text{ setx and } \Delta \vdash_\Sigma \sigma = \theta \in [\Gamma^-]$.

ACM Transactions on Computational Logic, Vol. V, No. N, Month 20YY.
(1) If $\Gamma \vdash_{\Sigma} M = N : A$ then $\Delta \vdash_{\Sigma^-} M[\sigma] = N[\theta] \in [A^-]$.
(2) If $\Gamma \vdash_{\Sigma} A = B : K$ then $\Delta \vdash_{\Sigma^-} A[\sigma] = B[\theta] \in [K^-]$.

The last step needed to establish completeness is to show that the identity substitution over a given context (written $id_\Gamma$) is related to itself:

**Lemma 25.** If $\vdash_{\Sigma} \Gamma$ ct$x$ then $\Gamma^- \vdash_{\Sigma^-} id_\Gamma = id_\Gamma \in [\Gamma^-]$.

**Theorem 6 (Definitionally equal terms are logically related).**
(1) If $\Gamma \vdash_{\Sigma} M = N : A$ then $\Gamma^- \vdash_{\Sigma^-} M = N \in [A^-]$.
(2) If $\Gamma \vdash_{\Sigma} A = B : K$ then $\Gamma^- \vdash_{\Sigma^-} A = B \in [K^-]$.

**Corollary 1 (Completeness).**
(1) If $\Gamma \vdash_{\Sigma} M = N : A$ then $\Gamma^- \vdash_{\Sigma^-} M \equiv N : A^-$.  
(2) If $\Gamma \vdash_{\Sigma} A = B : K$ then $\Gamma^- \vdash_{\Sigma^-} A \equiv B : K^-$.  
(3) If $\Gamma \vdash_{\Sigma} K = L : \text{kind}$ then $\Gamma^- \vdash_{\Sigma^-} K \equiv L : \text{kind}$.

Note that part 3 of Cor. 1 was omitted from HP05, but it is straightforward to prove by induction given parts 1 and 2, and algorithmic transitivity and symmetry.

### 3.4 Soundness

Soundness of algorithmic object (or type, or kind) equivalence means that if two well-formed objects (or type families, or kinds respectively) are algorithmically equivalent then they are also definitionally equivalent. For example, for objects, Thm. 2(1) states:

If $\Gamma^- \vdash_{\Sigma^-} M \equiv N : A^-$ and $\Gamma \vdash_{\Sigma} M : A$ and $\Gamma \vdash_{\Sigma} N : A$
then $\Gamma \vdash_{\Sigma} M = N : A$.

First, though, since the algorithmic judgments perform weak head reduction, we must show that weak head reduction preserves well-formedness:

**Lemma 26 (Subject reduction).** Suppose $M \xrightarrow{whr} M'$ and $\Gamma \vdash_{\Sigma} M : A$. Then $\Gamma \vdash_{\Sigma} M' : A$.

Naturally, since algorithmic and structural equivalences for objects and types are defined by simultaneous induction, we must also prove a simultaneous soundness property for the structural equivalence judgments. For example, to prove Thm. 2(1), we also need to show by simultaneous induction that:

If $\Gamma^- \vdash_{\Sigma^-} M \equiv N : \tau$ and $\Gamma \vdash_{\Sigma} M : A$ and $\Gamma \vdash_{\Sigma} N : B$
then $\Gamma \vdash_{\Sigma} M = N : A$ and $\Gamma \vdash_{\Sigma} A = B : \text{type} \quad \text{and} \quad \tau^- = \tau$ and $B^- = \tau$.

In contrast to completeness, the proof of soundness in HP05 proceeds by entirely syntactic techniques, by induction over the structure of algorithmic and structural derivations, using standard syntactic properties and subject reduction. Our initial formalization attempt followed the proofs given by HP05. However, we encountered two difficulties which were not addressed in the article. Both difficulties have to do with algorithmic rules for checking equivalence at function types (or function kinds) using extensionality. In the rest of this section, we first discuss and address a minor difficulty involving extensionality in the proof of Thm. 2(1). We then discuss a more serious complication in proving soundness at the level of types, and show how to fix the problem. We conclude by summarizing the soundness results.
Soundness for algorithmic object equivalence. In proving the soundness of algorithmic extensionality for objects arising in part 1 of Thm. 2, recall that we have a derivation of the form:

\[
(x, \tau_1); \Gamma^{-} \vdash \Sigma M x \leftrightarrow N x : \tau_2 \quad x \# (\Gamma^{-}, M, N)
\]

and we also know that \(\Gamma^{-} \vdash \Sigma M : A\) and \(\Gamma^{-} \vdash \Sigma N : A\) for some \(A\) with \(A^{-} = \tau_1 \rightarrow \tau_2\). In order to apply the induction hypothesis, we need to know that \(M x\) and \(N x\) are well-formed in an extended context \((x, A_1):\Gamma^{-}\). HP05’s proof begins by assuming that \(\Gamma^{-} \vdash \Sigma M : \Pi x : A_1, A_2\) and \(\Gamma^{-} \vdash \Sigma N : \Pi x : A_1, A_2\), and proceeding using inversion properties. However, it is not immediately clear that \(A^{-} = \tau_1 \rightarrow \tau_2\) implies that \(A = \Pi x : A_1, A_2\) for some \(A_1\) and \(A_2\); indeed, this can fail to be the case if \(A\) is not well-formed. Instead, we first need the following inversion principles for erasure:

**Lemma 27 (Erasure inversion).**

1. If \(\Gamma \vdash \Sigma A : \Pi x : B. K\) then \(\exists c. A^{-} = c^{-}\).
2. If \(\tau_1 \rightarrow \tau_2 = A^{-}\) and \(\Gamma \vdash \Sigma A : \text{type and } x \# A\) then \(\exists A_1 A_2. A = \Pi x : A_1, A_2\).
3. If \(\tau \rightarrow \kappa = K^{-}\) and \(x \# K\) then \(\exists A L K = \Pi x : A. L\).

**Proof.** Part 1 follows by induction on the derivation. Parts 2 and 3 follow by induction on the structure of \(A\) and \(K\) respectively. In the case for type applications \(A M\), clearly \(A\) has a \(\Pi\)-kind, but by part 1, \(A\) erases to a constant, contradicting the assumption that \(A^{-} = \tau_1 \rightarrow \tau_2\). So the case is vacuous. The remaining cases of part 2 are straightforward, as are the cases for part 3. \(\square\)

Using Lem. 27, we can complete the proof of the first part of Thm. 2 as described in HP05:

**Lemma 28 (Soundness of algorithmic object equivalence).**

1. If \(\Gamma^{-} \vdash \Sigma^{-} M \leftrightarrow N : A^{-}\) and \(\Gamma \vdash \Sigma M : A\) and \(\Gamma \vdash \Sigma N : A\) then \(\Gamma \vdash \Sigma M = N : A\).
2. If \(\Gamma^{-} \vdash \Sigma^{-} M \leftrightarrow N : \tau\) and \(\Gamma \vdash \Sigma M : A\) and \(\Gamma \vdash \Sigma N : B\) then \(\Gamma \vdash \Sigma M = N : A\) and \(\Gamma \vdash \Sigma A = B : \text{type and } A^{-} = \tau\) and \(B^{-} = \tau\).

Soundness for algorithmic type equivalence. The second problem we encountered arises in the proof of soundness for the extensionality rule in the algorithmic type equivalence judgment (part 3 of Thm. 2). In this case, we have a derivation of the form:

\[
(x, \tau); \Gamma^{-} \vdash \Sigma A x \leftrightarrow B x : \kappa \quad x \# (\Gamma^{-}, A, B)
\]

We can easily show that the induction hypothesis applies, using the same technique as above, ultimately deriving \((x, A'):\Gamma \vdash \Sigma A x = B x : K\) for some \(A'\) and \(K\). However, we cannot complete the proof of this case in the same way as for object extensionality, because HP05’s variant of LF does not include a type-level extensionality rule.
Fig. 6. Weak algorithmic type equivalence judgment

\[
\begin{align*}
\Delta \vdash_{\Sigma} A &= B : \kappa \\
(a, \kappa) &\in \Sigma \vdash \Sigma \text{ssig} \vdash \Delta \text{setz} \\
\Delta \vdash_{\Sigma} a &= a : \kappa \\
\Delta \vdash_{\Sigma} \kappa &= \Delta \vdash_{\Sigma} M \leftrightarrow N : \tau \quad \Delta \vdash_{\Sigma} A \equiv B : \kappa \\
\Delta \vdash_{\Sigma} \Pi \vdash_{\Pi} A_1 \equiv B_1 : \text{type}^- \quad \Delta \vdash_{\Sigma} A_2 \equiv B_2 : \text{type}^- \quad x \# (\Delta, A_1, B_1) \\
\Delta \vdash_{\Sigma} \Pi \vdash_{\Pi} A_1 \equiv B_1 : \text{type}^- \\
\Delta \vdash_{\Sigma} \Pi \vdash_{\Pi} A_2 \equiv B_2 : \text{type}^- \\
\end{align*}
\]

that would permit us to conclude that \( \Gamma \vdash_{\Sigma} A = B : \Pi x : C. K \).

It was not immediately clear to us whether the original proof could be repaired. There appear to be several ways to fix this problem by changing the definitional or algorithmic rules. One way is simply to add the above extensionality rule for types to the definitional system. Using our formalization, we were easily able to verify that this solves the problem and does not introduce any new complications. For this we had to make sure that every proof done earlier is either not affected by this additional rule or can be extended to include it.

A second solution, suggested by Harper\(^1\), is to observe that the original algorithmic rules were unnecessarily general. In the absence of type-level \( \lambda \)-abstraction, the weaker, syntax-directed type equivalence rules shown in Fig. 6 suffice. We can easily prove that these rules are sound with respect to definitional type equivalence:

**Lemma 29 (Soundness of weak type equivalence).**
If \( \Gamma^- \vdash_{\Sigma^-} A = B : \kappa \) and \( \Gamma^- \vdash_{\Sigma^-} A : K \) and \( \Gamma^- \vdash_{\Sigma^-} B : L \), then \( \Gamma^- \vdash_{\Sigma^-} A = B : K, \Gamma^- \vdash_{\Sigma^-} K = L : \text{kind}, K^- = \kappa \) and \( L^- = \kappa \).

**Proof.** Similar to the proof of soundness of algorithmic and structural type equivalence from HP05. Requires soundness of object equivalence (Lem 28).

With this change, we can prove completeness using a slightly modified logical relation: the type-level logical relation needs to be redefined as

\[
\Delta \vdash_{\Sigma} A \equiv B : \kappa = \Delta \vdash_{\Sigma} A \equiv B : \kappa .
\]

The first two solutions however establish soundness only for variants of the definitions in HP05. In particular, the first shows that the original algorithmic rules are sound with respect to a stronger notion of definitional equality, while the second gives a correct modified algorithm for the original definitional rules. Either solution appears reasonable, but neither tells us whether the original equivalence algorithm is sound with respect to the original definitional system in HP05. We felt it was important to determine whether or not a change to the definitions is truly necessary to recover soundness. In the rest of this section we show that the original results hold as stated.

\(^1\) personal communication

ACM Transactions on Computational Logic, Vol. V, No. N, Month 20YY.
Since we already established that weak type equivalence implies definitional equivalence (for well-formed terms), it suffices to show that the original algorithmic type equivalence judgments imply weak type equivalence. To do so, we need to show that weak type equivalence admits extensionality (Lem. 34 below). This is nontrivial: we first need to develop some syntactic properties of algorithmic equivalence for objects, in particular that if \( \Delta \vdash_{\Sigma} x \equiv x : \tau \) then \((x, \tau) \in \Delta\). This seems obvious, but the proof is slightly subtle because the algorithmic equivalence judgment is type-directed, not syntax-directed. Indeed, if we try to prove this directly by induction, then in the case where \( x \) has function type, the inductive hypothesis does not apply.

Instead, we need to show something more general: for any term \( M_0 \) of the form \( x \ y_1 \cdot \cdot \cdot y_n \), if \( M_0 \) is algorithmically equivalent to itself then every free variable of \( M_0 \) appears in \( \Delta \) with an appropriate type. We say that such an object \( M_0 \) is an applied variable, defined formally as follows:

\[
M_0 ::= x \mid M_0 x
\]

that is, it is a variable applied to a sequence of variables. Clearly, applied variables are weak head normal forms:

**Lemma 30.** If \( M_0 \) is an applied variable then \( M_0 \) is in weak head normal form.

We then introduce a weak well-formedness relation \( \Delta \vdash_0 M_0 : \tau \) for applied variables, defined as follows:

\[
\frac{(x, \tau) \in \Delta}{\Delta \vdash_0 x : \tau} \quad \frac{\Delta \vdash_0 M_0 : \tau_1 \rightarrow \tau_2 \quad (y, \tau_1) \in \Delta}{\Delta \vdash_0 M_0 y : \tau_2}
\]

It is easy to show that that \( \vdash_0 \) satisfies strengthening:

**Lemma 31.** If \((y, \tau') :\Delta \vdash_0 M_0 : \tau \) and \( y \not\equiv M_0 \) then \( \Delta \vdash_0 M_0 : \tau \).

Furthermore, if an applied variable is algorithmically or structurally equivalent to itself, then it is weakly well-formed:

**Lemma 32.** Suppose \( M_0 \) is an applied variable and \( \vdash \Delta \) sctx.

\( 1 \) If \( \Delta \vdash_{\Sigma} M_0 \equiv M_0 : \tau \) then \( \Delta \vdash_0 M_0 : \tau \).

\( 2 \) If \( \Delta \vdash_{\Sigma} M_0 \equiv M_0 : \tau \) then \( \Delta \vdash_0 M_0 : \tau \).

**Proof.** Induction on derivations. Lem. 30 is needed to show that the cases involving weak head reduction are vacuous. The only other interesting case is the case for an extensionality rule

\[
\frac{(x, \tau_1) :\Delta \vdash_{\Sigma} M_0 x \equiv M_0 x : \tau_2 \quad x \not\equiv (\Delta, M_0, M_0)}{\Delta \vdash_{\Sigma} M_0 \equiv M_0 : \tau_1 \rightarrow \tau_2}
\]

By induction, we have that \((x, \tau_1) :\Delta \vdash_0 M_0 x : \tau_2\). By inversion, we can show that \((x, \tau_1) :\Delta \vdash_0 M_0 : \tau_1 \rightarrow \tau_2\). To complete the proof, we use Lem. 31 to show that \( \Delta \vdash_0 M_0 : \tau_1 \rightarrow \tau_2 \), which follows since \( x \not\equiv M_0 \).

**Corollary 2.** If \( \Delta \vdash_{\Sigma} x \equiv x : \tau \) and \( \vdash \Delta \) sctx then \((x, \tau) \in \Delta\).

We also need to establish strengthening for weak algorithmic type equivalence:
Lemma 33 (Strengthening of weak type equivalence).
If \( \Delta' \vdash \Gamma \vdash \Sigma \) \( A \leftarrow B : \kappa \) and \( x \# (\Delta', A, B) \) then 
\( \Delta' \vdash \Gamma \vdash \Sigma \) \( A \leftarrow B : \kappa \).

Proof. Straightforward induction on derivations. Note that we need Lem. 19 here in the case for structural equivalence of type applications.

We now establish the admissibility of extensionality for weak type equivalence:

Lemma 34 (Extensionality of weak type equivalence).
If \( (x, \tau) : \Delta \vdash \Gamma \vdash \Sigma \) \( A \leftarrow B : \kappa \) and \( x \in \Gamma \vdash \Sigma \) then 
\( \Delta \vdash \Gamma \vdash \Sigma \) \( A \leftarrow B : \tau \rightarrow \kappa \).

Proof. By inversion, we have subderivations \( (x, \tau) : \Delta \vdash \Gamma \vdash \Sigma \) \( A \leftarrow B : \tau \rightarrow \kappa \) and \( (x, \tau) : \Delta \vdash \Gamma \vdash \Sigma \) \( x \equiv x : \tau' \) for some \( \tau' \). Using Cor. 2 on the second subderivation we have that \( (x, \tau') \in \Delta \) and using the validity of \( (x, \tau) : \Delta \) we know that \( \tau = \tau' \). Hence, \( (x, \tau) : \Delta \vdash \Gamma \vdash \Sigma \) \( A \leftarrow B : \tau \rightarrow \kappa \). Using Lem. 33 we conclude \( \Delta \vdash \Gamma \vdash \Sigma \) \( A \leftarrow B : \tau \rightarrow \kappa \).

Lemma 35. Suppose \( \Delta \vdash \Gamma \vdash \Sigma \). Then:
1. If \( \Delta \vdash \Gamma \vdash \Sigma \) \( A \leftarrow B : \kappa \) then \( \Delta \vdash \Gamma \vdash \Sigma \) \( A \leftarrow B : \kappa \).
2. If \( \Delta \vdash \Gamma \vdash \Sigma \) \( A \leftarrow B : \kappa \) then \( \Delta \vdash \Gamma \vdash \Sigma \) \( A \leftarrow B : \kappa \).

Proof. By induction on the structure of derivations. The case for the algorithmic type extensionality rule requires Lem. 34.

The proof of Thm. 2 is completed as follows.

Lemma 36 (Soundness of algorithmic type equivalence).
1. If \( \Gamma \vdash \Sigma \) \( A \leftarrow B : \kappa \) and \( \Gamma \vdash \Sigma \) \( A : K \) and \( \Gamma \vdash \Sigma \) \( B : K \) then 
\( \Gamma \vdash \Sigma \) \( A = B : K \).
2. If \( \Gamma \vdash \Sigma \) \( A \leftarrow B : \kappa \) and \( \Gamma \vdash \Sigma \) \( A : K \) and \( \Gamma \vdash \Sigma \) \( B : L \) then 
\( \Gamma \vdash \Sigma \) \( A = B : K \), \( \Gamma \vdash \Sigma \) \( K = L : \text{kind} \), \( \kappa = \kappa \), and \( \text{L} = \text{L} \).

Proof. Immediate using Lem. 35 and 29.

Lemma 37 (Soundness of algorithmic kind equivalence).
If \( \Gamma \vdash \Sigma \) \( K \leftarrow L : \text{kind} \) and \( \Gamma \vdash \Sigma \) \( K : \text{kind} \) and \( \Gamma \vdash \Sigma \) \( L : \text{kind} \) then \( \Gamma \vdash \Sigma \) \( K = L : \text{kind} \).

Proof. As in HP05, using Lem. 36 as necessary.

Thm. 2 follows immediately from Lem. 28, 36 and 37.

3.5 Algorithmic typechecking

After the soundness and completeness proof, HP05 introduces an algorithmic version of the typechecking judgment, proves additional syntactic properties of definitional equivalence, sketches proofs of decidability, and discusses quasicanonical forms and adequacy of LF encodings of object languages. We formalized many of these results and we will discuss them in the next few sections.

The typechecking algorithm in HP05 traverses terms, types and kinds in a syntax-directed manner, using the algorithmic equivalence judgment in certain places. The
definition of algorithmic typechecking in HP05 omitted explicit definitions of algorithmic signature and context validity. In our formalization, we added these (obvious) rules, as shown in Fig. 7. The remaining rules are the same as in HP05 except for a trivial typographical error in the rule for type constants. Proving the soundness and completeness of algorithmic typechecking is a (mostly) straightforward exercise using soundness and completeness of algorithmic equivalence and various syntactic properties:

**Theorem 7 (Soundness of Algorithmic Typechecking).**

1. If $\vdash \Sigma \Rightarrow \text{sig}$ then $\vdash \Sigma \Rightarrow \text{sig}$.
2. If $\vdash \Gamma \Rightarrow \text{ctx}$ then $\vdash \Gamma \Rightarrow \text{ctx}$.
If $\Gamma \vdash_{\Sigma} M \Rightarrow A$ then $\Gamma \vdash_{\Sigma} M : A$.
(4) If $\Gamma \vdash_{\Sigma} A \Rightarrow K$ then $\Gamma \vdash_{\Sigma} A : K$.
(5) If $\Gamma \vdash_{\Sigma} K \Rightarrow \text{kind}$ then $\Gamma \vdash_{\Sigma} K : \text{kind}$.

Theorem 8 (Completeness of algorithmic typechecking).
(1) If $\vdash_{\Sigma} \text{sig}$ then $\vdash_{\Sigma} \Rightarrow \text{sig}$.
(2) If $\vdash_{\Sigma} \Gamma \Rightarrow \text{ctx}$ then $\vdash_{\Sigma} \Gamma \Rightarrow \text{ctx}$.
(3) If $\Gamma \vdash_{\Sigma} M : A$ then $\exists A'. \Gamma \vdash_{\Sigma} M \Rightarrow A'$ and $\Gamma \vdash_{\Sigma} A = A' : \text{type}$.
(4) If $\Gamma \vdash_{\Sigma} A : K$ then $\exists K'. \Gamma \vdash_{\Sigma} A \Rightarrow K'$ and $\Gamma \vdash_{\Sigma} K = K' : \text{kind}$.
(5) If $\Gamma \vdash_{\Sigma} K : \text{kind}$ then $\Gamma \vdash_{\Sigma} K \Rightarrow \text{kind}$.

3.6 Strengthening and strong extensionality

The strengthening property states that all of the definitional judgments are preserved by removing an unused variable from the context. We already established strengthening for the algorithmic equivalence judgments (Lem. 19). In order to establish strengthening for the algorithmic typechecking judgments, we need a stronger freshness lemma for algorithmic typechecking, which was not discussed in HP05:

Lemma 38 (Strong algorithmic freshness). Let $\Gamma = \Gamma_1 \circ [(x, B)] \circ \Gamma_2$.
(1) If $\Gamma \vdash_{\Sigma} M \Rightarrow A$ and $x \neq (\Gamma_1, M)$ then $x \neq A$.
(2) If $\Gamma \vdash_{\Sigma} A \Rightarrow K$ and $x \neq (\Gamma_1, A)$ then $x \neq K$.

We can now prove strengthening for algorithmic typechecking by induction on derivations:

Theorem 9 (Strengthening of algorithmic typechecking).
Let $\Gamma = \Gamma_1 \circ [(x, B)] \circ \Gamma_2$.
(1) If $\vdash_{\Sigma} \Gamma \Rightarrow \text{ctx}$ and $x \neq \Gamma_1$ then $\vdash_{\Sigma} \Gamma_1 \circ \Gamma_2 \Rightarrow \text{ctx}$.
(2) If $\Gamma \vdash_{\Sigma} K \Rightarrow \text{kind}$ and $x \neq (\Gamma_1, K)$ then $\Gamma_1 \circ \Gamma_2 \vdash_{\Sigma} K \Rightarrow \text{kind}$.
(3) If $\Gamma \vdash_{\Sigma} A \Rightarrow K$ and $x \neq (\Gamma_1, A)$ then $\Gamma_1 \circ \Gamma_2 \vdash_{\Sigma} A \Rightarrow K$.
(4) If $\Gamma \vdash_{\Sigma} M \Rightarrow A$ and $x \neq (\Gamma_1, M)$ then $\Gamma_1 \circ \Gamma_2 \vdash_{\Sigma} M \Rightarrow A$.

Proof. The proof is straightforward, using strengthening for algorithmic equivalence; parts (1–4) need to be proved in the order stated above since we need strengthening for contexts everywhere, we need strengthening for kinds to prove strengthening for types, and so on. Lem. 38 is needed in the cases for object and type application. □

Finally, we can prove strengthening for the definitional system.

Theorem 10 (Strengthening). Let $\Gamma = \Gamma_1 \circ [(x, B)] \circ \Gamma_2$.
(1) If $\vdash_{\Sigma} \Gamma \Rightarrow \text{ctx}$ and $x \neq \Gamma_1$ then $\vdash_{\Sigma} \Gamma_1 \circ \Gamma_2 \Rightarrow \text{ctx}$.
(2) If $\Gamma \vdash_{\Sigma} K : \text{kind}$ and $x \neq (\Gamma_1, K)$ then $\Gamma_1 \circ \Gamma_2 \vdash_{\Sigma} K : \text{kind}$.
(3) If $\Gamma \vdash_{\Sigma} K = L : \text{kind}$ and $x \neq (\Gamma_1, K, L)$ then $\Gamma_1 \circ \Gamma_2 \vdash_{\Sigma} K = L : \text{kind}$.
(4) If $\Gamma \vdash_{\Sigma} A : K$ and $x \neq (\Gamma_1, A)$ then $\Gamma_1 \circ \Gamma_2 \vdash_{\Sigma} A : K$.
(5) If $\Gamma \vdash_{\Sigma} A = B : K$ and $x \neq (\Gamma_1, A, B)$ then $\Gamma_1 \circ \Gamma_2 \vdash_{\Sigma} A = B : K$.
(6) If $\Gamma \vdash_{\Sigma} M : A$ and $x \neq (\Gamma_1, M)$ then $\Gamma_1 \circ \Gamma_2 \vdash_{\Sigma} M : A$.
(7) If $\Gamma \vdash_{\Sigma} M = N : A$ and $x \neq (\Gamma_1, M, N)$ then $\Gamma_1 \circ \Gamma_2 \vdash_{\Sigma} M = N : A$. 

ACM Transactions on Computational Logic, Vol. V, No. N, Month 20YY.
Mechanizing the Metatheory of LF

Proof. The proof follows the sketch in the article, using algorithmic strengthening and soundness and completeness of the algorithmic judgments, but some care is needed. Part 1 is straightforward, but we must prove the remaining cases in the specific order listed: first kind validity, then kind equivalence, then type validity, etc. The reason is that to prove strengthening for the equivalence judgments, we need strengthening for the corresponding validity judgments because of the validity side-conditions on Thm. 2. In turn, to prove strengthening for the object and type validity judgments, we need strengthening for type and kind equivalence respectively, because of the respective type and kind equivalence judgments in the conclusions of Thm. 8. Lem. 38 is needed in parts (4) and (6). □

HP05 also sketched a proof of admissibility of a stronger version of the extensionality rule which omits the well-formedness checks:

\[
(x, A_1) : \Gamma \vdash \Sigma \; M \; x = N \; x : A_2 \quad x \neq (M, N)
\]

\[
\Gamma \vdash \Sigma \; M = N : \Pi x : A_1. \; A_2
\]

However, the short proof sketched in the article actually requires a substantial amount of work to formalize. The first two steps of their informal proof were as follows:

1. By validity, we have \((x, A_1) : \Gamma \vdash \Sigma \; M \; x : A_2\).
2. By inversion, we have \((x, A_1) : \Gamma \vdash \Sigma \; M : \Pi x : B_1. \; B_2\) and \((x, A_1) : \Gamma \vdash \Sigma \; x : B_1\).

However, step (2) above does not follow immediately from the inversion lemmas proved earlier. In particular, we only know that \(M\) will have a type of the form \(\Pi y : B_1. \; B_2\) for some \(y, B_1\) and \(B_2\) such that \((x, A_1) : \Gamma \vdash \Sigma \; M : \Pi y : B_1. \; B_2\) and \((x, A_1) : \Gamma \vdash \Sigma \; y : B_1\) and \((x, A_1) : \Gamma \vdash \Sigma \; A_2 = B_2[y := x] : type\). Moreover, in this case we cannot use the strong version of the inversion lemma to avoid this problem, because \(x\) is already in use in the context.

Although their proof looks rigorous and detailed, here Harper and Pfenning appear to employ implicit “without loss of generality” reasoning about inversion and renaming that is not easy to formalize directly. Instead we needed to show carefully that:

Lemma 39. If \((x, A_1) : \Gamma \vdash \Sigma \; M \; x : A_2\) and \(x \neq M\) then \(\Gamma \vdash \Sigma \; M : \Pi x : A_1. \; A_2\).

Proof. The proof proceeds by applying validity and inversion principles, as discussed above. One subtle freshness side-condition is the fact that \(x\) is fresh for \(\Pi y : B_1. \; B_2\), and this is proved by translating to the algorithmic typechecking system and using Lem. 38. □

Strong extensionality then follows essentially as in HP05, using Lem. 39 to fill the gap identified above:

Theorem 11 (Strong extensionality). If \((x, A_1) : \Gamma \vdash \Sigma \; M \; x = N \; x : A_2\) and \(x \neq (M, N)\) then \(\Gamma \vdash \Sigma \; M = N : \Pi x : A_1. \; A_2\).

3.7 Decidability

HP05 also sketches proofs of the decidability of the algorithmic judgments (and hence also the definitional system). Reasoning about decidability within Isabelle/HOL.
is not straightforward because Isabelle/HOL is based on classical logic. Thus, unlike constructive logics or type theories, we cannot infer decidability of $P$ simply by proving $P \lor \neg P$. Furthermore, given a relation $R$ definable in Isabelle/HOL, it is not clear how best to formalize the informal statement “$R$ is decidable”.

As a sanity check, we have shown that weak head reduction is strongly normalizing for well-formed terms. We write $M \downarrow$ to indicate that $M$ is strongly normalizing under weak head reduction. This proof uses techniques and definitions from the example formalization of strong normalization for the simply-typed lambda calculus in the Nominal Datatype Package.

**Theorem 12.** If $\Gamma \vdash_{\Sigma} M : A$ then $M \downarrow$.

**Proof.** We first show the (standard) property that if $M \downarrow N$ then $M \downarrow$. We then show that if $\Delta \vdash_{\Sigma} M \Rightarrow N : \tau$ then $M \downarrow$ by induction on derivations. The main result follows by reflexivity and Thm. 1. □

Turning now to the issue of formalizing decidability properties in Isabelle/HOL, we considered the following options:

**Formalizing computability theory.** It should be possible to define Turing machines (or some other universal model of computation) within Isabelle/HOL and derive enough of the theory of computation to be able to prove that the algorithmic equivalence and typechecking relations are decidable. It appears to be an open question how to formalize proofs of decidability in Isabelle/HOL, especially for algorithms over complex data structures such as nominal datatypes. Although this would probably be the most satisfying solution, it would also require a major additional formalization effort, including a great deal of work that is orthogonal to the issues addressed here. Another possibility would be to restrict Isabelle/HOL to a constructive fragment, but this seems even more difficult and time-consuming since Isabelle/HOL makes extensive use of choice principles and the law of excluded middle. We therefore view fully formalizing decidability in this way as beyond the scope of this article. Instead, we consider other techniques that stop short of full formalization while providing some convincing evidence for decidability.

**Bounded-height derivations.** We could define height-bounded versions of the algorithmic typechecking relations and prove that there is a computable bound on the height needed to derive any derivable judgment in the system. That is, there exists a computable $h$ such that for any inputs $x_1, \ldots, x_n$, there is a derivation of $J(x_1, \ldots, x_n)$ if and only if there is a derivation of height at most $h(x_1, \ldots, x_n)$.

This seems reasonable intuitively, but there are several problems. First, it is not obvious how to obtain a closed-form, recursively defined height bound for the number of steps needed for algorithmic equivalence for the same reason it is difficult to give an explicit termination measure for weak head normalization. Second, even if we could find such an $h$, this approach begs the question of how to prove that $h$ is computable. It is clearly not enough to simply require that some $h$ exists, because the Axiom of Choice can be used to define $h$ nonconstructively. Finally, inductively defined judgments in Isabelle/HOL may themselves involve nonconstructive features, including equality at or quantification over infinite types, negation of undecidable properties, and choice operators. Although the definitions
we have in mind do not use these facilities, there is no easy way to certify this within Isabelle/HOL.

**Inductive definability.** We have formalized what we believe is the essence of the decidability proof using the following methodology. For each inductively defined relation $R$ we wish to prove decidable, possibly under some constraints $P$:

1. Inductively define a complement relation $R'$.
2. (Exclusion) Prove that $\neg (R \land R')$.
3. (Exhaustion) Prove that $P$ implies $R \lor R'$.
4. Observe (informally) that $R$ and $R'$ are recursively enumerable since they are defined inductively by rules without recourse to nonconstructive features such as negation or universal quantification in the hypotheses. Conclude (informally) that $P$ implies $R$ is both r.e. and co-r.e., hence decidable.

This approach exploits an intuitive connection between inductively definable predicates and recursively enumerable sets in step (4). It is important to note that this intuition is not rigorously formalized. We argue that this approach does force us to perform all of the case analysis that would be necessary in a proper decidability proof, but the only way to be certain of this is to fully formalize a substantial amount of computability theory in Isabelle/HOL, which as we have discussed above would be a major undertaking in its own right.

We call a formula $R$ *quasidecidable* if both $R$ and its negation are equivalent to inductively defined relations, as described above. This is an informal (and intensional) property; we have not defined quasidecidability explicitly in Isabelle/HOL.

We have the following lemma, analogous to RW’s Theorem 6.1:

**Theorem 13 (Quasidecidability of algorithmic equivalence).**

1. If $\Delta \vdash_{\Sigma} M \iff \tau$ and $\Delta \vdash_{\Sigma} N \iff N' : \tau$ then $\Delta \vdash_{\Sigma} M \iff N : \tau$ is quasidecidable.
2. If $\Delta \vdash_{\Sigma} M \iff M' : \tau_1$ and $\Delta \vdash_{\Sigma} N \iff N' : \tau_2$ then $\exists \tau_3. \Delta \vdash_{\Sigma} M \iff N : \tau_3$ is quasidecidable.
3. If $\Delta \vdash_{\Sigma} A \iff A' : \kappa$ and $\Delta \vdash_{\Sigma} B \iff B' : \kappa$ then $\Delta \vdash_{\Sigma} A \iff B : \kappa$ is quasidecidable.
4. If $\Delta \vdash_{\Sigma} A \iff A' : \kappa_1$ and $\Delta \vdash_{\Sigma} B \iff B' : \kappa_2$ then $\exists \kappa_3. \Delta \vdash_{\Sigma} A \iff B : \kappa_3$ is quasidecidable.
5. If $\Delta \vdash_{\Sigma} K \iff K' : \text{kind}^-$ and $\Delta \vdash_{\Sigma} L \iff L' : \text{kind}^-$ then $\Delta \vdash_{\Sigma} K \iff L : \text{kind}^-$ is quasidecidable.

We further proved that the algorithmic typechecking judgments are quasidecidable, which is the key step in HP05’s Theorem 6.5. Proving exclusivity required establishing uniqueness of algorithmic typechecking.

**Lemma 40 (Uniqueness of algorithmic types).**

1. If $\Gamma \vdash_{\Sigma} M \Rightarrow A$ and $\Gamma' \vdash_{\Sigma} M \Rightarrow A'$ then $A = A'$.
2. If $\Gamma \vdash_{\Sigma} A \Rightarrow K$ and $\Gamma' \vdash_{\Sigma} A \Rightarrow K'$ then $K = K'$.

Equipped with Thm. 13 and the uniqueness lemma above, we can show a form of HP05’s Theorem 6.2. Note that uses of Thm. 13 are safe because we always call the algorithmic equivalence judgments on terms that are well-formed, and hence (by Thm. 2) algorithmically equivalent to themselves.
Theorem 14 (Quasidecidability of Algorithmic Typechecking).

1. For any $\Sigma, \Gamma \models \sigma$ is quasidecidable.
2. For any $\Sigma, \Gamma$, if $\Gamma \vdash \sigma$ holds then $\Gamma \vdash \sigma$ is quasidecidable.
3. For any $\Sigma, \Gamma, M$, if $\Gamma \vdash \sigma$ holds then $\exists A, \Gamma \vdash M \Rightarrow A$ is quasidecidable.
4. For any $\Sigma, \Gamma, A$, if $\Gamma \vdash \sigma$ holds then $\exists K, \Gamma \vdash A \Rightarrow K$ is quasidecidable.
5. For any $\Sigma, \Gamma, K$, if $\Gamma \vdash \sigma$ holds then $\Gamma \vdash K \Rightarrow \kind$ is quasidecidable.

3.8 Quasicanonical forms

Section 7 of HP05 discusses quasicanonical forms which can be used to study the adequacy, or correctness, of LF encodings. Quasicanonical forms are untyped $\lambda$-terms that correspond to the $\beta$-normal, $\eta$-long forms of well-typed LF terms. Quasicanonical forms $\bar{O}$ and quasitomatomic forms $\bar{O}$ are given by the grammar rules:

$$\bar{O} ::= O \mid \lambda x.\bar{O} \quad \bar{O} ::= x \mid e \mid \bar{O} \bar{O}$$

HP05 introduces instrumented algorithmic equivalence judgments that construct quasicanonical forms for algorithmically and structurally equivalent terms, respectively. The rules are shown in Fig. 8.

It is straightforward to show that quasi-canonical and quasi-atomic forms exist and are unique (provided that $\Sigma$ and $\Delta$ are valid).

Lemma 41 (Properties of Quasicanonical Forms).

1. If $\Delta \vdash \Sigma M \Rightarrow N : \tau \Rightarrow QC$. $\Delta \vdash \Sigma M \Rightarrow N : \tau \Rightarrow QC$.
2. If $\Delta \vdash \Sigma M \Rightarrow N : \tau \Rightarrow QA$. $\Delta \vdash \Sigma M \Rightarrow N : \tau \Rightarrow QA$.
3. If $\Delta \vdash \Sigma M \Rightarrow N : \tau \Rightarrow \bar{O}$ then $\Delta \vdash \Sigma M \Rightarrow N : \tau$.
4. If $\Delta \vdash \Sigma M \Rightarrow N : \tau \Rightarrow \bar{O}$ then $\Delta \vdash \Sigma M \Rightarrow N : \tau$.
5. If $\Delta \vdash \Sigma M \Rightarrow N : \tau \Rightarrow \bar{O}$ and $M \vdash A$ then $\Delta \vdash \Sigma M \Rightarrow N : \tau \Rightarrow \bar{O}$.
6. If $\Delta \vdash \Sigma M \Rightarrow N : \tau \Rightarrow \bar{O}$ and $N \vdash \bar{O}$ then $\bar{O} \equiv \bar{O}$.

Theorem 15 (Uniqueness of Quasicanonical Forms).

1. If $\Delta \vdash \setc$ and $\Gamma \vdash \ssig$ and $\Delta \vdash \Sigma M \Rightarrow N : \tau \Rightarrow \bar{O}_1$ and $\Delta \vdash \Sigma M \Rightarrow N \vdash \bar{O}_2$ then $\bar{O}_1 = \bar{O}_2$. 

ACM Transactions on Computational Logic, Vol. V, No. N, Month 20YY.
(2) If \( \vdash \Delta \text{ set } x \) and \( \vdash \Sigma \text{ ssig } \) and \( \Delta \vdash_{\Sigma} M \leftrightarrow N : \tau \downarrow \bar{O}_1 \) and \( \Delta \vdash_{\Sigma} M \leftrightarrow N : \tau' \downarrow \bar{O}_2 \) then \( \tau = \tau' \) and \( \bar{O}_1 = \bar{O}_2 \).

**Proof.** By induction on derivations, using Lem. 41(5,6) in the cases involving weak head reduction. \( \square \)

The main result about these forms in HP05 is that well-formed LF terms can be recovered from quasicanonical forms and type information. To show this, we write \( N \uparrow \bar{O} \) or \( N \downarrow \bar{O} \) for the relations that relate objects \( N \) with their quasicanonical forms \( \bar{O} \) or quasiatricial forms \( \bar{O} \), respectively, where the type-labels have been erased. (HP05 defined this notion as a partial function, which would be difficult to define with the Nominal Datatype Package at the time of writing.) These relations are defined as follows:

\[
\begin{array}{ccc}
x \downarrow x & c \downarrow c & M \downarrow \bar{O} \\
(M N) \downarrow \bar{O} \bar{O} & (\lambda x : A. M) \uparrow \lambda x \bar{O} & M \uparrow \bar{O}
\end{array}
\]

In the proof of the Quasicanonical Forms theorem (Theorem 7.1 of HP05) we found it necessary to prove several nontrivial auxiliary lemmas such as the admissibility of \( \eta \)-equivalence (which was not discussed in HP05):

**Lemma 42 (Eta-equivalence).** If \( x \notin \Gamma \) and \( \Gamma \vdash_{\Sigma} M : \Pi x : A_1. A_2 \) then \( \Gamma \vdash_{\Sigma} M = \lambda x : A_1. M x : \Pi x : A_1. A_2 \).

The following theorem is stated slightly differently than the corresponding theorem in HP05 (Theorem 7.1), but their version follows immediately from this version.

**Theorem 16 (Quasicanonical forms).**

1. If \( \Gamma^- \vdash_{\Sigma^-} M_1 \Rightarrow M_2 : A^- \uparrow \bar{O} \) and \( \Gamma \vdash_{\Sigma} M_1 : A \) and \( \Gamma \vdash_{\Sigma} M_2 : A \) then \( \exists N. N \uparrow \bar{O} \) and \( \Gamma \vdash_{\Sigma} N : A \) and \( \Gamma \vdash_{\Sigma} M_1 = N : A \) and \( \Gamma \vdash_{\Sigma} M_2 = N : A \).
2. If \( \Gamma^- \vdash_{\Sigma^-} M_1 \Rightarrow M_2 : \tau \downarrow \bar{O} \) and \( \Gamma \vdash_{\Sigma} M_1 = A_1 \) and \( \Gamma \vdash_{\Sigma} M_2 = A_2 \) then \( \Gamma \vdash_{\Sigma} A_1 = A_2 \) : type and \( A_1^- = \tau \) and \( A_2^- = \tau \) and \( (\exists N. N \downarrow \bar{O} \) and \( \Gamma \vdash_{\Sigma} N : A_1 \) and \( \Gamma \vdash_{\Sigma} M_1 = N : A_1 \) and \( \Gamma \vdash_{\Sigma} M_2 = N : A_2 \).

### 3.9 Adequacy

Conventionally, adequacy is the property that the terms of the object language are in a bijective correspondence with the well-formed LF terms of a given type, modulo LF equality. Moreover, the bijection should be compositional\(^2\) in the sense that substitution for the object language is preserved and reflected by substitution in LF. The exact statement of the adequacy theorem for a given language depends on the language and its definition of substitution. To illustrate how quasicanonical forms could be used for reasoning about adequacy, HP05 introduces a small example language of first-order terms \( t \) and formulas \( \varphi \), similar to the following:

\[
\begin{align*}
t, u & ::= x | f(t, u) \\
\varphi, \psi & ::= t = u | \varphi \land \psi | \forall x. \varphi
\end{align*}
\]

along with an appropriate LF signature \( \Sigma_{FO} \) with types \( t \) for first-order terms, \( o \) for first-order formulas, and constants

\(^2\)This term is used in HP05 without being defined, but this is the definition used in other articles which discuss adequacy, for example [Harper et al. 1993; Pfenning 2001].
signature parametrized by a signature that unlike most other judgments in this article the translations are bijections and then proving compositionality by induction over the structure of terms and formulas. Theorem \[PT as follows a \]

\[\begin{align*}
\Gamma \vdash t & \iff \bar{M} : \iota \\
(x, t) \in \Gamma & \quad \frac{\Gamma \vdash t_1 \iff \bar{M}_1 : \iota \quad \Gamma \vdash t_2 \iff \bar{M}_2 : \iota}{\Gamma \vdash f(t_1, t_2) \iff c_f \bar{M}_1 \bar{M}_2 : \iota}
\end{align*}\]

Fig. 9. Adequacy translation

\[
\begin{align*}
c_f : & \quad t \to t \to t \\
c_m : & \quad t \to t \to o \\
c_o : & \quad o \to o \to o \\
c_o : & \quad (t \to o) \to o
\end{align*}
\]

HP05 then defines translation judgments \(\Gamma \vdash t \iff M : \iota\) and \(\Gamma \vdash \varphi \iff M : o\) relating LF terms \(M\) with first-order terms and formulas \(t : \iota\) and \(\varphi : o\). Note that unlike most other judgments in this article, the translations are not implicitly parametrized by a signature \(\Sigma\) since they only refer to constants from the fixed signature \(\Sigma_{FO}\). The rules for the translation are shown in Fig. 9.

Harper and Pfenning then formulate the adequacy property for this language in their Theorem 7.2 as follows:

**Theorem 17 (Adequacy for Syntax of First-Order Logic).** Let \(\Gamma\) be a context of the form \(x_1 : \iota, \ldots, x_n : \iota\) for some \(n \geq 0\).

1. The relation \(\Gamma \vdash t \iff \bar{M} : \iota\) is a compositional bijection between terms \(t\) of first-order logic over variables \(x_1, \ldots, x_n\) and quasi-canonical forms \(\bar{M}\) of type \(\iota\) relative to \(\Gamma\).

2. The relation \(\Gamma \vdash \varphi \iff \bar{M} : o\) is a compositional bijection between formulas \(t\) of first-order logic over variables \(x_1, \ldots, x_n\) and quasi-canonical forms \(\bar{M}\) of type \(o\) relative to \(\Gamma\).

Their proof sketch involves first showing that (for all appropriate \(\Gamma\)) the translations are bijections, and then proving compositionality by induction over the structure of terms and formulas.

Unfortunately, the statement of this theorem is ambiguous or at least incomplete. The reason is that Harper and Pfenning do not explicitly define what it means for a bijection to be compositional. Even assuming the standard definition of compositionality as substitution preservation, HP05 did not provide a definition of substitution for quasicanonical forms.

If we wish to substitute a quasicanonical form for a variable \(y\) in another quasicanonical form, the result is not always quasicanonical. For example, if we substitute \(\lambda x.M\) for \(y\) in \(N\), we get \((\lambda x.M)\ N\), which is not quasicanonical. This illustrates that quasicanonical forms are not closed under substitution of quasicanonical forms for variables, because variables are quasianomic forms and substituting a \(\lambda\)-expression for a variable may introduce \(\beta\)-redexes.
It has been observed elsewhere (apparently first by Watkins et al. [2003]) that substitution can be defined for well-formed quasicanonical expressions in a hereditary way that recursively renormalizes any \( \beta \)-redexes introduced by substitution. Harper and Licata [2007] have shown how this idea can be used as the basis for a variant of LF called Canonical LF in which all expressions are maintained in canonical form.

In our initial formalization (reported in [Urban et al. 2008]) we misinterpreted the definition of the translation slightly by defining the adequacy translations to relate first-order terms and formulas to quasiatomic forms. It is easy to define substitution of quasiatomic forms for variables since no reduction can be introduced in doing so. Consequently, we proved a variant of HP05’s Theorem 7.2 with the word “quasicanonical” replaced by “quasiatomic”. However, even with this modification, the formal proof is not as easy as the sketch in HP05 suggests: for example, we needed to prove weakening, exchange, and substitution lemmas for the translation judgment in order to establish compositionality.

After we discovered and corrected the mismatch between our definition and the original translation, we were still able to prove that the translations are bijections. To establish compositionality, we also formalized hereditary substitution (using a simple form of Harper and Licata’s definition) and showed that the translation maps object-language substitution to hereditary substitution.

Formalizing HP05’s Theorem 7.2 thus appears to require either changing their translation or introducing hereditary substitution, a nontrivial concept that was not mentioned in HP05. The Canonical LF approach now appears to be the preferred starting point for research on extensions to LF. Developing a full and satisfying formalization of hereditary substitutions and adequacy properties (and relating HP05’s version of LF to Harper and Licata’s development of Canonical LF [2007]) would be a significant independent undertaking. Therefore, we prefer to leave further study of adequacy based on hereditary substitution for future work.

4. CODE GENERATION

Since type checking in LF can be part of the trusted code base of proof-carrying code, Appel et al. [2003] were very careful to implement it as cleanly as possible and in as few lines of code as possible. Their motivation was that a small and clean implementation can be manually inspected and hence can be made robust against, for example, Thompson-style attacks [Thompson 1984]. For this they explicitly set out to minimize the number of library functions they have to trust in order for their implementation to be correct. However, they relied upon the correctness of the type-checking algorithm in HP05.

In this paper we have formally proved that both the equivalence checking and type-checking algorithms from HP05 are sound and complete. Consequently, we can remove this aspect from our “trusted code base”. In this section we show how to obtain a verified executable ML-implementation of the type-checking algorithm from our proof of correctness.

Isabelle/HOL contains a code generator implemented by Berghofer and Nipkow [2002] which can translate inductive definitions into executable pure ML-code automatically. To be able to use this code generator, however, we need to invest
some further work. The present version of this code generator can only deal with rules involving datatypes, not nominal datatypes. To surmount this problem we translate our nominal representation of kinds, types and terms into a locally nameless representation [McKinna and Pollack 1999; Aydemir et al. 2008], which can be implemented as an ordinary Isabelle/HOL datatype. For the LF-syntax this gives rise to the definition:

\[
\text{Locally Nameless Kinds} \quad ::= \quad \text{type} \mid \Pi A. K \\
\text{Locally Nameless Types} \quad ::= \quad a \mid \Pi A_1. A_2 \mid A M \\
\text{Locally Nameless Objects} \quad ::= \quad c \mid x \mid n \mid \lambda A. M \mid M_1 M_2
\]

where terms contain de Bruijn indices \( n \) for bound variables [de Bruijn 1972]. In comparison with “pure” de Bruijn representations, in the locally nameless representation free variables still have names. This means we can continue using our implementation of signatures and contexts in judgments. With a “pure” de Bruijn representation, contexts would need to be referenced by numbers and positions.

While the locally nameless representation is straightforward to implement in Isabelle/HOL, the translations between the nominal and locally nameless representation involve quite a lot of formalisation work. First we have to define a well-formedness predicate that ensures that there are no loose de Bruijn indices. We also need three substitution operations, namely substituting (well-formed) terms for free variables, written \((-)[x := M]\), substituting terms for de Bruijn indices, written \((-)[n := M]\), and substituting de Bruijn indices for variables, written \((-)[x := n]\). In the latter we have to increase the de Bruijn index whenever the substitution moves under a binder. Also the translation functions between the nominal and locally nameless representations are non-trivial to define. In one direction the translation is a partial function and only total over well-formed locally nameless terms. In the other direction we use a translation depending on an explicit list of variables. The idea is to push a variable onto the list whenever the translation goes under a \( \lambda \)- or a \( \Pi \)-abstraction. Now the de Bruijn index for a variable occurrence is the position of the variable in this list. The translation, written \( \vert - \vert_{xs} \), can be formally defined as

\[
|\text{type}|_{xs} = \text{type} \\
|\Pi x. A. K|_{xs} = \Pi |A|_{xs}. |K|_{(x::xs)} \quad \text{provided } x \# xs \\
|a|_{xs} = a \\
|A M|_{xs} = |A|_{xs} |M|_{xs} \\
|\Pi x. A_1. A_2|_{xs} = \Pi |A_1|_{xs}. |A_2|_{(x::xs)} \quad \text{provided } x \# xs \\
|c|_{xs} = c \\
|x|_{xs} = \text{index } x \text{ } xs \text{ } 0 \\
|M N|_{xs} = |M|_{xs} |N|_{xs} \\
|\lambda x. A. M|_{xs} = \lambda |A|_{xs}. |M|_{(x::xs)} \quad \text{provided } x \# xs
\]

where the variable case is defined in terms of the auxiliary function \( \text{index } x \text{ } xs \text{ } n \):

\[
\text{index } x \text{ } [] \text{ } n = x \\
\text{index } x \text{ } (y::ys) \text{ } n = (\text{if } x = y \text{ then } n \text{ else } \text{index } y \text{ } ys (\text{Suc } n))
\]

The problem with this definition arises from the fact that inductions need to be appropriately generalised in order to take the potentially growing list of variables
into account. This is sometimes easy to do, but sometimes we needed a lot of ingenuity to find the right lemmas to get inductions through.

Having translated all our terms into the locally nameless representation, we solved the technical problem with the code generator in Isabelle/HOL. However, there is a further problem that needs to solved: the algorithms specified so far are not yet concrete enough to be translated directly into runnable ML-code. For this consider again the algorithmic equivalence rule

\[(x, \tau_1) \vdash \Delta \vdash x : \Sigma \Rightarrow (\Delta, M, N) \]

\[
\Delta \vdash \Sigma \Rightarrow N : \tau_1 \Rightarrow \tau_2
\]

from Fig. 4. This rule decides the equivalence between the terms \(M\) and \(N\) having function type. When read bottom-up, it states that we need to introduce a variable \(x\) (any will do) that is fresh for \(\Delta, M\) and \(N\). ML does not have any built-in facilities for choosing such a fresh name (unlike, for example, FreshML by Shinwell et al. [2003]). This means for an ML-implementation of type and equivalence checking that we need to make explicit which fresh name should be chosen. An obvious choice is to inspect all free variables occurring in \(\Delta, M\) and \(N\), and produce a variable with a higher index. In our case, it suffices to compute the maximum index of all variables in scope and increase by one to obtain a fresh variable index. We are able to compute this index because names in the Nominal Datatype Package have a natural number as index and thus can be ordered. This allows us to formulate algorithmic equivalence rules as follows

\[(x, \tau_1) \vdash \Delta_{ln} \vdash x : \Sigma \Rightarrow (\Delta_{ln}, M, N) \]

\[
\Delta_{ln} \vdash \Sigma \Rightarrow N : \tau_1 \Rightarrow \tau_2
\]

where \(fv\) is a polymorphic function producing a list of free variables of a term or context, and the function \(\text{maxi}\) scans through a list of variables and returns the highest variable increased by one.

In Fig. 10 we show the rules for type checking in the locally nameless representation and with the explicit choice of fresh variables. The locally nameless variants of these judgments are marked by the subscript \(ln\). We omit the locally nameless versions of the algorithmic equivalence rules but they are similar. The functions \(fi\) (\(-\)) and \(fe\) (\(-\)) calculate the free identifiers and free variables of their arguments, respectively.

It is important to note that it would be extremely inconvenient to build the concrete choice for a fresh variable into the rules that are used in the soundness and completeness proofs described in the earlier sections. The reason is that several of the proofs would not go through as stated in HP05 since the choice is not fresh enough for all entities considered in some lemmas (an example is the weakening property, where the variable \(x\) is assumed to be not just fresh for \(\Delta, M\) and \(N\), but also for a larger context \(\Delta'\)). It is however relatively straightforward to show the equivalence (i.e., they derive the same judgments, modulo translation) between the original rules and the rules with the concrete choice for fresh variables. We can show:

**Lemma 43 (Equivalence).**

(1) \(\vdash \Sigma \Rightarrow sig\) if and only if \(\vdash_{ln} \Sigma[0] \Rightarrow sig\).

ACM Transactions on Computational Logic, Vol. V, No. N, Month 20YY.
\[
\begin{align*}
\Gamma \vdash \Sigma &\Rightarrow \text{sig} \\
\Gamma \vdash \Sigma &\Rightarrow \text{sig} \quad \text{if } \Gamma \vdash \Sigma A \Rightarrow \text{type}, c \notin \text{fv } \Sigma \\
\Gamma \vdash (c, A) : \Sigma &\Rightarrow \text{sig} \\
\Gamma \vdash \Sigma &\Rightarrow \text{sig} \quad \text{if } \Gamma \vdash \Sigma K \Rightarrow \text{kind}, a \notin \text{fv } \Sigma \\
\Gamma \vdash (a, K) : \Sigma &\Rightarrow \text{sig} \\
\Gamma \vdash \Sigma &\Rightarrow \text{ctx} \\
\Gamma \vdash \Sigma &\Rightarrow \text{ctx} \quad \text{if } \Gamma \vdash \Sigma A \Rightarrow \text{type}, x \notin \text{fv } \Gamma \\
\Gamma \vdash \Sigma (x, A) : \Gamma &\Rightarrow \text{ctx} \\
\Gamma \vdash \Sigma M &\Rightarrow A \\
\Gamma \vdash \Sigma \Gamma \Rightarrow \text{ctx} \quad \text{if } (x, A) \in \Gamma \\
\Gamma \vdash \Sigma \Gamma \Rightarrow \text{ctx} \quad \text{if } (c, A) \in \Sigma \\
\Gamma \vdash \Sigma \Gamma \Rightarrow \text{ctx} \quad \text{if } x \in \Gamma \\
\Gamma \vdash \Sigma \Gamma \Rightarrow \text{ctx} \quad \text{if } A \in \Gamma \\
\Gamma \vdash \Sigma M &\Rightarrow \Pi A_2, A_1 \\
\Gamma \vdash \Sigma M_1 \Rightarrow A_1 \quad \Gamma \vdash \Sigma M_2 \Rightarrow A_2 \quad \Gamma \vdash \Sigma \Rightarrow A_1 : \text{type} \\
\Gamma \vdash \Sigma M_1 \Rightarrow A_1 [\theta := M_2] \\
\Gamma \vdash \Sigma A_1 &\Rightarrow \text{type} \\
\Gamma \vdash \Sigma M_2 [\theta := x] &\Rightarrow A_2 \\
x = \maxi (\text{fv } \Gamma \ominus \text{fv } A_1 \ominus \text{fv } A_2) \\
A_2' = A_2 [x := \theta] \\
\Gamma \vdash \Sigma \lambda A_1, M_2 \Rightarrow \Pi A_1, A_2' \\
\Gamma \vdash \Sigma A &\Rightarrow K \\
\Gamma \vdash \Sigma \Gamma \Rightarrow \text{ctx} \quad \text{if } (a, K) \in \Sigma \\
\Gamma \vdash \Sigma \Gamma \Rightarrow \text{ctx} \quad \text{if } (a, K) \in \Sigma \\
\Gamma \vdash \Sigma \Gamma \Rightarrow \text{ctx} \quad \text{if } x \in \Gamma \\
\Gamma \vdash \Sigma \Gamma \Rightarrow \text{ctx} \quad \text{if } A \in \Gamma \\
\Gamma \vdash \Sigma \Pi A_1, A_2 \Rightarrow \text{type} \\
\Gamma \vdash \Sigma A_1 \Rightarrow \text{type} \quad \text{if } (x, A_1) \vdash \Sigma A_2 [\theta := x] \Rightarrow \text{type} \\
x = \maxi (\text{fv } \Gamma \ominus \text{fv } A_1 \ominus \text{fv } A_2) \\
\Gamma \vdash \Sigma \Pi A_1, A_2 \Rightarrow \text{type} \\
\Gamma \vdash \Sigma K &\Rightarrow \text{kind} \\
\Gamma \vdash \Sigma \Gamma \Rightarrow \text{ctx} \quad \text{type } \Rightarrow \text{kind} \\
\Gamma \vdash \Sigma A &\Rightarrow \text{type} \quad \text{if } (x, A) \vdash \Sigma K [\theta := x] \Rightarrow \text{kind} \\
x = \maxi (\text{fv } \Gamma \ominus \text{fv } A \ominus \text{fv } K) \\
\Gamma \vdash \Sigma \Pi A, K \Rightarrow \text{kind}
\end{align*}
\]

Fig. 10. Algorithmic typechecking rules used for generating executable code.

\(2\) \(\vdash \Sigma \Gamma \Rightarrow \text{ctx} \) if and only if \(\Gamma \vdash \Sigma \| \Gamma \| \Rightarrow \text{ctx}\).

\(3\) \(\Gamma \vdash \Sigma M \Rightarrow A \) if and only if \(\Gamma \vdash \Sigma \| \Gamma \vdash \Sigma \| M \| \Rightarrow \| A \|\).

\(4\) \(\Gamma \vdash \Sigma A \Rightarrow K \) if and only if \(\Gamma \vdash \Sigma \| \Gamma \vdash \Sigma \| A \| \Rightarrow \| K \|\).

\(5\) \(\Gamma \vdash \Sigma K \Rightarrow \text{kind} \) if and only if \(\Gamma \vdash \Sigma \| \Gamma \vdash \Sigma \| K \| \Rightarrow \text{kind}\).

From the rules in Fig. 10 the code generator of Isabelle/HOL can generate ML-code. Of course the correctness of this code depends on the correctness of the generator. However it is relatively easy to inspect the generated ML-code and we are confident that it implements correctly the inductive definitions that have been proved to be
sound and complete with respect to their specification. We have used the extracted ML-code to type-check several LF example signatures.

5. DISCUSSION

It is difficult to argue objectively about the efficacy or usability of tools for mechanized metatheory about languages with name-binding, since there are substantial differences among systems, there are few experts in the use of more than one system, and each such formalization is a major undertaking. Nevertheless, we believe it is worthwhile to make some subjective observations about our experience formalizing LF using Nominal Isabelle/HOL, and identify aspects of the two systems that aided or hindered formalization.

Methodological observations. The formalization was performed by two of the authors; one is a developer of the Nominal Datatype Package and expert Isabelle/HOL user and the other had roughly three months’ experience with these tools prior to starting the formalization. We estimate that the total effort involved in conducting the formalizations in Sec. 3 was at most three person-months. We worked on the code generation part intermittently and therefore do not have detailed information about the time required. Although there is still room for improvement in both Isabelle/HOL and the Nominal Datatype Package, our experience suggests that these tools can now be used to perform significant formalizations within reasonable time-frames, at least by experienced users.

It took approximately six person-weeks to formalize everything up to the soundness proof (including pondering why the omitted case for type extensionality did not go through). However, once Harper and Pfenning confirmed that this case was indeed not handled correctly in their proof, one of the authors was able to check within 2 hours that adding a type-extensionality rule solves the problem. Re-checking the proof on paper would have meant reviewing approximately 31 pages of proofs. Subsequently we checked the validity of a solution suggested by Harper and found another solution for the problem. As a practical matter, the ability to rapidly evaluate the effects of changes to the system was essential for finding these solutions and evaluating other possibilities. In a similar formalization project, the first author showed that a central lemma in the informal proof in his PhD-thesis can be repaired [Urban and Zhu 2008].

Comparing the formalization and informal proof. In our formalization, we attempted to follow the syntax, definitions and proofs given in HP05 as closely as we could, and resisted the temptation to change their rules to make our task easier. We found that nominal techniques were usually able to state results almost exactly as they are presented on paper; the main differences tended to involve freshness or validity side-conditions that were left implicit in HP05. To illustrate this point, we have prepared this paper using Isabelle’s documentation facilities [Nipkow et al. 2002]. Most lemmas, theorems, and definitions in this paper have been generated directly from the formalization (the main exceptions are the quasidecidability and adequacy properties, which are paraphrased).

In this article, we have focused on the high-level ideas of the formalization and, in the main, downplayed the low-level details of proofs using the Nominal Datatype
Package. This is not because these details are embarrassing, but because (with a few clearly-marked exceptions) they are prosaic. For example, as one would expect, our formalization also required formally proving many properties of substitution, swapping, freshness, contexts, erasure and so on. We have not discussed these because they are routine, and rely upon techniques already covered in previous work on nominal techniques [Urban 2008]. However, we would like to point out here that the capability to define functions such as substitution and erasure as (nominal) primitive recursive functions, and use Isabelle/HOL's built-in simplifier to rewrite formulas involving these functions, was absolutely essential. This is not to say that these proofs were always easy, but that difficulties involving name-binding were usually not the dominant factor.

We have not explicitly stated when features such as strong nominal induction or inversion principles [Urban et al. 2007; Berghofer and Urban 2008] have been used (nor have we given complete explanations of these techniques), but our formalization relies upon them extensively. When these principles could be used, the paper proof was usually easy to translate to a formal proof step-by-step (although as is often the case with formalizations, an informal proof step often translated to many formal steps or necessitated additional lemmas). On the other hand, in a few cases nominal induction principles could not be applied, often because of subtleties involving binding. When this was the case, proof cases involving binding were often much more labor-intensive because they required explicit reasoning about choosing fresh names, alpha-equivalence, swapping and substitution (see, for example, the proof of transitivity of algorithmic equivalence).

Many of our proofs have been be written to match corresponding informal proofs closely using the Isar proof-language, as in an example by Urban [2008, Sec. 6] of a typical substitution property. However, writing readable Isar proofs is labor-intensive; the proof-script tactic language of classic Isabelle/HOL tends to be much easier to write but harder to read.

The interested, or skeptical, reader is welcome to consult the formalization for these details, replay the proofs of key properties, compare them with those in HP05, and form his or her own opinion.

**Metrics about the formalization.** In Table I, we report some simple metrics about our formalization such as the sizes, number of lines of text, and number of lemmas in each theory in the main formalization. As Table I shows, the core LF theory accounts for about 20% of the development. These syntactic properties are mostly straightforward, and their proofs merit only cursory discussion in HP05, but some lemmas have many cases which must each be handled individually. The Decidability theory accounts for another 15%; the quasidecidability proofs are verbose but largely straightforward. The LocallyN theory proves that the nominal datatypes version of LF is equivalent to a locally nameless formulation; this accounts for about 25% of the development. The effort involved in this part was therefore quite substantial: it can be explained by the lack of automatic infrastructure for the locally nameless representation of binders in Isabelle/HOL, but also by the inherent subtleties when working with this representation. A number of lemmas need to be carefully stated, and in a few cases in rather non-intuitive ways. The remaining theories account for at most 5–10% of the formalization each;
the WeakAlgorithm theory defines the weak algorithmic equivalence judgment and proves the additional properties needed for the third solution, and accounts for only around 2% of the total development.

The merit of metrics such as proof size or number of lemmas is debatable. We have not attempted to distinguish between meaningful lines of proof vs. blank or comment lines; nor have we distinguished between significant and trivial lemmas. Nevertheless, this information should at least convey an idea of the relative effort involved in each part of the proof.

Correctness of the representation. The facilities for defining and reasoning about languages with binding provided by the Nominal Datatype Package are convenient, but their use may not be persuasive to readers unfamiliar with nominal logic and abstract syntax. Thus, a skeptical reader might ask whether these representations, definitions and reasoning principles are really correct; that is, whether they are equivalent to the definitions in HP05, as formalized using some more conventional approach to binding syntax. For higher-order abstract syntax representations, this property is often called adequacy; this term appears to have been coined in the context of LF [Harper et al. 1993], due to the potential problems involved in reasoning about higher-order terms modulo alpha, beta and eta-equivalence.

Adequacy is also important for nominal techniques and deserves further study. We believe that the techniques explored in existing work on the semantics of nominal abstract syntax and its implementation in the Nominal Datatype Package [Gab-
bay and Pitts 2002; Pitts 2003; Cheney 2006; Pitts 2006; Urban 2008] suffices for
informally judging the correctness of our formalization. There has also been some
prior work on formalizing adequacy results for nominal datatypes via isomorphisms.
Urban [2008] proves a bijective correspondence between nominal datatypes and a
conventional named implementation of the λ-calculus modulo α-equivalence. Nor-
rish and Vestergaard [2007] have formalized isomorphisms between nominal and
de Bruijn representations, and they provide further citations to several other iso-
morphism results. Our proof of equivalence to a locally nameless representation
described in Sec. 4 also gives evidence for the correctness of the nominal datatype
representation.

In any case, our formalization has exposed some subtle issues which make sense
in the context of LF, independently of whether or not nominal datatypes in Is-
abelle/HOL really capture our informal intuitions about abstract syntax with bind-
ing.

Reflecting on formalizing LF. It has been observed (as discussed, for example, by
Pientka [2007]) that the process of formalization can suggest changes that both case
formalization and clarify the original system. Likewise, our formalization provides
a basis for reflecting on how the LF metatheory might be adapted to make it easier
to formalize. Most obviously, many of the problems we encountered with soundness
disappear if we simply add the omitted extensionality rule or change the equivalence
algorithm.

A more subtle complication we encountered was that since the algorithmic rules
in HP05 do not enforce well-formedness, it is not even guaranteed that a variable
appearing in one of the terms being compared also appears in the context Δ. This
necessitates extra freshness conditions on many rules and induction hypotheses to
ensure that strong nominal induction principles can be used safely. Building these
constraints into the algorithmic rules might make several of the proofs about the
equivalence algorithm cleaner.

Another practical consideration was that the syntax and rules of LF in HP05
exhibit redundancy, which leads to additional (albeit straightforward) formalization
effort. For example, constants, dependent products, and applications each appear
at more than one level of the syntax, resulting in proofs with redundant cases.
Similarly, because objects, kinds and types are defined by mutual recursion, each
inductive proof about syntax needs to have three inductive hypotheses and ten
cases. Likewise, any proof concerning the definitional judgments needs to state
eight simultaneous induction hypotheses and thirty-five cases. Collapsing the three
levels of LF syntax into one level, and collapsing the many definitional judgments
into a smaller number could make the formalization much less verbose, as in Pure
Type Systems [McKinna and Pollack 1999], at the cost of increasing the distance
between the paper version and the formalization. On the other hand, such an
approach could also make it easier to generalize proofs about LF to richer type
theories.

6. RELATED AND FUTURE WORK

McKinna and Pollack [1999]’s LEGO formalization of Pure Type Systems is prob-
bly the most extensive formalization of a dependent type theory in a theorem
mechanizing the metatheory of LF

prover. Their formalization introduced the locally nameless variant of de Bruijn’s name-free approach [de Bruijn 1972] and considered primarily syntactic properties of pure type systems with β-equivalence, including a proof of strengthening. Pollack [1995] subsequently verified the partial correctness of typechecking algorithms for certain classes of Pure Type Systems including LF.

Completely formalizing metatheoretic and syntactic proofs about languages and logics with name-binding has been a long-standing open problem in computational logic. We will not give a detailed survey of all of these techniques here, but mention a few recent developments. In the last five years, catalyzed by the POPLMark Challenge [Aydemir et al. 2005], there has been renewed interest in this area. Aydemir et al. [2008] have developed a methodology for formalizing metatheory in Coq using the locally nameless representation to manage binding, and using cofinite quantification to handle fresh names. Chlipala’s parametric higher-order abstract syntax is another recently developed technique for reasoning about abstract syntax in Coq, and has been applied to good effect in reasoning about compiler transformations [Chlipala 2008]. Westbrook et al. [2009] are developing CINIC, a variant of Coq that provides built-in support for nominal abstract syntax (generalizing a simple nominal type theory developed by Cheney [2009]). Gacek et al. [2008] have developed Abella, a proof assistant for reasoning about higher-order abstract syntax, inductive definitions, and generic quantification (similar to nominal logic’s fresh-name quantifier). Schürmann and Sarnat [2008] have recently discovered techniques for performing logical relations proofs in Twelf [Pfenning and Schürmann 1999]. Formalizing the results in this article using these or other emerging tools would provide a useful comparison of these approaches, particularly concerning decidability proofs, which ought to be easier in constructive logics.

Algorithms for equivalence and canonicalization for dependent type theories have been studied by several authors. Prior work on equivalence checking for LF has focused on first checking well-formedness with respect to simple types, then β- or βη-normalizing; these approaches are discussed in detail by Harper and Pfenning [2005]. Coquand’s algorithm [1991] is similar to Harper and Pfenning’s but operates on untyped terms. Goguen’s approach [2005b] involves first type-directed η-expansion and then β-normalization, and relies on standard properties such as the Church-Rosser theorem, strong normalization of β-reduction and strengthening. Goguen [2005a] extends this proof technique to show termination of Coquand’s and Harper and Pfenning’s algorithms, and gives a terminating type-directed algorithm for checking βη-equivalence in System F. It may be interesting to formalize these algorithms and proofs and compare with Harper and Pfenning’s proof.

Our formalization provides a foundation for several possible future investigations. We are interested in extending our formalization to include verifying Twelf-style meta-reasoning about LF specifications, following Harper and Licata’s detailed informal development of Canonical LF [2007]. Doing so could make it possible to extract Isabelle/HOL theorems from Twelf proofs, but as discussed earlier, formalizing Canonical LF, hereditary substitutions, and the rest of Harper and Licata’s work appears to be a substantial challenge.

It would also be interesting to extend our formalization to accommodate extensions to LF involving (ordered) linear logic, concurrency, proof-irrelevance, or
singleton kinds, as discussed by Harper and Pfenning [2005, Sec. 8]. We hope that anyone who proposes an extension to LF will be able to use our formalization as a starting point for verifying its metatheory.

7. CONCLUSIONS

LF is an extremely convenient tool for defining logics and other calculi involving binding syntax. It has many compelling applications and underlies the system Twelf, which has a proven record in formalizing many programming language calculi. Hence, it is of intrinsic interest to verify key properties of LF’s metatheory, such as the correctness and decidability of the typechecking algorithms. We have done so, using the Nominal Datatype Package for Isabelle/HOL. The infrastructure provided by this package allowed us to follow the proof of Harper and Pfenning closely.

For our formalization we had the advantage of working from Harper and Pfenning’s carefully-written informal proof, which withstood rigorous mechanical formalization rather well. Still we found in this informal proof one gap and numerous minor complications. We have shown that they can be repaired. We have also partially verified the decidability of the equivalence and typechecking algorithms, although some work remains to formally prove decidability per se. Formalizing decidability proofs of any kind in Isabelle/HOL appears to be an open problem, so we leave this for future work.

While verifying correctness of proofs is a central motivation for doing formalizations, it is not the only one. There is a second important benefit—they can be used to experiment with changes to the system rapidly. By replaying a modified formalization in a theorem prover one can immediately focus on places where the proof fails and attempt to repair them rather than re-checking the many cases that are unchanged. This capability was essential in fixing the soundness proof, and it illustrates one of the distinctive advantages of performing such a formalization. Had we attempted to repair the gap using only the paper proof, experimenting with different solutions would have required manually re-checking the roughly 31 pages of paper proofs for each change.

Our formalization is not an end in itself but also provides a foundation for further study in several directions. Researchers developing extensions to LF may find our formalization useful as a starting point for verifying the metatheory of such extensions. We plan to further investigate hereditary substitutions and adequacy proofs in LF and Canonical LF. More ambitiously, we contemplate formalizing the meaning and correctness of metatheoretic reasoning about LF specifications (as provided by the Twelf system) inside Isabelle/HOL, and extracting Isabelle/HOL theorems from Twelf proofs.

ELECTRONIC APPENDIX

The electronic appendix for this article can be accessed in the ACM Digital Library by visiting the following URL: http://www.acm.org/pubs/citations/journals/tocl/20YY-V-N/p1-URLend.
ACKNOWLEDGMENTS
We are extremely grateful to Bob Harper for discussions about LF and the proof. Benjamin Pierce and Stephanie Weirich have also made helpful comments on drafts of this paper.

REFERENCES

ACM Transactions on Computational Logic, Vol. V, No. N, Month 20YY.


Received October 2009; revised April 2010; accepted April 2010