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*Developing (Meta)Theory of -calculus* in the Theory of Contexts [1](#_bookmark0)

*Marino Miculan 2*

*Dipartimento di Matematica e Informatica, Universit a di Udine, Italy*

*Abstract*

*We present a case study on the formal development of a non trivial (meta)theory in the Theory of Contexts using the Coq proof assistant. The methodology underlying the Theory of Contexts for reasoning on systems presented in HOAS is based on an axiomatic syntactic standpoint. We feel that one of the main advantages of this approach, is that it requires a very low logical overhead.*

*The object system we focus on is the lazy, call-by-name -calculus ( cbn), both untyped and simply typed. We will see that the formal, fully detailed development of the theory of cbn in the Theory of Contexts introduces a small, sustainable overhead with respect to the proofs \on the paper". Moreover, this will allow for comparison with similar case studies developed in other approaches to the metathe- oretical reasoning in higher-order abstract syntax.*

*Keywords: higher-order abstract syntax, induction, logical frameworks.*

# *Introduction*

*In recent years there has been growing interest in developing systems for de n-* ing and reasoning on languages featuring -conversion. A promising line of approach has focused on Higher-Order Abstract Syntax (HOAS) [[13,](#_bookmark19) [24].](#_bookmark27) The gyst of this approach is to delegate to type-theoretic metalanguages the burden of dealing with binders. This approach however has some drawbacks. First of all, being equated to metalanguage variables, object level variables cannot be de ned inductively without introducing exotic terms [[7,](#_bookmark13) [20].](#_bookmark22) A similar diÆ- culty arises with contexts, which are rendered as functional terms. Reasoning by induction and de nition by recursion on object level terms is therefore problematic. Various approaches have been proposed to overcome these prob- lems based on di erent techniques such as functor categories, permutation models of ZF, etc. [[9,](#_bookmark15) [10,](#_bookmark16) [1](#_bookmark20)4, [11,](#_bookmark17) [19].](#_bookmark23)

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*2 Email:* [*miculan@dimi.uniud.it*](mailto:miculan@dimi.uniud.it)

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*In [15] another logical framework for reasoning on systems in HOAS is* presented, based on an axiomatic syntactic standpoint. This system stems from the technique originally used in [16] for formally deriving in Coq [17] the metatheory of strong late bisimilarity of the -calculus. This framework

*consists of a simple types theory a la Church extended with a set of axioms*

*called the Theory of Contexts, recursion operators and induction principles.* According to our experience, this framework is rather expressive. Higher Or- der Logic allows for the impredicative de nition of many relations, possibly functional, the recursors and induction principles allow for the de nition of many important functions and properties over contexts, and most notably the axioms in the Theory of Contexts allow for a smooth handling of schemata in HOAS. In fact, we feel that one of the main advantages of the axiomatic ap- proach of the Theory of Contexts, is that it requires a very low mathematical and logical overhead.

*Of course there are some tradeo s. One of the major theoretical problems* concerning any axiomatic approach is the consistency of the axioms. In fact, it is possible to prove that the Theory of Context is sound. We refer the reader to [4], where a full proof of consistency of the Theory of Contexts is given, using a model of functor categories along the line of [14].

*From a practical point of view, however, the applicability of this approach* has to be tested by means of several cases studies. These are particularly useful for discussing pragmatic issues which arise in developing real proofs in the Theory of Contexts, addressing possible solutions and suggesting directions for future developments. This is precisely the aim of this paper, where we develop a non trivial (meta)theory of the lazy, call-by-name -calculus ( cbn), both untyped and simply typed, in the Theory of Contexts within the Coq proof assistant. We choose cbn as the object of this case study for several reasons. First, it is a well-known logic, so much that most works about - calculus skim quickly standard de nitions and basic proofs, sweeping many details under the rug. We will see that the formal, fully detailed development of the theory of cbn in the Theory of Contexts introduces a small, sustainable overhead with respect to the proofs \on the paper". Moreover, cbn owns some features (as substitution of terms for variables, typing system,. . . ) which are somewhat complementary to those of -calculus, which has been the object of another large case study in the Theory of Context [16]. Finally, some variant of the -calculus has been always taken as the traditional benchmark/example of application of the many approaches to HOAS in the literature; see [13, 2, 7, 19, 14, 11, 12] among the others.

*It turns out that Theory of Contexts is quite successful in handling the* metatheory of cbn. The encoding of the syntax, the semantics and the type system is straightforward, and still we delegate the -conversion to the met- alevel. Only the encoding of substitution is not immediate, since we need to represent it as a relation. However, this will allow us to state and prove some fundamental results (i.e., functionality of substitution) which usually are

*taken for granted in informal works on the -calculus. Moreover, these proofs* cast some light on the limits, and suggest possible solutions, of the Theory of Contexts in Coq.

*The Coq code is available at* [*http://www.dimi.uniud.it/~miculan/HOAS/.*](http://www.dimi.uniud.it/~miculan/HOAS/) *Synopsis. In Section 1 we recall brie y (that is, as in most works is done) the object system cbn. In Section 2 we give a brief presentation of the type*

*theory CIC and its implementation Coq. The HOAS encoding of syntax and*

*semantics of cbn, and the formal development of its metatheory using the* Theory of Contexts, is described in Section 3. Practical issues which arise in developing the proofs are discussed and, when possible, solutions are proposed. In Section 4 we consider two extensions of the object system: applicative bisimulation and observational equivalence, and a simple type system for cbn. Comparison with related work and conclusions are in Sections 5, 6 respectively.

*1 The object system cbn*

*In this section we give an intentionally brief (and somewhat sloppy) de nition* of the lazy call-by-name -calculus cbn, as it is usually given in most papers. This will allow us to enlighten, in the following sections, how the formal rep- resentation of the theory does not introduce a substantial overhead despite the high level of detail required. We assume the reader familiar with the basic notions of -calculus; for an introduction and a comprehensive development of the theory of the -calculus, see [3].

*The set of terms of cbn is de ned by the following grammar:*

*M; N ::= x j (MN) j x:M*

*where x; y; z;::: range over an in nite set of variables. Terms are taken up-* to -equivalence. We denote by M[N=x] the capture-avoiding substitution of N for x in M. Contexts, i.e. terms with holes, are denoted by M( ). A term is said to be a value if it is not an application. The notion of \free variables" (FV ) is de ned as usual. For X a nite set of variables, we de ne

*X , fM 2 j FV (M) Xg. By 0 we denote ;.*

*We consider two lazy operational semantics. The reduction (or small-step* semantics) is the smallest relation M ! N de ned by the following rules

*M ! M0*

*( x:M) N ! M[N=x] (M N) ! (M0 N)*

*We denote by ! the re exive and transitive closure of !.*

*The evaluation (or big-step semantics) is the smallest relation M + N* de ned by the following rules:

*x:M + x:M*

*M + x:M0 M0[N=x] + V* M N + V

# *2 The Calculus of Inductive Constructions*

*The Calculus of Inductive Constructions is an extension of the Calculus of* Constructions (CC), which can be de ned as the PTS C of Barendregt's - cube, with two sorts, Prop and Set. Under the proposition-as-types, proofs-as- terms paradigm, there is an isomorphism between propositions of intuitionistic higher-order logic and types of sort Prop. If A has type Prop then it represents a logical proposition; the fact that A is inhabited by a term M represents the fact that A holds. Each term M inhabiting A represents a proof of A. On the other hand, the sort Set is supposed to be the type of datatypes, such as naturals, lists, trees, booleans, etc. These types di er from those inhabiting Prop for their constructive contents.

*Therefore, CC, as many similar Type Theories, can be fruitfully used* as a general logic speci cation language, i.e. as a Logical Framework (LF) [13, 22, 23]. In an LF, we can represent faithfully and uniformly all the rel- evant concepts of the inferential process in a logical system (syntactic cate- gories, terms, variables, contexts, assertions, axiom schemata, rule schemata, instantiation, tactics, etc.).

*The Calculus of Inductive Constructions (CIC) (implemented in the Coq* system [17]) extends CC with some special constants which represent the de nition, introduction and elimination of inductive types. For instance, the following de nition of natural numbers (written in Gallina, Coq's speci cation language)

*Inductive nat : Set := O : nat | S : nat -> nat*

*allows to de ne terms by \case analysis", like the following function:*

*Definition pred := [n:nat]Cases n of O => O | (S u) => u end.*

*where [n:nat] is Gallina notation for abstraction n : nat. Using these elim-* ination schemata, Coq automatically states and proves the induction principle for each inductively de ned type. For instance, the above de nition yields the Peano induction principle \for free":

*nat\_ind : (P:nat->Prop)(P O) ->*

*((n:nat)(P n)->(P (S n))) -> (n:nat)(P n) where (n:nat) is the notation for dependent product Qn:nat. This feature has been extensively used in the de nition of logical connectives: we need only to*

*specify the introduction rules, and we can prove the elimination rules from*

*the elimination principle the system automatically provides us.*

*However, allowing for any inductive de nition in CIC would yield non-* normalizing terms, thus invalidating the standard proof of consistency of the system. Hence, inductive de nitions are subject to the positivity condition, which (roughly) requires that the type we are de ning does not occur in neg- ative position in the type of any argument of any constructor. This condition ensures the soundness of the system, but it rules out also many sound inductive

*de nitions. For instance, the following de nition of -terms in higher-order* abstract syntax

*Inductive L : Set := lam : (L->L) -> L | app : L -> L -> L.*

*is not well-formed, due to the negative occurrence of L in the type L->L of the* argument of lam.

*Another problem arising from the use of higher order abstract syntax to-* gether with inductive types is that of exotic terms. These are -terms which do not correspond to any object \on the paper", despite their types corre- spond to some syntactic category. Exotic terms are generated when a type has a higher-order constructor over an inductive type. A simple example is the following fragment of rst-order logic:

*Inductive i : Set := zero : i | one : i.*

*Inductive o : Set := ff : o | eq : i->i->o | forall : (i->o)->o.*

*Definition weird : o := (forall [x:i](Cases x of*

*zero => ff*

*| one => (eq zero zero) end)).*

*The term weird does not correspond to any proposition of rst order logic:* there is no formula 8x such that f0=xg and f1=xg are syntactically equal to

*\ " and \0 = 0", respectively. Exotic terms are problematic in establishing* the faithfulness of the formalization; usually, they have to be ruled out by means of auxiliary \validity" judgements [7, 27]. Another approach, which will be used in Section 3.1 is to have the higher order constructors to range over types which are not de ned as inductive, so that there is no Cases to use as above.

*A common implementation of CIC is Coq, an interactive proof assistant* developed by the INRIA and other institutes. For a complete description, we refer to [17]. Coq is an editor for interactively searching for an inhabitant of a type, in a top-down fashion by applying tactics step-by-step, backtracking if needed, and for verifying correctness of typing judgements. A proof search starts by entering

*Lemma ident : goal.*

*where goal is the type representing the proposition to prove. At this point,* Coq waits for commands from the user, in order to build the proof term which inhabits goal (i.e., the proof). To this end, Coq o ers a rich set of tactics, e.g., introduction and application of assumptions, application of rules and previously proved lemmata, elimination of inductive objects, inversion of (co)inductive hypotheses and so on. These tactics allow the user to proceed in his proof search much like he would do informally. At every step, the type checking algorithm ensures the soundness of the proof. When the proof term is completed, it can be saved (by the command Qed) for future applications.

# *3 Formalizing and reasoning on cbn in CIC*

*3.1 Encoding the syntax of cbn*

*The HOAS representation of the syntax of cbn is the following: Parameter Var : Set.*

*Inductive tm : Set := var : Var -> tm*

*| app : tm -> tm -> tm*

*| lam : (Var -> tm) -> tm.*

*Coercion var : Var >-> tm.*

*Declaring var as a coercion allows us to inject implicitly terms from type Var* into tm, so that in the following this constructor may be omitted from terms.

*Remark 3.1 We do not de ne Var as an inductive set. In fact, this is not* required by the syntax of cbn, so there is no reason to bring in unnecessary assumptions, i.e., the induction and recursion principles. Actually, these un- wanted principles are not harmless, because they can be exploited for de ning exotic terms; hence, taking Var as inductive would be simply wrong.

*Remark 3.2 Notice that lam is a higher-order constructor, that is it takes* a functional term as argument. In particular, terms of type Var->tm rep- resent exactly the capture-avoiding contexts of the -calculus. This tech- nique allows to inherit the -equivalence on terms from the metalanguage, and still to have an inductive de nition for terms. For instance, x:(xx) and

*y:(yy) are represented by (lam [x:Var](app (var x) (var x))) and (lam*

*[y:Var](app (var y) (var y))), respectively, which are the same term up-* to -conversion. At the same time we can de ne functions by rst-order re- cursion or case analysis on the syntax of terms, like the following:

*Definition isvalue := [M:tm]Cases M of*

*(var x) => False*

*| (lam t) => True*

*| (app t1 t2) => False*

*end.*

*The adequacy of this encoding is a consequence of [15, Theorem 1]. For*

*X = fx1;::: ; xng a nite set of variables, let us de ne*

*X , fx1 : Var;::: ; xn : Varg[ fdij : ~(xi = xj) j 1 i < j ng tmX , fM j X ` M : tm;M in long -normal formg:*

*Proposition 3.3 For all X nite set of variables, there is a bijection X* between X and tmX . Moreover, this bijection is compositional, in the sense that if M 2 X;x and N 2 X, then X(M[N=x]) = X;x(M)[ X (N)=(var x)]:

*As a corollary, a (capture-avoiding) context M( ) 2 X is naturally en-* coded as [z:Var] X;z(M(z)), where the fresh variable z acts as a \placeholder" for the hole. In fact, a bijection like in Proposition 3.3 can be established be- tween contexts and terms of type Var->tm.

*3.2 The Theory of Contexts for cbn*

*Often, a HOAS encoding of an object system is not suÆcient for handling the* metatheory of the system, that is to prove properties on the object system itself. Since we aim to prove several results about cbn, we need to introduce the corresponding Theory of Contexts.

*Given the signature of the syntax, the Theory of Contexts is composed* by two parts. The rst contains the de nitions of \occurrence" predicates. These de nitions are immediately derived from the signature of the language, following the pattern in [16, 15].

*Inductive notin [x:Var] : tm -> Prop := notin\_var : (y:Var)~x=y->(notin x y)*

*| notin\_app : (M,N:tm)(notin x M) -> (notin x N)*

*-> (notin x (app M N))*

*| notin\_lam : (M:Var->tm)((y:Var)~x=y->(notin x (M y)))*

*-> (notin x (lam M)).*

*Inductive isin [x:Var] : tm -> Prop := isin\_var : (isin x x)*

*| isin\_app1: (M,N:tm)(isin x M) -> (isin x (app M N))*

*| isin\_app2: (M,N:tm)(isin x N) -> (isin x (app M N))*

*| isin\_lam : (M:Var->tm)((y:Var)(isin x (M y)))*

*-> (isin x (lam M)).*

*The only thing we need to know about names (variables), is that equality* over Var is decidable. However, we do not need a full blown classical logic: it is suÆcient to have a classical behaviour on the occurrence check predicates.

*Axiom LEM\_OC: (M:tm)(x:Var)(isin x M)\/(notin x M). This implies the decidability of (eq Var).*

*The second part of the Theory of Contexts consist of a set of axiom* schemata, which re ect at the theory level some fundamental properties of the intuitive notion of \context" and \occurrence" of variables. Their infor- mal meaning is the following:

*Unsaturability of variables: no term can contain all variables; i.e., there exists always a variable which does not occur free in a given term;*

*Extensionality of contexts: two contexts are equal if they are equal on a* fresh variable; that is, if M(x) = N(x) and x 62 M( );N ( ), then M = N.

*More formally, these are the axioms of the Theory of Contexts we need: Axiom unsat : (M:tm)(Ex [x:Var](notin x M)).*

*Axiom ext\_tm : (M,N:Var->tm)(x:Var)*

*(notin x (lam M)) -> (notin x (lam N)) -> (M x)=(N x) -> M=N.*

*Axiom ext\_tm1 : (M,N:Var->Var->tm)(x:Var)*

*(notin x (lam [z:Var](lam (M z)))) ->*

*(notin x (lam [z:Var](lam (M z)))) -> (M x)=(N x) -> M=N.*

*The following are immediate consequences of the Theory of Contexts and* the induction principles over tm.

*Lemma differ : (x:Var)(Ex [y:Var]~x=y).*

*Lemma* [*isin\_notin\_absurd*](#_bookmark21) *: (x:Var)(M:tm)(isin x M)->(notin x M)->False.*

*Remark 3.4 In [15] also another axiom schema, called -expansion, is pre-* sented. Informally, -exp states that given a term M and a variable x, there is a context N( ) such that N(x) = M and x does not occur in N( ). This has been used several times in the development of the metatheory of

*-calculus [16]. On the other hand, it has not been needed in the present*

*work on cbn. A possible motivation is that here we are allowed for higher-* order induction, while in [16] we had to recover it from induction over plain,

*rst-order terms.*

*Another useful application of -exp which we have not used in this work is* the representation of variable-capturing contexts in HOAS. In general, this is diÆcult because bound variables are not accessible from \outside" the abstrac- tion, not even their names. In the Theory of Contexts, a context C[ ] capturing x can be represented as a term of type (var->tm)->tm, and the instantiation requires a -expansion of the inserted term. For instance, x:([ ] x) is repre- sented as C' = [N:(var->tm)](lam [x:Var](app (N x) (var x))). Con- sider a term M with a free variable x which has to be captured: let M0( ) the context obtained by -expansion over x (i.e., such that M0(x) = M and x does not appear free in M0). Then, the variable-capturing instantiation C[M] is rendered as (C' M').

*Remark 3.5 As described in Section 2, Coq and similar systems provide* support for inductive types. However, this does not hold for higher-order types: there is no induction principle over A->B, even if A and/or B are inductive. This is because the intended meaning of A->B (usually, a function space) is not an initial algebra. Thus, most proof editors give no induction principles, case analysis, inversion predicates and similar tools for reasoning on terms of type Var->tm, i.e., contexts. Nevertheless, it is possible to prove that types of the form Var->...->Var->tm do have recursion and induction principles [14,4,15]. Hence, beside the simple Axioms of the Theory of Contexts above, we can safely assume higher-order induction and recursion principles as needed, like the following induction over Var->tm:

*Axiom tm\_ind1 : (P:(Var->tm)->Prop) (P var) ->*

*((y:Var)(P [\_:Var](var y))) ->*

*((M,N:Var->tm)(P M)->(P N)->(P [x:Var](app (M x) (N x)))) ->*

*((M:Var->Var->tm)*

*((y:Var)(P [x:Var](M x y)))->(P [x:Var](lam (M x))))*

*-> (M:Var->tm)(P M).*

*(notice how there are two base cases). In the following we may introduce also* others of these principles,

*3.3 Formalizing the substitution*

*A drawback of using using a speci c type for variables (a \weak HOAS" encod-* ing), is that we cannot delegate the substitution to the metalanguage. Instead, we need to de ne it by hand, as a parametric relation between contexts and terms:

*Inductive subst [N:tm] : (Var->tm) -> tm -> Prop := subst\_var : (subst N var N)*

*| subst\_void : (y:Var)(subst N [\_:Var]y y)*

*| subst\_app : (M1,M2:Var->tm)(M1',M2':tm)*

*(subst N M1 M1') -> (subst N M2 M2') ->*

*(subst N [y:Var](app (M1 y) (M2 y)) (app M1' M2'))*

*| subst\_lam : (M:Var->Var->tm)(M':Var->tm)*

*((z:Var)(subst N [y:Var](M y z) (M' z))) ->*

*(subst N [y:Var](lam (M y)) (lam M')).*

*Thus, a term M0 is syntactically equal to the substitution M(x)[N=x] i (subst N M M') holds. More formally:*

*Proposition 3.6 Let X be a nite set of variables and x a variable not in*

*X. Let N; M0 2 X and M 2 X]fxg. Then:*

*M[N=x] = M0 () X ` : (subst X(N) [x:Var] X]fxg(M) X(M0))*

*Capture-avoiding substitution is naturally de ned as a function, but in* fact its de nition is seldom given in full detail|and we made no exception in Section 1. Actually, the de nition which is usually intended is not determin- istic a priori, since it requires an arbitrary -conversion of bound variables of the context in order to avoid capturing free variables in the substituted term. More complex languages (e.g., dynamic logic, Hoare logic [20]) may require nonstandard substitutions involving contrived notions of conversion, not sim- ply -conversion. Representing the substitution in CIC as a relation, in fact, gives raise to the possibility that it may be not total, that is for some N; M there is no M0 such that M0 = M[N=x]. The fact that such a de nition does give a functional (i.e., deterministic and total) relation is a property which we are going to prove explicitly using the Theory of Contexts.

*Determinism of substitution*

*The property we want to prove is the following: Parameter N:tm.*

*Lemma subst\_is\_det: (M:Var->tm)(M1:tm)(subst N M M1) ->*

*(M2:tm)(subst N M M2) -> (M1 = M2).*

*We give two proofs of this property. The rst goes by induction on the deriva-* tion of (subst N M M1). This gives rise to four cases:

*N : tm*

*M : var->tm M2 : tm*

*H : (subst N Var M2)*

*============================ N=M2*

*subgoal 2 is: (y)=M2*

*subgoal 3 is: (app M1' M2')=M0*

*subgoal 4 is: (lam M')=M2*

*each of which should be dealt by inverting the hypothesis H (or corresponding).* Usually, such an inversion would eliminate automatically all absurd cases, but this does not work when the terms which have to be discriminate are higher- order. This is indeed the case, since the second argument of subst has type Var->tm. The Inversion H tactic gives us four cases for the rst goal, only one of which is trivially true and the other are absurd:

*subgoal 1 is: N : tm*

*M : Var->tm*

*M2 : tm*

*H : (subst N var M2) H0 : var=var*

*H1 : N=M2*

*============================ M2=M2*

*...*

*subgoal 2 is: N : tm*

*M : Var->tm M2 : tm*

*H : (subst N var M2) y : Var*

*H1 : ([\_:var](y))=var H0 : (y)=M2*

*============================ N=(y)*

*Absurd cases are (tediously) eliminated by using the Theory of Contexts, in* particular the axiom of extensionality. The whole proof is 95 lines long, most of which are dealing with the elimination of absurd cases.

*Determinism of substitution, again*

*A much shorter proof can be obtained by proving a suitable higher-order* inversion lemma for substitution. In Coq, inversion lemmata are automatically synthesized and proved on-the- y [from](#_bookmark11) recursion principles by the Inversion tactic, using the algorithm originally implemented by Murthy with subsequent elaboration by Cornes and Terrasse [6]. However, this algorithm fails to give the right inversion predicate when the datatype, which we have to discriminate over, is higher-order, because usual [inductiv](#_bookmark9)[e](#_bookmark21) type theories do not recognize a higher-order type as inductive. Nevertheless, we know that types of the form Var->tm do have recursion principles [14, 4, 15]. Hence, we can consistently introduce these principles (as Axioms) for the de nition of the recursive map needed in the inversion predicate:

*Parameter subst\_inv\_fun : tm -> (Var->tm) -> tm -> Prop.*

*Axiom subst\_inv\_fun\_var0 : (N,M:tm)(subst\_inv\_fun N var M)==(N=M). Axiom subst\_inv\_fun\_var1 :*

*(y:Var)(B,N:tm)(subst\_inv\_fun N [\_:Var]y B)==((var y)=B).*

*Axiom subst\_inv\_fun\_app : (A1,A2:Var->tm)(B,N:tm) (subst\_inv\_fun N [x:Var](app (A1 x) (A2 x)) B) ==*

*(EX B1 | (EX B2 | (app B1 B2)=B /\ (subst N A1 B1)*

*/\ (subst N A2 B2))).*

*Axiom subst\_inv\_fun\_lam : (A:Var->Var->tm)(B,N:tm) (subst\_inv\_fun N [x:Var](lam (A x)) B) ==*

*(EX A1 | (lam A1)=B /\ (y:Var)(subst N [x:Var](A x y) (A1 y))).*

*Then, the higher-order inversion principle is \mechanically" claimed and* proved as follows:

*Lemma subst\_inv : (A:Var->tm)(B,N:tm)(subst N A B) -> (subst\_inv\_fun N A B). Intros; Inversion\_clear H.*

*Rewrite subst\_inv\_fun\_var0; Reflexivity. Rewrite subst\_inv\_fun\_var1; Reflexivity.*

*Rewrite subst\_inv\_fun\_app; Exists M1'; Exists M2'; Auto. Rewrite subst\_inv\_fun\_lam; Exists M'; Auto.*

*Qed.*

*Using this inversion lemma, the proof of determinism of substitution is* much easier|in fact, we \lift" at the level of context the syntactic machinery of inversion tactics that Coq provides at the level of terms:

*Lemma subst\_is\_det': (M:Var->tm)(M1:tm)(subst N M M1) ->*

*(M2:tm)(subst N M M2) -> (M1 = M2).*

*Induction 1; Intros.*

*Generalize (subst\_inv ? ? ? H0); Rewrite subst\_inv\_fun\_var0; Trivial. Generalize (subst\_inv ? ? ? H0); Rewrite subst\_inv\_fun\_var1; Trivial. Generalize (subst\_inv ? ? ? H4); Rewrite subst\_inv\_fun\_app; Intros.*

*Inversion\_clear H5; Inversion\_clear H6; Inversion\_clear H5; Inversion\_clear H7. Rewrite (H1 ? H5); Rewrite (H3 ? H8); Assumption.*

*Generalize (subst\_inv ? ? ? H2); Rewrite subst\_inv\_fun\_lam; Intros. Inversion\_clear H3; Inversion\_clear H4; Inversion\_clear H3.*

*Replace x with M'; Auto.*

*Elim (unsat (app (lam M') (lam x))). Intros; Inversion\_clear H3.*

*Apply ext\_tm with x0; Auto. Qed.*

*As one can see, in this proof we used also the axioms of the Theory of* Contexts (unsat and ext tm).

*Totality of substitution*

*The proof of totality is tricky due to some peculiarities of CIC. The lemma* we want to prove is

*Lemma subst\_is\_total : (M:Var->tm)(EX M' | (subst N M M')).*

*Our intent is to prove this by higher-order induction over M. This fails in the* case of the lambda abstraction, which appears as follows:

*N : tm*

*M : Var->tm*

*M0 : Var->Var->tm*

*H : (y:Var)(EX M':tm | (subst N [x:Var](M0 x y) M'))*

*============================*

*(EX M':tm | (subst N [x:Var](lam (M0 x)) M'))*

*The suitable term should be obtained from the hypothesis H. However, Coq* does not allow us to eliminate a Proposition (like H) to build a term in a Set (M' in tm). Such \eliminations of strong -types" may lead to inconsistencies, and hence are ruled out by the type theory CIC [5].

*The solution we adopt is to move the whole proof in the Set realm, and* then to lift the result to Prop. Therefore, we introduce a Set-typed version of the induction principle|which, equivalently, can be seen as a recursor with dependent types:

*Axiom tm\_rec1 : (P:(Var->tm)->Set) (P var) ->*

*((y:Var)(P [\_:Var](var y))) ->*

*((M,N:Var->tm)(P M)->(P N)->(P [x:Var](app (M x) (N x)))) ->*

*((M:Var->Var->tm)*

*((y:Var)(P [x:Var](M x y)))->(P [x:Var](lam (M x))))*

*->*

*(M:Var->tm)(P M).*

*Then, we prove the totality in Set by higher-order dependent recursion: Lemma sit: (N:tm)(M:Var->tm){M':tm | (subst N M M')}.*

*Intros; Pattern M; Apply tm\_rec1; Intros; Clear M.*

*Split with N; Apply subst\_var. Exists (var y); Apply subst\_void.*

*(Inversion\_clear H; Inversion\_clear H0).*

*Split with (app x x0); Apply subst\_app; Assumption. Exists (lam [y:Var](proj1\_sig tm ? (H y))).*

*Apply subst\_lam; Intros. Apply proj2\_sig.*

*Qed.*

*Notice that in the case of lambda, the required term is built by eliminating* (projecting) the -type in the hypothesis H instantiated on a locally bound (and hence, fresh) variable y.

*Then, the totality theorem is just the extraction of the logical part from* the -type (sit M):

*Lemma subst\_is\_total : (M:Var->tm)(Ex [M':tm](subst N M M')). Intros. Exists (proj1\_sig ? ? (sit M)).*

*Apply proj2\_sig.*

*Qed.*

*Extracting the substitution function*

*Lemma sit can be seen as the speci cation of the substitution function.* We can make it explicit by extracting the rst component of the -type (sit N M):

*Lemma subst\_f : tm->(Var->tm)->tm.*

*Intros N M; Exact (proj1\_sig ? ? (sit N M)). Qed.*

*which, sweetened by a bit of syntactic sugar, takes the familiar form [ ], like* in the following \veri cation" and congruence properties:

*Lemma subst\_f\_prop : (N:tm)(M:Var->tm)(subst N M M[N]). Lemma subst\_f\_var : (N:tm)(var[N])=N.*

*Lemma subst\_f\_void : (N:tm)(y:Var)(([\_:Var]y)[N])=y.*

*Lemma subst\_f\_app : (N:tm)(M1,M2:Var->tm)*

*(([x:Var](app (M1 x) (M2 x)))[N])=(app M1[N] M2[N]).*

*Lemma subst\_f\_lam : (N:tm)(M:Var->Var->tm)*

*(([x:Var](lam (M x)))[N]) = (lam ([y:Var](([x:Var](M x y))[N]))).*

*An interesting property of substitution is composition: for M; N; P terms* and x 6= y, we have that (P [Q=y])[M=x] = (P [M=x])[Q[M=x]=y]. The formal- ization of this statement requires a context with 2 holes:

*Lemma subst\_f\_comp : (M:tm)(Q:Var->tm)(P:Var->Var->tm)*

*(([x:Var]((P x)[(Q x)]))[M]) = ([y:Var]([x:Var](P x y))[M])[Q[M]]).*

*Beside using axioms ext\_tm and |unsat|, the proof of this property goes* by structural induction over the structure of P ; thus we need to assume the corresponding induction principle on Var->Var->tm:

*Axiom tm\_ind2 : (P:(Var->Var->tm)->Prop) (P [x,y:Var]x) ->*

*(P [x,y:Var]y) ->*

*((z:Var)(P [\_;\_:Var](var z))) ->*

*((M,N:Var->Var->tm)(P M)->(P N)->(P [x,y:Var](app (M x y) (N x y)))) ->*

*((M:Var->Var->Var->tm)*

*((z:Var)(P [x,y:Var](M x y z)))->(P [x,y:Var](lam (M x y))))*

*->*

*(M:Var->Var->tm)(P M).*

*3.4 Formalizing the semantics of cbn*

*The representation of both operational semantics is straightforward. Inductive red : tm -> tm -> Prop :=*

*red\_beta: (N:tm)(M:Var->tm)*

*(red (app (lam M) N) (subst\_f N M))*

*| red\_head: (M,N,M':tm)*

*(red M M') -> (red (app M N) (app M' N)).*

*Inductive trred : tm -> tm -> Prop :=*

*| trred\_ref : (M:tm)(trred M M)*

*| trred\_trs : (M,N:tm)(red M N)->(P:tm)(trred N P)->(trred M P).*

*Inductive eval : tm -> tm -> Prop := eval\_var : (x:Var)(eval x x)*

*| eval\_lam : (M:Var->tm)(eval (lam M) (lam M))*

*| eval\_app : (M,N,V:tm)(M':Var->tm)*

*(eval M (lam M')) -> (eval M'[N] V) -> (eval (app M N) V).*

*Proposition 3.7 Let X be a nite set of variables; for all M; N 2 X, we have:*

*(i) M ! N () X ` : (red X(M) X(N))*

*(ii) M ! N () X ` : (trred X(M) X(N))*

*(iii) M + N () X ` : (eval X(M) X(N))*

*Most interesting properties of small-step and big-step semantics can be* proved without using the Theory of Contexts. These properties include the progress lemma, determinism of semantics, equivalence of big-step and small- step semantics:

*Definition closed : tm -> Prop := [M:tm](x:Var)(notin x M).*

*Lemma progress : (M:tm)(closed M)->(isvalue M)\/(EX N | (red M N)). Lemma red\_is\_det : (M,V1:tm)(red M V1)->(V2:tm)(red M V2)->V1=V2.*

*Lemma eval\_is\_det : (M,V1:tm)(eval M V1)->(V2:tm)(eval M V2)->V1=V2. Lemma red\_eval : (M,N:tm)(red M N)->(V:tm)(eval N V)->(eval M V).*

*Lemma trred\_eval : (M,V:tm)(trred M V)->(isvalue V)->(eval M V). Lemma eval\_trred : (M,N:tm)(eval M N) -> (trred M N).*

*These properties are proved by simple induction on the syntax of M and the derivation of (red M V1), (eval M V1), (red M N), (trred M V), (eval M N), respectively.*

# *4 Extending the (meta)theory*

*In this section we consider two extensions of the cbn: applicative bisimulation* and observational equivalence, and a simple type system. This allows us to test the modularity of the Theory of Contexts. It turns out that, while in the rst case the Theory of Contexts previously introduced works ne, in the latter case we have to modify slightly the unsat axiom, in order to take into account the new behaviour of variables brought in by the type system.

*4.1 Applicative Bisimulation and Observational Equivalence*

*In this section we extend the theory and the metatheory of cbn by considering* two well-known equivalences over cbn [1]:

*De nition 4.1 The observational equivalence is the relation o over 0 de-*

*ned as follows: M o N i for all C[ ] 2 0, if C[M]+ then C[N]+.*

*The applicative bisimulation is the relation a over 0 de ned as follows:* M a N i if M + xP for some P , then there exists Q such that N + xQ and for all R 2 0: P [R=x] a Q[R=x].

*Notice that the de nition of the applicative bisimulation is coinductive.* There is also a \linearized" de nition of the same relation, which we denote

*by 0 : M 0 N i for all n and R1;::: ; Rn 2 0: if (MR1 ::: Rn)+ then*

*a a*

*(NR1 ::: Rn)+.*

*It is quite clear that a= 0 . A more interesting and important result is* the so called operational extensionality, that is a= o [1]. The proof sketch given in [1] consists in the proof of the following technical lemma:

*a*

*M N ) 8n:8C 2 0:C[M]+n ) C[N]+n (1)*

*a*

*where +n is a \indexed" version of the evaluation semantics. The intended* meaning of the index is the number of substitution performed in the evalua- tion. The rules for +n are the following:

*M +m x:M0 M0[N=x] +n V*

*x:M +0 x:M*

*M N +m+n+1 V*

*Our aim is to encode these relations in CIC and to prove formally their* equivalence. The formalization of a and o is not problematic; in particular, we can take advantage of Coinductive types for encoding a:

*CoInductive appsim : tm -> tm -> Prop := appsim\_coind : (M,N:tm)*

*((M':Var->tm)(eval M (lam M')) ->*

*(EX N' | (eval N (lam N')) /\*

*(L:tm)(closed L) -> (appsim M'[L] N'[L])*

*-> (appsim M N).*

*Definition conv := [M:tm](EX V | (eval M (lam V))). Definition obseq : tm -> tm -> Prop := [M,N:tm](C:Var->tm)*

*(closed (lam C))-> (conv C[M]) -> (conv C[N]).*

*For 0 , on the other hand, we need to introduce the datatype of applicative* lists, and the operation of list application:

*a*

*Inductive ltm : Set := nil : ltm | larg : ltm -> tm -> ltm. Fixpoint lapp [M:tm;L:ltm] : tm :=*

*Cases L of nil => M*

*| (larg L' N) => (app (lapp M L') N) end.*

*Definition appsim' : tm -> tm -> Prop := [M,N:tm]*

*(L:ltm)(lclosed L)-> (conv (lapp M L)) -> (conv (lapp N L)).*

*Then, two implications are proved without using the Theory of Contexts:*

*Lemma obseq\_appsim' : (M,N:tm)(obseq M N) -> (appsim' M N). Lemma appsim'\_appsim : (M,N:tm)(appsim' M N) -> (appsim M N).*

*The former is proved by induction on the applicative list in the de nition of* appsim'. The latter is proved by coinduction: using the tactic Cofix we can

*\assume" the conclusion and apply the coinductive rule:*

*appsim'\_appsim : (M,N:tm)(appsim' M N)->(appsim M N)*

*M : tm*

*N : tm*

*H : (appsim' M N) P : Var->tm*

*H0 : (eval M (lam P))*

*============================*

*(EX Q:Var->tm |*

*(eval N (lam Q))/\((R:tm)(closed R)->(appsim P[R] Q[R])))*

*The proof proceeds then by elimination of the hypothesis H. Notice that for* these proofs we do not need the hypothesis that M,N are closed.

*More diÆcult is the proof of the third inclusion, namely*

*Variable M,N: tm.*

*Hypothesis closedN : (closed N). Hypothesis closedM : (closed M).*

*Lemma appsim\_obseq : (appsim M N) -> (obseq M N).*

*For this end, we need to encode +n and prove the property (1): Inductive neval : nat -> tm -> tm -> Prop :=*

*neval\_lam : (M:Var->tm)(neval O (lam M) (lam M))*

*| neval\_app : (M,N,V:tm)(M':Var->tm)(n,m:nat)*

*(neval n M (lam M')) -> (neval m M'[N] V) ->*

*(neval (S (plus n m)) (app M N) V).*

*[...]*

*Lemma Context : (n:nat)(C:Var->tm)(closed (lam C)) ->*

*(V:tm)(neval n C[M] V) -> (conv C[N]).*

*Following [1], the proof is by induction on n. Induction over Var->tm is used* for destructing the context C in order to obtain the two cases mentioned in [1]:

*C[ ] ( xP [ ])(Q[ ])R[ ]*

*C[ ] [ ](Q[ ])R[ ]*

*Beside these we obtain also other four cases which have been omitted in [1],* and which are easily dealt with. The proof proceeds by several technical manipulations of applicative lists and some structural properties of indexed evaluation, like the following

*Lemma neval\_one\_step : (P:Var->tm)(Q:tm)(R:ltm)(V:tm)(n:nat)*

*(neval (S n) (lapp (app (lam P) Q) R) V) ->*

*(neval n (lapp P[Q] R) V).*

*In many points, the Theory of Contexts is used to prove easily equivalences* between contexts.

*It should be noticed that the burden of the proofs is in the manipulation* of applicative lists, rather than in dealing with contexts. Many properties of lists which are usually taken for granted, here must be spelled out and proved in full detail.

*4.2 Typing system*

*In this section we extend the theory and the metatheory of cbn by adding* simple types. Simple types are de ned by the grammar ::= u j ! , where u; v range over type variables. The typing judgement has the form ` M : , where is the typing base, that is a nite set of pairs x1 : 1;::: ; xn : n. The usual typing rules are the following:

*(x : ) 2*

*` x :*

*` M : ! ` N :*

*` (M N) :*

*;x : ` M :*

*` x:M : !*

*x 62 dom( )*

*The syntax of simple types is encoded trivially: Parameter tyVar : Set.*

*Inductive ty : Set := tvar : tyVar -> ty | arr : ty -> ty -> ty.*

*Coercion tvar : tyVar >-> ty.*

*The introduction of a typing system has a bearing on the structure of Var. In* the previous section, we assumed Var to be simply any set with the required properties, i.e. the unsat axiom and, ultimately, decidability of equality. The typing system, however, requires that every free variable is given a type. This is re ected in the encoding by adding more structure to Var, i.e. by assuming the existence of a type assignment and by requiring that every fresh variable introduced by unsat must be given a type:

*Parameter typevar : Var -> ty.*

*Axiom unsat\_t : (M:tm)(s:ty)(EX x | (notin x M) /\ (typevar x)=s). Then, the encoding of the typing system is straightforward:*

*Inductive type : tm -> ty -> Prop :=*

*type\_var : (x:Var)(type (var x) (typevar x))*

*| type\_app : (M,N:tm)(s,t:ty)(type M (arr s t)) -> (type N s) -> (type (app M N) t)*

*| type\_lam : (M:Var->tm)(s,t:ty)*

*((x:Var)((typevar x)=s) -> (type (M x) t))*

*-> (type (lam M) (arr s t)).*

*Notice that unsat\_t entails unsat, so the results previously proved, still hold* with this axiom.

*The rst important property we need to prove is that substitution preserves* types of terms:

*Lemma subst\_preserves\_types : (E:Var->tm)(N,M:tm)(subst N E M) -> (s,t:ty)(type (lam E) (arr s t)) -> (type N s) -> (type M t).*

*This can be proved by induction on the derivation of (subst N E M), using* unsat\_t for introducing fresh names with the right types and the following lemma of type invariance under replacement of free variables:

*Lemma type\_invar : (M:Var->tm)(s,t:ty)*

*(x:Var)((typevar x)=s) -> (type (M x) t) ->*

*(y:Var)((typevar y)=s) -> (type (M y) t).*

*This lemma states a property of contexts, so it is natural to proceed \by higher-* order induction on M". Indeed, using the higher-order induction principle tm\_ind1, the lemma type\_invar can be proved straightforwardly. Then, all

*subject reductions properties are simple consequences of subst\_preserves\_types: Lemma SR\_eval : (M,V:tm)(eval M V)->(s:ty)(type M s)->(type V s).*

*Induction 1; Clear H V M; Intros; Try Assumption.*

*Inversion\_clear H4; Apply H3.*

*Apply subst\_preserves\_types with s:=s0 1:=H1; Auto. Qed.*

*Lemma SR\_red : (M,N:tm)(red M N)->(s:ty)(type M s)->(type N s).*

*Lemma SR\_trred : (M,N:tm)(trred M N) -> (s:ty)(type M s) -> (type N s). The proofs of the latter properties are similar to former's.*

# *5 Related work*

*The case study presented in this paper should be compared with similar de-* velopments on the -calculus in HOAS. Due to the lack of space, here we can discuss brie y only some of them. Despeyroux et al. in [7] adopted an approach similar to ours for reasoning on the (call-by-value) -calculus. The main di erence is that variables are represented by an inductive set (such as nat). This allows to avoid to assume the properties of the Theory of Contexts as axioms, but at the price to cope with exotic terms. These are ruled out by means of a well-formedness predicate valid ; all arguments are then carried out on terms which are extensionally equivalent to some valid term. Since CIC is not extensional, this equivalence has to be embedded into valid explicitly. Dealing with well-formedness predicats introduces a substantial overhead with respect to informal proofs, although it is conceivable that much can be au- tomatized by means of ad hoc tactics. The Coq code of [7] (covering syntax, substitution, big-steps semantics, typing system and proof of subject reduc- tion) is 500 lines long; the same theory, developed in the Theory of Contexts, takes less than 300 lines.

*On the other hand, Rockl et al. proved recently that the Theory of Con-* texts (for the -calculus) can be derived from well-formedness predicates in Isabelle [27]. In some sense, therefore, the Theory of Contexts can be seen as a core set of basic properties capturing the essence of what a context is, without assuming unnecessary assumptions. Further case studies like the present one are needed, in order to verify the expressive power of this approach.

*In [26], Pitts introduced the Nominal Logic, a rst-order logic speci cally* designed for reasoning on syntax involving variable bindings. The axioms of Nominal Logic express the key properties of the FM-model of syntax intro- duced in [11]. The main idea is to express and deal only with properties whose validity is invariant under swapping of bindable names. It is interesting to see that many principles are common to Nominal Logic and the Theory of Con- texts (e.g., unsaturability of names, \structural induction modulo ", ... ). The exact connection between the two theories is still to be investigated.

*As already pointed out, most nowadays proof editors, and in particular all* those based on type theory, lack of induction on higher order types. The prob- lem of combining HOAS and induction, avoiding the arising of exotic terms, has been addressed radically in [9, 8], where modal -calculi are proposed as metalanguages in place of usual type theories. In fact, this approach is best seen as a step towards a brand new generation of proof assistants, rather than a way for dealing with HOAS in nowadays proof editors, as the Theory of Contexts is intended to be.

*In all these approaches, we reason on objects of the metalogic (CIC,* HOL,... ), in the metalogic itself. A di erent perspective is to add explicitly an extra logical level for reasoning over metalogics. One of these meta-metalogic is F O N [19], a higher-order intuitionistic logic extended with de nitions and higher order quanti cation over simply typed -terms. Induction on types is recovered from induction on natural numbers via appropriate notions of mea- sure. Di erently from the approach adopted in this work and in [7], in F O N it is possible to delegate even the substitution to the metalanguage. F O N has been successfully used to reason with typing and evaluation judgements for the call-by-name -calculus, among other case studies. However, F O N is more in the streamline of logic programming: it does not support a notion of \proof object", nor the typical judgements-as-types paradigm. Actually, all the properties on cbn proved in [19] have been proved also in the present work using the Theory of Contexts and simple (i.e., structural) induction over proofs. Due to its logic programming avour, F O N seems more suited for a complete automatization, i.e. the implementation of a theorem prover.

*A similar attitude, but with di erent aims, is behind Schurmann's M2 [25],* which is a constructive rst-order logic based on the Edinburgh LF. At the meta-metalevel, M2 o ers higher-order induction and recursion for reasoning over (possibly open) objects of a LF encoding. M2 is aimed to a complete au- tomatization (it is implemented in the theorem prover Twelf ), hence it is diÆ- cult to compare with interactive approaches like the ones previously discussed.

# *6 Conclusions*

*In this paper we have presented a non trivial case study of the (meta)theory* of cbn using the Theory of Contexts in the Coq proof environment. This approach allowed for a smooth treatment of the syntax up-to -conversion, substitution, small-step and big-step semantics and typing system of cbn. We have formally proved several metatheoretical properties such as functionality of substitution, determinism of big-step semantics, equivalence of big-step and small-step semantics, subject reductions for both semantics, equivalence of applicative bisimulation and observational equivalence, etc.

*In our opinion, the case study has been successful. The logical overhead* which is required to the user is acceptable, since the encodings are straigth- forward and the user can directly transpose his/her intuition and hand-made proofs about contexts in the proof editor. This case study has pointed out also some weak points of the Theory of Contexts in the Coq system, in par- ticular in connection with higher-order inversion principles. We have shown, by means of an example, how suitable inversion principles over higher-order types can be stated and derived.

*Although in this work we have focused on the Coq system, all arguments* should be applicable to any other proof assistant based on inductive type theories close to CIC, such as LEGO or Plastic. On the other hand, the Theory of Contexts is inconsistent with the Axiom of Unique Choice (AC!) [14]. In particular, this means that the approach we have adopted in this paper cannot be adopted in Isabelle/HOL because the Description Axiom entailes AC!. For a comparison of formalizations of languages with variable bindings in Isabelle, see [21]. Nevertheless, it is still possible to use the Theory of Contexts within classical HOL; see [15, 4] for an example metalanguage with full classical higher-order logic, and the proof of its consistency.

*Future work.*

*The present development of the metatheory of cbn can be extended in* many directions. A possible future work could be the generalization of the inversion algorithms presented in [6] to suitable higher-order types. From a practical point of view, this would be particularly useful.

*On the theoretical side, at least two interesting issues has arisen. The rst* is that we have not needed the whole Theory of Contexts, since the axiom of -expansion has not been introduced. This seems to point out that the properties of cbn we dealt with do not rely on such kind of property. The second issue is that, due to soundness constraints imposed by CIC, in order to prove totality of substitution we introduced higher-order recursion with dependent types. Known models of the Theory of Contexts validate plain higher-order recursion; it is an open question if these models can be extended to dependent type theory.

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