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Developing (Meta) Theory of λ -calculus in the Theory of Contexts

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A common scenario

- represent formally (encode) syntax and semantics of an object language (e.g., λ -, π -calculus) in some logical framework for doing formal (meta)reasoning.
- derive some results interaction in a goal-directed manner, using tactics in some general-purpose theorem prover/proof assistant

Problem: how to render binding operators (e.g, λ , ν) efficiently?

In interactive development,

efficiently \cong "formal proofs should look like on paper"

Many approaches, with pros and cons: de Bruijn indexes, first-order abstract syntax, higher-order abstract syntax . . . [HHP87, Hue94, DFH95, GM96, MM01, . . .].

They have to be tested on *real* case studies, in *real* proof assistants.

In this talk

We focus on

call-by-name λ -calculus in type-theory based proof assistants (viz., Coq), using (weak) HOAS and the Theory of Contexts.

Why λ -calculus?

- complementary to π -calculus (higher-order binders, terms-for-variables substitution, . . .) which has been already done [HMS01]
- well-known (meta)theory. Too well, maybe.
- customary benchmark for formal treatments of binders ⇒ allows for comparison with other approaches ([Momigliano et al. 2001] for a survey)

Claim: the formal, fully detailed development of the theory of λ_{cbn} in the Theory of Contexts introduces a small, sustainable overhead with respect to the proofs "on the paper".

Outline of the talk

- ullet Definition of λ_{cbn} "on the paper"
- ullet Encoding of syntax and semantics of λ_{cbn} in HOAS
- Some formally proved results.
- Extending the language: type systems. More results.
- Discussion
- Related work
- Future work

A typical definition of λ_{cbn} in 1 slide

Syntax The set Λ is defined by Λ : $M, N := x \mid (MN) \mid \lambda x.M$ where x, y, z, \ldots range over an infinite set of variables. Terms are taken up-to α -equivalence. We denote by M[N/x] the capture-avoiding substitution of N for x in M. Free variables (FV) are defined as usual. For X a finite set of variables, we define $\Lambda_X \triangleq \{M \in \Lambda \mid FV(M) \subseteq X\}$.

Contexts, i.e. terms with holes, are denoted by $M(\cdot)$. A (closed) term is said to be a value if it is not an application.

Small-step semantics (or *reduction*) is the smallest relation $M \longrightarrow N$ defined by

$$\frac{M \longrightarrow M'}{(\lambda x.M) \ N \longrightarrow M[N/x]} \qquad \frac{M \longrightarrow M'}{(M \ N) \longrightarrow (M' \ N)}$$

We denote by \longrightarrow^* the reflexive and transitive closure of \longrightarrow .

Big-step semantics (or *evaluation*) is the smallest relation $M \Downarrow N$ defined by

$$\frac{1}{x \Downarrow x} \frac{M \Downarrow \lambda x.M' \quad M'[N/x] \Downarrow V}{\lambda x.M \Downarrow \lambda x.M}$$

Formalizing the theory of $\lambda_{\mbox{cbn}}$

Encoding of the syntax

The general methodology: define a datatype for each syntactic class of the language.

Two classes: variables and terms

What we put in place of ... and for Var depends on the approach we will follow:

- first-order
- higher-order

First-order approaches

deep embedding: write the encoding in the framework

First-order abstract syntax Var is an inductive set (e.g., nat)

$$\lambda \quad \leadsto \quad \text{lam} : \quad \text{Var} \rightarrow \text{tm} \rightarrow \text{tm}$$
 $\lambda x. \lambda y. (xy) \quad \leadsto \quad \text{lam x (lam y (app x y))}$

 \spadesuit Needs to implement and validate lots of machinery about α -equivalence, substitution, . . .

de Bruijn indexes Var=1, the initial object

$$\lambda \hspace{0.2cm}
ightharpoonup \hspace{0.1cm} \operatorname{lam}: \hspace{0.1cm} \operatorname{tm} \hspace{0.1cm} ext{-> tm} \ \lambda x. \lambda y. (xy) \hspace{0.2cm}
ightharpoonup \hspace{0.1cm} \operatorname{lam} \hspace{0.1cm} (\operatorname{lam} \hspace{0.1cm} (\operatorname{app} \hspace{0.1cm} 1 \hspace{0.1cm} 0))$$

- \heartsuit Good at α -equivalence
- ♠ Not immediate to understand and needs even more technical machinery for capture-avoiding substitution than FOAS

We respect the rules of the game \Rightarrow Coq and Isabelle/HOL automatically provide induction principles to reason over processes

Higher-order approaches

Shallow embedding: Change the rules, and write the encoding within the framework!

Full HOAS [HHP87] Var = tm

```
\lambda \longrightarrow \lim : (tm \rightarrow tm) \rightarrow tm
\lambda x. \lambda y. (xy) \longrightarrow \lim [x:tm] (lam [y:tm] (app x y))
```

- \heartsuit all aspects of variables management are delegated successfully to the metalanguage (α -conversion, capture-avoiding substitution, generation of fresh names,...)
- incompatible with inductive types: the definition

```
Inductive tm : Set := app : tm -> tm -> tm \mid \text{lam} : (tm -> tm) -> tm.
```

is not acceptable due to the negative occurrence of tm.

Higher-order approaches (cont.)

(Weak) Higher Order Abstract Syntax Var is not tm, and

```
\lambda \longrightarrow \lim : (Var \rightarrow tm) \rightarrow tm \lambda x. \lambda y. (xy) \longrightarrow \lim [x:Var](lam [y:Var](app (var x) (var y)))
```

- \heartsuit it delegates successfully many aspects of names management to the metalanguage (α -conversion, capture-avoiding substitution of names/variables, generation of fresh names,...)
- \heartsuit compatible with inductive types \Rightarrow we can define functions and reason by case analysis on the syntax
- if Var is defined as inductive then exotic terms (= not corresponding to any real process of the object language) will arise!

```
? \rightsquigarrow lam [x:nat](Cases x of 0 => x | _ => (app (var x) (var x)) end)
```

metatheoretic analysis is difficult/impossible; e.g., structural induction over higher-order terms (contexts, terms with holes) is not provided

The Theory of Contexts addresses these problems from an "axiomatic standpoint".

Encoding the syntax: avoiding exotic terms

Exotic terms arise only when a binding constructor has an inductive type in negative position (lam : (Var -> tm) -> tm).

Occam razor: Var is not required to be an inductive set

- ⇒ there is no reason to bring in induction/recursion principles and case analysis, which can be exploited for defining exotic terms
- \Rightarrow leave Var as an "open" set. Just assume it has the needed properties.

Complete definition (properties on Var will come later on):

Proposition 1 For all X finite set of variables, there is a bijection ϵ_X between Λ_X and canonical terms of type tm with free variables in X.

Moreover, this bijection is compositional, in the sense that if $M \in \Lambda_{X,x}$ and $N \in \Lambda_X$, then $\epsilon_X(M[N/x]) = \epsilon_{X,x}(M)[\epsilon_X(N)/(\text{var }x)]$.

Encoding of substitution

Substitution of terms for variables is no longer delegated to the metalevel.

It is represented as a (functional) relation, whose derivations are syntax-driven.

The judgement "(subst N M M')" represents "M' = M[N]":

Proposition 2 Let X be a finite set of variables and x a variable not in X. Let $N, M' \in \Lambda_X$ and $M \in \Lambda_{X \uplus \{x\}}$. Then:

```
M[N/x] = M' \iff \Gamma_X \vdash \_ : (\text{subst } \epsilon_X(N) \ [x:Var] \epsilon_{X \uplus \{x\}}(M) \ \epsilon_X(M'))
```

Encoding of semantics

Straightforward. The only remark is about the use of the substitution judgement.

The encoding is adequate; e.g.:

Proposition 3 Let X be a finite set of variables; for all $M, N \in \Lambda_X$, we have $M \Downarrow N \iff \Gamma_X \vdash _ : (\text{eval } \epsilon_X(M) \epsilon_X(N)).$

Formalization of the MetaTheory of λ_{cbn}

Following the methodology developed in [HMS98] and fully generalized in [HMS01]:

- Definition of occurrence predicates.
 Driven by the signature of the object language.
- Axiomatization of the Theory of Contexts. Parametric in the occurrence predicates.
- Development of theory (Have fun!)

Occurrence predicates

```
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)).

Roughly, "(isin x M)" means "x occurs free in M".

Dually for (notin x M): "x does not occur free in M".
```

The Theory of Contexts

A set of axiom schemata, which reflect at the theory level some fundamental properties of the intuitive notion of "context" and "occurrence" of variables. Their informal meaning is the following:

- **Decidability of occurrence:** every variable either occurs or does not occur free in a term (generalizes decidability of equality on Var). Unnecessary if we are in a classical setting;
- 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; (cfr. axiom F4 in Pitts' nominal logic)
- **Extensionality of contexts:** two contexts are equal if they are equal on a fresh variable; that is, if M(x) = N(x) and $x \notin M(\cdot), N(\cdot)$, then M = N.
- β -expansion: given a term M and a variable x, there is a context $C_M(\cdot)$, obtained by abstracting M over x

The Theory of Contexts for λ_{cbn}

What of the Theory of Contexts we need in the present development:

Notice that we do not need β -expansion.

Scared by axioms? Axioms are our friends!

The axiomatic approach helps us to split the problem in two (quite orthogonal) issues:

- 1. isolating a core set of fundamental properties of contexts, and to play with them in order to check their expressivity and "efficiency"
- 2. proving the soundness of these properties, or even deriving them from more basic (but possibly less natural) notions (like, e.g., in [Röckl et al., 2001])

Consistency of these axioms in Classical Higher Order Logic has been proved in [BHHMS01], by building a model following Hofmann's idea [Hof99]. The model is a classical tripos in a category of covariant presheaves...but this is another story.

Moreover, this model justifies also *recursion and induction principles* over higherorder types, which can be therefore safely assumed as needed

Induction over Var -> tm

```
(P \lambda x : v \cdot (var x))
       \forall y : Var.(P \ \lambda x : v.(var \ y))
       \forall M_1: v \to \Lambda, M_2: v \to \Lambda.(P M_1) \land (P M_2) \Rightarrow (P \lambda x: v.(app (M_1 x) (M_2 x)))
      \forall M_1: v \to v \to \Lambda.(\forall y: v.(P \ \lambda x: v.(M_1 \ x \ y))) \Rightarrow (P \ \lambda x: v.(\lambda(M_1 \ x)))
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))) \rightarrow (P [x:Var](lam (M x))))
         -> (M:Var->tm)(P M).
but for all n, a similar schemata over Var^n->tm can be defined [HMS01b].
Similarly for recursions (recursors and equivalence (reduction) rules).
Compare it with "structural induction mod \alpha" in Pitts' nominal logic.
```

Some results formally proved in Coq

- subst is deterministic (easier with higher-order inversion)
- subst is total (higher-order recursion)
- generation lemma for terms
- generation lemma for contexts (higher-order induction)
- substitution preserves free variables
- evaluation preserves free variables
- determinism (confluence) of evaluation
- determinism (confluence) of reduction
- equivalence of evaluation and reduction

• . . .

```
Lemma subst_is_det: (M:Var->tm)(M1:tm)(subst N M M1) ->
                     (M2:tm)(subst N M M2) \rightarrow (M1 = M2).
Lemma sit: (N:tm)(M:Var->tm){M':tm | (subst N M M')}.
Lemma subst_is_total : (N:tm)(M:Var->tm)(EX M' | (subst N M M')).
Lemma subst_isin : (M:Var->tm)(N,M':tm)(subst N M M') -> (x:Var)(isin x M') ->
                    (isin x N)\/(isin x (lam M)).
Lemma subst notin : (M:Var->tm)(N,M':tm)(subst N M M') -> (x:Var)(notin x N) ->
                     (notin x (lam M)) -> (notin x M').
Lemma closed_generation : (M:tm)(closed M)->(EX C | (EX L | M=(lapp C L))).
Lemma closedschema_generation : (M:Var->tm)(closed (lam M))->
                   (EX C: Var \rightarrow tm \mid (EX L: Var \rightarrow ltm \mid M=[x:Var](lapp (C x) (L x)))).
Lemma reducts_are_values : (M,N:tm)(eval M N)->(isvalue N).
Lemma values_do_not_reduce : (N:tm)(isvalue N)->(eval N N).
Lemma eval_is_det : (M,V1:tm)(eval M V1) -> (V2:tm)(eval M V2) -> V1=V2.
Lemma eval_isin : (M,N:tm) (eval M N) -> (x:Var) (isin x N) -> (isin x M).
Lemma eval_notin : (M,N:tm) (eval M N) -> (x:Var) (notin x M) -> (notin x N).
Lemma values_do_not_red : (V:tm)(isvalue V)->(M:tm)(red V M)->False.
Lemma red is det : (M,V1:tm)(red M V1) \rightarrow (V2:tm)(red M V2) \rightarrow 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).
```

Functionality of substitution: some pragmatics

The proof goes by induction on the derivation of (subst N M M1).

This gives rise to four cases:

For each case, inversion on H gives 4 subcases, 3 of which are absurd

```
subgoal 2 is:
subgoal 1 is:
                                    N: tm
 N: tm
                                    M : Var->tm
 M : Var->tm
                                    M2:tm
 M2:tm
                                    H : (subst N var M2)
 H: (subst N var M2)
                                    y : Var
 HO: var=var
                                    H1 : ([_:var](y))=var
 H1: N=M2
                                    HO : (y) = M2
 _______
  M2=M2
                                       ______
                                     N=(\lambda)
```

The inversion algorithm fails to eliminate absurd cases because the terms to discriminate on are higher-order. Absurd cases are (tediously) eliminated by using the Theory of Contexts (in particular tm_{ext}) and plain (i.e., first order) recursion.

The whole proof is 95 lines long, most of which are for dealing with the elimination of absurd cases.

Functionality of substitution: higher-order inversion

Higher-order inversion lemmata can be (mechanically) proved from higher-order recursion principles (over Type).

Extending the object language: typing system

We extend the object language with a theory of simple types. Common definition: Types are defined by $\tau := u \mid \tau \to \tau$ where u, v range over type variables.

Typing judgement: $\Gamma \vdash M : \tau$, where Γ is the typing base, that is a finite set of pairs $x_1 : \tau_1, \ldots, x_n : \tau_n$. The usual typing rules are the following:

$$\frac{(x:\tau) \in \Gamma}{\Gamma \vdash x:\tau} \qquad \frac{\Gamma \vdash M:\sigma \to \tau \quad \Gamma \vdash N:\sigma}{\Gamma \vdash (M\ N):\tau} \qquad \frac{\Gamma,x:\sigma \vdash M:\tau}{\Gamma \vdash \lambda x.M:\sigma \to \tau} x \not\in dom(\Gamma)$$

The syntax of simple types is encoded trivially:

```
Parameter TVar : Set.

Inductive T : Set := tvar : TVar -> T | arr : T -> T -> T.

Coercion tvar : TVar >-> T.
```

Modularity of the Theory of Contexts

The introduction of a typing system has a bearing on the structure of Var.

- before: Var may be any set satisfying unsat axiom and decidability of equality
- now: we require that every free variable is given a type, by assuming that
 - the existence of a type assignment: a map from variables to types
 - every fresh variable introduced by unsat must be given a type

Since the locally assumed x is fresh, the assumption (typevar x)=s is safe

More results formally proved in Coq

- preservation of types under renaming of variables (higher-order induction)
- preservation of types under substitution
- subject reduction for evaluation
- subject reduction for reduction (small-step semantics)

Discussion

About the development

- Most of these proofs use built-in inductions (on plain terms and derivations),
 and the axioms unsat, LEM_OC, ext_tm, ext_tm1
- Some proofs required higher order induction (induction over contexts)
- Totality of substitution: higher-order recursion (induction in Set)
- Powerful higher-order inversion principles can be derived from higher-order recursion
- No proof has needed β -expansion replaced by higher-order induction?

Discussion (cont.)

The Theory of Contexts turned out to be successful

- smooth handling of schemata in HOAS
- on need of well-formedness predicate for ruling out exotic terms
- V low mathematical and logical overhead: "proofs looks (almost) like on the paper". Almost, because of the explicit handling of substitution.

Weak points:

- compatible with Classical HOL but not with the Axiom of Unique Choice (AC!)
 - ⇒ not easily portable to metalogics containing AC!
 - ⇒ weak expressive power at the level of functions (which can be nevertheless recovered at the level of predicates)
- no automatization of inversion lemmata, yet

Related work

[Despeyroux, Felty, Hirschowitz 1995]: closest to ours, but Var=nat.

- + no need of axioms
- well-formedness predicate (valid); all arguments are then carried out on terms which are extensionally equivalent to some valid term ⇒ substantial overhead.
 E.g., for syntax, substitution, big-steps semantics, typing system and subject reduction: 500 lines in [DFH95], vs < 300 lines within the Theory of Contexts.

[Momigliano, Ambler, Crole 2001] (good survey!): very similar theory and issues

- weak HOAS on an inductive set $Var=\{x,y\} \Rightarrow$ well-formedness predicates
- overhead mitigated by automatization (higher in Isabelle than in Coq)
- totality of substitution requires the description axiom, which entails AC!, which is inconsistent with the Theory of Contexts [Hof99]

Related work: meta-meta-logics

In previous approaches: we reason on objects of the metalogic (CIC, HOL,...), in the metalogic itself.

A different perspective: add an extra logical level for reasoning over metalogics.

 $FO\lambda^{\Delta N}$ [McDowell, Miller, 1997]:

- ullet a higher-order intuitionistic logic extended with definitions, for reasoning on representations in simply typed λ -calculus
- it is possible to delegate the substitution to the metalanguage
- induction on types is recovered from induction on natural numbers via appropriate notions of measure
- it does not support a notion of "proof object" (and in the Theory of Contexts many properties of λ_{cbn} are derived by plain structural induction over proofs)

Related work: meta-meta-logics

 \mathcal{M}_2 [Pfenning and Schürmann, 2000]

- constructive first-order logic (based on ELF) for reasoning over (possibly open) objects of a LF encoding
- supporting higher-order induction and recursion
- ullet aimed to a complete automatization \Rightarrow difficult to compare with interactive approaches
- implemented in the theorem prover *Twelf*

Work in progress

Abramsky's applicative bisimulation

ullet neatly encoded as a *coinductive predicate* (like strong late bisimulation in π -calculus)

 equivalence between applicative bisimulation and observational equivalence: at a good stage to its completion

Work in progress (2)

Equivalence between different notions of α -equivalence (Scagnetto):

• "Standard" (i.e., Barendregt's book) definition:

$$\frac{M \equiv_{\alpha} M' \quad N \equiv_{\alpha} N'}{(MN) \equiv_{\alpha} (M'N')} \quad \frac{\lambda x.M \equiv_{\alpha} \lambda y.M[y/x]}{\chi x.M} \notin FV(M)$$

Alternative (Gabbay and Pitts) definition:

$$\frac{1}{x\sim_{\alpha}x}\frac{M\sim_{\alpha}M'}{(MN)\sim_{\alpha}(M'N')}\frac{(zx)\cdot M\sim_{\alpha}(zy)\cdot N}{\lambda x.M\sim_{\alpha}\lambda y.N}z \text{ does not occur in }M,N$$
 where $(zx)\cdot M$ swaps all occurrences of x by z .

- $\equiv_{\alpha} \subset \sim_{\alpha}$: done
- $\sim_{\alpha} \subseteq \equiv_{\alpha}$: in progress (difficulty: transitivity of \equiv_{α} , not trivial)

Other minor/work in progress case studies

First Order Logic full theory: validity judgement, substitution; metatheory: functionality of substitution.

spi calculus full theory; metatheory: some algebraic laws

 ν -calculus theory

 $\lambda \sigma$ -calculus theory; some metatheoretic result

Ambient calculus language, congruence, logic, some result

Future work:

Higher-order inversion generalization of the Murthy-Cornes-Terrasse algorithm