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## Reduction Under Substitution

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**Abstract.** The Reduction-under-Substitution Lemma (RuS), due to van Daalen [Daa80], provides an answer to the following question concerning the lambda calculus: given a reduction  $M[x:=L] \to N$ , what can we say about the contribution of the substitution to the result N. It is related to a not very well-known lemma that was conjectured by Barendregt in the early 70's, addressing the similar question as to the contribution of the argument M in a reduction  $FM \to N$ . The origin of Barendregt's Lemma lies in undefinablity proofs, whereas van Daalen's interest came from its application to the so-called Square Brackets Lemma, which is used in proofs of strong normalization.

In this paper we compare various forms of RuS. We strengthen RuS to multiple substitution and context filling and show how it can be used to give short and perspicuous proofs of undefinability results. Most of these are known as consequences of Berry's Sequentiality Theorem, but some fall outside its scope. We show that RuS can also be used to prove the sequentiality theorem itself. To that purpose we give a further adaptation of RuS, now also involving "bottom" reduction rules, sending unsolvable terms to a bottom element and in the limit producing Böhm trees.

#### 1 Introduction

The Reduction-under-Substitution Lemma (RuS) addresses the following question concerning the  $\lambda$ -calculus: given a reduction  $M[x:=L] \to N$ , what is the contribution of the substitution to the result N? Or, equivalently: how much of N can be produced already by M, independently of the substitution? The answer to the second question will turn out to be: a prefix of N. Thus there is a natural inverse correspondence with the so-called prefix property, cf. [BKV00] or [Ter03], Ch. 8.

RuS was formulated by Diederik van Daalen [Daa80] as a slightly strengthened version of an observation of Barendregt [Bar74], addressing the same questions as to the contribution of the argument M in a reduction FM oup N. We will study Barendregt's Lemma (BL) in Section 2. Because of its more general form, van Daalen's formulation allowed for an easier and more elegant proof than BL. RuS found its way into Barendregt's book on the  $\lambda$ -calculus [Bar84], where it ended up as Exercise 15.4.8. This literally seemed to be the end of the story, as subsequently little more attention has been paid in the literature to either BL or RuS. Unjustly so, as we hope to make clear in this paper.

The origin of Barendregt's Lemma lies in undefinability. In accordance, Exercise 15.4.8 in [Bar84] is employed there as one of two methods to obtain the

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undefinability of Church's  $\delta$  (using a particular encoding of numerals), the other method using a Böhm-out technique. In [Vri87] Barendregt's Lemma was used for a quick proof of the undefinability of surjective pairing in the  $\lambda$ -calculus, which was one of the early results of Barendregt in [Bar74], there proved using the technique of underlining.

Van Daalen's interest in reduction under substitution derived from the fact that it implied the so-called Square Brackets Lemma (SqBL), a structural lemma on the contribution of a substitution in a reduction to abstractor form. The SqBL was the key to van Daalen's new and original method for proving strong normalization. Use has been made of this method in [Daa80], [Lév75], [Bar84], Ch. 14, and [Oos97]. It is also discussed in [Vri07], to which we refer for a detailed historical account of Barendregt's Lemma and reduction under substitution.

The aim of this paper is twofold. First, to give a cogent exposition of reduction under substitution. Thereto the first two sections are explanatory in character. The second goal is to explore the potential of RuS for producing new insights, proof methods and results in the  $\lambda$ -calculus, starting by generalizing RuS to multiple substitution, and later also extending it to filling holes in contexts. The essential difference is that hole filling may introduce variables that are captured by a binder, whereas substitution may not.

We will present new elementary proofs of undefinability results that are sometimes presented as applications of Berry's Sequentiality Theorem (BST), [Ber78, Ber79], [Bar84]. BST is in terms of Böhm trees, and therefore it is intrinsically infinitary, whereas RuS is just a structural observation on finite reductions. We also use RuS to prove the Perpendicular Lines Theorem for open terms with respect to  $\beta$ -conversion, thereby confirming a conjecture from [BS99]. Finitary proofs of classic undefinability results have also been obtained in [BKOV99]. In Section 5 we will briefly discuss the relation to our approach.

We will also pay attention to the issue of sequentiality itself. In Section 7 we first prove a new sequentiality result that is purely in terms of  $\beta$ -reduction. Then we tackle the original BST, adapting RuS to cover also the Böhm-reduction rules, sending unsolvable terms to a bottom element and in the limit producing Böhm trees. We note that some of our results fall outside the scope of BST.

#### 1.1 Outline

In Section 2 we start out by a discussion of Barendregt's Lemma. We illustrate the use of BL by giving short proofs for the undefinability of surjective pairing in the  $\lambda$ -calculus and for the Genericity Lemma. We generalize the Genericity Lemma to a form that is not implied by BST.

Then in Section 3 the Reduction-under-Substitution Lemma (RuS) is introduced and its relation to Barendregt's Lemma indicated. The use of RuS is illustrated by the Square Brackets Lemma.

A proof of RuS will be given in Section 4, at the same time generalizing it to multiple substitutions.

Then in Section 5 a couple of undefinability results are presented, related to the sequential nature of the  $\lambda$ -calculus.

In Section 6 we indicate how our analysis can be extended from substitutions to subterms within an arbitrary context. As an application we prove a form of the Perpendicular Lines Theorem.

Finally in Section 7 we turn to the theme of sequentiality. First a new sequentiality result is established as a corollary to RuS and then we use RuS in an analysis of Berry's Sequentiality Theorem.

We conclude by assessing our results in Section 8, giving links to relevant related work and pointing out possible lines for further research.

#### 1.2 Preliminaries

We are concerned with the pure  $\lambda$ -calculus, with which we assume familiarity. We adopt the notations and conventions of the standard text [Bar84]. In particular, we use  $\to$  to denote one-step  $\beta$ -reduction,  $\to$  for the reflexive, transitive closure of  $\to$ , and = for  $\beta$ -convertibility. Moreover,  $\equiv$  stands for syntactive equivalence modulo  $\alpha$ -conversion.

For terms t, s and a position p in t we use  $t|_p$  for the subterm of t at position p, and  $t[s]_p$  denotes the result of replacing the subterm at position p in t by s. The empty context is denoted by  $[\ ]$ . Note that in particular  $C[[\ ]]_p$  denotes the result of placing a hole at position p in the context C.

## 2 Barendregt's Lemma

At the end of [Bar72], a handwritten note of Henk Barendregt on the undefinability of Church's  $\delta$  in combinatory logic (CL), one finds a statement that seems to be added just as an afterthought. It is not widely known, probably just by a group of insiders, who refer to it as Barendregt's Lemma (BL). We quote [Bar72] verbatim:

**Theorem 12.** If  $CL \vdash FM \twoheadrightarrow N$ , then there are subterm occurrences  $A_i$  of N such that  $CL \vdash Fx \twoheadrightarrow N'$  where N' is the result of substituting  $xN_i$  for the subterm occurrence  $A_i$  and such that  $CL \vdash [x/M]N' \twoheadrightarrow N$ .

*Proof.* Same method as the proof of 9.

Here "Same method as the proof of 9" refers to the method used earlier in the manuscript, an intricate syntactic analysis using the technique of underlining.

We will now give a rendering of BL for the  $\lambda$ -calculus that is in several aspects somewhat more explicit.

First, the prefix that remains invariant in passing from N' to N can be specified as a multi-hole context C (with 0 or more holes!), such that we have  $N \equiv C[A_1, \ldots, A_n]$  and  $N' \equiv C[x\mathbf{N_1}, \ldots, x\mathbf{N_n}]$ , with  $n \geq 0$ .

Secondly, the notation  $xN_i$  should be elucidated. Define an x-vector as a term of the form  $xP_1 \dots P_k$   $(k \ge 0)$ . Then what is meant is that each  $xN_i$  is an x-vector, that is, a term  $xN_i \equiv xN_{i,1} \dots N_{i,k_i}$ .

Thirdly, we can be more specific about the reduction  $N'[x := M] \to N$ . It takes place below the prefix C, so it can be divided into reductions  $(xN_i)[x := M] \to A_i$ . Making this explicit rules out syntactic accidents.

**Lemma 1** (Barendregt's Lemma). Let FM o N and let x be a variable not occurring in F. Then there are a term N', an n-hole context C (with  $n \ge 0$ ), x-vectors  $B_1, \ldots, B_n$  and terms  $A_1, \ldots, A_n$ , such that  $Fx o N' \equiv C[B_1, \ldots, B_n]$ ,  $B_i[x := M] o A_i$  ( $1 \le i \le n$ ) and  $N \equiv C[A_1, \ldots, A_n]$ . See Fig. 1.

*Proof.* In the next section we will see that this lemma follows immediately from Lem. 6, the Reduction-under-Substitution Lemma.  $\Box$ 

The lemma is depicted in Fig. 1, where we use the notations  $B_i^* \equiv B_i[x := M]$  and  $B_i \mapsto B_i^*$ .

$$Fx \twoheadrightarrow N' \equiv C[B_1, \dots, B_n]$$

$$\downarrow \dots \downarrow$$

$$C[B_1^*, \dots, B_n^*]$$

$$\downarrow \dots \downarrow$$

$$C[A_1, \dots, A_n] \equiv N$$

Fig. 1. Barendregt's Lemma, pictorial

Heuristically, BL describes the contribution of the argument M to the result N in a reduction  $FM \to N$ . Namely, the result N can be decomposed in two parts:

- (i) A prefix C of N that is independent of M.
- (ii) Subterm occurrences  $A_i$ , immediately below C, that depend on M in an essential way, namely as reducts of x-vectors in which M has been substituted for x.

We now give two typical applications of Barendregt's Lemma.

### 2.1 Undefinability of Surjective Pairing

A surjective pairing would consist of a triple of lambda terms  $D, D_1, D_2$ , such that for arbitrary M, N we have:

$$D_1(DMN) = M$$
  $D_2(DMN) = N$   $D(D_1M)(D_2M) = M$ 

The undefinability of surjective pairing in the  $\lambda$ -calculus is the central result of [Bar74], where it is proved via underlining. Here we present the short proof from [Vri87] using Barendregt's Lemma.

We recall the notion of terms of order 0, see [Bar84], 17.3.2-3.

**Definition 2.** A term Z has order 0 if it does not reduce to a term in abstraction form, that is if  $\neg \exists P \colon Z \twoheadrightarrow \lambda x.P$ 

For a term Z of order 0 we have the following implication:

$$ZM_1 \dots M_p \twoheadrightarrow N \Rightarrow N \equiv Z'M'_1 \dots M'_p, Z \twoheadrightarrow Z', M_i \twoheadrightarrow M'_i$$
 (1)

The paradigmatic example of a term of order 0 is  $\Omega \equiv (\lambda x.xx)\lambda x.xx$ , and in this case we even have the stronger implication:

$$\Omega M_1 \dots M_p \twoheadrightarrow N \Rightarrow N \equiv \Omega M'_1 \dots M'_p, \ M_i \twoheadrightarrow M'_i$$
 (2)

The same holds for the case that Z is a variable or an x-vector.

**Theorem 3.** In the  $\lambda$ -calculus a surjective pairing does not exist.

Proof. Assume there were  $D, D_1, D_2$  satisfying the equations for surjective pairing. Define  $F \equiv \lambda x. D(D_1\Omega)(D_2x)$ . Then  $F\Omega = D(D_1\Omega)(D_2\Omega) = \Omega$  and hence by the Church–Rosser Theorem the terms  $F\Omega$  and  $\Omega$  have a common reduct, which can only be  $\Omega$  itself. So  $F\Omega \twoheadrightarrow \Omega$  and BL can be applied to yield an N' with the ascribed properties (taking  $M \equiv N \equiv \Omega$ ). Since for  $\Omega$  we have (2), one easily verifies that there are only two possibilities for N', namely either  $N' \equiv \Omega$  or  $N' \equiv x$ . We investigate both cases.

Case 1  $N' \equiv \Omega$ . Then  $Fx \to \Omega$  and so  $Fx = \Omega$  and by substitutivity of conversion  $FM = \Omega$  for an arbitrary term M. So for any M we have  $D_2M = D_2(D(D_1\Omega)(D_2M)) = D_2(FM) = D_2\Omega$  and hence for arbitrary N we have  $N = D_2(DNN) = D_2\Omega$ . It follows that all terms are equal, contradicting consistency of the  $\lambda$ -calculus.

Case 2  $N' \equiv x$ . Then  $Fx \to x$  and so Fx = x and we have FM = M for an arbitrary term M. Hence  $D_1M = D_1(FM) = D_1(D(D_1\Omega)(D_2M)) = D_1\Omega$  for any M. From this a contradiction is derived in the same way as in Case 1.  $\square$ 

## 2.2 Genericity

The following theorem is due to Barendregt [Bar84]. As far as we know the observation that it follows from Barendregt's Lemma is new.

Theorem 4 (Genericity). If  $F\Omega = I$ , then Fx = I.

*Proof.* Apply BL to a reduction  $F\Omega \to I$ , which exists according to the Church-Rosser Theorem. We get the following situation.

$$Fx \twoheadrightarrow N' \equiv C[\dots, xM_1 \dots M_p, \dots]$$

$$\downarrow C[\dots, \Omega M_1^* \dots M_p^*, \dots]$$

$$\downarrow C[\dots, \Omega M_1' \dots M_p', \dots] \equiv I$$

Since the term I contains no occurrence of  $\Omega$ , the context C must have zero holes, hence  $N' \equiv C \equiv I$ . It follows that Fx = I.

By inspecting the proof one sees that the Genericity Lemma can be generalized to arbitrary order-zero terms, if they do not occur in the result of the reduction.

**Theorem 5 (Generalized Genericity).** If FZ N for a term Z of order zero and  $Z \not N$  for all subterms S of N, then Fx = N.

*Proof.* Applying BL to a reduction FZ woheadrightarrow N, we get the following situation. Since the term Z is of order zero and does not rewrite to any subterm of N, the context C must have zero holes, hence  $C \equiv N$ . It follows that Fx = N.

It is interesting to note that, in contrast with the original Thm. 4, this generalized Genericity Theorem does not follow from Berry's Sequentiality Theorem. An example of an application of Thm. 5 that is not in the scope of Berry's Sequentiality Theorem can be obtained by taking Z and N to be both unsolvable terms, e.g.  $Z \equiv \Omega\Omega$  and  $N \equiv \Omega$ . If  $F(\Omega\Omega) = \Omega$ , then  $Fx = \Omega$  by Thm. 5, but the Böhm trees of Z as well as N are just  $\bot$ .

#### 3 Reduction Under Substitution

Barendregt's Lemma can be cast in a different way, in terms of substitution instead of function application. This is the form that originates with Diederik van Daalen [Daa80] and that found its way into the book [Bar84], as Exercise 15.4.8. It is slightly stronger than BL and easier to prove.

$$M \twoheadrightarrow N' \equiv C[B_1, \dots, B_n]$$

$$\downarrow \cdots \downarrow$$

$$C[B_1^*, \dots, B_n^*]$$

$$\downarrow \cdots \downarrow$$

$$C[A_1, \dots, A_n] \equiv N$$

Fig. 2. Reduction under substitution, pictorial

**Lemma 6 (Reduction under Substitution).** Let M[x := L] woheadrightarrow N. Then there are a term N', an n-hole context C (with  $n \ge 0$ ), x-vectors  $B_1, \ldots, B_n$  and terms  $A_1, \ldots, A_n$ , such that  $M woheadrightarrow N' \equiv C[B_1, \ldots, B_n]$ ,  $B_i[x := L] woheadrightarrow A_i$  for all  $1 \le i \le n$  and  $N \equiv C[A_1, \ldots, A_n]$ . See Fig. 2.

*Proof.* In Sec. 4 we will prove the Reduction-under-Substitution Lemma for multiple substitution, Thm. 13, of which the present form is just a special case.  $\Box$ 

So the proof will be postponed, but we already point out that Lem. 1 immediately follows from Lem. 6 by taking Fx for M and M for L.

It should be remarked that the context C and the x-vectors  $B_i$  are in general not unique. Consider for example  $M \equiv xzx$  with the substitution  $[x := \lambda y.y]$  together with the reduction  $M[x := \lambda y.y] \rightarrow z(\lambda y.y)$ . Then we have

- (i)  $M \twoheadrightarrow C_1[B_1]$  with  $C_1 \equiv [], B_1 \equiv xzx, B_1^* \twoheadrightarrow z(\lambda y.y)$
- (ii)  $M \rightarrow C_2[B_2, B_3]$  with  $C_2 \equiv [\ ][\ ], B_2 \equiv xz, B_3 \equiv x, B_2^* \rightarrow z, B_3^* \rightarrow \lambda y.y$

In the second factorization the context  $C_2$  shows more of the stucture of the result  $z(\lambda y.y)$  than  $C_1$  does, namely that it is an application term. We call  $C_2$  finer than  $C_1$ , and  $C_1$  coarser,  $C_1 \triangleleft C_2$ .

Van Daalen's interest in the substitution variant of BL was because of the Square Brackets Lemma, which he used in his proof of strong normalization.<sup>1</sup>

**Lemma 7 (Square Brackets Lemma).** Let  $M[x := L] \rightarrow \lambda y.P.$  Then we have one of the following two cases.

- 1.  $M \rightarrow \lambda y.P'$  for a P' such that  $P'[x := L] \rightarrow P$ 2.  $M \rightarrow xQ$  and  $(xQ)[x := L] \rightarrow \lambda y.P$
- z.  $M \twoheadrightarrow x \mathbf{y}$  and  $(x \mathbf{y})[x L] \twoheadrightarrow \lambda y.I$

*Proof.* The prefix C found by Lem. 6 can either be of the form  $\lambda y.C'$  or it must be the empty context. If  $C \equiv \lambda y.C'$  then  $N' \equiv \lambda y.P'$  for some P' and we are in Case 1. If  $C \equiv []$  then N' is an x-vector and we are in Case 2.

It is noted in [Daa80] that the lemma can be generalized to situations where the outer shape of the reduct is not an abstraction. In [Oos97] a similar lemma is stated for arbitrary patterns, the generalization is called there "Invert".

## 4 Reduction Under Multiple Substitution

We now prove the Reduction-under-Substitution Lemma for multiple substitutions. Throughout this section, and in some of the following ones, we will work with a fixed substitution  $[\boldsymbol{x} := \boldsymbol{L}]$  with  $\boldsymbol{x} = x_1, \ldots, x_m$  and  $\boldsymbol{L} = L_1, \ldots, L_m$   $(m \ge 0)$ . We tacitly assume that no lambdas binding the variables  $x_i$  are used (this can always be achieved by  $\alpha$ -renaming), so that occurrences of  $x_1, \ldots, x_m$  will always be free.

The following definition sums up some technical notions and convenient notations (some of which we already used in the previous sections).

#### Definition 8

- 1. An x-vector is a term of the form  $x_i P_1 \dots P_k$  with  $1 \le i \le m$  and  $k \ge 0$ .
- 2.  $M^*$  denotes  $M[\boldsymbol{x} := \boldsymbol{L}]$ .
- 3.  $M \mapsto N$  when  $N \equiv M^*$ .
- 4.  $C \triangleleft M$  if context C is a prefix of term (or context) M.
- 5.  $C \blacktriangleleft M$  if  $C \triangleleft M$ ,  $x_1, \ldots, x_m \notin FV(C)$  and  $M \equiv C[B_1, \ldots, B_n]$  for some x-vectors  $B_i$ .
- 6.  $M \leadsto_C C[A_1, \ldots, A_n]$  if  $C \blacktriangleleft M$  as in 5 and moreover  $B_i^* \twoheadrightarrow A_i$  for i = 1, ..., n
- 7.  $M \rightsquigarrow N$  if there exists a context C such that  $M \rightsquigarrow_C N$

<sup>&</sup>lt;sup>1</sup> Why "square brackets"? The lemma analyses the contribution of the substitution in a reduction to an abstraction term. In the notation of Automath square brackets were used to denote lambda abstraction.

**Lemma 9.** We have  $M \rightsquigarrow N$  if and only if one of the following four cases applies:

- (i) M is an x-vector with  $M^* \rightarrow N$
- (ii)  $M \equiv N \equiv y$  for some variable y with  $y \not\equiv x_1, \dots, y \not\equiv x_m$
- (iii)  $M \equiv M_1 M_2$  and  $N = N_1 N_2$  with  $M_1 \rightsquigarrow N_1$  and  $M_2 \rightsquigarrow N_2$
- (iv)  $M \equiv \lambda y.M'$  and  $N \equiv \lambda y.N'$  with  $M' \rightsquigarrow N'$

As a consequence, if  $M \leadsto_C N$  then  $M|_p \leadsto_{C|_p} N|_p$  for every position p in C.

*Proof.* Follows directly from the definition.

**Lemma 10.** Let  $C \triangleleft M$  and  $C' \triangleleft M$  with  $C' \triangleleft C$ , then  $\leadsto_C \subseteq \leadsto_{C'}$ .

Proof. Let  $B_i$ ,  $B'_j$  be x-vectors such that  $M \equiv C[B_1, \ldots, B_n] \equiv C'[B'_1, \ldots, B'_{n'}]$ . Then  $C[B_1^*, \ldots, B_n^*] \equiv C'[B'_1^*, \ldots, B'_{n'}]$  since  $x_1, \ldots, x_m \notin FV(C) \cup FV(C')$  and all occurrences of  $x_1, \ldots, x_m$  are free. Now  $\leadsto_C \subseteq \leadsto_{C'}$  follows since the  $B_i^*$  are disjoint, and each of them is a subterm of some  $B'_i^*$ .

**Lemma 11.** If  $y \not\equiv x_1, \dots, y \not\equiv x_m$ , then

$$M \leadsto M', \, N \leadsto N' \Rightarrow M[y := N] \leadsto M'[y := N']$$
.

*Proof.* Let  $\sigma$  be shorthand for [y := N],  $\sigma'$  for [y := N'] and  $\sigma^*$  for  $[y := N^*]$ . We use induction over the structure of M according to Lem. 9:

- (i) If M is an x-vector, then  $M\sigma$  is and  $(M\sigma)^* \equiv M^*\sigma^*$  since  $y \not\equiv x_1, \ldots, x_m$ . From  $M^* \twoheadrightarrow M'$  and  $N^* \twoheadrightarrow N'$  follows  $M^*\sigma^* \twoheadrightarrow M'\sigma'$  and  $M\sigma \leadsto M'\sigma'$ .
- (ii) If  $M \equiv M' \equiv z$  for a variable z with  $z \not\equiv x_1, \ldots, x_m$ , then either  $z \equiv y$  and  $M\sigma \equiv N \leadsto N' \equiv M'\sigma'$ , or  $z \not\equiv y$  and  $M\sigma \equiv z \leadsto z \equiv M'\sigma'$ .
- (iii) If  $M \equiv M_1 M_2$  and  $M' \equiv M'_1 M'_2$  with  $M_i \rightsquigarrow M'_i$ , then  $M_i \sigma \rightsquigarrow M'_i \sigma'$  by IH and since  $M \sigma \equiv M_1 \sigma(M_2 \sigma)$  and  $M' \sigma' \equiv M'_1 \sigma'(M_2 \sigma')$  we get  $M \sigma \rightsquigarrow M' \sigma'$ .
- (iv) If  $M \equiv \lambda z.M_1$  and  $M' \equiv \lambda z.M_1'$  with  $M_1 \rightsquigarrow M_1'$ , then either  $z \equiv y$  and  $M\sigma \equiv M \rightsquigarrow M' \equiv M'\sigma'$ , or  $z \not\equiv y$ ,  $M\sigma \equiv \lambda z.M_1\sigma \rightsquigarrow^{\mathrm{IH}} \lambda z.M_1'\sigma' \equiv M'\sigma'$ .

## Lemma 12. $\rightsquigarrow \cdot \rightarrow \subseteq \rightarrow \cdot \rightsquigarrow$

*Proof.* By induction it suffices to show  $\leadsto \cdot \to \subseteq \to \cdot \leadsto$ . Let  $M \leadsto N \to O$ , then there are a context C,  $\boldsymbol{x}$ -vectors  $B_i$  and terms  $A_i$  such that:  $M \equiv C[B_1, \ldots, B_n]$ ,  $B_i \mapsto B_i^* \twoheadrightarrow A_i$  for all  $1 \le i \le n$ ,  $N \equiv C[A_1, \ldots, A_n]$ , and a step  $\rho : N \to O$  at position p. Note that  $M^* \twoheadrightarrow_C N$  where  $\twoheadrightarrow_C$  means that all steps are below C.

Assume  $\rho$  is entirely in C. Then we have  $M|_p \equiv (\lambda y.M_1)M_2 \to M_1[y:=M_2]$  and  $N|_p \equiv (\lambda y.N_1)N_2 \to N_1[y:=N_2] \equiv O|_p$  with  $M_1 \leadsto_{C|_{p_{11}}} N_1$ ,  $M_2 \leadsto_{C|_{p_2}} N_2$  by Lem. 9. Hence  $M_1[y:=M_2] \leadsto_{C'} N_1[y:=N_2]$  for some context C' by Lem. 11. Let  $M' \equiv M[M_1[y:=M_2]]_p$  then  $M \to M' \leadsto_{C[C']_p} O$ .

If  $\rho$  is below C, then it is contained in one of the  $\boldsymbol{x}$ -vectors  $B_i$  and 'absorbed' by  $\leadsto$ , that is,  $M \leadsto_C O$ . Finally if  $\rho$  is neither in C nor below C, then  $C|_p \equiv [\ ]C'$ . Then  $M|_p$  is an  $\boldsymbol{x}$ -vector since  $C \blacktriangleleft M$  and therefore  $M|_{p1}$  is an  $\boldsymbol{x}$ -vector. Hence  $C[[\ ]]_p \blacktriangleleft M$  and  $\leadsto_C \subseteq \leadsto_{C[[\ ]]_p}$  by Lem. 10. Observe that  $\rho$  is below  $C[[\ ]]_p$ , a case that we have already considered,  $M \leadsto_{C[[\ ]]_p} O$ .

**Theorem 13 (RuS).** If  $M^* N$ , then  $M C[B_1, ..., B_n] CN$  for some context C and x-vectors  $B_1, ..., B_n$ . See Fig. 2.

*Proof.* Follows from  $M \rightsquigarrow M^* \to N$  and an application of Lem. 12.

## 5 Undefinability Proofs

In this section we use reduction under substitution to give new proofs of some well-known consequences of Berry's Sequentiality Theorem.

Given  $\mathbf{x} = x_1, \dots, x_m$ , we define the following notions relative to this choice of variables, that are assumed to be free.

**Definition 14.** An occurrence of  $x_i$  in M is leading if M contains no  $x_j$ -vector of the form  $x_j P$  such that the occurrence of  $x_i$  is in P. A variable  $x_i$  is leading if it has a leading occurrence. LV(M) denotes the set of leading variables in M.

**Lemma 15.** For terms M, N we have

- (i) If at least one of the variables  $x_1, \ldots, x_m$  occurs in M, then  $LV(M) \neq \emptyset$ .
- (ii) If  $C \triangleleft M$  and  $M \equiv C[y_1P_1, \dots, y_nP_n]$ , then  $LV(M) \subseteq \{y_1, \dots, y_n\}$ .
- (iii) If M woheadrightarrow N, then  $LV(N) \subseteq LV(M)$ .

*Proof.* (i) Take an outermost occurrence of  $x_i P$ , then  $x_i \in LV(M)$ .

- (ii) Directly from the definition together with the fact that  $x_1, \ldots, x_n \notin FV(C)$ .
- (iii) Note that if a variable  $x_i$  is leading in a term M[y := N] then it must have been leading in M or N and hence in  $(\lambda y.M)N$ . The claim follows by closure under contexts and induction on the reduction length.  $\square$

We start by showing the undefinability of Gustave's function.

**Theorem 16.** There is no lambda term G such that:

$$G01x = x$$
  $G1x0 = x$   $Gx01 = x$ 

Proof. We employ RuS with  $M \equiv Gxyz$  and x = x, y, z. We have  $G01\Omega = \Omega$  and  $G01\Omega \twoheadrightarrow \Omega$  by confluence. By RuS there exists  $N_z$  with  $M \twoheadrightarrow N_z \leadsto \Omega$ . If z is leading variable in  $N_z$ , then  $N_z \equiv z$ , otherwise every  $\leadsto$ -reduct of  $N_z$  would contain  $\Omega$  at a non-root position. But if  $N_z \equiv z$  then we would have  $G1x0 \twoheadrightarrow 0$ . Hence  $z \notin LV(N_z)$  and likewise there exist  $N_x$  and  $N_y$  with  $M \twoheadrightarrow N_x$ ,  $M \twoheadrightarrow N_y$  and  $x \notin LV(N_x)$ ,  $y \notin LV(N_y)$ . By confluence  $N_x$ ,  $N_y$  and  $N_z$  have a common reduct N with  $LV(N) = \varnothing$  and then by Lem. 15 none of the variables x, y, z occur in N. Therefore we obtain  $\forall L : M[x := L] \twoheadrightarrow N[x := L] \equiv N$ , and hence x = G01x = N = G01y = y, contradicting consistency of the  $\lambda$ -calculus.

Remark 1. For a variant of Gustave's function where x is replaced by Z ranging over all closed terms the proof stays valid. For a variant where the right-hand sides are closed terms A, B, C we refer to the Perpendicular Lines Theorem (Thm. 22).

It is interesting to note that Thm. 16 is obtained in [BKOV99] by a different argument, involving an analysis of residuals along head reductions. Their Lemma 5.2, on the undefinability of a general form of the G of Thm. 16, can be proved by our method in the same way as Thm. 16. The undefinability of the other two variants of G mentioned in this remark are not covered by Lemma 5.2 in [BKOV99].

Before continuing we state a few lemmas that capture the common essence of the following undefinability results. Fig. 3 illustrates Lem. 17 and 18 applied to "parallel or" (Por). If  $x_i$  is substituted by  $\Omega$  in M and M rewrites to a normal form, then  $x_i$  cannot have been leading in M. If such a reduction exists for every  $x_i$  then all  $M[\mathbf{x} := \mathbf{L}]$  (and hence all reducts) are convertible for arbitrary  $\mathbf{L}$ .

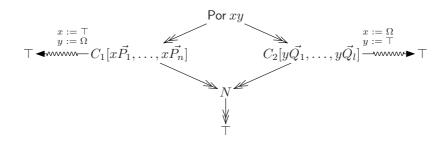


Fig. 3. Lem. 17 and Lem. 18 at the example of "parallel or"

**Lemma 17.** If for i = 1, ..., m there exist  $N_i$  with  $M = N_i$  and  $x_i \notin LV(N_i)$ , then there exists an N such that  $LV(N) = \emptyset$  and  $\forall L : M[\mathbf{x} := L] \to N$ .

*Proof.* By confluence the terms  $M, N_1, \ldots, N_m$  have a common reduct N and by Lem. 15(iii) we have  $LV(N) \subseteq LV(N_1) \cap \ldots \cap LV(N_m) = \emptyset$ . So by Lem. 15(i) the variables  $x_1, \ldots, x_m$  do not occur in N. Hence for arbitrary L we have  $M[x := L] \twoheadrightarrow N[x := L] \equiv N$ .

**Lemma 18.** If for i = 1, ..., m there are normal forms  $N_i$  and  $\mathbf{L}^i$  with  $L_i^i \equiv \Omega$  such that  $M[\mathbf{x} := \mathbf{L}^i] \to N_i$ , then  $N_1 \equiv ... \equiv N_m$  and  $\forall \mathbf{L} : M[\mathbf{x} := \mathbf{L}] \to N_1$ .

Proof. Let  $i \in \{1, \ldots, m\}$  arbitrary. An application of RuS to  $M[\boldsymbol{x} := \boldsymbol{L}^i] \twoheadrightarrow N_i$  yields that there exist a term  $N_i'$ , a context C and  $\boldsymbol{x}$ -vectors  $B_1, \ldots, B_n$  such that  $M \twoheadrightarrow N_i' \equiv C[B_1, \ldots, B_n] \leadsto_C N_i$ . None of the  $B_j$ 's can be an  $x_i$ -vector. For suppose it were, then every reduct of  $B_j^*$  and hence also  $N_i$  would contain  $\Omega$ , contradicting  $N_i$  being a normal form. We conclude by Lem. 15(ii) that  $x_i \notin LV(N_i')$ . Since i was arbitrary, by Lem. 17 there exists an N such that  $\forall \boldsymbol{L} : M[\boldsymbol{x} := \boldsymbol{L}] \twoheadrightarrow N$ . Hence  $N_1 = \ldots = N_m$ . By confluence and the fact that all  $N_i$  are normal forms we get  $M \twoheadrightarrow N_1 \equiv \ldots \equiv N_m$ .

#### 5.1 Undefinability of "Parallel or"

We can now show the undefinability of "parallel or".

**Theorem 19.** There are no lambda terms Por and normal forms  $T \not\equiv \bot s.t.$ :

$$\operatorname{Por} \top x = \top \qquad \qquad \operatorname{Por} x \top = \top \qquad \qquad \operatorname{Por} \bot \bot = \bot$$

*Proof.* Assume that Por exists, we consider  $M \equiv \text{Por } xy$  with  $\boldsymbol{x} = x, y$ . Since Por  $\Omega \top \twoheadrightarrow \top$  and Por  $\top \Omega \twoheadrightarrow \top$ , we get  $\forall L : \text{Por } xy[\boldsymbol{x} := \boldsymbol{L}] \twoheadrightarrow \top$  by Lem. 18. Then in particular  $F \bot \bot \twoheadrightarrow \top \not\equiv \bot$  contradicting the assumption.

The following is a variant of "parallel or" from [Bar84], that is also undefinable.

**Theorem 20.** There is no lambda term F s.t. for arbitrary closed M, N:

$$FMN = I$$
 if  $M$  or  $N$  is solvable  $FMN = \Omega$  otherwise

*Proof.* Assuming there is such an F, we consider  $M \equiv Fxy$  with  $\mathbf{x} = x, y$ . Since  $F\Omega I \to I$  and  $FI\Omega \to I$ , we get  $\forall L : Fxy[\mathbf{x} := \mathbf{L}] \to I$  by Lem. 18. Then in particular  $F\Omega\Omega \to I \not\equiv \Omega$  contradicting the assumption.

## 6 Extension to Context Filling

We extend reduction under multiple substitution to context filling; the difference being that variables of the arguments might get bound.

**Corollary 1.** Let  $C[L_1, ..., L_m] N$ . Let  $\mathbf{x} = x_1, ..., x_m$  be fresh variables. For i = 1, ..., m let  $\mathbf{y_i}$  be a vector consisting of all variables that are bound at the i-th hole of C. Then there are a context D,  $\mathbf{x}$ -vectors  $B_1, ..., B_n$  and terms  $A_1, ..., A_n$ , such that:

$$C[x_1 \mathbf{y_1}, \dots, x_m \mathbf{y_m}] \twoheadrightarrow D[B_1, \dots, B_n]$$

$$\downarrow \dots \qquad \downarrow \qquad [x_1 := \lambda \mathbf{y_1}.L_1, \dots, x_m := \lambda \mathbf{y_m}.L_m]$$

$$D[B_1^*, \dots, B_n^*]$$

$$\downarrow \dots \qquad \downarrow$$

$$D[A_1, \dots, A_n] \equiv N$$

*Proof.* Let  $\sigma$  be shorthand for  $[x_1 := \lambda y_1, L_1, \dots, x_m := \lambda y_m, L_m]$  and we define  $M \equiv C[x_1y_1, \dots, x_my_m]$ . Then clearly  $M\sigma \twoheadrightarrow C[L_1, \dots, L_m] \twoheadrightarrow N$ . As a consequence of Reduction under Multiple Substitution there exist a context D and x-vectors  $B_1, \dots, B_n$  such that:  $M \twoheadrightarrow D[B_1, \dots, B_n] \leadsto_C N$ .

**Lemma 21.** If for i = 1, ..., m there are a term  $N_i$  with  $z \notin N_i$  and terms  $\mathbf{L}^i$  with  $L_i^i \equiv z$  such that  $C[\mathbf{L}^i] = N_i$ , then  $\forall \mathbf{L}: C[\mathbf{L}] = N_1 = ... = N_m$ .

*Proof.* After an application of Thm. 1 the proof continues analogously to the proof of Lem. 18, from  $z \notin N_i$  follows that no  $B_j$  is an  $x_i$ -vector.

#### 6.1 Perpendicular Lines Theorem

The Perpendicular Lines Theorem is a result from [Bar84], Ch. 14, stated there in terms of Böhm equivalence, together with a suggestion to extend it to  $\beta$ -equality. In [BS99] a counterexample is given to PPL with respect to  $\beta$ -equality, which, however, concerns the variant where the equations are only required to hold for substitutions of a closed term for the variable z. They added a suggestion to try to use [Bar84], Exercise 15.4.8, for the open variant. Indeed, it turns out that we can use RuS to prove the following theorem.

**Theorem 22 (PPL).** Assume that for lambda terms  $M_{ij}$ ,  $N_i$  with  $z \notin N_i$ :

$$C[M_{11}, M_{12}, \dots, M_{2n-1}, z] = N_1$$

$$C[M_{21}, M_{22}, \dots, z, M_{2n}] = N_2$$

$$\vdots \qquad \vdots \qquad \vdots$$

$$C[z, M_{n2}, M_{n3}, \dots, M_{nn}] = N_n$$

Then

$$-N_1 = N_2 = \ldots = N_n = N$$
  
- For all  $Z_1, \ldots, Z_n$  we have  $C[\mathbf{Z}] = N$ 

*Proof.* Follows from an application of Lem. 21 to the above equations.

## 7 Sequentiality

Berry's Sequentiality Theorem (BST) is about Böhm trees and these can be obtained as infinite normal forms with respect to  $\beta$ -reduction extended with the Böhm reduction rules. To be able to deal with this we will have to adapt the Reduction-under-Substitution Lemma to this extended notion of reduction. But before doing so, we formulate a strictly finitary sequentiality result for  $\beta$ -reduction alone. We give the version for multiple substitution, but a functional and a context-filling version can be straightforwardly derived.

**Theorem 23.** Let  $M[\mathbf{x} := \mathbf{L}] \to N$  with  $\mathbf{x} = x_1, \dots x_m$ . Then N can be written as  $N \equiv C[A_1, \dots, A_n]$  in such a way that:

- 1. The prefix C is independent of the substitution, that is, for any  $P=P_1, \ldots P_m$  we have  $M[x:=P] \rightarrow C[\ldots]$ .
- 2. Each  $A_i$  depends on exactly one of the substituted terms  $L_j$  in the sense that at the position of  $A_i$  any term B can be realized by an appropriate replacement Q of  $L_j$ , regardless of the choice of the other substituted terms. That is,

$$(\forall i)(\exists j)(\forall B)(\exists Q)(\forall P): P_j \equiv Q \Rightarrow M[x := P] \rightarrow C[\dots, B, \dots]$$
  
where  $1 \le i \le n, 1 \le j \le m$  and with  $B$  at position  $i$  of  $C$ .

*Proof.* This is an immediate consequence of RuS, Thm. 6. If  $B_i$  is an x-vector  $x_j K_1 \ldots K_k$  then Q can be chosen as  $\lambda y_1 \ldots y_k . B$ .

Undefinability results like the ones mentioned earlier can also be obtained by applying this new sequentiality theorem.

Now we turn to BST. We consider  $\Lambda(\perp)$ , the  $\lambda$ -calculus enriched with the constant  $\perp$  (bottom). The Böhm rewrite relation  $\rightarrow_{\beta\perp} = \rightarrow_{\beta} \cup \rightarrow_{\perp}$  on  $\Lambda(\perp)$  consists of  $\beta$ -reduction  $\rightarrow_{\beta}$  together with  $\rightarrow_{\perp}$  defined by:

$$\bot M \to \bot$$
  $\lambda y. \bot \to \bot$   $u \to \bot$  if  $u$  is an unsolvable

For  $\rightarrow_{\beta\perp}$  we have to adapt the definition of  $\boldsymbol{x}$ -vector. Let  $\boldsymbol{x}=x_1,\ldots,x_m$ . The set of  $\boldsymbol{x}$ -clusters is inductively defined as follows:

- $-x_1,\ldots,x_m$  are  $\boldsymbol{x}$ -clusters
- if B is an x-cluster and  $M \in \Lambda(\bot)$  a term, then BM is an x-cluster
- if B is an x-cluster and  $y \not\equiv x_1, \dots, y \not\equiv x_m$ , then  $\lambda y.B$  is an x-cluster

Note that for every x-cluster B we have  $B[x := \bot] \twoheadrightarrow_{\beta \bot} \bot$ . We tacitly assume that all occurrences of the variables  $x_1, \ldots, x_m$  are free.

We adapt the notation from Def. 8 to Böhm reduction by exchanging  $\twoheadrightarrow_{\beta\perp}$ ,  $\leadsto_{\beta\perp}$ ,  $\blacktriangleleft_{\beta\perp}$  and x-clusters for  $\twoheadrightarrow$ ,  $\leadsto$ ,  $\blacktriangleleft$  and x-vectors, respectively. Likewise we obtain lemmas  $9^{\perp}$ - $11^{\perp}$  for  $\twoheadrightarrow_{\beta\perp}$  identical to Lem. 9-11 for  $\twoheadrightarrow$ . In order to lift Lem. 12 to Böhm reduction, the proof has to be adopted and extended.

Lemma 24. 
$$\rightsquigarrow \cdot \rightarrow \rightarrow_{\beta \perp} \subseteq \rightarrow_{\beta \perp} \cdot \rightsquigarrow$$

*Proof.* By induction  $\leadsto_{\beta\perp} \cdot \leadsto_{\beta\perp} \subseteq \leadsto_{\beta\perp} \cdot \leadsto_{\beta\perp}$  suffices. Let  $M \leadsto_{\beta\perp} N \to_{\beta\perp} O$ , then there are a context C, x-clusters  $B_i$  and terms  $A_i$  such that:  $M \equiv C[B_1, \ldots, B_n]$ ,  $B_i \mapsto B_i^* \twoheadrightarrow_{\beta\perp} A_i$  for all  $1 \le i \le n$ ,  $N \equiv C[A_1, \ldots, A_n]$ , and a step  $\rho: N \to_{\beta\perp} O$  at position p. The case of  $\beta$ -steps  $\rho$  is analogous to the proof of Lem. 12.

Hence let  $\rho$  be a  $\perp$ -step according to one of the three  $\perp$ -rules: (i)  $\rho: \perp M \to \perp$ , (ii)  $\rho: \lambda y. \perp \to \perp$ , or (iii)  $\rho: u \to \perp$  if u is an unsolvable.

If  $\rho$  is below C, then it is contained in one of the x-clusters  $B_i$  and 'absorbed' by  $\leadsto_{\beta\perp}$ , that is,  $M \leadsto_{\beta\perp,C} O$ . Therefore assume  $\rho$  is not below C.

First we consider the  $\perp$ -rules (i) and (ii). If the redex pattern of  $\rho$  is entirely in C, then we have  $M \to_{\beta\perp} M[\perp]_p \leadsto_{\beta\perp,C[\perp]_p} O$ . Otherwise  $\rho$  is neither in C nor below C, that is,  $\rho$  is overlapping in-between. Then in case of (i)  $C|_p \equiv [\ ]C'$  and (ii)  $C|_p \equiv \lambda y.[\ ]$ . In both cases it follows that  $M|_p$  is an x-cluster since  $M|_{p1}$  is an x-cluster. Then we are done since  $C[[\ ]]_p \blacktriangleleft_{\beta\perp} M, \leadsto_{\beta\perp,C} \subseteq \leadsto_{\beta\perp,C[[\ ]]_p}$  by Lem.  $10^\perp$  and  $\rho$  is now below  $C[[\ ]]_p$ .

The remaining case is  $\perp$ -rule (iii) with redex position in C. Note that if  $U \to U'$  and U' is unsolvable then U is unsolvable. Thus  $M^*|_p$  is unsolvable; either  $M|_p$  is unsolvable, then  $M \to_{\beta\perp} M[\perp]_p \leadsto_{\beta\perp,C[\perp]_p} O$ , or the head reduction sequence  $M|_p \to M'$  yields a term M' having an  $x_i$  as head. Then M' is an x-cluster with  $M' \leadsto_{\beta\perp,[\cdot]} \perp$ , hence  $M \to M[M']_p \leadsto_{\beta\perp,C[\cdot]_p} O$ .

**Theorem 25.** Let  $M[\mathbf{x} := \mathbf{L}] \to_{\beta \perp} N$ . Then there exist an n-hole context C,  $\mathbf{x}$ -clusters  $B_1, \ldots, B_n$  and terms  $A_1, \ldots, A_n$ , such that  $M \to_{\beta \perp} C[B_1, \ldots, B_n]$ ,  $B_i[\mathbf{x} := \mathbf{L}] \to_{\beta \perp} A_i$  for all  $1 \le i \le n$ , and  $N \equiv C[A_1, \ldots, A_n]$ .

*Proof.* The statement of the theorem is equivalent to  $M^* \twoheadrightarrow_{\beta \perp} N \Rightarrow M \twoheadrightarrow_{\beta \perp} N$ .  $\rightsquigarrow_{\beta \perp} N$ , which follows from  $M \leadsto_{\beta \perp} M^* \twoheadrightarrow_{\beta \perp} N$  and an application of Lem. 24.

**Theorem 26.** Let  $M[\mathbf{x} := \bot, ..., \bot] \twoheadrightarrow_{\beta \bot} N$  with  $\mathbf{x} = x_1, ..., x_m$ . Then N can be written as  $N \equiv C[A_1, ..., A_n]$  in such a way that:

- 1. The prefix C is independent of the substitution, that is, for any  $P=P_1, \ldots P_m$  we have  $M[\mathbf{x} := P] \rightarrow C[\ldots]$ .
- 2. Each  $A_i$  depends on exactly one of the substituted terms  $\perp$  in the sense that:
  - A refinement of the corresponding  $\bot$  to a free variable will give rise to a reduction to  $C[\ldots, A'_i, \ldots]$  where  $A'_i \not\rightarrow_{\beta \bot} \bot$ , regardless of the choice of the other substituted terms. That is,

$$(\forall i)(\exists j)(\forall \mathbf{P}) \colon P_j \equiv x \Rightarrow M[\mathbf{x} := \mathbf{P}] \twoheadrightarrow_{\beta \perp} C[\dots, A'_i, \dots], A'_i \not \twoheadrightarrow_{\beta \perp} \bot$$

- At the position of  $A_i$  a  $\perp$  can be realized regardless of the choice of the other substituted terms. That is,

$$(\forall i)(\exists j)(\forall P): P_j \equiv \bot \Rightarrow M[x := P] \twoheadrightarrow_{\beta \bot} C[\dots, \bot, \dots]$$

*Proof.* This is an immediate consequence of Thm. 25, noting that an  $x_i$ -cluster with  $\bot$  substituted for  $x_i$  rewrites to  $\bot$ .

Berry's Sequentiality Theorem can be derived as a corollary of Thm. 26 in the following way.

Let  $M \equiv C[\bot, \ldots, \bot]$  and let B be the Böhm tree of M. For arbitrary depths  $d \in \mathbb{N}$  there exists a reduction  $M \twoheadrightarrow_{\beta \bot} N$  such that N is in  $\twoheadrightarrow_{\beta \bot}$ -normal form up to depth d; then N coincides with B up to depth d. An application of Thm. 26 to  $M \equiv (C[x_1, \ldots, x_m])[\boldsymbol{x} := \bot, \ldots, \bot] \twoheadrightarrow_{\beta \bot} N$  yields  $N \equiv D[A_1, \ldots, A_n]$ . For all  $A_i$  above depth d we have  $A_i \equiv \bot$ , since they are  $\boldsymbol{x}$ -clusters with  $\bot$  substituted for the leading variable in normal form. Now a  $\bot$  in the Böhm tree B above depth d is either (a) one of the  $A_i$  or (b) it is in the context D. In case (b) the  $\bot$  is independent from all substituted  $\bot$ 's, and will be at this position in the Böhm tree of every C[L] for arbitrary L. In case (a) the  $A_i$  depends on exactly one of the substituted  $\bot$ 's from the input. If this  $\bot$  is refined to a free variable, then the Böhm tree will no longer have a  $\bot$  at this position. On the other hand, refining all other  $\bot$ 's from M will not affect the  $\bot$  in the Böhm tree at this position.

## 8 Concluding Remarks

On intuitive grounds it seems plausible that there is an "inverse" correspondence of Barendregt's Lemma and the reported properties of reduction under substitution with the notions of tracing and origin tracking, and especially with the prefix property, see [BKV00]. This relation was already indicated in [BKV00] and, with the SqBL in the place of BL, also in [Oos97] and [Ter03], Sec. 8.6. It would be interesting to investigate this correspondence in more detail and to compare the techniques of dynamic labelling used in tracing and origin tracking with the special underlining techniques that were employed in [Bar72] and [Bar74].

It seems likely that reduction under substitution can contribute to a better understanding of sequentiality, a direction that merits further investigation. The same holds for the connection with work on stability, semi-standardization and factorization, see e.g. [GK94], [Mel97, Mel98] and [Ter03], Ch. 8.

Although we didn't need it in order to obtain a sequentiality result concerning the, potentially infinite, Böhm tree of the output, it might be possible to prove also an infinitary version of RuS. This is an objective of further investigation.

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