

# Binding and Substitution

Susmit Sarkar and Peter Sewell and Francesco Zappa Nardelli

October 18, 2007

We explain the binding specifications used in Ott in this document. The explanation is for a fragment of Ott, not including the list forms. The concrete substitution and free variable functions generated by Ott are defined in this document. We also give a more mathematical treatment by defining a notion of alpha-equivalence on abstract syntax terms for arbitrary binding specification. We then prove that under appropriate conditions, the concrete substitution functions respect alpha-equivalence. Further, we show that concrete substitutions coincides with capture-avoiding substitutions.

## 1 Grammar

The metavariables used in the following are:

*index, i, i', j, j', k, k', l, l', m, m', n, n', o, o', q, q'*  
*terminal, t*  
*metavarroot, mvr*  
*nontermroot, ntr*  
*suffix, suff*  
*variable, var*  
*auxfn, f*  
*prodname, pn*

The grammar of mini-Ott is:

<i>metavar, mv</i>	::=	<i>metavarroot suffix</i>	
<i>nonterm, nt</i>	::=	<i>nontermroot suffix</i>	
<i>element, e</i>	::=	<i>terminal</i>   <i>metavar</i>   <i>nonterm</i>	Elements of production rules
<i>mse</i>	::=	{}   <i>mse</i> $\cup$ <i>mse'</i>   <i>metavar</i>   <i>auxfn(nonterm)</i>	Metavariable set expressions
<i>mSES</i>	::=	[ <i>mse</i> <sub>1</sub> .. <i>mse</i> <sub><i>n</i></sub> ]	Lists of metavariable set expressions

<i>bindspec, bs</i>	::=   <code>bind mse in nonterm</code>   <code>auxfn = mse</code>	
<i>prod, p</i>	::=   <code>  element<sub>1</sub> .. element<sub>m</sub> :: :: prodname (+ bindspec<sub>1</sub> .. bindspec<sub>n</sub> +)</code>	Grammar productions
<i>rule, r</i>	::=   <code>nontermroot :: ' ' ::= prod<sub>1</sub> .. prod<sub>m</sub></code>	
<i>grammar_rules, g</i>	::=   <code>grammar rule<sub>1</sub> .. rule<sub>m</sub></code>	

Abstract syntax terms from the above grammar with concrete variables are defined as

<i>sorted_var, v</i>	::=   <code>var:mvr</code>
<i>concrete_abstract_syntax_term, cast</i>	::=   <code>v</code>   <code>prodname ( cast<sub>1</sub> , .. , cast<sub>m</sub> )</code>

We will have a simple type structure on the above grammar to ensure some basic sanity properties. These use the following types:

<i>auxfn_type, aut</i>	::=   <code>nontermroot<sub>1</sub> .. nontermroot<sub>n</sub> → metavarroot</code>
<i>auxfn_type_env, Φ</i>	::=
<i>cast_type, ct</i>	::=   <code>ntr</code>   <code>mvr</code>

Our substitutions are defined as a list of simultaneous substitutions of *cast* for *var* at particular sorts:

<i>substitution, s</i>	::=   <code>{ cast<sub>1</sub> / v<sub>1</sub> , .. , cast<sub>n</sub> / v<sub>n</sub> }</code>
------------------------	--

Finally, our interpretations will use the following auxiliary notions:

<i>ntmv</i>	::=   <code>nt</code>   <code>mv</code>	
<i>ntmv_list</i>	::=   <code>ntmv<sub>1</sub> , .. , ntmv<sub>i</sub></code>	
<i>occurrence, oc</i>	::=   <code>[]</code>   <code>n :: oc</code>	Lists of natural number indices, picking out path in syntax tree
<i>oc_set</i>	::=	Sets of occurrences
<i>oc_reln</i>	::=	PER's over occurrences, represented as sets of sets of occurrences

$var\_set ::=$  Sets of sorted variables

## 2 Rules

### 2.1 Utility functions and relations

We first define some utility relations (many of which are in fact defining primitive recursive partial functions) to work on syntactic objects.

$p \in g(ntr)$

$$\frac{\begin{array}{l} 1 : g = \text{grammar } r_1 .. r_l \\ 2 : r_i = ntr :: ' ' ::= p_1 .. p_m \\ 3 : j \text{ INDEXES } p_1 .. p_m \end{array}}{p_j \in g(ntr)} \quad \text{FUNSPEC\_LOOKUP\_P\_PRODS}$$

$\text{remove\_suffix}(ntmv) = ct$

$$\frac{}{\text{remove\_suffix}(ntr \text{ suff}) = ntr} \quad \text{FUNSPEC\_REMOVE\_SUFFIX\_NT}$$

$$\frac{}{\text{remove\_suffix}(mvr \text{ suff}) = mvr} \quad \text{FUNSPEC\_REMOVE\_SUFFIX\_MV}$$

$\text{remove\_terminals}(e_1 .. e_n) = ntmv\_list$

$$\frac{}{\text{remove\_terminals}(\ ) = []} \quad \text{FUNSPEC\_REMOVE\_TERMINALS\_NIL}$$

$$\frac{1 : \text{remove\_terminals}(e_1 .. e_n) = ntmv\_list}{\text{remove\_terminals}(t_m e_1 .. e_n) = ntmv\_list} \quad \text{FUNSPEC\_REMOVE\_TERMINALS\_TM}$$

$$\frac{1 : \text{remove\_terminals}(e_1 .. e_n) = ntmv\_list}{\text{remove\_terminals}(mv e_1 .. e_n) = mv, ntmv\_list} \quad \text{FUNSPEC\_REMOVE\_TERMINALS\_MV}$$

$$\frac{1 : \text{remove\_terminals}(e_1 .. e_n) = ntmv\_list}{\text{remove\_terminals}(nt e_1 .. e_n) = nt, ntmv\_list} \quad \text{FUNSPEC\_REMOVE\_TERMINALS\_NT}$$

$\text{binding\_mses} \forall j. (bs_j) \in ntmv \Rightarrow mses$

$$\frac{}{\text{binding\_mses} \in nt \Rightarrow [ ]} \quad \text{FUNSPEC\_BINDING\_MSES\_NT\_NIL}$$

$$\frac{1 : \text{binding\_mses} \forall j. (bs_j) \in nt \Rightarrow mses}{\text{binding\_mses} \text{ bind } mse \text{ in } nt \forall j. (bs_j) \in nt \Rightarrow mse \text{ mses}} \quad \text{FUNSPEC\_BINDING\_MSES\_NT\_CONS\_T}$$

$$\frac{\begin{array}{l} 1 : \text{binding\_mses} \forall j. (bs_j) \in nt \Rightarrow mses \\ 2 : \neg(\exists mse, bs = \text{bind } mse \text{ in } nt) \end{array}}{\text{binding\_mses } bs \forall j. (bs_j) \in nt \Rightarrow mses} \quad \text{FUNSPEC\_BINDING\_MSES\_NT\_CONS\_F}$$

$$\frac{}{\text{binding\_mses} \forall j. (bs_j) \in mv \Rightarrow [ ]} \quad \text{FUNSPEC\_BINDING\_MSES\_MV}$$

$\text{cast}@oc = \text{cast}'$

$$\frac{}{\text{cast}@[] = \text{cast}} \quad \text{FUNSPEC\_TERM\_AT\_NIL}$$

$$\frac{1 : \text{cast}_i @ oc = \text{cast}}{pn(\forall j. (\text{cast}_j)) @ i :: oc = \text{cast}} \quad \text{FUNSPEC\_TERM\_AT\_CONS}$$

$\text{cast} \simeq \text{cast}' \text{ at } oc$

$$\begin{array}{c}
1 : \text{cast}_1 @ oc = v \\
2 : \text{cast}_2 @ oc = v \\
\hline
\text{cast}_1 \simeq \text{cast}_2 \text{ at } oc \quad \text{NODE\_IDENT\_VAR} \\
\\
1 : \text{cast}_1'' @ oc = \text{pn}(\forall i. (\text{cast}_i)) \\
2 : \text{cast}_2'' @ oc = \text{pn}(\forall i. (\text{cast}_i')) \\
\hline
\text{cast}_1'' \simeq \text{cast}_2'' \text{ at } oc \quad \text{NODE\_IDENT\_APP}
\end{array}$$

We also define several relations that characterise operations on occurrences, sets thereof and relations thereupon.

**head**  $oc = i$

$$\frac{}{\text{head}(i :: oc) = i} \quad \text{FUNSPEC\_OC\_HEAD\_T}$$

**oc\_set subset oc\_set'**

Axiomatic definition of the subset relation on sets of occurrences

$$\frac{1 : \forall oc, (oc \in oc\_set \Rightarrow oc \in oc\_set')}{oc\_set \text{ subset } oc\_set'} \quad \text{OC\_SUBSET\_DEF}$$

**oc**  $\in$  **support**  $oc\_reln$

Whether an occurrence is in the support of a relation

$$\frac{1 : oc \in oc\_set \\ 2 : oc\_set \in oc\_reln}{oc \in \text{support } oc\_reln} \quad \text{OC\_IN\_IN\_DEF}$$

**is\_PER**  $oc\_reln$

A  $oc\_reln$  is a proper PER (partial equivalence relation) iff it is a set of disjoint sets (these sets are the equivalence classes).

$$\frac{1 : \forall oc\_set, \forall oc\_set', ((oc\_set \in oc\_reln \wedge oc\_set' \in oc\_reln) \Rightarrow \neg(\exists oc, (oc \in oc\_set \wedge oc \in oc\_set')))}{\text{is\_PER } oc\_reln} \quad \text{OC\_IS\_PE}$$

**oc\_reln refines oc\_reln'**

A PER  $oc\_reln$  refines another  $oc\_reln'$  iff being related by  $oc\_reln$  implies being related by  $oc\_reln'$ . Since  $oc\_reln'$  relates more pairs of elements than  $oc\_reln$ ,  $oc\_reln'$  is coarser than  $oc\_reln$ .

$$\frac{1 : \forall oc\_set, (oc\_set \in oc\_reln \Rightarrow \exists oc\_set', (oc\_set' \in oc\_reln' \wedge oc\_set \text{ subset } oc\_set'))}{oc\_reln \text{ refines } oc\_reln'} \quad \text{OC\_REFINES\_DEF}$$

**union\_closure**  $oc\_reln_1 \ oc\_reln_2 = oc\_reln_3$

The union-closure of  $oc\_reln_1$  and  $oc\_reln_2$  is the finest PER that is coarser than both  $oc\_reln_1$  and  $oc\_reln_2$ . In other words (if equivalence relations are considered as traditional sets of pairs), it is the smallest partial equivalence relation containing the union of  $oc\_reln_1$  and  $oc\_reln_2$ .

$$\frac{1 : \text{is\_PER } oc\_reln_3 \\ 2 : oc\_reln_1 \text{ refines } oc\_reln_3 \\ 3 : oc\_reln_2 \text{ refines } oc\_reln_3 \\ 4 : \forall oc\_reln', ((\text{is\_PER } oc\_reln' \wedge (oc\_reln_1 \text{ refines } oc\_reln' \wedge oc\_reln_2 \text{ refines } oc\_reln')) \Rightarrow oc\_reln_3 \text{ refines } oc\_reln')}{\text{union\_closure } oc\_reln_1 \ oc\_reln_2 = oc\_reln_3}$$

<< no parses (char 48): :oc\_reln.select: oc\_reln = { oc\_set in oc\_reln' \*\*\*'|' formula } >>

$$\begin{array}{l}
1: \forall oc\_set, (oc\_set \in oc\_reln \Rightarrow oc\_set \in oc\_reln') \\
2: \forall oc\_set, (oc\_set \in oc\_reln \Rightarrow formula) \\
3: \forall oc\_set, ((oc\_set \in oc\_reln' \wedge formula) \Rightarrow oc\_set \in oc\_reln) \\
\hline
oc\_reln = \{ oc\_set \in oc\_reln' \mid formula \}
\end{array}
\quad \text{OC\_RELN\_SELECT\_DEF}$$

$$\boxed{oc\_set = \mathbf{eponymous} \text{ } oc \text{ } cast}$$

$$\begin{array}{l}
1: cast@oc = v \\
2: \forall oc', (oc' \in oc\_set \Leftrightarrow cast@oc' = v) \\
\hline
oc\_set = \mathbf{eponymous} \text{ } oc \text{ } cast
\end{array}
\quad \text{OC\_SET\_EPONYMOUS\_DEF}$$

## 2.2 Sanity checks

We will define typing judgements that check for sanity properties, such as the fact that production names are not repeated for different productions of a non-terminal, that there is a unique definition for a non-terminal, and that if an auxiliary function is defined for a non-terminal, every production clause must define the function.

$$\boxed{\Phi \vdash f : aut}$$

$$\frac{}{\Phi, f : aut \vdash f : aut} \quad \text{SANITY\_AUXFN\_HEAD}$$

$$\begin{array}{l}
1: \Phi \vdash f : aut \\
2: \neg(f = f') \\
\hline
\Phi, f' : aut' \vdash f : aut
\end{array}
\quad \text{SANITY\_AUXFN\_SKIP}$$

$$\boxed{\Phi; e_1 .. e_n \vdash mse : metavarroot}$$

$$\frac{}{\Phi; e_1 .. e_n \vdash \{ \} : mvr} \quad \text{SANITY\_MSE\_EMPTY}$$

$$\begin{array}{l}
1: \Phi; e_1 .. e_n \vdash mse : mvr \\
2: \Phi; e_1 .. e_n \vdash mse' : mvr \\
\hline
\Phi; e_1 .. e_n \vdash mse \cup mse' : mvr
\end{array}
\quad \text{SANITY\_MSE\_UNION}$$

$$\begin{array}{l}
1: \exists!j \in 1..n. e_j = mvr \text{ } suff \\
\hline
\Phi; e_1 .. e_n \vdash mvr \text{ } suff : mvr
\end{array}
\quad \text{SANITY\_MSE\_MV}$$

$$\begin{array}{l}
1: \Phi \vdash f : ntr_1 .. ntr_m \rightarrow mvr \\
2: \exists!j \in 1..n. (e_j = nt \wedge nt = ntr_i \text{ } suff) \\
\hline
\Phi; e_1 .. e_n \vdash f(nt) : mvr
\end{array}
\quad \text{SANITY\_MSE\_F}$$

$$\boxed{\Phi; e_1 .. e_n : ntr \vdash bs \mathbf{ok}}$$

$$\begin{array}{l}
1: \Phi; e_1 .. e_n \vdash mse : mvr \\
2: \exists!j \in 1..n. e_j = nt \\
\hline
\Phi; e_1 .. e_n : ntr \vdash \mathbf{bind} \text{ } mse \text{ } \mathbf{in} \text{ } nt \text{ } \mathbf{ok}
\end{array}
\quad \text{SANITY\_BS\_BIND}$$

$$\begin{array}{l}
1: \Phi; e_1 .. e_n \vdash mse : mvr \\
2: \Phi \vdash f : ntr_1 .. ntr_n \rightarrow mvr \\
3: ntr = ntr_i \\
\hline
\Phi; e_1 .. e_n : ntr \vdash f = mse \mathbf{ok}
\end{array}
\quad \text{SANITY\_BS\_AUXFN}$$

$$\boxed{\Phi \vdash prod : ntr}$$

$$\begin{array}{l}
1: \forall i \in 1..m. \Phi; e_1 .. e_n : ntr \vdash bs_i \mathbf{ok} \\
2: prod = | e_1 .. e_n :: : prodname (+ bs_1 .. bs_m +) \\
3: \forall f \in \text{dom}(\mathbf{Phi}), (\Phi \vdash f : ntr_1 .. ntr_q \text{ } ntr \text{ } ntr'_1 .. ntr'_q \rightarrow mvr \Rightarrow \exists!i \in 1..m. \exists mse, bs_i = f = mse) \\
\hline
\Phi \vdash prod : ntr
\end{array}
\quad \text{SANITY\_PROD\_}$$

$\Phi \vdash \text{rule ok}$

1 :  $\text{rule} = \text{ntr} :: ' ' ::= \text{prod}_1 .. \text{prod}_m$   
 2 :  $\forall i \in 1..m. \Phi \vdash \text{prod}_i : \text{ntr}$   
 3 :  $\forall i \in 1..m. \forall j \in 1..m. ((\text{prod}_i = | e_1 .. e_m :: :: \text{pn} (+ bs_1 .. bs_n +) \wedge \text{prod}_j = | e'_1 .. e'_{m'} :: :: \text{pn} (+ bs'_1 .. bs'_{n'} +)) \Rightarrow i = j)$   


---

 $\Phi \vdash \text{rule ok}$

$\Phi \vdash \text{grammar\_rules ok}$

1 :  $\text{grammar\_rules} = \text{grammar rule}_1 .. \text{rule}_m$   
 2 :  $\forall i \in 1..m. \Phi \vdash \text{rule}_i \text{ ok}$   
 3 :  $\forall i \in 1..m. \forall j \in 1..m. ((\text{rule}_i = \text{ntr} :: ' ' ::= \text{prod}_1 .. \text{prod}_m \wedge \text{rule}_j = \text{ntr} :: ' ' ::= \text{prod}'_1 .. \text{prod}'_n) \Rightarrow i = j)$   


---

 $\Phi \vdash \text{grammar\_rules ok}$  SANIT

$g \vdash \text{cast} : \text{cast\_type}$

SANITY\_CAST\_VAR

$\overline{g \vdash v : \text{mvr}}$

1 :  $| e_1 .. e_n :: :: \text{pn} (+ bs_1 .. bs_o +) \in g(\text{ntr})$   
 2 :  $\text{remove\_terminals}(e_1 .. e_n) = \text{ntmv}_1, .., \text{ntmv}_q$   
 3 :  $\text{remove\_suffix}(\text{ntmv}_1) = \text{ct}_1 .. \text{remove\_suffix}(\text{ntmv}_q) = \text{ct}_q$   
 4 :  $g \vdash \text{cast}_1 : \text{ct}_1 .. g \vdash \text{cast}_q : \text{ct}_q$   


---

 $g \vdash \text{pn}(\text{cast}_1, .., \text{cast}_q) : \text{ntr}$  SANITY\_CAST\_APP

$v \in \text{dom}(s)$

$\overline{v \in \text{dom}(\{\forall i. (\text{cast}_i / v_i), \text{cast} / v, \forall j. (\text{cast}'_j / v'_j)\})}$  SANITY\_INDOM\_LIST

## 2.3 Concrete substitutions

Now, for well-typed grammar rules, we are ready to give rules for the concrete interpretation of  $\text{mse}$  on a  $\text{cast}$ , which is the set of variables picked out by  $\text{mse}$  on  $\text{cast}$ .

$\text{concrete} \llbracket \text{mse} \rrbracket g(\text{cast}) \Rightarrow \text{var\_set}$

FUNSPEC\_CONCRETE\_EMPTY

$\overline{\text{concrete} \llbracket \{\} \rrbracket g(\text{cast}) \Rightarrow \{\}}$

1 :  $\text{concrete} \llbracket \text{mse} \rrbracket g(\text{cast}) \Rightarrow \text{var\_set}$   
 2 :  $\text{concrete} \llbracket \text{mse}' \rrbracket g(\text{cast}) \Rightarrow \text{var\_set}'$   


---

 $\text{concrete} \llbracket \text{mse} \cup \text{mse}' \rrbracket g(\text{cast}) \Rightarrow \text{var\_set} \cup \text{var\_set}'$  FUNSPEC\_CONCRETE\_UNION

1 :  $| e_1 .. e_n :: :: \text{pn} (+ bs_1 .. bs_o +) \in g(\text{ntr})$   
 2 :  $\text{remove\_terminals}(e_1 .. e_n) = \text{ntmv}_1, .., \text{ntmv}_q$   
 3 :  $\text{ntmv}_l = \text{mv}$   
 4 :  $\text{cast}_l = v'$   


---

 $\text{concrete} \llbracket \text{mv} \rrbracket g(\text{pn}(\text{cast}_1, .., \text{cast}_q)) \Rightarrow \{v'\}$  FUNSPEC\_CONCRETE\_MV

1 :  $| e_1 .. e_n :: :: \text{pn} (+ bs_1 .. bs_o +) \in g(\text{ntr})$   
 2 :  $\text{remove\_terminals}(e_1 .. e_n) = \text{ntmv}_1, .., \text{ntmv}_q$   
 3 :  $\text{ntmv}_l = \text{nt}$   
 4 :  $\text{nt} = \text{ntr}' \text{ suff}'$   
 5 :  $\text{cast}_l = \text{pn}'(\text{cast}'_1, .., \text{cast}'_{q'})$   
 6 :  $| e'_1 .. e'_{n'} :: :: \text{pn}' (+ bs'_1 .. bs'_o +) \in g(\text{ntr}')$   
 7 :  $bs'_k = f = \text{mse}'$   
 8 :  $\text{concrete} \llbracket \text{mse}' \rrbracket g(\text{cast}_l) \Rightarrow \text{var\_set}$   


---

 $\text{concrete} \llbracket f(\text{nt}) \rrbracket g(\text{pn}(\text{cast}_1, .., \text{cast}_q)) \Rightarrow \text{var\_set}$  FUNSPEC\_CONCRETE\_F

In the case that  $mse$  is a single metavariable  $mv$  (INTERP\_MSE\_CONC\_3), we pick out the variable at the corresponding position. In the case that  $mse$  is  $f(nt)$  (INTERP\_MSE\_CONC\_4), we look at the production for the non-terminal  $nt$  that we have, and perform the calculation of the auxfn definition.

With these interpretations in hand, we can define the concrete substitution and free variable functions generated by Ott.

$$\boxed{\text{subst } s \in \text{cast} = \text{cast}'}$$

$$\frac{}{\text{subst } s \in v = v} \text{CONCRETE\_SUBST\_VAR}$$

$$\frac{}{\text{subst } \{ \forall i. (\text{cast}_i / v_i), \text{cast} / v, \forall j. (\text{cast}'_j / v'_j) \} \in \text{pn}(v) = \text{cast}} \text{CONCRETE\_SUBST\_IN}$$

$$\frac{1 : \neg(v \in \mathbf{dom}(s))}{\text{subst } s \in \text{pn}(v) = \text{pn}(v)} \text{CONCRETE\_SUBST\_OUT}$$

$$\frac{\begin{array}{l} 1 : \text{cast} = \text{pn}(\forall k. (\text{cast}_k)) \\ 2 : \neg(\exists v, \text{cast} = \text{pn}(v)) \\ 3 : | e_1 .. e_n :: :: \text{pn}(+bs_1 .. bs_m +) \in g(\text{ntr}) \\ 4 : \mathbf{remove\_terminals}(e_1 .. e_n) = \forall k. (\text{ntmv}_k) \\ 5 : \forall k. (\mathbf{binding\_mSES} bs_1 .. bs_m \in \text{ntmv}_k \Rightarrow \text{mSES}_k) \\ 6 : \mathbf{concrete} [\bigcup \text{mSES}_k] g(\text{cast}) \Rightarrow \text{var\_set}_k \\ 7 : \forall k. (s_k = \mathbf{filter} \text{var\_set}_k \text{ from } s) \\ 8 : \forall k. (\text{subst } s_k \in \text{cast}_k = \text{cast}'_k) \\ 9 : \text{cast}' = \text{pn}(\forall k. (\text{cast}'_k)) \end{array}}{\text{subst } s \in \text{cast} = \text{cast}'} \text{CONCRETE\_SUBST\_APP}$$

$$\boxed{\mathbf{fv} \text{ ntr mvr of } \text{cast} = \text{var\_set}}$$

$$\frac{\begin{array}{l} 1 : | e_1 .. e_n :: :: \text{pn}(+bs_1 .. bs_o +) \in g(\text{ntr}') \\ 2 : \neg(\text{ntr} = \text{ntr}') \end{array}}{\mathbf{fv} \text{ ntr mvr of } \text{pn}(v) = \{ \}} \text{CONCRETE\_FV\_OUT\_NT}$$

$$\frac{\begin{array}{l} 1 : | e_1 .. e_n :: :: \text{pn}(+bs_1 .. bs_o +) \in g(\text{ntr}) \\ 2 : \neg(\text{mvr} = \text{mvr}') \end{array}}{\mathbf{fv} \text{ ntr mvr of } \text{pn}(v') = \{ \}} \text{CONCRETE\_FV\_OUT\_MV}$$

$$\frac{1 : | e_1 .. e_n :: :: \text{pn}(+bs_1 .. bs_o +) \in g(\text{ntr})}{\mathbf{fv} \text{ ntr mvr of } \text{pn}(v) = \{ v \}} \text{CONCRETE\_FV\_IN}$$

$$\frac{}{\mathbf{fv} \text{ ntr mvr of } v = \{ \}} \text{CONCRETE\_FV\_VAR}$$

$$\frac{\begin{array}{l} 1 : \text{cast} = \text{pn}(\forall k. (\text{cast}_k)) \\ 2 : \neg(\exists v, \text{cast} = \text{pn}(v)) \\ 3 : | e_1 .. e_n :: :: \text{pn}(+bs_1 .. bs_m +) \in g(\text{ntr}) \\ 4 : \mathbf{remove\_terminals}(e_1 .. e_n) = \forall k. (\text{ntmv}_k) \\ 5 : \forall k. (\mathbf{binding\_mSES} bs_1 .. bs_m \in \text{ntmv}_k \Rightarrow \text{mSES}_k) \\ 6 : \forall k. (\mathbf{concrete} [\bigcup \text{mSES}_k] g(\text{cast}) \Rightarrow \text{var\_set}_k) \\ 7 : \forall k. (\mathbf{fv} \text{ ntr mvr of } \text{cast}_k = \text{var\_set}'_k) \\ 8 : \text{var\_set} = \bigcup \{ \forall k. (\text{var\_set}'_k - \text{var\_set}_k) \} \end{array}}{\mathbf{fv} \text{ ntr mvr of } \text{cast} = \text{var\_set}} \text{CONCRETE\_FV\_APP}$$

Notice that we treat only variables wrapped in a singleton constructor as free, or subject to substitution.

In the case that this is a compound term (SUBST\_3), we first check to see that we do not fall into the singleton variable case. Next, we look up the production in our grammar, and remove the terminals to get elements that can appear in abstract terms. We look at all the bind clauses of the form  $\mathbf{bind} \text{ mse}' \text{ in } nt$ , and filter out the interpretation of  $\text{mse}'$  from the substitution before applying it to the corresponding subterm.

## 2.4 Mathematical definition

We now turn to the definition of alpha-equivalence on the concrete terms. This is defined as follows:

$$\boxed{\llbracket mse \rrbracket g (cast) = oc\_set}$$

$$\frac{}{\overline{\llbracket \{\} \rrbracket g (cast) = \{\}}} \text{FUNSPEC\_INTERP\_MSE\_EMPTY}$$

$$\begin{array}{l} 1 : \llbracket mse \rrbracket g (cast) = oc\_set \\ 2 : \llbracket mse \rrbracket g (cast') = oc\_set' \end{array}$$

$$\frac{}{\llbracket mse \cup mse' \rrbracket g (cast) = oc\_set \cup oc\_set'} \text{FUNSPEC\_INTERP\_MSE\_UNION}$$

$$\begin{array}{l} 1 : | e_1 .. e_n :: :: pn (+ bs_1 .. bs_o +) \in g (ntr) \\ 2 : \mathbf{remove\_terminals} (e_1 .. e_n) = ntmv_1, \dots, ntmv_q \\ 3 : ntmv_l = mv \\ 4 : cast_l = v' \end{array}$$

$$\frac{}{\llbracket mv \rrbracket g (pn (cast_1, \dots, cast_q)) = \{ l :: [] \}} \text{FUNSPEC\_INTERP\_MSE\_MV}$$

$$\begin{array}{l} 1 : | e_1 .. e_n :: :: pn (+ bs_1 .. bs_o +) \in g (ntr) \\ 2 : \mathbf{remove\_terminals} (e_1 .. e_n) = ntmv_1, \dots, ntmv_q \\ 3 : ntmv_l = nt \\ 4 : nt = ntr' \mathit{suff}' \\ 5 : cast_l = pn' (cast'_1, \dots, cast'_q) \\ 6 : | e'_1 .. e'_n :: :: pn' (+ bs'_1 .. bs'_o +) \in g (ntr') \\ 7 : bs'_k = f = mse' \\ 8 : \llbracket mse' \rrbracket g (cast_l) = oc\_set \end{array}$$

$$\frac{}{\llbracket f(nt) \rrbracket g (pn (cast_1, \dots, cast_q)) = l :: oc\_set} \text{FUNSPEC\_INTERP\_MSE\_F}$$

$$\boxed{\llbracket auxfn \rrbracket g (cast) = oc\_set}$$

$$\begin{array}{l} 1 : cast = pn (cast_1, \dots, cast_q) \\ 2 : | e_1 .. e_n :: :: pn (+ bs_1 .. bs_o +) \in g (ntr) \\ 3 : bs_j = f = mse \\ 4 : \llbracket mse \rrbracket g (cast) = oc\_set \end{array}$$

$$\frac{}{\llbracket f \rrbracket g (cast) = oc\_set} \text{FUNSPEC\_INTERP\_AUXFN\_DEF}$$

$$\boxed{\Phi \vdash f \mathbf{accepts} ntr}$$

$$\frac{1 : \Phi \vdash f : ntr_1 .. ntr_m ntr ntr'_1 .. ntr'_n \rightarrow mvr}{\Phi \vdash f \mathbf{accepts} ntr} \text{F\_ACCEPTS\_ARG}$$

$$\boxed{\Phi \vdash g (ntr) \mathbf{at} cast \mathbf{reveals} oc}$$

$$\begin{array}{l} 1 : \Phi \vdash f \mathbf{accepts} ntr \\ 2 : \llbracket f \rrbracket g (cast) = oc\_set \\ 3 : oc \in oc\_set \end{array}$$

$$\frac{}{\Phi \vdash g (ntr) \mathbf{at} cast \mathbf{reveals} oc} \text{NTR\_REVEALS\_F}$$

$$\boxed{\Phi \vdash \mathbf{equiv\_both} g (cast) = \langle \mathbf{closed} : oc\_reln_1, \mathbf{open} : oc\_reln_2 \rangle}$$



- 1 :  $\Phi \vdash g \text{ ok}$
- 2 :  $cast = pn(\forall i. (cast_i))$
- 3 :  $| e_1 .. e_n :: :: pn(+ bs_1 .. bs_m +) \in g(ntr)$
- 4 :  $\text{remove\_terminals}(e_1 .. e_n) = \forall i. (ntmv_i)$
- 5 :  $\forall i. (\text{binding\_mses } bs_1 .. bs_m \in ntmv_i \Rightarrow mses_i)$
- 6 :  $\forall i. (\llbracket \bigcup mses_i \rrbracket g(cast) = oc\_set_i)$
- 7 :  $\forall i. (\Phi \vdash \text{equiv\_both } g(cast_i) = \langle \text{closed} : oc\_reln_{1\ i}, \text{open} : oc\_reln_{2\ i} \rangle)$
- 8 :  $oc\_reln_1 = \bigcup \{ \forall i. (i :: oc\_reln_{1\ i}) \}$
- 9 :  $oc\_reln_2 = \bigcup \{ \forall i. (i :: oc\_reln_{2\ i}) \}$
- 10 :  $oc\_reln_3 = \{ ((\text{eponymous } oc_0 \text{ cast} \cap \bigcup \{ \forall i. (oc\_set_i) \}) \cup \bigcup \{ \forall i. (\{ oc \in \text{eponymous } oc_0 \text{ cast} \mid \text{head } oc = i \wedge oc \in oc\_set_i \}) \}) \}$
- 11 :  $\text{union\_closure } oc\_reln_2 \text{ } oc\_reln_3 = oc\_reln_4$
- 12 :  $oc\_reln_5 = \{ oc\_set' \in oc\_reln_4 \mid \exists oc, (\Phi \vdash g(ntr) \text{ at } cast \text{ reveals } oc \wedge oc \in oc\_set') \}$
- 13 :  $oc\_reln_6 = oc\_reln_1 \cup (oc\_reln_4 - oc\_reln_5)$

---


$$\Phi \vdash \text{equiv\_both } g(cast) = \langle \text{closed} : oc\_reln_6, \text{open} : oc\_reln_5 \rangle$$

For the definition of the equivalence classes (EQUIVS\_CAST\_1), we start in steps 1--4 by looking up the production name in our grammar, and removing the terminals. In steps 5--6, we extract the set of binding occurrences as given by the bindspec clauses:  $oc\_set_i$  is the set of binding occurrences of variables that bind in subterm  $i$ . In step 7--9, we recursively calculate closed and binding equivalence relations for all subterms.

In step 10, we iterate over all binding occurrences  $oc_0$  of any variable  $var:mvr$ , and build the equivalence class of that occurrence. This equivalence class has the form  $(C(var:mvr) \cup \bigcup_i (i :: D_i(var:mvr))) - U$ , where:

- $C(var:mvr)$  is the set of binding occurrences of  $var:mvr$ , computed as the occurrences of  $var:mvr$  (i.e., **eponymous**  $oc_0 \text{ cast}$ ) that are binding;
- $D_i(var:mvr)$  is the set of bound occurrences of  $var:mvr$  inside subterm  $i$ ;  $D_i(var:mvr)$  is built directly as the occurrences of  $var:mvr$  whose head is some  $i$  such that  $var:mvr$  is bound in subterm  $i$  (note that the bindspec clause that makes  $var:mvr$  bound in subterm  $i$  might mention an occurrence  $oc$  which is different from  $oc_0$ );
- $U$  is the set of occurrences that are already bound in the subterm, as recorded in  $oc\_reln_1$ .

In step 11, we take the equivalence closure of this set with the open binding sets of subterms. Finally, we pick out all equivalence classes such that they pick out something within the domain of an auxfn (which means they can potentially be bound later), calling that the open bound set, and the remaining equivalence closures of bound variable occurrences are called the closed binding set of this term.

$$\boxed{\Phi; g \vdash cast_1 \equiv_\alpha cast_2}$$

- 1 :  $\Phi \vdash \text{equiv\_both } g(cast_1) = \langle \text{closed} : oc\_reln_1, \text{open} : oc\_reln_2 \rangle$
- 2 :  $\Phi \vdash \text{equiv\_both } g(cast_2) = \langle \text{closed} : oc\_reln_3, \text{open} : oc\_reln_4 \rangle$
- 3 :  $oc\_reln_1 = oc\_reln_3$
- 4 :  $\forall oc, ((\neg oc \in \text{support } oc\_reln_1) \Rightarrow ((\exists cast'_1, cast_1 @ oc = cast'_1) \Leftrightarrow (\exists cast'_2, cast_2 @ oc = cast'_2)))$
- 5 :  $\forall oc, (((\neg oc \in \text{support } oc\_reln_1) \wedge ((\exists cast'_1, cast_1 @ oc = cast'_1) \wedge (\exists cast'_2, cast_2 @ oc = cast'_2))) \Rightarrow cast_1 \simeq cast_2 \text{ a})$

---


$$\Phi; g \vdash cast_1 \equiv_\alpha cast_2$$

Two terms are said to be alpha-equivalent if they have the same closed binding sets, and for each occurrence not in the closed binding set, the occurrence is defined for one term if it is for the other, and the subterms at that occurrence are node-identical.

$$\boxed{\Phi; g \vdash s \text{ ok}}$$

- 1 :  $\forall i. (\Phi \vdash \text{equiv\_both } g(cast_i) = \langle \text{closed} : oc\_reln_{1\ i}, \text{open} : \{ \} \rangle)$
- 2 :  $\forall i. (\forall oc, ((\exists v, cast_i @ oc = v) \Rightarrow oc \in \text{support } oc\_reln_{1\ i}))$
- 3 :  $\forall i. (\forall pn, \forall ntr, ((g \vdash pn(var_i:mvr_i) : ntr) \Rightarrow (g \vdash cast_i : ntr \vee \exists pn', g \vdash pn'(cast_i) : ntr)))$
- 4 :  $\forall i. (\neg (\exists ntr', ((\exists pn, g \vdash pn(cast_i) : ntr') \wedge ((\exists f, \Phi \vdash f : ntr_1 .. ntr_n \text{ ntr}'_1 .. \text{ ntr}'_m \rightarrow mvr_i) \wedge (\exists pn', g \vdash pn'(cast_i) : ntr')))))$

---


$$\Phi; g \vdash \{ \forall i. (cast_i / var_i : mvr_i) \} \text{ ok}$$

Well-typed substitutions always substitute closed terms (ie all occurrences of variables are within the closed binding relation calculated in step 1). Next (step 3), we ensure that for all possible substitution positions, the result makes sense. Finally, we impose a sanity condition which ensures that substitution matches the notion on alpha-equivalence in step 4. This sanity condition says that we disallow substitutions which substitute terms such that the result of the substitution can itself be picked out by auxfns (to be bound later, presumably).

$$\boxed{\Phi; g \vdash \mathbf{c\_a\_subst} s \in \mathit{cast} = \mathit{cast}''}$$

$$\frac{}{\Phi; g \vdash \mathbf{c\_a\_subst} s \in v = v} \text{SUBST\_SPEC\_VAR}$$

$$\frac{}{\Phi; g \vdash \mathbf{c\_a\_subst} \{ \forall i. (\mathit{cast}_i / v_i), \mathit{cast} / v, \forall j. (\mathit{cast}'_j / v'_j) \} \in \mathit{pn}(v) = \mathit{cast}} \text{SUBST\_SPEC\_IN}$$

$$\frac{1 : \neg(v \in \mathbf{dom}(s))}{\Phi; g \vdash \mathbf{c\_a\_subst} s \in \mathit{pn}(v) = \mathit{pn}(v)} \text{SUBST\_SPEC\_OUT}$$

$$\frac{\begin{array}{l} 1 : \mathit{cast} = \mathit{pn}(\forall k. (\mathit{cast}_k)) \\ 2 : \neg(\exists v, \mathit{cast} = \mathit{pn}(v)) \\ 3 : | e_1 .. e_n :: :: \mathit{pn}(+ bs_1 .. bs_m +) \in g(ntr) \\ 4 : \mathbf{remove\_terminals}(e_1 .. e_n) = \forall k. (\mathit{ntmv}_k) \\ 5 : \forall k. (\Phi; g \vdash \mathit{cast}'_k \equiv_{\alpha} \mathit{cast}_k \wedge (\forall oc, \forall v, (v \in \mathbf{dom}(s) \Rightarrow \neg(\mathit{cast}'_k @ oc = v)))) \\ 6 : \forall k. (\mathbf{subst} s_k \in \mathit{cast}'_k = \mathit{cast}''_k) \\ 7 : \forall k. (\Phi; g \vdash \mathit{cast}''_k \equiv_{\alpha} \mathit{cast}'''_k) \\ 8 : \mathit{cast}' = \mathit{pn}(\forall k. (\mathit{cast}'''_k)) \end{array}}{\Phi; g \vdash \mathbf{c\_a\_subst} s \in \mathit{cast} = \mathit{cast}'} \text{SUBST\_SPEC\_APP}$$

### 3 Relating concrete binding and alpha-equivalence

**Lemma 3.1** (Substitutions on node-identical occurrences produce node-identical results). *Suppose  $\mathit{cast}_1 \simeq \mathit{cast}_2$  at  $oc$ . Then for any substitution  $s$ , if  $\mathbf{subst} s \text{ in } \mathit{cast}_1 = \mathit{cast}'_1$ , and  $\mathbf{subst} s \text{ in } \mathit{cast}_2 = \mathit{cast}'_2$ , then  $\mathit{cast}'_1 \simeq \mathit{cast}'_2$  at  $oc$ .*

*Proof.* By induction on the cases for substitution and node-equality.  $\square$

We introduce a bit of notation. Call an occurrence  $oc$  defined for a term  $\mathit{cast}$  if there is a subterm at  $oc$ , ie if there exists a  $\mathit{cast}'$  such that  $\mathbf{termat} oc \mathit{cast} = \mathit{cast}'$ .

Also, call an occurrence  $oc$  closed bound in a term  $\mathit{cast}$  if  $\Phi \vdash \mathbf{equiv\_both} g(\mathit{cast}) = \langle \mathbf{closed} : oc\_reln_1, \mathbf{open} : oc\_reln_2 \rangle$  and  $oc \in \mathbf{union}\{oc\_set | oc\_set \in oc\_reln_1\}$ .

**Lemma 3.2** (Binding occurrences are not substituted). *For any  $s, \Psi, g, \mathit{cast}_1, \mathit{cast}_2$  and  $mse$ , if  $\Phi; g \vdash s \mathbf{ok}, g \vdash \mathit{cast}_1 : \mathit{cast\_type}, \mathbf{subst} s \text{ in } \mathit{cast}_1 = \mathit{cast}_2$  and if  $oc \in \llbracket mse \rrbracket g(\mathit{cast}_1)$  then  $oc$  is defined for  $\mathit{cast}_2$  and is the same term as in  $\mathit{cast}_1$ .*

*Proof.* This is proved by induction on the structure of  $mse$ . For  $mse = \{ \}$ , this is immediate. For  $mse = mse_1 \mathbf{union} mse_2$ , the inductive hypothesis on the two sets  $\llbracket mse_1 \rrbracket$  and  $\llbracket mse_2 \rrbracket$  give us the required results.

Now consider if  $mse = mv$ . Then the subterm at that occurrence to be well-typed must be  $var : mvr$ . Notice that bare variables are not substituted for by the concrete substitution function. Thus this case is covered.

The final case is if  $mse = f(nt)$ . Looking at the definition of the concrete substitution function, this occurrence is defined in the result. It is always the same subterm, except when this variable occurrence is wrapped in a singleton production. Assume then for purpose of contradiction that this variable occurrence is wrapped in a singleton production  $prodname$  for some nonterminal root  $ntr$ . Since it was picked up by an auxfn, there must be a auxfn  $f$  which takes  $ntr$  to the sort of metavariables in  $mse$ , ie  $mvr$ . But this is impossible for well-typed substitutions, since then there must be a singleton production for the substituent for the same nonterminal, and this nonterminal is in the domain of an auxfn. Thus we have the required contradiction.  $\square$

**Lemma 3.3** (Closed bound occurrences are not substituted). *For any  $s, \Psi, g, cast_1$  and  $cast_2$ , if  $\Phi; g \vdash s \mathbf{ok}, g \vdash cast_1 : cast\_type, \mathbf{subst} s \mathbf{in} cast_1 = cast_2$ , and an occurrence  $oc$  is closed bound in the term  $cast_1$ , then  $oc$  is defined for  $cast_2$  and in fact is closed bound in the term  $cast_2$ .*

*Proof.* We perform induction on the structure of the term, and look at the calculation of the closed binding set. We notice that an occurrence can turn out to be closed bound in one of three ways.

First, the occurrence might be a lift of an occurrence already closed bound on a subterm. This case goes through by inductive hypothesis, since the subterm is smaller.

Second, the occurrence might be of a variable  $var : mvr$  in the subtree corresponding to  $nt$ , where a bindspec clause  $\mathbf{bind} mse \mathbf{in} nt$  present attached to the production. We will call these occurrences bound occurrences. The variable  $var : mvr$  must lie within the  $var\_set$  which is the concrete interpretation  $\mathbf{concrete} \llbracket mse \rrbracket$  of the term  $cast_1$ . Looking at the definition of concrete substitutions, this set is filtered out from the domain of substitution, and thus the occurrence remains unchanged in the result of substitution.

Third, the occurrence might lie within  $\llbracket mse \rrbracket$  for a bindspec clause  $\mathbf{bind} mse \mathbf{in} nt$ . We will call these occurrences binding occurrences. In this case we defer to the lemma 3.2. □

**Lemma 3.4** (Substitution preserves closed bound equivalence classes). *For any  $s, \Psi, g, cast_1$  and  $cast_2$ , if  $\Phi; g \vdash s \mathbf{ok}, g \vdash cast_1 : cast\_type, \mathbf{subst} s \mathbf{in} cast_1 = cast_2$ . Say that  $\Phi \vdash \mathbf{equiv\_both} g ( cast_1 ) = \langle \mathbf{closed} : oc\_reln_{11}, \mathbf{open} : oc\_reln_{12} \rangle$  and  $\Phi \vdash \mathbf{equiv\_both} g ( cast_2 ) = \langle \mathbf{closed} : oc\_reln_{21}, \mathbf{open} : oc\_reln_{22} \rangle$ . Then  $oc\_reln_{11} \subseteq oc\_reln_{21}$ .*

*Proof.* We argue by induction on the term, and looking at the calculation of the closed equivalence relation. By induction, the closed equivalence classes of the subterms are still present in the result. Further, for any occurrence which is closed bound, the subterm is not changed by substitution, by lemma 3.3. Thus each occurrence previously closed bound will still be picked up. No new occurrence will be picked up, since well-typedness of substitution ensures that the substituents are closed. Since the set of auxfn's have not changed, no occurrence which was previously closed bound will become open-bound, or vice versa. □

**Theorem 3.5.** *For any  $s, \Psi, g, cast_1$  and  $cast_2$ , if  $\Phi; g \vdash s \mathbf{ok}, g \vdash cast_1 : cast\_type, g \vdash cast_2 : cast\_type, \Phi; g \vdash cast_1 \equiv_\alpha cast_2, \mathbf{subst} s \mathbf{in} cast_1 = cast'_1$ , and  $\mathbf{subst} s \mathbf{in} cast_2 = cast'_2$ , then  $\Phi; g \vdash cast'_1 \equiv_\alpha cast'_2$ .*

*Proof.* We prove this by looking at the definition of  $\equiv_\alpha$ , knowing that  $\Phi; g \vdash cast_1 \equiv_\alpha cast_2$ .

There are now two cases for an occurrence  $oc$  which is defined for  $cast_1$ . Either it is within closed bound in  $cast_1$ , or it is not. We will look at these cases in turn.

In the case that it is closed bound, since the two closed binding relations have to be the same for alpha-equivalent terms, the same occurrence must be defined and indeed closed bound for  $cast_2$  (Note that the variable at that occurrence need not be identical). We know by lemma 3.3 that the applied substitutions do not touch these occurrences, and that the corresponding equivalence class remains within the set of closed equivalence relations for the results of the substitution.

In the case that it is not closed bound, the subterms of the two terms at that occurrence are node-identical. The result of substitution on these subterms are therefore themselves node-identical, by lemma 3.1.

Using these facts, we now show that the results are themselves  $\alpha$ -equivalent. This involves two steps.

First, we have to show that the closed equivalence relations are identical for the two resultant terms. We follow the construction of the closed equivalence relation at each node of the syntax tree of  $cast'_1$ . If this subterm was already present in  $cast_1$ , then all pre-existing closed equivalence classes must still be present in the new equivalence relation, by lemma 3.4. Further, the only new additions can be due to new subterms created by the substitution. Notice however that substitutions only changed the structure of the term at occurrences which are not closed bound. In these cases the subterms at occurrences were node-identical. Thus only identical equivalence classes of closed occurrences are added to the closed equivalence relations of both terms. Further, since well-typed substitutions substitute only closed terms, we get that there are no additional equivalence classes of open bound occurrences.

Second, all occurrences which are not closed bound in the result are defined for both resultant terms if it is defined for any one resultant term, and the terms at such occurrences are node-identical. So consider

an occurrence which is not closed bound. If this occurrence was defined in the initial term, it cannot have been closed bound, since the closed equivalence relation of the result includes that of the initial term, by lemma 3.4. Thus by the previous statements, it is defined and node-identical in both terms. If on the other hand, it is an occurrence not defined in the initial term, since the substitution only acted on node-identical terms, it must be defined and identical in both resultant terms.  $\square$

**Theorem 3.6** (Correspondence of concrete and capture-avoiding substitution). *For any  $s, \Psi, g, cast$  and  $cast'$ , if  $\Phi; g \vdash s \text{ ok}$ ,  $g \vdash cast : cast\_type$ ,  $\text{subst } s \text{ in } cast = cast'$ , then  $\Phi; g \vdash \text{c\_a\_subst } s \text{ in } cast = cast'$ .*

*Proof.* This theorem is proved by induction on the structure of the term.

For the cases where the term is a variable, or a singleton production containing a variable, concrete substitution and capture-avoiding substitutions are defined identically.

For a non-singleton production, capture avoiding substitution carries on by alpha-renaming all bound variables to fresh ones. The concrete substitution on the other hand filters out bound variables. We thus pick some fresh variable (that is, one not appearing in the term at all) and performing the alpha-renaming. Since we have countably infinite variables, this can always be done. Now, by theorem 3.5, we get that the result of applying the concrete substitution is alpha-equivalent to the capture-avoiding substitution performed by our chosen renaming. Looking at the rule CA\_SUBST\_3, this allows us to match up with the premise 7. This completes the case.  $\square$