# Global Control for Partial Deduction through Characteristic Atoms and Global Trees

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#### Abstract

Recently, considerable advances have been made in the (on-line) control of logic program specialisation. A clear conceptual distinction has been established between local and global control and on both levels concrete strategies as well as general frameworks have been proposed. For global control in particular, recent work has developed concrete techniques based on the preservation of characteristic trees (limited, however, by a given, arbitrary depth bound) to obtain a very precise control of polyvariance. On the other hand, the concept of an m-tree has been introduced as a refined way to trace "relationships" of partially deduced atoms, thus serving as the basis for a general framework within which global termination of partial deduction can be ensured in a non ad hoc way.

Blending both, formerly separate, contributions, in this paper, we present an elegant and sophisticated technique to globally control partial deduction of normal logic programs. Leaving unspecified the specific local control one may wish to plug in, we develop a concrete global control strategy combining the use of characteristic atoms and trees with global (m-)trees. We thus obtain partial deduction that always terminates in an elegant, non ad hoc way, while providing excellent specialisation as well as fine-grained (but reasonable) polyvariance.

We conjecture that a similar approach may contribute to improve upon current (on-line) control strategies for functional program transformation methods such as (positive) supercompilation.

**Keywords:** Partial Deduction, Online Control, Global Control, Characteristic Trees, Termination

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Abstract. Recently, considerable advances have been made in the (online) control of logic program specialisation. A clear conceptual distinction has been established between local and global control and on both levels concrete strategies as well as general frameworks have been proposed. For global control in particular, recent work has developed concrete techniques based on the preservation of characteristic trees (limited, however, by a given, arbitrary depth bound) to obtain a very precise control of polyvariance. On the other hand, the concept of an m-tree has been introduced as a refined way to trace "relationships" of partially deduced atoms, thus serving as the basis for a general framework within which global termination of partial deduction can be ensured in a non ad hoc way.

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#### 1 Introduction

A major concern in the specialisation of functional ([4, 13, 30]) as well as logic programs ([21, 15, 8, 27, 5]) has been the issue of control: How can the transformation process be guided in such a way that termination is guaranteed and results are satisfactory?

This problem has been tackled from two (until now) largely separate angles: the so-called off-line versus on-line approaches. Partial evaluation of functional

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programs ([4, 13]) has mainly stressed the former, while supercompilation of functional ([30, 31, 29]) and partial deduction of logic programs ([10, 28, 2, 3, 22, 25, 17]) have concentrated on on-line control. (Some exceptions are [32, 26, 16, 14].) It is within this on-line control tradition that the present work provides a novel and important contribution.

In partial deduction of logic programs, one distinguishes two levels of control ([8, 25]): the local and the global level. In a nutshell, the local level decides on how SLD(NF)-trees for individual atoms should be built. The (leaves of the) resulting trees allow to construct specialised clauses for the given atoms ([21, 1]). At the global level on the other hand, one typically attends to the overall correctness of the resulting program (satisfying the closedness condition in [21]) and strives to achieve the "right" amount of polyvariance, producing sufficiently many (but not too much) specialised versions for each predicate definition in the original program.

Gallagher in [8] writes that providing adequate global control seems much harder than handling the local level. So, in this paper, it is to the latter, global, level that we (again) turn our attention. In recent work, both authors of the present paper have already, separately, investigated issues in global control of partial deduction. [25] and its extended and slightly revised version [24] focus on termination and provide a quite general, refined framework for global control, different instances of which can be taken as the core of practical systems. [17] on the other hand starts from the central role of characteristic trees in preserving specialisation and determining polyvariance (as first proposed in [10]). It shows how partial deduction can be governed through the use of characteristic atoms, combining the usual atoms to be partially deduced with the characteristic trees to be enforced upon them. Global termination, however, is guaranteed at the cost of imposing an arbitrary, ad hoc depth bound on characteristic trees (as in all earlier partial deduction based on characteristic trees, see e.g. [10, 7, 18]).

In the present paper, we endeavour to obtain the best of both worlds, blending (a slightly adapted version of) the general framework in [25, 24] with the use of characteristic atoms and trees as in [17]. We thus obtain a very elegant, sophisticated and precise apparatus for on-line global control of partial deduction.

Below, we first recapitulate some necessary background material and provide motivating examples for our approach in Sect. 2. Sect. 3, subsequently, contains the formal elaboration of our method, leading to the presentation of a partial deduction algorithm, parameterised by its local control, the particular choice of which is left open in this paper. Next, in Sect. 4, we return to the examples in Sect. 2, showing how indeed the method developed in Sect. 3 deals properly with them and leads to greatly improved practical specialisation results. Finally, a possible drawback of the presented approach as well as some connections with related work in supercompilation are briefly discussed. We conclude the paper in Sect. 5.

Proofs are assembled in App. A.

# 2 Ecological Partial Deduction and the Depth Bound Problem

In what follows, we assume the reader to be familiar with the basic concepts of logic programming and partial deduction, as they are presented in e.g. [20, 21]. Throughout, unless stated explicitly otherwise, the terms "(logic) program" and "goal" will refer to a *normal* logic program and goal, respectively.

Given a program P and a goal G, partial deduction produces a new program P' which is P "specialised" to the goal G. The underlying technique is to construct "incomplete" SLDNF-trees for a set of atoms  $\mathcal A$  to be specialised and extract the program P' from these incomplete search trees by taking resultants (for each atom in  $\mathcal A$  a different specialised predicate definition will thus be generated). An incomplete SLDNF-tree is an SLDNF-tree which, in addition to success and failure leaves, may also contain leaves where no literal has been selected for a further derivation step. Leaves of the latter kind will be called dangling. Under the conditions stated in [21], namely closedness and independence, correctness of the specialised program is guaranteed.

In the context of partial deduction, incomplete SLDNF-trees are obtained by applying an unfolding rule, defined as follows:

**Definition 1.** An unfolding rule U is a function which given a program P and a goal G returns a finite (possibly incomplete) SLDNF-tree<sup>3</sup> for  $P \cup \{G\}$ .

### 2.1 Ecological Partial Deduction

The problem of controlling polyvariance in partial deduction boils down to finding a terminating procedure to produce a finite set of atoms  $\mathcal{A}$  which satisfies the correctness conditions of [21] while at the same time being as precise as possible (usually the more fine-grained and instantiated the set  $\mathcal{A}$  is, the better the potential for specialisation is). Most approaches in the literature so far are based on the syntactic structure of the atoms to be specialised, but it can be shown (see e.g. [18, 17]) that this provides insufficient detail.

[10, 7] therefore introduced the notion of a *characteristic tree*, capturing how atoms are specialised and as such constituting a more refined basis for polyvariance. The following definitions are adapted from [7, 17, 18].

**Definition 2.** Let  $G_1$  be a goal and let P be a program the clauses of which are numbered. Let  $G_1, \ldots, G_n$  be a finite, incomplete SLDNF-derivation of  $P \cup \{G_1\}$ . The *characteristic path* of the derivation is the sequence  $(l_1, c_1), \ldots, (l_{n-1}, c_{n-1})$ , where  $l_i$  is the position of the selected literal in  $G_i$ , and  $c_i$  is defined as:

- if the selected literal is an atom, then  $c_i$  is the number of the clause chosen to resolve with  $G_i$ .
- if the selected literal is  $\neg p(\bar{t})$ , then  $c_i$  is the predicate p. The set of all characteristic paths for a given goal G and program P will be denoted by chpaths(G, P).

<sup>&</sup>lt;sup>3</sup> We even allow a trivial SLDNF-tree, i.e. one whose root is a dangling leaf.

**Definition 3.** Let G be a goal, P a program and U an unfolding rule. Then the characteristic tree  $\tau$  of G (in P) via U is the set of characteristic paths of the non-failing derivations of the incomplete SLDNF-tree obtained by applying U to G (in P). We introduce the notation  $chtree(G,P,U)=\tau$ . We also say that  $\tau$  is a characteristic tree of G (in P) if it is the characteristic tree for some unfolding rule U. Also  $\tau$  is a characteristic tree if it is a characteristic tree of some G in some P.

Note that the characteristic path of an empty derivation is the empty path (), and the characteristic tree of a trivial SLDNF-tree is {()}. Characteristic trees are an interesting abstraction of SLDNF-trees because they capture the specialisation performed locally by partial deduction. If two atomic goals have the same characteristic tree then the same branches have been pruned by partial deduction and the atoms have been unfolded in the same way (i.e. to the same depth and the same clauses have been resolved with literals in the same position). Also, in principle a single predicate definition can be used. For more details about the interest and relevance of characteristic trees, we refer to [10, 7, 18, 17].

When using characteristic trees to control polyvariance, the atoms to be specialised are classified according to their characteristic tree. The basic idea is to have only one specialised version for each characteristic tree. If several atoms have the same characteristic tree, then they are abstracted by a single more general atom. Earlier approaches to partial deduction using characteristic trees [7, 10] have been limited by not being able to preserve characteristic trees in that abstraction process (implying that the generalisation has a different local specialisation behaviour). As shown in [17, 18], this can lead to important precision losses as well as non-termination.

The problem has been solved in [17] by simply *imposing* characteristic trees on the generalised atoms. <sup>4</sup> This amounts to associating characteristic trees with the atoms to be specialised, thus allowing the preservation of characteristic trees without having to construct intricate generalisations. The rest of this subsection recapitulates and adapts the necessary material from [17].

From now on, throughout the rest of this paper, we implicitly assume the existence of some given finite underlying language  $\mathcal{L}$  in which atoms and terms, goals and programs are expressed.

We first introduce the crucial notion of a characteristic atom.

**Definition 4.** A *P-characteristic atom*, for a given program P, is a couple  $(A, \tau)$  consisting of an atom A and a characteristic tree  $\tau$  with  $\tau \subseteq chpaths(\leftarrow A, P)$ .

Often, when the context allows it, we will drop the P annotation and simply refer to *characteristic* atoms. Also note that  $\tau$  is not necessarily a characteristic tree of  $\leftarrow A$  in P. The following definition associates a set of concretisations with each characteristic atom.

<sup>&</sup>lt;sup>4</sup> Another solution is presented in [18], which is however limited to definite programs and certain unfolding rules, but enjoys a better overall precision. The core ideas of the present paper can also be used to enhance the [18] method in order to eliminate a similar depth bound problem.

**Definition 5.** An atom A is a precise concretisation of a P-characteristic atom  $(A', \tau')$  iff A is an instance of A' and for some unfolding rule U we have that  $chtree(\leftarrow A, P, U) = \tau'$ . An atom B is a concretisation of  $(A', \tau')$  iff it is an instance of a precise concretisation of  $(A', \tau')$ .

A P-characteristic atom can thus be seen as standing for a (possibly infinite) set of atoms, namely the concretisations according to the above definition. A characteristic atom  $(A, \tau)$  also uniquely determines a set of resultants:

**Definition 6.** Let  $(A, \tau)$  be a P-characteristic atom. If  $\tau \neq \{()\}$  then  $\delta(P, (A, \tau))$  is the set of all (necessarily non-failing) SLDNF-derivations for  $P \cup \{\leftarrow A\}$  such that their characteristic paths are in  $\tau$ . If  $\tau = \{()\}$  then  $\delta(P, (A, \tau))$  is the set of all non-failing SLD-derivations for  $P \cup \{\leftarrow A\}$  of length 1.

**Definition 7.** Let  $(A, \tau)$  be a P-characteristic atom. Let  $\{\delta_1, \ldots, \delta_n\}$  be the SLDNF-derivations in  $\delta(P, (A, \tau))$  and let  $\leftarrow G_1, \ldots, \leftarrow G_n$  be the goals in the leaves of these derivations. Let  $\theta_1, \ldots, \theta_n$  be the computed answers of the derivations from  $\leftarrow A$  to  $\leftarrow G_1, \ldots, \leftarrow G_n$  respectively. Then the set of resultants  $\{A\theta_1 \leftarrow G_1, \ldots, A\theta_n \leftarrow G_n\}$  is called the partial deduction of  $(A, \tau)$  in P. Every atom occurring in some of the  $G_i$  will be called a body atom (in P) of  $(A, \tau)$ . We will denote the set of such body atoms by  $BA_P(A, \tau)$ .

The approach in [17] generates a partial deduction not for a set of atoms but for a set of characteristic atoms. As such, the same atom A might occur in several characteristic atoms with entirely different characteristic trees. In order to guarantee correctness of the specialised program, renaming (as well as filtering, see also [9]) is added in [17]. Then, given the following coveredness condition, correctness of the specialised program is established in [17].

**Definition 8.** Let P be a program and A a set of characteristic atoms. Then A is called P-covered iff for every characteristic atom in A each of its body atoms in P is a concretisation of a characteristic atom in A.

#### 2.2 The Depth Bound Problem

When, for the given program, query and unfolding rule, the above sketched method generates a finite number of different characteristic trees, its global control regime guarantees termination and correctness of the specialised program as well as "perfect" polyvariance: For every predicate, exactly one specialised version is produced for each of its different associated characteristic trees. Now, [17], as well as all earlier approaches based on characteristic trees ([10, 7, 18]), achieves the mentioned finiteness condition at the cost of imposing an ad hoc (typically very large) depth bound on characteristic trees. However, for a fairly

<sup>&</sup>lt;sup>5</sup> The reason behind the special treatment of the case  $\tau = \{()\}$  is that at least one unfolding step is needed to avoid the problematic resultant  $A \leftarrow A$  in Definition 7.

<sup>&</sup>lt;sup>6</sup> W.r.t. local precision, see [18, 17].

<sup>&</sup>lt;sup>7</sup> I.e. a characteristic tree associated to an atom with this predicate symbol.

large class of realistic programs (and unfolding rules), the number of different characteristic trees generated, is not naturally bounded. In those cases, the underlying depth bound will have to ensure termination, meanwhile propagating its ugly, ad hoc nature into the resulting specialised program. We illustrate this problem through some examples, setting out with a slightly artificial, but very simple one.

Example 1. The following is the well known reverse with accumulating parameter where a list type check on the accumulator has been added.

```
\begin{array}{l} (1) \ rev([], Acc, Acc) \leftarrow \\ (2) \ rev([H|T], Acc, Res) \leftarrow ls(Acc), rev(T, [H|Acc], Res) \\ (3) \ ls([]) \leftarrow \\ (4) \ ls([H|T]) \leftarrow ls(T) \end{array}
```

As can be noticed in Fig. 1, (determinate ([10, 7, 18]) and well-founded ([3, 23, 22]), among others) unfolding produces an infinite number of different characteristic atoms, all with a different characteristic tree. Imposing a depth bound of say 100, we obtain termination, but the algorithm produces 100 different reverse versions and the specialised program looks like:

This program is certainly far from optimal and clearly exhibits the ad hoc nature of the depth bound.

Situations like the above typically arise when an accumulating parameter influences the computation, because then the growing of the accumulator causes a corresponding growing of the characteristic trees. To be fair, it must be admitted that with most simple programs, this is not the case. For instance, in the standard reverse with accumulating parameter, the accumulator is only copied in the end, but never influences the computation. As illustrated by Example 1 above, this state of affairs will often already be changed when one adds type checking in the style of [11] to even the simplest logic programs.

Among larger and more sophisticated programs, cases like the above become more and more frequent, even in the absence of type checking.<sup>8</sup> For instance,

<sup>&</sup>lt;sup>8</sup> Especially since efficiently written programs often use accumulating parameters.

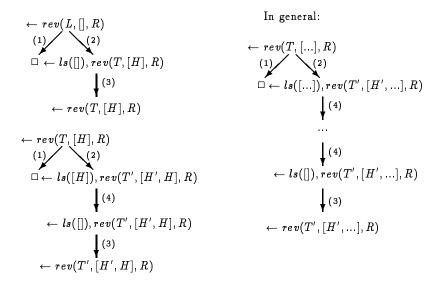


Fig. 1. SLD-trees for Example 1

in an explicit unification algorithm, one accumulating parameter is the substitution built so far. It heavily influences the computation because new bindings have to be added and checked for compatibility with the current substitution. Another example is the "mixed" meta-interpreter of [12, 19] (sometimes called InstanceDemo; part of it is depicted in Fig. 2) for the ground representation in which the goals are "lifted" to the non-ground representation for resolution. To perform the lifting, an accumulating parameter is used to keep track of the variables that have already been encountered. This accumulator influences the computation: Upon encountering a new variable, the program inspects the accumulator.

Example 2. Let  $A = l\_mng(Lg, Ln, [sub(N, X)], S)$  and P be the program of Fig. 2 (this situation arose in a real-life experiment). As can be seen in Fig. 3, unfolding A (e.g. using well-founded measures) causes the addition of the atom  $l\_mng(Tg, Tn, [sub(N, X), sub(J, Hn)], S)$  at the global (control) level. Notice that the third argument has grown (i.e. we have an accumulator).

So, when in turn unfolding  $l\_mng(Tg, Tn, [sub(N, X), sub(J, Hn)], S)$ , we will obtain a deeper characteristic tree (because mng traverses the third argument and thus needs one more step to reach the end) which will have as one of its leaves the atom  $l\_mng(Tg', Tn', [sub(N, X), sub(J, Hn), sub(J', Hn')], S)$ . An infinite sequence of ever growing characteristic trees results and again, as in Example 1, we obtain non-termination without a depth bound, and very unsatisfactory (ad hoc) specialisations with it.

```
Program:
(1) make\_non\_ground(GrTerm, NgTerm) \leftarrow
        mng(GrTerm, NgTerm, [], Sub)
(2) mng(var(N), X, [], [sub(N, X)]) \leftarrow
(3) mng(var(N), X, [sub(N, X)|T], [sub(N, X)|T]) \leftarrow
(4) mng(var(N), X, [sub(M, Y)|T], [sub(M, Y)|T1]) \leftarrow
        not(N = M), mng(var(N), X, T, T1)
(5) mng(struct(F, GrArgs), struct(F, NgArgs), InSub, OutSub) \leftarrow
        l\_mng(GrArgs, NgArgs, InSub, OutSub)
(6) l\_mng([], [], Sub, Sub) \leftarrow
(7) l\_mng([GrH|GrT], [NgH|NgT], InSub, OutSub) \leftarrow
        mng(GrH, NgH, InSub, InSub1),
        l\_mng(GrT, NgT, InSub1, OutSub)
Example query:
        \leftarrow make\_non\_ground(struct(f, [var(1), var(2), var(1)]), F)
            \sim c.a.s. \{F/struct(f, [Z, V, Z])\}
```

Fig. 2. Lifting the ground representation

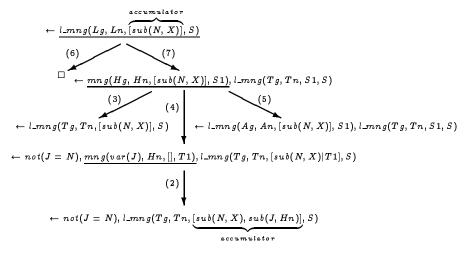


Fig. 3. Accumulator growth in Example 2

Summarising, computations influenced by one or more growing data structures are by no means rare and will, very often, lead to ad hoc behaviour of partial deduction where the global control is founded on characteristic trees with a depth bound. In the next section, we show how this annoying depth bound can be lifted without endangering termination.

# 3 Partial Deduction using Global Trees

#### 3.1 Introduction

A general framework for global control, not relying on any depth bounds, is proposed in [25, 24]. Marked trees (m-trees) are introduced to register descendency relationships among atoms at the global level. The overall tree is then kept finite through ensuring monotonicity of well-founded measure functions and termination of the algorithm follows, provided the generalisation operation (on atoms) is similarly well-founded. It is to this framework that we now turn for inspiration on how to solve the depth bound problem uncovered in Subsect. 2.2.

The basic idea will be to watch over the evolution of characteristic trees associated to atoms along the branches of the global tree. Obviously, just measuring the depth of characteristic trees would be far too crude: Global branches would be cut off prematurely and entirely unrelated atoms could be mopped together through generalisation, resulting in completely unacceptable specialisation losses. No, as can be seen in Fig. 1, we need a more refined measure which would somehow spot when a characteristic tree (piecemeal) "contains" characteristic trees appearing earlier in the same branch of the global tree. If such a situation arises (as it indeed does in Example 1), it seems reasonable to stop expanding the global tree, generalise the offending atoms and produce a specialised procedure for the generalisation instead.

However, a closer look at the following variation of Example 2 shows that also this approach would sometimes overgeneralise and consequently fall short of providing sufficiently detailed polyvariance.

Example 3. Reconsider the program in Fig. 2, and suppose that local control uses determinate unfolding. Let us now start partial deduction for the atom A = mng(G, struct(cl, [struct(f, [X, Y])|B]), [], S) (also this situation arose in a real-life experiment). When unfolding A (see Fig. 4), we obtain an SLDNF-tree containing the atom mng(H, struct(f, [X, Y]), [], S1) in one of its leaves. If we subsequently (determinately) unfold the latter atom, we obtain a tree that is "larger" than its predecessor, also in the more refined sense. Potential non-termination would therefore be detected and a generalisation operation executed. However, the atoms in the leaves of the second tree are more general than those already met, and simply continuing partial deduction without generalisation will lead to natural termination without any depth bound intervention.

Example 3 demonstrates that only measuring growth of characteristic trees, even in a refined way, does not always lead to satisfactory specialisation. Luckily, the same example also suggests a solution to this problem: Rather than measuring and comparing characteristic trees, we will scrutinise entire characteristic

<sup>&</sup>lt;sup>9</sup> In fact, whenever the (local) unfolding rule does not unfold "as deeply as possible" (for whatever reason), then a growing characteristic tree might simply be caused by splitting the "maximally deep tree" in such a way that the second part "contains" the first part.

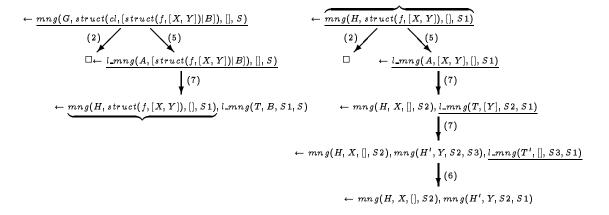


Fig. 4. SLD-trees for Example 3

atoms, comparing both the syntactic content of the ordinary atoms they contain and the associated characteristic trees. Accordingly, the global tree nodes will not be labeled by plain atoms as in [25, 24], but by entire characteristic atoms.

The rest of this section, then, contains the formal elaboration of this new approach.

### 3.2 More on Characteristic Atoms

Generalising Characteristic Atoms. We extend the notions of variants, instances and generalisations, familiar for ordinary atoms, <sup>10</sup> to characteristic trees and atoms:

**Definition 9.** A characteristic tree  $\tau_1$  is more general than another characteristic tree  $\tau_2$ , denoted by  $\tau_1 \leq \tau_2$ , iff  $\tau_2$  can be obtained by attaching subtrees to the leaves of  $\tau_1$ . A characteristic atom  $(A_1, \tau_1)$  is more general than another characteristic atom  $(A_2, \tau_2)$ , denoted by  $(A_1, \tau_1) \leq (A_2, \tau_2)$ , iff  $A_1 \leq A_2$  and  $\tau_1 \leq \tau_2$ . Also  $(A_1, \tau_1)$  is a variant of  $(A_2, \tau_2)$ , denoted by  $(A_1, \tau_1) \equiv (A_2, \tau_2)$ , iff  $(A_1, \tau_1) \leq (A_2, \tau_2)$  and  $(A_2, \tau_2) \leq (A_1, \tau_1)$ . Finally,  $CA_1 \leq CA_2$  holds when  $CA_1 \leq CA_2$  but not  $CA_1 \equiv CA_2$ .

Note that  $\{()\}$ , a characteristic tree containing a single, empty path, can be extended into a more specific characteristic tree, while the empty characteristic tree  $\emptyset = \{\}$  cannot.

Example 4. Given  $\tau_1 = \{((1,3))\}, \tau_2 = \{((1,3),(2,4))\}$  and  $\tau_3 = \{((1,3)),((1,4))\}$  we have that  $\tau_1 \preceq \tau_2$  and  $\tau_1 \prec \tau_2$  but not that  $\tau_1 \preceq \tau_3$  nor  $\tau_2 \preceq \tau_3$ .

The following proposition shows that the above definition makes sense wrt the set of ordinary atoms represented by characteristic atoms.

For ordinary atoms,  $A_1 \leq A_2$  will denote that  $A_1$  is more general than  $A_2$ .

**Proposition 10.** Let  $CA_1, CA_2$  be two characteristic atoms such that  $CA_1 \leq CA_2$ . Then every atom A which is a concretisation of  $CA_2$  is also a concretisation of  $CA_1$ .

Finally, we extend the notion of most specific generalisation (msg) to characteristic trees and atoms:

**Definition 11.** Let  $\tau_1, \tau_2$  be two P-characteristic trees. Then  $msg(\tau_1, \tau_2)$  is the most specific characteristic tree which is more general than both  $\tau_1$  and  $\tau_2$ . Let  $(A_1, \tau_1), (A_2, \tau_2)$  be two characteristic atoms. Then  $msg((A_1, \tau_1), (A_2, \tau_2)) = (msg(A_1, A_2), msg(\tau_1, \tau_2))$ .

Note that the above msg for characteristic atoms is still unique up to variable renaming. Its further extension to sets of characteristic atoms (rather than just pairs) is straightforward, and will not be included explicitly.

```
Example 5. Given \tau_1 = \{((1,3))\}, \ \tau_2 = \{((1,3),(2,4))\}, \ \tau_3 = \{((1,3),((1,4))\}, \ \tau_4 = \{((1,3),(2,4)),((1,3),(2,5))\}, \ \text{we have that} \ msg(\tau_1,\tau_2) = \tau_1, \ msg(\tau_1,\tau_3) = msg(\tau_2,\tau_3) = \{()\} \ \text{and} \ msg(\tau_2,\tau_4) = \tau_1.
```

Ordering Characteristic Atoms. We now proceed to introduce an order relation on characteristic atoms. It will be instrumental in guaranteeing termination of the partial deduction method to be presented.

**Definition 12.** A set  $V, \leq_V$  is called well-quasi-ordered (wqo) iff for any infinite sequence of elements  $e_1, e_2, \ldots$  in V there are i < j such that  $e_i \leq_V e_j$ . We also say that  $\leq_V$  is a well-quasi order (wqo) on V.

An interesting wqo is the homeomorphic embedding relation  $\leq$  of [29] (where it is adapted from [6]).

**Definition 13.** The homeomorphic embedding relation  $\leq$  on atoms and terms<sup>11</sup> is defined inductively as follows:

- 1.  $X \triangleleft Y$  for all variables X, Y
- 2.  $s \leq f(t_1, \ldots, t_n)$  if  $s \leq t_i$  for some i
- 3.  $f(s_1, ..., s_n) \triangleleft f(t_1, ..., t_n) \text{ if } \forall i \in \{1, ..., n\} : s_i \triangleleft t_i$ .

Example 6. We have:  $p(a) \unlhd p(f(a))$ ,  $X \unlhd X$ ,  $p(X) \unlhd p(f(Y))$ ,  $p(X, X) \unlhd p(X, Y)$  and  $p(X, Y) \unlhd p(X, X)$ .

Proposition 14. The relation ≤ is a wqo on the set of atoms and terms.

Expressed in the language  $\mathcal{L}$  which we implicitly assume underlying the programs and queries under consideration. Remember that it contains only finitely many constant, function and predicate symbols! This property is of crucial importance for the proofs in App. A.

The intuition behind Definition 13 is that when some structure re-appears within a larger one, it is homeomorphically embedded by the latter. As is argued in [29], this provides a good starting point for detecting growing structures created by (hence) possibly non-terminating processes.

However, as can be observed in Example 6, the homeomorphic embedding relation  $\leq$  as defined in Definition 13 is rather crude wrt variables. In fact, all variables are treated as if they were the same variable, a practice which is clearly undesirable in a logic programming context. Intuitively, in the above example,  $p(X,Y) \leq p(X,X)$  is acceptable, while  $p(X,X) \leq p(X,Y)$  is not. 12

To remedy the problem, we refine the above introduced homeomorphic embedding as follows:

**Definition 15.** Let A, B be atoms or terms. Then B (strictly homeomorphically) embeds A, written as  $A \leq^* B$ , iff  $A \leq B$  and A is not a strict instance of B.

Example 7. We now have that  $p(X,Y) \preceq^* p(X,X)$  but not  $p(X,X) \preceq^* p(X,Y)$ . Note that still  $X \preceq^* Y$  and  $X \preceq^* X$ .

**Proposition 16.** The relation  $\triangleleft^*$  is a wgo on the set of atoms and terms.

We now extend the embedding relation of Definition 15 to characteristic atoms. One way to obtain a wqo is to first define a term representation of characteristic trees and then use the embedding relation  $\preceq^*$  with this term representation.

**Definition 17.** By  $\lceil . \rceil$  we denote an injective, monotonic  $^{13}$  mapping from characteristic trees to (ordinary) atoms.

Such a mapping can be easily constructed by representing leaves of the tree by variables. For example we could have  $\lceil \{((1,3))\} \rceil = select(1, [match(3,X)])$  and  $\lceil \{((1,3),(2,4))\} \rceil = select(1, [match(3,select(2, [match(4,X)]))])$ .

**Definition 18.** Let  $(A_1, \tau_1)$ ,  $(A_2, \tau_2)$  be characteristic atoms. We say that  $(A_2, \tau_2)$  embeds  $(A_1, \tau_1)$ , denoted by  $(A_1, \tau_1) \preceq^* (A_2, \tau_2)$ , iff  $A_1 \preceq^* A_2$  and  $[\tau_1] \preceq^* [\tau_2]$ .

**Proposition 19.** Let A be a set of P-characteristic atoms. Then  $A, \preceq^*$  is well-quasi-ordered.

Finally, we consider the relationship between  $\preceq^*$  and  $\preceq$  on characteristic atoms.

**Proposition 20.** Let  $CA_1, CA_2, CA_3$  be characteristic atoms such that  $CA_3 \leq CA_2$ . Then  $CA_1 \leq^* CA_3 \Rightarrow CA_1 \leq^* CA_2$ .

 $<sup>\</sup>overline{^{12}}$  p(X,X) can be seen as standing for something like and(eq(X,Y),p(X,Y)) which clearly embeds p(X,Y), but the reverse does not hold.

<sup>&</sup>lt;sup>13</sup> I.e. if  $\tau_1 \prec \tau_2$  then  $\lceil \tau_1 \rceil \prec \lceil \tau_2 \rceil$ .

<sup>&</sup>lt;sup>14</sup> Note that  $\{((1,3))\} \prec \{((1,3),(2,4))\}$  and indeed  $[\{((1,3))\}] \prec [\{((1,3),(2,4))\}]$ .

So, a generalisation of a given characteristic atom will only embed characteristic atoms already embedded by the given one.

**Proposition 21.** Let  $CA_1$ ,  $CA_2$  be characteristic atoms such that  $CA_2 \leq CA_1$ . Then  $CA_1 \leq^* CA_2$  iff  $CA_1 \equiv CA_2$ .

**Proposition 22.** Let  $CA_1, \ldots, CA_n$  be characteristic atoms and assume that  $M = msg(CA_1, \ldots, CA_n)$ . Then the following three statements are equivalent (where  $1 \leq i \leq n$ ):

- 1.  $CA_i \triangleleft^* M$
- 2.  $CA_i \equiv M$
- 3.  $CA_i \leq CA_1, \ldots, CA_i \leq CA_n$

Properties 20 and 22 will be used to prove termination of the partial deduction algorithm in Sect. 3.4. Note that Propositions 21 and 22 do not hold for the ⊴ relation (which makes ⊴ less suitable for ensuring termination of partial deduction).

### 3.3 Global Trees

In this subsection, we adapt and instantiate the m-tree concept presented in [25, 24] according to our particular needs in this paper.

**Definition 23.** A global tree  $\gamma_P$  for a program P is a (finitely branching) tree where nodes can be either marked or unmarked and each node carries a label which is a P-characteristic atom.

In other words, a node in a global tree  $\gamma_P$  will look as follows:  $(n, mark, (A, \tau_A))$ , where n is the node identifier, mark an indicator that can take the values u or m designating whether the node is marked or not, and the P-characteristic atom  $(A, \tau_A)$  is the node's label. Informally, a marked node corresponds to a characteristic atom which has already been treated by the partial deduction algorithm. We will often omit the P subscript when it is either clear from or not relevant in the particular context we are considering.

In the sequel, we consider a global tree  $\gamma$  partially ordered through the usual  $ancestor\_node >_{\gamma} descendent\_node$  relationship. Given a node  $n \in \gamma$ , we denote by  $Anc_{\gamma}(n)$  the set of its  $\gamma$  ancestor nodes (including itself).

Let  $\gamma_P$  be a global tree. Then we will henceforth denote as  $L_{\gamma_P}$  the set of its labels. And for a given node n in a tree  $\gamma$ , we will refer to its label by  $l_n$ .

**Definition 24.** Let  $\gamma$  be a global tree. Then we define its associated label mapping  $f_{\gamma}$  as the one-to-one mapping  $f_{\gamma}: \gamma, >_{\gamma} \to L_{\gamma}, \underline{\triangleleft}^*$  such that  $n \mapsto l_n$ .  $f_{\gamma}$  will be called non-monotonic iff  $\exists n_1, n_2$  such that  $n_1 >_{\gamma} n_2$  and  $l_{n_1} \underline{\triangleleft}^* l_{n_2}$ .

**Definition 25.** We call a global tree  $\gamma$  well-quasi-ordered if  $f_{\gamma}$  is not non-monotonic.

**Theorem 26.** A global tree  $\gamma$  is finite if it is well-quasi-ordered.

As we in fact already did in the pair-wise case, we slightly abuse notation by not writing  $msg(\{CA_1,\ldots,CA_n\})$ , while that is of course actually what is intended.

### 3.4 An Algorithm for Partial Deduction

In this subsection, we present the actual partial deduction algorithm where global control is imposed through characteristic atoms in a global tree.

We first introduce the following definition:

**Definition 27.** Let A be an ordinary atom, U an unfolding rule and P a program. Then  $chatom(A, P, U) = (A, \tau)$  where  $chtree(\leftarrow A, P, U) = \tau$ .

A formal description of the algorithm can be found in Fig. 5. Please note that it is parameterised by an unfolding rule U, thus leaving the particulars of local control unspecified. Without loss of generality, we suppose the initial goal to consist of a single atom.

```
Algorithm 28.
Input
   a normal program P and goal \leftarrow A
Output
   a set of characteristic atoms A
Initialisation
   \gamma := \{(1, u, (A, \tau_A))\}
While γ contains an unmarked leaf do
  let n be such an unmarked leaf in \gamma: (n, u, (A_n, \tau_{A_n}))
   \max n
   \mathcal{B} := \{ chatom(B, P, U) | B \in BA_P(A_n, \tau_{A_n}) \}
   For each (B, \tau_B) \in \mathcal{B} do
      If \mathcal{H} = \{(C, 	au_C) \in Anc_{\gamma}(n) | (C, 	au_C) \leq^* (B, 	au_B)\} = \emptyset
         Then add (n_B, u, (B, \tau_B)) to \gamma as a child of n
         Else If \{(D, \tau_D) \in Anc_{\gamma}(n) | (D, \tau_D) \leq (B, \tau_B)\} = \emptyset
                Then add (n_B, u, msg(\mathcal{H} \cup \{(B, \tau_B)\})) to \gamma as a child of n
   Endfor
Endwhile
\mathcal{A} := L_{\gamma}
```

Fig. 5. Partial deduction with global trees.

As in e.g. [8, 25, 17], Algorithm 28 does not output a specialised program, but rather a set of (characteristic) atoms from which the actual code can be generated in a straightforward way. Most of the algorithm is self-explanatory, except perhaps the For-loop. In  $\mathcal{B}$ , all the characteristic atoms are assembled, corresponding to the atoms occurring in the leaves of the SLDNF-tree built (locally, of course) for  $A_L$  according to  $\tau_{A_L}$ . Elements of  $\mathcal{B}$  are subsequently inserted into  $\gamma$  as (unmarked) child nodes of L if they do not embed the label of n or any of its ancestor nodes. If one does, and it is an instance of n's label or that of an

ancestor of n, then it is simply not added to  $\gamma$ . Finally, if a characteristic atom  $(B, \tau_B) \in \mathcal{B}$  does embed an ancestor label, but there is no more general characteristic atom to be found labelling any of the ancestor nodes, then n receives a child node carrying as label the most specific generalisation of  $(B, \tau_B)$  and all embedded ancestor labels. The latter case is of course the most interesting: Simply adding a node labelled  $(B, \tau_B)$  would endanger termination. Adding the msg label instead secures finiteness, while trying to preserve as much information as seems possible. We obtain the following theorems:

Theorem 29. Algorithm 28 always terminates.

**Theorem 30.** Let P be a program, input to Algorithm 28, and A the corresponding set of characteristic atoms produced as output. Then A is P-covered.

From Theorem 30, correctness of the specialisation follows as in [17].

Finally, we have developed a post-processing phase reducing the polyvariance to some minimal level without removing any of the specialisation performed by the partial deduction described in Algorithm 28. Due to space limitations a description thereof could not be included.

# 4 Experimental Results and Discussion

Creating a fully fledged implementation of Algorithm 28 and the above described post-processing is the subject of ongoing work. However, to preliminarily check whether the developed ideas actually lead to improved practical results, we enhanced the system used for ecological partial deduction in [17] with global control through embedding and generalisation on characteristic atoms. We experimented with the result (denoted by eco-embed), comparing its performance with ecological partial deduction as in [17]. In the latter case, various depth bounds were imposed on the (local) SLDNF-trees in order to ensure termination (hence the notation  $eco-db_{--}$ ). Finally, in the experiments described below, local control is always based on the embedding relation on the atoms in the proof tree structure (i.e. it checks whether selected literals in covering ancestors, see [3], are embedded), possibly cut off by the imposed depth bound.

We report on three experiments. In the first one, we specialised the reverse (with type checking) program of Example 1 for the atom rev(L, [], R). The second and third experiment involved the "lifting" solve meta-interpreter ([12, 19]). The program depicted in Fig. 2 is actually an excerpt from its code. Experiment 2 consisted in specialising this program for solve(["c1","c2", U], [struct(fa, [X, Y])]), where "e" denotes the ground representation of an expression e, c1 denotes the clause  $fa(X, Y) \leftarrow p(X, Y), m(X)$  and c2 the clause  $mo(X, Y) \leftarrow p(X, Y), f(X)$ . Finally, in Experiment 3, we specialised the same solve for the atom  $solve(["c1","c2","p(a,b)\leftarrow","m(a)\leftarrow"], [struct(fa, [X, Y])])$ .

Further enhancing precision through even more cautious generalisation will be a topic of future research.

The first two experiments illustrate the problems encountered in Examples 1 and 2, and have to rely on a depth-bound for termination when using ecological partial deduction as in [17]. The third experiment does not require a depth bound, but illustrates another (well-known) adverse effect of using depth bounds.

The results are summarised in Tables 1, 2 and 3. The experiments were performed using Prolog by BIM on a Sparc Classic running Solaris. The size of the compiled code is expressed in units, 1 unit corresponding to 4.08 bytes on a Sparc Classic. The (compiled code) run times were obtained by using the time/2 predicate of Prolog by BIM on an extensive number of queries.

Experiment 1 shows that the additional polyvariance produced by using a depth bound to ensure termination does not pay off in efficiency but increases the code size unnecessarily. Experiment 2 illustrates this even more poignantly. The amount of polyvariance produced by the method eco-db50 was even so big that we could not complete the partial deduction.<sup>17</sup>

In Experiment 3, it is interesting to note that, even with a depth bound of 50 and for this very simple object program, we do not yet get the optimal result! So, for Experiment 2, the depth bound of 50 generates way too much polyvariance, while for Experiment 3, the depth bound of 50 is not sufficient to guarantee optimal specialisation of the same program! Concluding, it seems very likely that the global control improvements proposed in this paper will indeed pay off in partial deduction practice.

Note that the current system (eco-embed) does not yet structure the characteristic atoms in a global tree, but still just puts them in a set as in [17]. For the above described experiments, this had no influence, but generalisation with non-ancestors may in general severely limit specialisation potential.

A possible drawback of the global control method as laid out in Sect. 3, might be its considerable complexity. Indeed, first, ensuring termination through a well-quasi-ordering is structurally much more costly than the alternative of using a well-founded ordering. The latter only requires comparison with a single "ancestor" object and can be enforced without any search through "ancestor lists" (see [22]). Testing for well-quasi-ordering, however, unavoidably does entail such searching and repeated comparisons with several ancestors. Moreover, in our particular case, checking  $\leq$  on characteristic atoms is in itself a quite costly operation, adding considerably to the innate complexity of maintaining a well-quasi-ordering. It remains therefore to be seen whether a global control such as the one above can be used (or approximated in an efficient way) in circumstances where speed (or complexity) of the transformation is an important factor.

We conclude this section with a brief discussion on the relation between our global control and what may be termed thus in supercompilation ([30, 31, 29]). We already pointed out that the inspiration for using  $\unlhd$  derives from [29]. In that paper, a generalisation strategy for positive supercompilation (no negative information propagation while driving) is proposed. It uses  $\unlhd$  to compare nodes in a marked partial process tree (a notion roughly corresponding to marked or

<sup>&</sup>lt;sup>17</sup> After running for over several hours, producing 134 different predicates and generalising 80 times, eco-db50 overflowed the heap limit of 4.5 Megabytes.

Method	Run Time	#Clauses/#Predicates	Compiled Code Size
original	6.7 s	4/2	20 <b>3</b> u
eco-embed	6.7 s	6/3	331 u
eco-db10	6.7 s	23/12	1 955 u
eco-db50	7.1 s	103/52	29 573 u
eco-db100	7.5 s	203/102	122 <b>3</b> 91 u

Table 1. Experiment 1, rev program

Method	Run Time	#Clauses/#Predicates	Compiled Code Size
original	3.07 s	16/8	1 328 u
eco-embed	1.42 s	138/26	26 <b>39</b> 0 u
eco-db10	1.84 s	328/68	65 <b>8</b> 63 u
eco-db50	- s	-/ ≥1 <b>3</b> 4	- u

Table 2. Experiment 2, solve program

Method	Run Time	#Clauses/#Predicates	Compiled Code Size
original	2.44 s	16/8	1 328 u
eco-embed	0.04 s	1/1	77 u
eco-db10	1.63 s	34/19	4 164 u
eco-db50	0.06 s	8/4	1 062 u

Table 3. Experiment 3, solve program for another query

global trees in partial deduction). These nodes, however, only contain syntactical information. It is our current understanding that both the addition of something similar to characteristic trees and the use of the refined  $\leq$ \* embedding can lead to improvements of the method proposed in [29]. Finally, we return to an observation made in [24]: Neighbourhoods of order "n" in (full) supercompilation ([31]), are essentially the same as classes of atoms (or goals) with an identical depth n characteristic tree. Adapting our technique for supercompilation would therefore probably allow to remove the depth bound on neighbourhoods.

# 5 Conclusion

In this paper, we have developed a sophisticated on-line global control technique for partial deduction of normal logic programs. Importing and adapting m-trees from [25, 24], we have overcome the need for a depth bound on characteristic trees to guarantee termination of partial deduction as proposed in [17]. Plugging in a depth bound free local control strategy (see e.g. [3, 22]), we thus obtain a fully automatic, concrete partial deduction method that always terminates and produces precise and reasonable polyvariance, without resorting to any ad hoc techniques. To the best of our knowledge, this is the very first such method.

Along the way, we have defined generalisation and embedding on characteristic atoms, refining the homeomorphic embedding relation ≤ from [29] into ≤\*, and showing that the latter is more suitable in a logic programming setting. Initial experiments with a partial implementation of the method showed its great practical value; A fully fledged implementation and further experimentation are the subjects of ongoing work.

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# A Appendix: Proofs

#### A.1 Proposition 10

**Proposition10.** Let  $CA_1, CA_2$  be two characteristic atoms such that  $CA_1 \leq CA_2$ . Then every atom A which is a concretisation of  $CA_2$  is also a concretisation of  $CA_1$ .

Proof. Let  $CA_1=(A_1,\tau_1)$  and  $CA_2=(A_2,\tau_2)$ . Let A be a concretisation of  $CA_2$ . Then A must be an instance of some precise concretisation B of  $CA_2$ , i.e.  $chtree(\leftarrow B,P,U)=\tau_2$  for some U. We know by definition 9 that  $\tau_2$  can be obtained from  $\tau_1$  by extending leaves. This means that we can find an unfolding rule U' such that  $chtree(\leftarrow B,P,U')=\tau_1$ . Hence A is also a concretisation of  $CA_1$ .

### A.2 Proposition 14

Proposition 14. The relation ≤ is a wgo on the set of atoms and terms.

*Proof.* (Proofs similar to this one, are standard in the literature. We include it for completeness.) We define the relation  $\leq$  on the set  $\mathcal{S} = \mathcal{V} \cup \mathcal{F}$  of symbols, containing the set of variables  $\mathcal{V}$  and the set of functors and predicates  $\mathcal{F}$ , as the least relation satisfying:

```
- x \leq y \text{ if } x \in \mathcal{V} \land y \in \mathcal{V} \\ - f \prec f \text{ if } f \in \mathcal{F}
```

This relation is a wqo on S and hence by Kruskal's theorem (see [6]) its embedding extension to terms,  $\leq_{emb}$ , which is identical to  $\leq$ , is a wqo on the set of atoms and terms.

### A.3 Proposition 16

The following definitions and lemmas are needed to prove Proposition 16.

**Definition 31.** Let Term and Atom denote the sets of terms and atoms, respectively, in a language  $\mathcal{L}$ . We define the function  $s: Term \cup Atom \rightarrow I\!\!N$ , counting the number of symbols in a term or an atom, by:

```
\begin{array}{l} \text{If } t=f(t_1,\ldots,t_n), n>0 \\ \text{then } s(t)=1+s(t_1)+\cdots+s(t_n) \\ \text{else } s(t)=1 \end{array}
```

Let the number of distinct variables in a term or atom t be v(t). Define the function  $h: Term \cup Atom \rightarrow \mathbb{N}, h(t) = s(t) - v(t)$ .

This definition is taken from [9, 24]. Note that h(t) > 0 for any non-variable t. The following lemma is proven in [9].

**Lemma 32.** If A and B are atoms or terms such that  $B \prec A$ , then h(A) > h(B).

It follows that, for every atom or term A, there are no infinite chains of strictly more general atoms or terms. In order to prove Proposition 16 we however need an even stronger property, namely that there are only a finite number of atoms (up to variable renaming) more general than any atom or term A. At this point, we repeat that we pre-suppose a finite underlying language (i.e. it contains only a finite number of constant, function and predicate symbols — the number of variables might still be infinite). This assumption is crucial in the remainder of this appendix.

**Lemma 33.** For every natural number  $n \geq 0$  there are only a finite number of distinct (up to variable renaming) atoms A such that h(A) = n.

*Proof.* (Sketch) We define the function  $c: Term \cup Atom \rightarrow IN$ , counting the number of function and constant symbols in a term or an atom, by:

If 
$$t = f(t_1, \ldots, t_n), n \geq 0$$
  
then  $c(t) = 1 + c(t_1) + \cdots + c(t_n)$   
else  $c(t) = 0$ 

Trivially, we have that  $\forall t: s(t) \geq h(t) \geq c(t)$ . Also, because the underlying language contains only a finite number of predicate, function and constant symbols, we have that for every  $n \geq 0$  there are only a finite number of atoms or terms t (up to variable renaming) such that c(t) = n (first prove this by induction for atoms and terms without repeated variables — the full result then follows because there is only a finite number of ways to substitute these variables for each other). This implies that for every  $n \geq 0$  there are only a finite number of atoms or terms t (up to variable renaming) such that  $c(t) \leq n$ . Finally, we can conclude that the set of atoms and terms such that h(t) = n is finite (up to variable renaming) since this set is contained in the finite set  $\{t \mid c(t) \leq n\}$  (because n = h(t) > c(t)).

**Lemma 34.** For each atom A there are only a finite number of distinct (up to variable renaming) atoms more general than A.

*Proof.* The result follows from Lemmas 32 and 33.

**Definition 35.** Let  $\sigma$  be a sequence of atoms (or terms). Then  $\sigma^*$  is defined recursively as follows:

- $-\epsilon^*=\epsilon$
- $-(A.\rho)^* = A.(\rho_A)^*$  where  $\rho_A$  is the subsequence of  $\rho$  containing all atoms which are not strictly more general than A.

**Lemma 36.** Let  $\sigma$  be a sequence of atoms (or terms). If  $\sigma$  is infinite and does not contain an infinite number of variants then  $\sigma^*$  is also infinite.

**Proof.** Because by Lemma 34, for each atom A there is only a finite number of atoms M (up to variable renaming) more general than A, and because for each such M we only have a finite number of variants in  $\sigma$ , we can deduce that at

each application of step 2 of Definition 35, only a finite number of atoms are removed. This means that we can indefinitely keep on applying step 2 and thus  $\sigma^*$  will be an infinite sequence.

We can now actually prove Proposition 16.

**Proposition16.** The relation  $\leq^*$  is a wqo on the set of atoms and terms.

Proof. Suppose that we have an infinite sequence  $\sigma$ . If  $\sigma$  contains an infinite number of variants, then we take the subsequence containing these variants. For this subsequence,  $\unlhd$  is identical to  $\unlhd^*$ , and therefore we can find i < j such that  $\sigma_i \unlhd^* \sigma_j$  (actually by definition of  $\unlhd^*$  and  $\unlhd$ , this will hold for any i < j in the subsequence). Otherwise, we consider the subsequence  $\sigma^*$  which by the above Lemma 36 is still infinite. For this subsequence,  $\unlhd$  is again identical to  $\unlhd^*$ , and therefore we can find i < j such that  $\sigma_i \unlhd^* \sigma_j$ .

## A.4 Proposition 19

**Proposition19.** Let A be a set of P-characteristic atoms. Then  $A, \preceq^*$  is well-quasi-ordered.

*Proof.* Let us take as our vocabulary  $\mathcal{F}$  the set of terms and atoms. By proposition 16,  $\leq^*$  is a wqo on  $\mathcal{F}$ . Hence by Kruskal's theorem (see e.g. [6]), its embedding extension to terms constructed from  $\mathcal{F}$  is also a wqo. We restrict ourselves to one binary functor c/2 and to terms c(A,T) constructed by using this functor exactly once such that A is an atom and T the representation of some characteristic tree. For this special case, this embedding coincides with Definition 18 and hence  $\mathcal{A}, \triangleleft^*$  is well-quasi-ordered.

## A.5 Propositions 20, 21 and 22

**Proposition20.** Let  $CA_1, CA_2, CA_3$  be characteristic atoms such that  $CA_3 \leq CA_2$ . Then  $CA_1 \leq^* CA_3 \Rightarrow CA_1 \leq^* CA_2$ .

*Proof.* We first prove the property for arbitrary terms. From that, the result follows immediately for the (ordinary) atom component.

So, let  $t_1, t_2, t_3$  be terms (in the underlying language) such that  $t_3 \leq t_2$  and  $t_1 \leq^* t_3$ . We have to argue that  $t_1 \leq^* t_2$ . First, clearly,  $t_1$  cannot be a strict instance of  $t_2$ . The proof that also  $t_1 \leq t_2$  is through induction on the structure of  $t_3$ . If  $t_3$  is a variable, then  $t_1$  and  $t_2$  also are, and the result follows. Finally, if  $t_3 = f(t_{31}, \ldots, t_{3n})$ , then also  $t_2 = f(t_{21}, \ldots, t_{2n})$  and  $t_{31} \leq t_{21}, \ldots, t_{3n} \leq t_{2n}$ . Irrespective of whether  $t_1 = f(t_{11}, \ldots, t_{1n})$  or is some other term, we obtain the desired result through the induction hypothesis.

Next, by monotonicity of  $\lceil . \rceil$   $\tau_3 \leq \tau_2$  implies that  $\lceil \tau_3 \rceil \leq \lceil \tau_2 \rceil$ . Hence the property for the characteristic tree component follows from the result for arbitrary terms. Finally, as  $(A_3, \tau_3) \leq (A_2, \tau_2)$  implies by definition both  $A_3 \leq A_2$  and  $\tau_3 \leq \tau_2$ , we have proven the result for characteristic atoms.

**Proposition21.** Let  $CA_1, CA_2$  be characteristic atoms such that  $CA_2 \leq CA_1$ . Then  $CA_1 \leq^* CA_2$  iff  $CA_1 \equiv CA_2$ .

*Proof.* Let  $CA_1 = (A_1, \tau_1)$  and  $CA_2 = (A_2, \tau_2)$ .

- $(\Rightarrow)$ :  $CA_1 \preceq^* CA_2$  implies that  $A_1 \preceq A_2$  and that  $A_1$  is not a strict instance of  $A_2$ . Hence  $A_1$  must be a non strict instance, i.e. a variant of  $A_2$ . For the characteristic tree part we know that  $\tau_1 \preceq \tau_2$  and that  $\lceil A_1 \rceil$  is not a strict instance of  $\lceil A_2 \rceil$ . By monotonicity of  $\lceil . \rceil$  we know that  $\tau_1$  must be identical to  $\tau_2$ .
- ( $\Leftarrow$ ): Trivial because  $CA_2$  is not strictly more general than  $CA_1$  and because two variants  $V_1, V_2$  always homeomorphically embed each other (i.e.  $V_1 \unlhd V_2 \land V_2 \unlhd V_1$ ).

**Proposition22.** Let  $CA_1, \ldots, CA_n$  be characteristic atoms and assume that  $M = msg(CA_1, \ldots, CA_n)$ . Then the following three statements are equivalent (where  $1 \leq i \leq n$ ):

- 1.  $CA_i \leq^* M$
- 2.  $CA_i \equiv M$
- 3.  $CA_i \leq CA_1, \ldots, CA_i \leq CA_n$

*Proof.* First observe that, by definition,  $M \leq CA_i$ . We then obtain:

- $1 \Rightarrow 2$  Immediate from the only-if part in Proposition 21.
- $2 \Rightarrow 3$  Trivial by definition of msg.
- $3 \Rightarrow 1$  Statement 3 implies that  $CA_i \leq msg(CA_1, \ldots, CA_{i-1}, CA_{i+1}, \ldots, CA_n)$ . It follows that  $CA_i \equiv M$  and we obtain statement 1 through the if part of Proposition 21.

A.6 Theorem 26

**Theorem26.** A global tree  $\gamma$  is finite if it is well-quasi-ordered.

Proof. Assume that  $\gamma$  is not finite. Then it contains (König's Lemma) at least one infinite branch  $n_1 >_{\gamma} n_2 >_{\gamma} \dots$  Consider the corresponding infinite sequence of elements  $l_{n_1}, l_{n_2}, \dots \in L_{\gamma}, \leq^*$ . From Proposition 19, we know that  $L_{\gamma}, \leq^*$  is woo and therefore, there must exist  $l_{n_i}, l_{n_j}, i < j$  in the above mentioned sequence such that  $l_{n_i} \leq^* l_{n_i}$ . But this implies that  $f_{\gamma}$  is non-monotonic.

#### A.7 Theorem 29

Theorem29. Algorithm 28 always terminates.

**Proof.** Upon each iteration of the while-loop in Algorithm 28, exactly one node in  $\gamma$  is marked, and zero or more (unmarked) nodes are added to  $\gamma$ . Moreover, Algorithm 28 never deletes a node from  $\gamma$ , neither does it ever "unmark" a marked node. Hence, since all branchings are finite, non-termination of the algorithm must result in the construction of an infinite branch. It is therefore sufficient to argue that after every iteration of the while-loop,  $\gamma$  is a wgo global tree.

First, this holds after initialisation. Also, obviously, a global tree will be converted into a new global tree through the while-loop. Now, a while-iteration adds zero or more, but finitely many, child nodes to a particular leaf n in the tree, thus creating a (finite) number of new branches that are extensions of the old branch leading to n. We prove that on none of the new branches,  $f_{\gamma}$  is non-monotonic. The branch extensions are actually constructed in the for-loop (which terminates trivially), (at most) one for every element of  $\mathcal{B}$ . So, let us take an arbitrary characteristic atom  $(B, \tau_B) \in \mathcal{B}$ , then there are three cases to consider:

- Either  $(B, \tau_B)$  does not embed any label on the branch (up) to (and including) n. It is then added in a fresh leaf. Obviously,  $f_{\gamma}$  will not be non-monotonic on the newly created branch.
- Or some such label is embedded, but there is also a more (or equally) general label already in some node on the branch to n. Then, no corresponding leaf is inserted in the tree, and there is nothing left to prove.
- Or, finally, some labels on the branch are embedded, but none are more general. The fresh leaf will then be labelled by the  $msg\ M$  of  $(B, \tau_B)$  and all the labels on the branch it embeds. In that case, Propositions 20 and 22 together imply that M embeds none of the labels on the branch to n.

#### A.8 Theorem 30

**Theorem 30.** Let P be a program, input to Algorithm 28, and A the corresponding set of characteristic atoms produced as output. Then A is P-covered.

Proof. First, it is straightforward to prove that throughout the execution of Algorithm 28, any unmarked node in  $\gamma$  must be a leaf. It therefore suffices to show that after each while-loop iteration, only unmarked leaves in  $\gamma$  possibly carry a non-covered label. Trivially, this property holds after initialisation. Now, in the while-loop, one unmarked leaf n is selected and marked. The forloop then precisely proceeds to incorporate (unmarked leaf) nodes into  $\gamma$  such that all body atoms of n's label are concretisations of at least one label in the new, extended  $\gamma$ .

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<sup>&</sup>lt;sup>18</sup> I.e. a label with at least one body atom (in P) that is not a concretisation of any label in  $\gamma$ .