Unfolding in CHR

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Program transformation is an appealing technique which allows to improve run-time efficiency, space-consumption and more generally to optimize a given program. Essentially it consists of a sequence of syntactic program manipulations which preserves some kind of semantic equivalence. One of the basic operations which is used by most program transformation systems is unfolding which consists in the replacement of a procedure call by its definition. While there is a large body of literature on transformation and unfolding of sequential programs, very few papers have addressed this issue for concurrent languages and, to the best of our knowledge, no other has considered unfolding of CHR programs.

This paper defines a correct unfolding system for CHR programs. We define an unfolding rule, show its correctness and discuss some conditions which can be used to delete an unfolded rule while preserving the program meaning. We prove that confluence and termination properties are preserved by the above transformations.

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1. INTRODUCTION

Program transformation was initially developed as a technique which assist in writing correct and efficient programs [Burstall and Darlington 1977]. Said technique consists of many intermediate transformation steps until the final one is reached. Every transformed program is equivalent (gives the same results) of the initial one, when an input is fixed. The transformation between various algorithms which compute Fibonacci succession can be considered as an example of program transformation. In fact, the time complexity of the previous succession ranges from the exponential to the logarithmic depending on the chosen algorithm

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CHR is a general purpose declarative, concurrent, committed-choice constraint logic programming language, consisting of guarded rules, which transform multisets of atomic formulas (constraints) into simpler ones to the point of exhaustion [Frühwirth 2006], that was initially designed for writing constraint solvers [Frühwirth 1998; Frühwirth and Abdennadher 2003]. There is nowadays a very large literature on CHR, ranging from theoretical aspects to implementations and applications. In fact, the website http://www.cs.kuleuven.ac.be/~dtai/projects/CHR/ reports more than 1000 papers mentioning CHR. However, only a few papers, notably [Frühwirth and Holzbaur 2003] [Frühwirth 2004] Sneyers et al. 2005, consider source to source transformation of CHR programs. This is not surprising, since program transformation is in general very difficult for (logic) concurrent languages and in case of CHR it is even more complicated, as we discuss later.

While [Frühwirth 2004] focuses on specialization of a program for a given goal, here we consider unfolding. This is a basic operation of any source to source transformation (and specialization) system and essentially consists in the replacement of a procedure call by its definition. While this operation can be performed rather easily for sequential languages, and indeed in the field of logic programming it was first investigated by Tamaki and Sato more than twenty years ago [Tamaki and Sato 1984], when considering logic concurrent languages it becomes quite difficult to define reasonable conditions which ensure its correctness. This is mainly due to three problems. The first one is the presence of guards in the rules. Intuitively, when unfolding a rule \( r \) by using a rule \( v \) (i.e. when replacing in the body of \( r \) a “call” of a procedure by its definition \( v \)) it could happen that some guard in \( v \) is not satisfied “statically” (i.e. when we perform the unfold), even though it could become satisfied later when the unfolded rule is actually used. If we move the guard of \( v \) in the unfolded version of \( r \) we can then loose some computations (because the guard is anticipated). This means that if we want to preserve the meaning of a program we cannot replace the rule \( r \) by its unfolded version, and we have to keep both the rules. The second source of difficulties consists in matching substitution mechanism. Only the variables in the atoms of the head of a rule \( r \) can be instantiated to become equal to the goal terms following the previous mechanism. From the other side, the unification mechanism permits also the instantiation of the variables in the atoms of the goal. Considering the matching substitution, the deletion of \( r \), when a rule \( v \) could be used to unfold \( r \) if strong enough hypotheses would be considered, can cause computation loss also if \( r \) is unfolded by another rule \( v' \). Finally, for CHR, the situation is further complicated by the presence of multiple heads in the rules. In fact, let \( B \) be the body of a rule \( r \) and let \( H \) be the (multiple) head of a rule \( v \), which can be used to unfold \( r \), we cannot be sure that at run-time all the atoms in \( H \) will be used to rewrite \( B \), since in general \( B \) could be in a conjunction with other atoms even though the guards are satisfied. This technical point, that one can legitimately find obscure now, will be further clarified in Chapter 5.

Despite these technical problems, the study of unfolding techniques for concurrent languages, and for CHR in particular, is important as it could lead to significant improvements in the efficiency and in non-termination analysis of programs.
In this paper we then define an unfolding rule for CHR programs and show that it preserves the semantics of the program in terms of qualified answers, a notion already defined in the literature [Frühwirth 1998]. We also provide a syntactic condition which allows to replace in a program a rule by its unfolded version while preserving qualified answers. Even though the idea of the unfolding is straightforward, its technical development is complicated by the presence of guards, multiple heads and matching substitution, as previously mentioned. In particular, it is not immediate to identify conditions which allow to replace the original rule by its unfolded version. Moreover, a further reason of complication comes from the fact that we consider the reference semantics (called $\omega_t$) defined in [Duck et al. 2004] which avoids trivial non termination by using a so-called token store or history. Due to the presence of this token store, in order to define correctly the unfolding we have to slightly modify the syntax of CHR programs by adding to each rule a local token store. The resulting programs are called annotated and we define their semantics by providing a (slightly) modified version of the semantics $\omega_t$, which is proven to preserve the qualified answers. Finally, the maintenance of confluence and termination of property between the original and the ones, which are modified following the above techniques, is proven.

The remaining of this paper is organized as follows. Next section contains some notations used in the paper and the syntax of CHR. The operational semantics of $\omega_t$ [Duck et al. 2004] and of the modified semantics $\omega'_t$ are presented in Section 3. Section 4 defines the unfolding rule and prove its correctness. Section 5 discuss the problems related to the replacement of a rule by its unfolded version and gives a correctness condition which holds for a specific class of rules. Then Section 6 proves that confluence and termination are preserved by the program modifications introduced. Finally Section 8 concludes by discussing also some related work.

2. PRELIMINARIES

In this section we introduce the syntax of CHR and some notations and definitions we will need in the paper. CHR uses two kinds of constraints: the built-in and the CHR ones, also called user-defined.

Built-in constraints are defined by

$$c ::= d \mid c \land c \mid \exists x c$$

where $d$ is an atomic built-in constraint. These constraints are handled by an existing solver and we assume given a (first order) theory $CT$ which describes their meaning. We assume also that built-in constraints contain $=$ which is described, as usual, by the Clark Equality Theory.

We use $c, d$ to denote built-in constraints, $h, k, s, p, q$ to denote CHR constraints and $a, b, g, f$ to denote both built-in and user-defined constraints (we will call these generically constraints). We also denote by $\text{false}$ any inconsistent (conjunction of) constraints and by $\text{true}$ the empty set of constraints. The capital versions will be used to denote multisets (or sequences) of constraints.

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1We could consider more generally first order formulas as built-in constraints, as far as the results presented here are concerned.
The notation $\exists_{-V} \phi$, where $V$ is a set of variables, denotes the existential closure of a formula $\phi$ with the exception of the variables in $V$ which remain unquantified. $Fv(\phi)$ denotes the free variables appearing in $\phi$. Moreover, if $t = t_1, \ldots, t_m$ and $t' = t'_1, \ldots, t'_m$ are sequences of terms then the notation $p(t) = p'(t')$ represents the set of equalities $t_1 = t'_1, \ldots, t_m = t'_m$ if $p = p'$, and it is undefined otherwise. Analogously, if $H = h_1, \ldots, h_k$ and $H' = h'_1, \ldots, h'_k$ are sequences of constraints, the notation $H = H'$ represents the set of equalities $h_1 = h'_1, \ldots, h_k = h'_k$. Finally, multiset union is represented by symbol $\uplus$.

2.1 CHR syntax

As shown by the following definition, a CHR program consists of a set of rules which can be divided into three types: simplification, propagation and simpagation rules. The first kind of rules is used to rewrite CHR constraints into simpler ones, while second one allows to add new redundant constraints which may cause further simplification. Simpagation rules allow to represent both simplification and propagation rules.

Definition 2.1. CHR Syntax [Frühwirth 1998]. A CHR program is a finite set of CHR rules. There are three kinds of CHR rules:

A simplification rule has the form:

$$r@H \Leftrightarrow C | B$$

A propagation rule has the form:

$$r@H \Rightarrow C | B$$

A simpagation rule has the form:

$$r@H_1 \setminus H_2 \Leftrightarrow C | B,$$

where $r$ is a unique identifier of the rule, $H$, $H_1$ and $H_2$ are sequences of user-defined constraints (called heads), $C$ is a possibly empty multiset of built-in constraints (guard) and $B$ is a possibly empty multiset of (built-in and user-defined) constraints (body). A CHR goal is a multiset of (both user-defined and built-in) constraints.

A simpagation rule can simulate both simplification and propagation rule by considering, respectively, either $H_1$ or $H_2$ empty (with $(H_1, H_2) \neq \emptyset$). In the following we will then consider in the formal treatment only simpagation rules.

When considering unfolding we need to consider a slightly different syntax, where rule identifiers are not necessarily unique, atoms in the body are associated with an identifier, that is unique in the rule, and where each rule is associated with a local token store $T$. More precisely, we define an identified CHR constraint (or identified atom) $h\#i$ as a CHR constraint $h$, associated with an integer $i$ which allows to distinguish different copies of the same constraint.

Definition 2.2. CHR Annotated syntax. Let us define a token as an object of the form $r@i_1, \ldots, i_l$, where $r$ is the name of a rule and $i_1, \ldots, i_l$ is a sequence of identifiers. A token store (or history) is a set of tokens.
An annotated rule has then the form:

\[ r \circ H_1 \setminus H_2 \leftrightarrow C \mid \hat{B}; T \]

where \( r \) is an identifier, \( H_1 \) and \( H_2 \) are sequences of user-defined constraints, \( \hat{B} \) is a sequence of built-in and identified CHR constraints such that different (occurrences of) CHR constraints have different identifiers, and \( T \) is a token store, called the local token store of rule \( r \). An annotated CHR program is a finite set of annotated CHR rules.

We will also use the functions \( \text{chr}(h \# j) = h \) and the overloaded function \( \text{id}(h \# j) = i \), [and \( \text{id}(r \circ j_1, \ldots, j_l) = \{i_1, \ldots, i_l\} \)] possibly extended to sets and sequences of identified CHR constraints [or tokens] in the obvious way. Given a goal \( G \), we denote by \( \hat{G} \) one of the possible identified versions of \( G \). Goals is the set of all (possibly identified) goals.

Intuitively, identifiers are used to distinguish different occurrences of the same atom in a rule. The identified atoms can be obtained by using a suitable function which associates a (unique) integer to each atom. More precisely, let \( B \) be a goal which contains \( m \) CHR-constraints. We assume that the function \( I_{n+m}^m(B) \) identifies each CHR constraint in \( B \) by associating to it a unique integer in \( [n+1, m+n] \) according to the lexicographic order.

On the other hand, the token store allows to memorize some tokens, where each token describes which (propagation) rule has been used for reducing which identified atoms. As we discuss in the next section, the use of this information was originally proposed in [Abdennadher 1997] and then further elaborated in the semantics defined in [Duck et al. 2004] in order to avoid trivial non termination arising from the repeated application of the same propagation rule to the same constraints. Here we simply incorporate this information in the syntax, since we will need to manipulate it in our unfolding rule.

Given a CHR program \( P \), by using the function \( I_{n+m}^m(B) \) and an initially empty local token store we can construct its annotated version as the next definition explains.

**Definition 2.3.** Let \( P \) be a CHR program. Then its annotated version is defined as follows:

\[
\text{Ann}(P) = \{ r \circ H_1 \setminus H_2 \leftrightarrow C \mid I_0^m(B); \emptyset \mid r \circ H_1 \setminus H_2 \leftrightarrow C \mid B \in P \text{ and } m \text{ is the number of CHR-constraints in } B \}.
\]

**Notation**

In the following examples, given a (possibly annotated) rule

\[ r \circ H_1 \setminus H_2 \leftrightarrow C \mid B(\cdot; T), \]

we write it as

\[ r \circ H_2 \leftrightarrow C \mid B(\cdot; T), \]

if \( H_1 \) is empty and we write it as

\[ r \circ H_1 \Rightarrow C \mid B(\cdot; T), \]

if \( H_2 \) is empty.
Table I. The transition system $T_{\omega t}$ for the $\omega t$ semantics

| Solve | $CT \models c \land C \leftrightarrow C'$ and $c$ is a built-in constraint |
| Introduce | $h$ is a user-defined constraint |
| Apply | $\langle B \cup G, \bar{S}, ((\text{chr}(\bar{H}_1, \bar{H}_2) = (H'_1, H'_2)) \land C) \rangle_n \rightarrow_{\omega t} \langle B \cup G, \bar{S}, (\text{chr}(\bar{H}_1, \bar{H}_2) = (H'_1, H'_2)) \land C, T' \rangle_n$ |

where $r@id(\bar{H}_1, \bar{H}_2) \notin T$ and $T' = T \cup \{r@id(\bar{H}_1, \bar{H}_2)\}$ if $\bar{H}_2 = \emptyset$ otherwise $T' = T$.

That is, we maintain also the notation previously introduced for simplification and propagation rules. Moreover, if $C = \text{true}$, then $\text{true} \mid$ is omitted. Finally, if in an annotated rule the token store is empty we simply omit it.

3. CHR OPERATIONAL SEMANTICS

This section introduces the reference semantics $\omega_t$ [Duck et al. 2004], in particular the variant that modifies the token set only after the application of a propagation rule (for the sake of simplicity, we omit indexing the relation with the name of the program).

Afterward we define a slightly different operational semantics, called $\omega'_t$, which considers annotated programs and which will be used to prove the correctness of our unfolding rules (via some form of equivalence between $\omega'_t$ and $\omega_t$).

We describe the operational semantics $\omega_t$, introduced in [Duck et al. 2004], by using a transition system

$T_{\omega_t} = (\text{Conf}_t, \rightarrow_{\omega_t})$.

Configurations in $\text{Conf}_t$ are tuples of the form $\langle G, \bar{S}, c, T \rangle_n$ with the following meaning. The goal $G$ is a multiset of constraints to be evaluated. The CHR constraint store $\bar{S}$ is the set of identified CHR constraints that can be matched with the head of the rules in the program $P$. The built-in constraint store $c$ is a conjunction of built-in constraints. The propagation history $T$ is a set of tokens of the form $r@i_1, \ldots, i_l$, where $r$ is the name of the applied propagation rule and $i_1, \ldots, i_l$ is the sequence of identifiers associated to the constraints to which the head of the rule is applied. This is needed to prevent trivial non-termination for propagation rules. If one do not consider tokens (as in the original semantics of [Fruhwirth 1998]) it is clear from the transition system that if a propagation rule can be applied once it can be applied infinitely many times thus originating an infinite computation (no fairness assumptions are made here). On the other hand, by using tokens one can
ensure that a propagation rule is used to reduce a sequence of constraints only if
the same rule has not been used before on the same sequence of constraints, thus
avoiding trivial infinite computations (arising from the application of the same rule
to the same constraints). As previously mentioned, the first idea of using a token
store to avoid trivial non termination was described in [Abdennadher 1997]. Finally
the \textit{counter} \( n \) represents the next free integer which can be used to number a CHR
constraint.

Given a goal \( G \), the \textit{initial configuration} has the form
\[
(G, \emptyset, \text{true}, \emptyset)_1.
\]
A \textit{final configuration} has either the form \((G', \tilde{S}, \text{false}, T)_n\) when it is \textit{failed} or it
has the form \((\emptyset, \tilde{S}, c, T)_n\) when it represents a successful termination (since there
are no more applicable rules).

The relation \( \longrightarrow_{\omega_t} \) (of the transition system of the operational semantics \( \omega_t \)) is
defined by the rules in Table I: the \textbf{Solve} rule moves a built-in constraint from goal
store to the built-in constraint store; the \textbf{Introduce} identifies and moves a CHR
(or used defined) constraint from the goal store to the CHR constraint store and
the \textbf{Apply} rule chooses a program rule \( r \), for which matching between constraints
in CHR store and the ones in the head of \( r \) exists, it checks that the guard of \( r \) is
entailed by the built-in constraint store, considering the matching substitution, and
it verifies that the token that would be eventually added by \textbf{Apply} in the token
store is not already present, than it fires the rule. After the application of \( r \) the
constraints which match with the right hand side of the head of \( r \) are deleted from
\( \tilde{S} \), the body of \( r \) is added to the CHR constraint store and the matching substitution
between the head of \( r \) and the atoms in \( \tilde{S} \) is added to the built-in constraint store.

3.1 The modified semantics \( \omega'_t \)
We now define the semantics \( \omega'_t \) which considers annotated rules. This semantics
differs from \( \omega_t \) in two aspects.

First, in \( \omega'_t \) the goal store and the CHR store are fused in a unique generic \textit{store},
where CHR constraints are immediately labeled. As a consequence, we do not need
anymore the \textbf{Introduce} rule and every CHR constraint in the body of an applied
rule is immediately utilizable for rewriting.

The second difference concerns the shape of the rules. In fact, each annotated
rule \( r \) has a local token store (which can be empty) that is associated to it and
which is used to keep trace of the propagation rules that are used to unfold the
body of \( r \). Note also that here, differently from the case of the propagation history
in \( \omega_t \), the token store associated to the real computation can be updated by adding
more tokens at once (because an unfolded rule with many token in its local token
store has been used).

In order to define formally \( \omega'_t \) we need a function \( \text{inst} \) which updates the formal
identifiers of a rule to the actual computation ones and it is defined as follows.

\textit{Definition 3.1.} Let Token be the set of all possible token set and let \( \mathbb{N} \) be the
set of natural numbers. We denote by \( \text{inst} : \text{Goals} \times \{\text{Token}\} \times \mathbb{N} \rightarrow \text{Goals} \times \{\text{Token}\} \times \mathbb{N} \) the function such that \( \text{inst}(B, T, n) = (B', T', m) \), where
\( \tilde{B} \) is an identified CHR goal,
Table II. The transition system $T_{\omega'}$ for the $\omega'$ semantics

\[ CT \models c \land C \leftrightarrow C' \text{ and } c \text{ is a built-in constraint} \]
\[ \langle \{c\} \cup G, C, T \rangle_n \rightarrow_{\omega'} \langle G, C', T \rangle_n \]

Apply'  \hspace{2cm}  \langle H_1 \cup H_2 \cup G, C, T \rangle_n \rightarrow_{\omega'} \langle B' \cup \tilde{H}_1 \cup G, \text{chr}(\tilde{H}_1, \tilde{H}_2) = (H'_1, H'_2) \land C, T' \rangle_m \]

where $(\tilde{B}', T', m) = \text{inst}(\tilde{B}, T, n) ; r@id(\tilde{H}_1, \tilde{H}_2) \not\in T$ and $T' = T \cup \{r@id(\tilde{H}_1, \tilde{H}_2)\} \cup T'_m$ if $\tilde{H}_2 = \emptyset$ otherwise $T' = T \cup T'_m$.

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$(\tilde{B}', T')$ is obtained from $(\tilde{B}, T)$ by incrementing each identifier in $(\tilde{B}, T)$ with $n$ and $-m$ is the greatest identifier in $(\tilde{B}', T')$.

We describe now the operational semantics $\omega'$ for annotated CHR programs by using, as usual, a transition system

$T_{\omega'} = (Conf', \rightarrow_{\omega'})$.

Configurations in $Conf'$ are tuples of the form $\langle \tilde{S}, c, T \rangle_n$ with the following meaning. $\tilde{S}$ is the set of identified CHR constraints that can be matched with rules in the program $P$ and built-in constraints. The built-in constraint store $c$ is a conjunction of built-in constraints and $T$ is a set of tokens, while the counter $n$ represents the last integer which was used to number the CHR constraints in $\tilde{S}$.

Given a goal $G$, the initial configuration has the form

$\langle I_0^m(G), \text{true}, \emptyset \rangle_m$,

where $m$ is the number of CHR constraints in $G$. A final configuration has either the form $\langle \tilde{S}, \text{false}, T \rangle_n$ when it is failed or it has the form $\langle \tilde{S}, c, T \rangle_n$ when it represents a successful termination, since there are no more applicable rules.

The relation $\rightarrow_{\omega'}$ (of the transition system of the operational semantics $\omega'$) is defined by the rules in Table II. Let us discuss briefly the rules.

$\text{Solve'}$ moves a built-in constraint from the store to the built-in constraint store;

$\text{Apply'}$ uses the rule $r@H'_1 \setminus H'_2 \Leftrightarrow D \mid \tilde{B}; T_r$ provided that exists a matching substitution $\theta$ such that $\text{chr}(\tilde{H}_1, \tilde{H}_2) = (H'_1, H'_2)\theta$. $D$ is entailed by the built-in constraint store of the computation and $r@id(\tilde{H}_1, \tilde{H}_2) \not\in T$; $\tilde{H}_2$ is replaced by $\tilde{B}$, where the identifier are suitably incremented by $\text{inst}$ function and $\text{chr}(\tilde{H}_1, \tilde{H}_2) = (H'_1, H'_2)$ is added to built-in constraint store.
In order to show the equivalence of the semantics \( \omega_t \) and \( \omega'_t \) we now define the notion of observables that we consider: these are the “qualified answers” (already used in Frühwirth 1998).

**Definition 3.2. (Qualified answers)**. Let \( P \) be a CHR program and let \( G \) be a goal. The set \( QA(P) \) of qualified answers for the query \( G \) in the program \( P \) is defined as follows:

\[
QA(P) = \\
\{ \exists F_v(G) \exists K \wedge d \mid \langle G, 0, \text{true}, 0 \rangle_1 \rightarrow^*_{\omega} \langle 0, K, d, T \rangle_n \neq_{\omega_t} \} \\
\cup \\
\{ \text{false} \mid \langle G, 0, \text{true}, 0 \rangle_1 \rightarrow^*_{\omega} \langle G', K, \text{false}, T \rangle_n \}.
\]

Analogously we can define the qualified answer of an annotated program.

**Definition 3.3. (Qualified answers for annotated programs)**. Let \( P \) be an annotated CHR program and let \( G \) be a goal with \( m \) CHR constraints. The set \( QA'(P) \) of qualified answers for the query \( G \) in the annotated program \( P \) is defined as follows:

\[
QA'(P) = \\
\{ \exists F_v(G) \exists K \wedge d \mid \langle I^m_0(G), 0, \text{true}, 0 \rangle_m \rightarrow^*_{\omega} \langle \tilde{K}, d, T \rangle_n \neq_{\omega'_t} \} \\
\cup \\
\{ \text{false} \mid \langle I^m_0(G), 0, \text{true}, 0 \rangle_m \rightarrow^*_{\omega} \langle \tilde{G'}, K, \text{false}, T \rangle_n \}.
\]

The following definition is introduced to describe the equivalence of two intermediate states and it is used only in the proofs. We consider two state equivalent when they are identical up to renaming of local variables and renaming of identifiers and logical equivalence of built-in constraints.

**Definition Interval-semantics State equivalence.** Let \( \sigma = \langle (H_1, C), \tilde{H}_2, D, T \rangle_n \in \text{Conf}_t \) be a state in the transition system \( \omega_t \) and let \( \sigma' = \langle (\tilde{K}, C), D, T' \rangle_m \in \text{Conf}'_t \) be a state in the transition system \( \omega'_t \).

\( \sigma \) and \( \sigma' \) are equivalent (and we write \( \sigma \equiv \sigma' \)) if:

1. there exist \( \tilde{K}_1 \) and \( \tilde{K}_2 \), such that \( \tilde{K} = \tilde{K}_1 \cup \tilde{K}_2 \), \( H_1 = \text{chr}(\tilde{K}_1) \) and \( \text{chr}(\tilde{H}_2) = \text{chr}(\tilde{K}_2) \),
2. for each \( l \in id(\tilde{K}_1) \), \( l \) does not occur in \( T' \),
3. there exists a renaming of identifier \( \rho \) s.t. \( T \rho = T' \) and \( \tilde{H}_2 \rho = \tilde{K}_2 \).

The following result shows the equivalence of the two introduced semantics proving the equivalence (w.r.t. Definition 3.2) of intermediate states. The proof is easy by definition of \( \omega_t \) and \( \omega'_t \).

**Lemma 3.5.** Let \( P \) and \( \text{Ann}(P) \) be respectively a CHR program and its annotated version. Moreover, let \( \sigma \in \text{Conf}_t \) and let \( \sigma' \in \text{Conf}'_t \) such that \( \sigma \equiv \sigma' \). Then the following holds

1. there exists a derivation \( \delta = \sigma \rightarrow^*_{\omega} \sigma_1 \) in \( P \) if and only if there exists a derivation \( \delta' = \sigma' \rightarrow^*_{\omega} \sigma'_1 \) in \( \text{Ann}(P) \) such \( \sigma_1 \equiv \sigma'_1 \),
2. the number of \text{Solve} (Apply) transition steps in \( \delta \) and the number of \text{Solve}' (Apply') transition steps in \( \delta' \) are equal.
Proof. We show that any transition step from any state in one system can be imitated from a (possibly empty) sequence of transition steps from an equivalent state in the other system to achieve an equivalent state. Moreover there exists a Solve (Apply) transition step in $\delta$ if and only if there exists a Solve' (Apply') transition step in $\delta'$.

Then the proof follows by a straightforward inductive argument.

Let $\sigma = \langle (H_1, C), H_2, D, T \rangle_n \in \text{Conf}_1$ and let $\sigma' = \langle (K, C), D, T' \rangle_m \in \text{Conf}'_1$ such that $\sigma \equiv \sigma'$.

Solve and Solve': they move a built-in constraint from the Goal store or the Store respectively to the built-in constraint store. In this case let $C = C' \cup \{c\}$. By definition of the two transition systems

$$\sigma \rightarrow_{\text{Solve}} \langle (H_1, C'), H_2, D \land c, T \rangle_n \quad \text{and} \quad \sigma' \rightarrow_{\text{Solve}'} \langle (K, C'), D \land c, T' \rangle_m.$$

By definition of $\equiv$, it is easy to check that $\langle (H_1, C'), H_2, D \land c, T \rangle_n \equiv \langle (K, C'), D \land c, T' \rangle_m$.

Introduce:. this kind of transition exists only in $\omega_1$ semantics and its application labels a CHR constraint in the goal store and moves it in the CHR store. In this case let $H_1 = H'_1 \cup \{h\}$ and $H_2 = H'_2 \cup \{h\#n\}$.

$$\sigma \rightarrow_{\text{Introduce}} \langle (H'_1, C), H'_2, D \land \{h\#n\}, D, T \rangle_{n+1}.$$ Let us denote $\tilde{H}_2 \cup \{h\#n\}$ by $\tilde{H}'_2$. By definition of $\equiv$, there exist $\tilde{K}_1$ and $\tilde{K}_2$, such that $\tilde{K} = \tilde{K}_1 \cup \tilde{K}_2$, $H_1 = \text{chr}(\tilde{K}_1)$ and $\text{chr}(\tilde{H}_2) = \text{chr}(\tilde{K}_2)$. Therefore there exists an identified atom $h\#m \in \tilde{K}_1$. Let $n' = \rho(n)$ (where $n' = n$ if $n$ is not in the domain of $\rho$). By construction and by hypothesis, $\tilde{K}'_1 = \tilde{K}_1 \{h\#m\}$ and $\tilde{K}'_2 = \tilde{K}_2 \{h\#m\}$ are such that $\tilde{K} = \tilde{K}'_1 \cup \tilde{K}'_2$, $\tilde{H}'_1 = \text{chr}(\tilde{K}'_1)$ and $\text{chr}(\tilde{H}'_2) = \text{chr}(\tilde{K}'_2)$.

Moreover, by definition of $\equiv$, for each $l \in \text{id}(\tilde{K}_1)$, $l$ does not occur in $T'$. Therefore, since by construction $\tilde{K}'_1 \subseteq \tilde{K}_1$, we have that for each $l \in \text{id}(\tilde{K}'_1)$, $l$ does not occur in $T'$.

Now, to prove that $\sigma' \equiv \langle (H'_1, C), \tilde{H}'_2, D, T \rangle_{n+1}$, we have only to prove that there exists a renaming $\rho'$, such that $T\rho' = T'$ and $\tilde{H}'_2\rho' = \tilde{K}'_2$. We can consider the new renaming $\rho' = \rho \circ \{n'/m, m/n\}$. By definition $\rho'$ is a renaming of identifiers. Since by construction, $m \notin \text{id}(\tilde{K}_2)$, we have that if there exists $m'/m \in \rho$, then $m' \notin \text{id}(\tilde{H}_2)$. Moreover, since $m \notin \text{id}(\tilde{K}_2)$, if there is no $m/m' \in \rho$ then $m \notin \text{id}(\tilde{H}_2)$. By the previous observations, we have that $\tilde{H}'_2\rho' = \tilde{H}_2\rho \cup \{h\#n\} \{n/m\} = \tilde{K}'_2$. Finally, since $n$ does not occur in $T$, we have that $T\rho' = T\rho\{m/n'\} = T\{m/n'\}$, where the last equality follows by hypothesis. Moreover since $m \in \text{id}(\tilde{K}_1)$, we have that $m$ does not occur in $T'$. Therefore $T\{m/n'\} = T'$ and then the thesis.

Apply and Apply': Let $r @ F \setminus F'' \Leftarrow D_1 | B, C_1 \in P$ and $r @ F \setminus F'' \Leftarrow D_1 | \tilde{B}, C_1 \in \text{Ann}(P)$ be its annotated version which can be applied to the considered state $\sigma' = \langle (K, C), D, T' \rangle_m$. In particular $F', F''$ match respectively with $\tilde{P}_1$ and $\tilde{P}_2$.

Without loss of generality, by using a suitable number of Introduce steps, we can assume that $r @ F \setminus F'' \Leftarrow D_1 | B, C_1 \in P$ can be applied to $\sigma = \langle (H_1, C), H_2, D, T \rangle_n$. In particular, we can assume for $i = 1, 2$, there exists $Q_i \subseteq H_2$ such that $Q_i \rho = \tilde{P}_i$ and $F', F''$ match respectively with $Q_1$ and $Q_2$. 
By definition of $\equiv$, there exist $\tilde{P}_1$ and $\tilde{Q}_3$ such that $\tilde{Q}_3 \rho = \tilde{P}_1 \cup \tilde{P}_2 \cup \tilde{P}_3$, $\tilde{H}_2 = \tilde{Q}_1 \cup \tilde{Q}_2 \cup \tilde{Q}_3$ and let $x = F v(\tilde{P}_1, \tilde{P}_2) = F v(\tilde{Q}_1, \tilde{Q}_2)$.

By construction, since $T \rho = T'$ and $(\tilde{P}_1, \tilde{P}_2) = (\tilde{Q}_1, \tilde{Q}_2) \rho$, we have that

\[
- r @ id(\tilde{P}_1, \tilde{P}_2) \notin T' \text{ if and only if } - r @ id(\tilde{Q}_1, \tilde{Q}_2) \notin T \text{ and }
- \exists \sigma (((F', F'') = chr(\tilde{P}_1, \tilde{P}_2)) \land D_1) \text{ if and only if } \exists \sigma (((F', F'') = chr(\tilde{Q}_1, \tilde{Q}_2)) \land D_1).
\]

Therefore, by definition of $\text{Apply}$ and of $\text{Apply'}$

\[
\sigma \xrightarrow{\omega'_{\text{Apply}}} (\{H_1, C\} \cup \{B, C_1\}, (\tilde{Q}_1, \tilde{Q}_2), ((F', F'') = chr(\tilde{Q}_1, \tilde{Q}_2)) \land D, T_1)_n
\]

if and only if

\[
\sigma' \xrightarrow{\omega'_{\text{Apply'}}} ((K_1, \tilde{P}_1, \tilde{P}_3, C, B', C_1), ((F', F'') = chr(\tilde{P}_1, \tilde{P}_2)) \land D, T'_1)_o,
\]

where

\[
- T' = T \cup \{r @ id(\tilde{Q}_1)\} \text{ if } \tilde{Q}_2 = \emptyset, \text{ otherwise } T_1 = T,
- (B', \emptyset, o) = \text{inst}(B, \emptyset, m) \text{ and }
- T'_1 = T' \cup \{r @ id(\tilde{P}_1)\} \text{ if } \tilde{Q}_2 = \emptyset, \text{ otherwise } T'_1 = T'.
\]

Let $\sigma_1 = ((\{H_1, C\} \cup \{B, C_1\}, (\tilde{Q}_1, \tilde{Q}_3), ((F', F'') = chr(\tilde{Q}_1, \tilde{Q}_2)) \land D, T_1)_n$ and $\sigma'_1 = ((K_1, \tilde{P}_1, \tilde{P}_3, B', C, C_1), ((F', F'') = chr(\tilde{P}_1, \tilde{P}_2)) \land D, T'_1)_o$.

Now, to prove the thesis, we have to prove that $\sigma_1 \equiv \sigma'_1$.

The following holds.

(1) There exist $K'_1 = (K_1, B')$ and $K'_2 = (\tilde{P}_1, \tilde{P}_3)$, such that $(K_1, \tilde{P}_1, \tilde{P}_3, B') = K'_1 \cup K'_2$ and $H_1 \cup B = chr(K'_1)$ and $chr(K'_1, Q_3)$.

(2) Since for each $l \in id(K_1)$, $l$ does not occur in $T'$, $\tilde{P}_1 \subseteq K_2$ and by definition of $\text{Apply'}$ transition, we have that for each $l \in id(K'_1) = id(K_1, B')$, $l$ does not occur in $T'_1$.

(3) By construction and since $T \rho = T'$, we have that $T_1 \rho = T'_1$. Moreover, by construction $(Q_1, Q_3) \rho = (\tilde{P}_1, \tilde{P}_3) = K'_2$.

By definition, we have that $\sigma_1 \equiv \sigma'_1$ and then the thesis.

\[
\Box
\]

**Proposition 3.6.** Let $P$ and $\text{Ann}(P)$ be respectively a CHR program and its annotated version. Then, for every goal $G$,

\[
\mathcal{Q}A_P(G) = \mathcal{Q}A'_{\text{Ann}(P)}(G)
\]

holds.

**Proof.** By definition of $\mathcal{Q}A$ and of $\mathcal{Q}A'$, the initial states of the two transition system are equivalent. Then the proof follows by Lemma 3.23.

### 4. THE UNFOLDING RULE

In this section we define the *unfold operation* for CHR simpagination rules. As a particular case we obtain also unfolding for simplification and propagation rules, as these can be seen as particular cases of the former.

The unfolding allows to replace a conjunction $S$ of constraints (which can be seen as a procedure call) in the body of a rule $r$ by the body of a rule $v$, provided that
the head of \( v \) matches with \( S \), by assuming the built-in constraints in the guard and in the body of the rule \( r \). More precisely, assume that the built-in constraints in the guard and in the body of the rule \( r \) imply that the head \( H \) of \( v \), instantiated by a substitution \( \theta \), matches with the conjunction \( S \) (in the body of \( r \)). Then the unfolded rule is obtained from \( r \) by performing the following steps: 1) the new guard in the unfolded rule is the conjunction of the guard of \( v \), the latter instantiated by \( \theta \) and without those constraints that are entailed by the built-in constraints which are in \( r \); 2) the body of \( v \) and the equality \( H = S \) are added to the body of \( r \); 3) the conjunction of constraints \( S \) can be removed, partially removed or left in the body of the unfolded rule, depending on the fact that \( v \) is a simplification, a simpagation or a propagation rule, respectively; 4) as for the local token store \( T \), associated to every rule \( r \), this is updated consistently during the unfolding operations in order to avoid that a propagation rule is used twice to unfold the same sequence of constraints.

Before formally defining the unfolding we need to define the function

\[
\text{clean} : \text{Goals} \times \text{Token} \rightarrow \text{Token},
\]

as follows: \( \text{clean} (\tilde{B}, T) \) deletes from \( T \) all the tokens for which at least one identifier is not present in the identified goal \( \tilde{B} \). More formally

\[
\text{clean} (\tilde{B}, T) = \{ t \in T \mid t = r \otimes i_1, \ldots, i_k \text{ and } i_j \in \text{id} (\tilde{B}) \text{, for each } j \in [1, k] \}.
\]

Recall also that we defined \( \text{chr} (h \# i) = h \).

**Definition 4.1. (Unfold).** Let \( P \) be an annotated CHR program and let \( r, sp \in P \) be two annotated rules such that:

\[
\begin{align*}
&v \otimes H_1 \setminus H_2 \Leftrightarrow D \mid \tilde{K}, \tilde{S}_1, \tilde{S}_2, C; T \quad \text{and} \\
v \otimes H'_1 \setminus H'_2 \Leftrightarrow D' \mid \tilde{B}; T'
\end{align*}
\]

where \( C \) is the conjunction of all the built-in constraints in the body of \( r \) and \( CT \models (C \land D) \rightarrow \text{chr} (\tilde{S}_1, \tilde{S}_2) = (H'_1, H'_2) \theta \), that is, the constraints \( H'_1 \) in the head of rule \( v \) match with \( \text{chr} (\tilde{S}_1) \) and \( H'_2 \) matches with \( \text{chr} (\tilde{S}_2) \) by using the substitution \( \theta \), once the built-in constraints in \( r \) are assumed. Furthermore assume that \( m \) is the greatest identifier which appears in the rule \( r \) and that \( (\tilde{B}_1, T_1, m_1) = \text{inst} (\tilde{B}, T', m) \). Then the **unfolded** rule is:

\[
\begin{align*}
&v \otimes H_1 \setminus H_2 \Leftrightarrow D, (D'' \theta) \mid \tilde{K}, \tilde{S}_1, \tilde{S}_2, C, \text{chr} (\tilde{S}_1, \tilde{S}_2) = (H'_1, H'_2); T''
\end{align*}
\]

where \( v \otimes \text{id}(\tilde{S}_1, \tilde{S}_2) \notin T, V \subseteq D' \) is the greatest set of built-in constraints \( c \), such that \( CT \models C \land D \rightarrow c \theta \), \( D'' = D' \setminus V \), the constraint \( (D, (D'' \theta)) \) is satisfiable and

- if \( H'_2 = \emptyset \) then \( T'' = \text{clean} ((\tilde{K}, \tilde{S}_1), T) \cup T_1 \cup \{ v \otimes \text{id} (\tilde{S}_1) \} \)
- if \( H'_2 \neq \emptyset \) then \( T'' = \text{clean} ((\tilde{K}, \tilde{S}_1), T) \cup T_1 \).

Note that we use the function \( \text{inst} \) (Definition 5.1) in order to increment the value of the identifiers associated to atoms in the unfolded rule. This allows us to distinguish the new identifiers introduced in the unfolded rule from the old ones. Note also that the condition on the token store is needed to obtain a correct rule. Consider for example a ground annotated program \( P = \{ r_1 \otimes \theta \Leftrightarrow k, r_2 \otimes k \Rightarrow \tilde{s}, r_3 \otimes s, s \Leftrightarrow \tilde{B} \} \) and let \( h \) be the start goal. In this case the unfolding could
change the semantics if the token store were not used. In fact, according to the semantics proposed in Table I or II we have the following computation: \( h \rightarrow (r_1) k \leftarrow (r_k) \bar{h}, \bar{s} \not= \omega_1 \). On the other hand, considering an unfolding without the update of the token store one would have \( r_1 \odot h \iff k, \bar{s}, \bar{t} \). So, starting from the constraint \( h \) we could arrive to constraint \( k, B \), that is not possible in the original program (the clause obtained after the wrongly applied unfolding rule is underlined).

As previously mentioned, the unfolding rules for simplification and propagation can be obtained as particular cases of Definition 4.1, by setting \( H_1 = \emptyset \) and \( H'_2 = \emptyset \), respectively, and by considering accordingly the resulting unfolded rule. In the following examples we will use \( \odot \) to denote both \( \iff \) and \( \Rightarrow \).

**Example 4.2.** The following program \( P = \{r_1, r_2, \bar{r}_2\} \) deduces information about genealogy. Predicate \( f \) is considered as father, \( g \) as grandfather, \( gs \) as grandson and \( gg \) as great-grandfather. The following rules are such that we can unfold some constraints in the body of \( r_1 \) using the rule \( r_2 \) [\( \bar{r}_2 \)].

\[
\begin{align*}
r_1 & @ f(X, Y), f(Y, Z), f(Z, W) \odot g(X, Z) \#1, f(Z, W) \#2, gs(Z, X) \#3. \\
r_2 & @ g(X, Y), f(Y, Z) \odot gs(X, Z) \#1. \\
\bar{r}_2 & @ g(X, Y) \setminus f(Y, Z) \iff gg(X, Z) \#1.
\end{align*}
\]

Now we unfold the body of rule \( r_1 \) by using the rule \( r_2 \) where we assume \( \odot \iff \) (so we have a simplification rule). We use \( \text{inst}(gg(X, Z) \#1, @, 3) = (gg(X, Z) \#4, 0, 4) \) and a renamed version of \( r_2 \)

\[ r_2 \odot g(X', Y'), f(Y', Z') \iff gg(X', Z') \#1. \]

in order to avoid variable clashes. So the new unfolded rule is:

\[
\begin{align*}
r_1 & @ f(X, Y), f(Y, Z), f(Z, W) \odot gg(X', Z') \#4, gs(Z, X) \#3, X' = X, Y' = Z, Z' = W. \\
\end{align*}
\]

Now, we unfold the body of rule \( r_1 \) by using the simpagation rule \( \bar{r}_2 \). As before,

\[ \text{inst}(gg(X, Z) \#1, @, 3) = (gg(X, Z) \#4, 0, 4) \]

and a renamed version of \( \bar{r}_2 \)

\[ \bar{r}_2 \odot g(X', Y') \setminus f(Y', Z') \iff gg(X', Z') \#1. \]

is used to avoid variable clashes. The new unfolded rule is:

\[
\begin{align*}
r_1 & @ f(X, Y), f(Y, Z), f(Z, W) \odot gg(X', Z') \#1, \quad gg(X', Z') \#4, gs(Z, X) \#3, X' = X, Y' = Z, Z' = W. \\
\end{align*}
\]

Finally we unfold the body of \( r_1 \) by using the \( r_2 \) rule where \( \odot \iff \Rightarrow \) is assumed (so we have a propagation rule). As usual, \( \text{inst}(gg(X, Z) \#1, @, 3) = (gg(X, Z) \#4, 0, 4) \) and a renamed version of \( r_2 \) is used to avoid variable clashes:

\[ r_2 \odot g(X', Y'), f(Y', Z') \Rightarrow gg(X', Z') \#1. \]

and so the new unfolded rule is:

\[
\begin{align*}
r_1 & @ f(X, Y), f(Y, Z), f(Z, W) \odot g(X, Z) \#1, \\
f(Z, W) \#2, gs(Z, X) \#3, gg(X', Z') \#4, X' = X, Y' = Z, Z' = W; \{r_2 \odot 1, 2\}. \\
\end{align*}
\]
The following example considers more specialized rules with guards which are not true.

**Example 4.3.** The following program \( P = \{ r_1, r_2, \bar{r}_2 \} \) specializes the rules introduced in Example 4.2 to the genealogy of Adam. So here we remember that Adam was father of Seth; Seth was father of Enosh; Enosh was father of Kenan. As before, we consider the predicate \( f \) as father, \( g \) as grandfather, \( gs \) as grandson and \( gg \) as great-grandfather.

\[ r_1 @ (f(X,Y), f(Y,Z), f(Z,W) \circ X = Adam, Y = Seth) \]
\[ g(X,Z) \# 1, f(Z,W) \# 2, gs(Z,X) \# 3, Z = Enosh. \]
\[ r_2 @ (g(X,Y), f(Y,Z) \circ X = Adam, Y = Enosh | gg(X,Z) \# 1, Z = Kenan. \]
\[ \bar{r}_2 @ (g(X,Y), f(Y,Z) \leftarrow X = Adam, Y = Enosh | gg(X,Z) \# 1, Z = Kenan. \]

If we unfold \( r_1 \) by using (a suitable renamed version of) \( r_2 \), where we assume \( \circ = \Leftarrow \), we obtain:

\[ r_1 @ (f(X,Y), f(Y,Z) f(Z,W) \circ X = Adam, Y = Seth | gg(X', Z') \# 4, Z' = Kenan, \]
\[ gs(Z,X) \# 3, Z = Enosh, X' = X, Y' = Z, Z' = W. \]

When \( \bar{r}_2 \) is considered to unfold \( r_1 \) we have

\[ r_1 @ (f(X,Y), f(Y,Z) f(Z,W) \circ X = Adam, Y = Seth | g(X,Z) \# 1, gg(X', Z') \# 4, \]
\[ Z' = Kenan, gs(Z,X) \# 3, Z = Enosh, X' = X, Y' = Z, Z' = W. \]

Finally if we assume \( \circ \Rightarrow \) in \( r_2 \) from the unfolding we obtain

\[ r_1 @ (f(X,Y), f(Y,Z) f(Z,W) \circ X = Adam, Y = Seth | g(X,Z) \# 1, f(Z,W) \# 2, \]
\[ gs(Z,X) \# 3, gg(X', Z') \# 4, Z' = Kenan, Z = Enosh, X' = X, Y' = Z, \]
\[ Z' = W; \{ \bar{r}_2 @ 1, 2 \}. \]

Note that \( X' = Adam, Y' = Enosh \) are not added to the guard of the unfolded rule because \( X' = Adam \) is entailed by the guard of \( r_1 \) and \( Y' = Enosh \) is entailed by the built-in constraints in the body of \( r_1 \).

We prove now the correctness of our unfolding definition. Before the introduction of the proposition which proves the correctness of our unfolding, three new definitions are given. The first one presents the concept of built-in free state. Said state either has no built-in constraints in the first component or the built-in store is unsatisfiable.

**Definition** Built-in Free State. Let \( \sigma = \langle G, \tilde{S}, D, T \rangle_o \in Conf \_ \) (\( \sigma = \langle \tilde{G}, D, T \rangle_o \in Conf^\prime \_ \)). The state \( \sigma \) is built-in free if either \( D = false \) or \( G (\tilde{G}) \) is a multiset of (identified) CHR-constraints.

The second definition introduces the state equivalence between states in \( Conf^\prime \_ \). Note that in such definition, the equivalence operator is represented with the symbol \( \simeq \).

**Definition** State Equivalence. Let \( \sigma = \langle \tilde{G}, D, T \rangle_o \) and \( \sigma' = \langle \tilde{G}', D', T' \rangle_o \) be states in \( Conf^\prime \_ \). \( \sigma \) and \( \sigma' \) are equivalent and we write \( \sigma \simeq \sigma' \) if one of the following facts hold.

- either \( D = false \) and \( D' = false \)
—or $G = G'$, $CT \vdash D \leftrightarrow D'$ and $clean(G, T) = clean(G', T)$.

Finally the third definition presents the normal derivation. A derivation is called normal if no other \textbf{Solve} (\textbf{Solve}') transition are possible when an \textbf{Apply} (\textbf{Apply}') one happens.

\textbf{Definition} Normal Derivation. Let $P$ be a (possibly annotated) CHR program and let $\delta$ be a derivation in $P$. We say that $\delta$ is normal if it uses a transition \textbf{Solve} (\textbf{Solve}') as soon as possible, namely it is possible to use a transition \textbf{Apply} (\textbf{Apply}') on a state $\sigma$ only if $\sigma$ is built-in free.

Note that, by definition, given a CHR program $P$, $QA(P)$ can be calculated by considering only normal derivations. Analogously for an annotated CHR program $P'$. The proof of the following proposition is straightforward and hence it is omitted.

\textbf{Proposition 4.7.} Let $P$ be CHR program and let $P'$ an annotated CHR program. Then

\[ QA_P(G) = \{ \exists_F \cdot (G) K \land d \mid \delta = \langle G, \emptyset, true, 0 \rangle_1 \rightarrow^* \omega_1 \langle \emptyset, K, d, T \rangle_n \not\vdash^\omega_1 \text{ and } \delta \text{ is normal} \} \]

and

\[ QA'_P(G) = \{ \exists_F \cdot (G) K \land d \mid \delta = \langle \exists^n_{F'}(G), true, 0 \rangle_m \rightarrow^* \omega_1 \langle \emptyset, K, d, T \rangle_n \not\vdash^\omega_1 \text{ and } \delta \text{ is normal} \} \]

\textbf{Proposition 4.8.} Let $r, v$ be annotated CHR rules and $r'$ be the result of the unfolding of $r$ with respect to $v$. Let $\sigma$ be a generic built-in free state such that we can use the transition \textbf{Apply} with the clause $r'$ obtaining the state $\sigma'_{r'}$ and then the built-in free state $\sigma'^f_{r'}$. Then we can construct a derivation which uses at most the clauses $r$ and $v$ and obtain a built-in free state $\sigma^f$ such that $\sigma'^f_{r'} \succeq \sigma^f$.

\textbf{Proof.} Assume that

\[ \sigma \rightarrow r' \sigma_{r'} \rightarrow^{\text{Solve}^*} \sigma'_{r'} \]

\[ \not\vdash^r \sigma_r \rightarrow^{\text{Solve}^*} \sigma^f_{r'} \rightarrow^{\text{Solve}^*} \sigma^f_{v'} \]

The labeled arrow $\rightarrow^{\text{Solve}^*}$ means that only solve transitions are applied. Moreover

— if $\sigma^f$ has the form $\langle \tilde{G}, false, T \rangle$ then the derivation between the parenthesis is not present and $\sigma^f = \sigma^f_{\tilde{G}}$.

— the derivation between the parenthesis is present and $\sigma^f = \sigma^f_{\tilde{G}}$, otherwise.

\textbf{Preliminaries:} Let $\sigma = \langle (\tilde{H}_1, \tilde{H}_2, \tilde{H}_3), C, T \rangle$ be a built-in free state and let $r \in (\tilde{H}_1 \setminus \tilde{H}_2) \Leftrightarrow D_r \mid \tilde{K}, \tilde{S}_1, \tilde{S}_2, C_r; T_r$ and $v \in S'_1 \setminus S'_2 \Leftrightarrow D_v \mid P, C_v; T_v$ where $C_r$ is the
conjunction of all the built-in constraints in the body of \( r \) and
\[
CT \models (D_r \land C_r) \rightarrow \text{chr}(\tilde{S}_1, \tilde{S}_2) = (S'_1, S'_2)\theta. \quad (1)
\]
Furthermore assume that \( m \) is the greatest identifier which appears in the rule \( r \) and that \( \text{inst}(P, T_v, m) = (\tilde{P}_1, T_1, m_1) \). Then the *unfolded* rule is:
\[
r' \odot H'_1 \oslash H'_2 \Leftrightarrow D_r, (D'_v \theta) \mid \tilde{K}, \tilde{S}_1, \tilde{P}_1, C_r, C_v, \text{chr}(\tilde{S}_1, \tilde{S}_2) = (S'_1, S'_2); T_r
\]
where \( v \odot \text{id}(\tilde{S}_1, \tilde{S}_2) \notin T_r \), \( V \subseteq D_v \) is the greatest set of built-in constraints \( c \), such that \( CT \models (D_r \land C_r) \rightarrow c \theta, D'_v = D_v \setminus V \), the constraint \( (D_r, (D'_v \theta)) \) is satisfiable and

- if \( S'_2 = \emptyset \) then \( T_{r'} = \text{clean}((\tilde{K}, \tilde{S}_1), T_r) \cup T_1 \cup \{ v \odot \text{id}(\tilde{S}_1) \} \)
- if \( S'_2 \neq \emptyset \) then \( T_{r'} = \text{clean}((\tilde{K}, \tilde{S}_1), T_r) \cup T_1 \).

By previous observations, we have that
\[
CT \models (D_r \land C_r) \rightarrow V \theta. \quad (2)
\]

**The proof:** By definition of the transition \textbf{Apply}\(^*\), we have that
\[
CT \models C \rightarrow \exists x ((\text{chr}(\tilde{H}_1, \tilde{H}_2) = (H'_1, H'_2)) \land D_r \land (D'_v \theta)), \quad (3)
\]
where \( x = \text{Fv}(H'_1, H'_2) \) and
\[
\sigma_{r'} = \langle \tilde{Q}, C_r, C_v, \text{chr}(\tilde{S}_1, \tilde{S}_2) = (S'_1, S'_2), \text{chr}(\tilde{H}_1, \tilde{H}_2) = (H'_1, H'_2) \land C, T_3 \rangle_{j+m_1},
\]
where \( \tilde{Q} = (\tilde{H}_1, \tilde{H}_2, \tilde{H}_3) \), with \( \text{inst}((\tilde{K}, \tilde{S}_1, \tilde{P}_1), T_{r'}, j) = (\tilde{Q}, T'_{r'}, j + m_1) \) and

- if \( H'_2 = \emptyset \) then \( T_3 = T \cup T'_{r'} \cup \{ r \odot \text{id}(\tilde{H}_1) \} \)
- if \( H'_2 \neq \emptyset \) then \( T_3 = T \cup T'_{r'} \).

Therefore, by definition
\[
\sigma'_{r'} = \langle \tilde{Q}, C'_{r'}, T_3 \rangle_{j+m_1},
\]
where
\[
CT \models C_{r'} \leftrightarrow C_r \land C_v \land \text{chr}(\tilde{S}_1, \tilde{S}_2) = (S'_1, S'_2) \land \text{chr}(\tilde{H}_1, \tilde{H}_2) = (H'_1, H'_2) \land C.
\]

On the other hand, since by (3),
\[
CT \models C \rightarrow \exists x ((\text{chr}(\tilde{H}_1, \tilde{H}_2) = (H'_1, H'_2)) \land D_r)
\]
by definition of the transition \textbf{Apply}\(^*\), we have that
\[
\sigma_r = \langle \tilde{Q}_2, C_r, \text{chr}(\tilde{H}_1, \tilde{H}_2) = (H'_1, H'_2) \land C, T_4 \rangle_{j+m},
\]
where \( \tilde{Q}_2 = (H_1, H_3, \tilde{K}', \tilde{S}_1', \tilde{S}_2') \), \((\tilde{K}', \tilde{S}_1', \tilde{S}_2'), T_2, j + m \) = \( \text{inst}((\tilde{K}, \tilde{S}_1, \tilde{S}_2), T_r, j) \) and

- if \( H'_2 = \emptyset \) then \( T_4 = T \cup T_2 \cup \{ r \odot \text{id}(\tilde{H}_1) \} \)
- if \( H'_2 \neq \emptyset \) then \( T_4 = T \cup T_2 \).

Therefore, by definition
\[
\sigma'_r = \langle \tilde{Q}_2, C'_r, T_4 \rangle_{j+m}.
\]
where
\[
CT \models C'_f \iff C_r \land \text{chr}(\tilde{H}_1, \tilde{H}_2) = (H'_1, H'_2) \land C.
\] (4)

Now, we have two possibilities

\( (C'_f = \text{false}) \). In this case, by construction we have that \( C'_f = \text{false} \). Therefore \( \sigma'_v \simeq \sigma_f \) and then the thesis.

\( (C'_f \neq \text{false}) \). By definition, since \( \text{chr}(\tilde{S}_1, \tilde{S}_2) = \text{chr}(\tilde{S}'_1, \tilde{S}'_2) \), by (1), (2) and (3), we have that
\[
CT \models (C_r \land \text{chr}(\tilde{H}_1, \tilde{H}_2) = (H'_1, H'_2) \land C) \rightarrow (\exists y (\text{chr}(\tilde{S}_1, \tilde{S}_2) = (S'_1, S'_2)) \land D_v),
\]
where \( y = \text{Fv}(S'_1, S'_2) \). Therefore by (4)
\[
CT \models C'_f \rightarrow (\exists y (\text{chr}(\tilde{S}_1, \tilde{S}_2) = (S'_1, S'_2)) \land D_v)
\]
and
\[
\sigma_v = \langle (Q_3, C_r), \text{chr}(\tilde{S}_1, \tilde{S}_2) = (S'_1, S'_2) \land C_r \land \text{chr}(\tilde{H}_1, \tilde{H}_2) = (H'_1, H'_2) \land C, T_5 \rangle_{m_1},
\]
where \( Q_3 = (\tilde{H}_1, \tilde{H}_3, \tilde{K}'', S''_1, \tilde{P}_2) \), with \( \text{inst}(\tilde{P}, T_v, j + m) = (\tilde{P}_2, T'_v, m_1) \) and

- if \( S'_2 = \emptyset \) then \( T_5 = T_4 \cup T'_v \cup \{ v @ id(S''_1) \} \)
- if \( S'_2 \neq \emptyset \) then \( T_5 = T_4 \cup T'_v \).

Finally by definition, we have that
\[
\sigma'_v = \langle (Q_3, C'_f, T_5) \rangle_{m_1},
\]
where
\[
C'_f \iff C_v \land \text{chr}(\tilde{S}_1, \tilde{S}_2) = (S'_1, S'_2) \land C_r \land \text{chr}(\tilde{H}_1, \tilde{H}_2) = (H'_1, H'_2) \land C.
\]

If \( C'_f = \text{false} \) then the proof is analogous to the previous case and hence it is omitted. Otherwise, observe that by construction, \( Q = (\tilde{H}_1, \tilde{H}_3, \tilde{Q}_1) \), where \( \tilde{Q}_1 \) is obtained from \( (\tilde{K}, \tilde{S}_1, \tilde{P}_1) \) by adding the natural \( j \) to each identifier in \( (\tilde{K}, \tilde{S}_1) \) and by adding the natural \( j + m \) to each identifier in \( \tilde{P} \). Analogously, by construction, \( Q_3 = (\tilde{H}_1, \tilde{H}_3, \tilde{K}'', S''_1, \tilde{P}_2) \), where \( (\tilde{K}'', S''_1) \) are obtained from \( (\tilde{K}, \tilde{S}_1) \) by adding the natural \( j \) to each identifier in \( (\tilde{K}, \tilde{S}_1) \) and \( \tilde{P}_2 \) is obtained from \( \tilde{P} \) by adding the natural \( j + m \) to each identifier in \( \tilde{P} \).

Therefore \( Q = Q_3 \) and then, to prove the thesis, we have only to prove that
\[
\text{clean}(\tilde{Q}, T_3) = \text{clean}(\tilde{Q}, T_5).
\]

Let us introduce the function \( \text{inst}' : \{ \text{Token} \} \times \mathbb{N} \rightarrow \mathbb{N} \) as the restriction of the function \( \text{inst} \) to token sets and natural numbers, namely \( \text{inst}'(T, n) = T' \), where \( T' \) is obtained from \( T \) by incrementing each identifier in \( T \) with \( n \). So, since \( T'_2 = \text{inst}'(T_2, j) \), \( T_2 = \text{clean}((\tilde{K}, \tilde{S}_1), T_r) \cup T_1 \cup \{ v @ id(\tilde{S}_1) \mid \text{if } S_2 = \emptyset \} \) and \( T_1 = \text{inst}'(T_v, m) \), we have that
\[
T_3 = T \cup T'_2 \cup \{ r @ id(\tilde{H}_1) \mid \text{if } H_2 = \emptyset \}
= T \cup \text{inst}'(\text{clean}((\tilde{K}, \tilde{S}_1), T_r), j) \cup \text{inst}'(T_v, j + m) \cup \text{inst}'(\{ v @ id(\tilde{S}_1) \mid \text{if } S_2 = \emptyset \}, j) \cup \{ r @ id(\tilde{H}_1) \mid \text{if } H_2 = \emptyset \}
\]
Analogously, \( T_4 = T \cup T'_v \cup \{ v@id(\bar{H}_1) | \text{if } H_2 = \emptyset \} \), \( T'_5 = \text{inst}'(T_r, j) \) and \( T'_v = \text{inst}'(T_v, j + m) \), we have that
\[
T_5 = T_4 \cup T'_v \cup \{ v@id(\bar{S}_1^n) | \text{if } S_2^n = \emptyset \}
\]
\[
= T \cup \text{inst}'(T_v, j) \cup \{ r@id(\bar{H}_1) | \text{if } H_2 = \emptyset \} \cup \text{inst}'(T_v, j + m) \cup \{ v@id(\bar{S}_1^n) | \text{if } S_2^n = \emptyset \}
\]

Now, since by construction \((S_1^n, S_2^n)\) is obtained from \((S_1, S_2)\) by adding the natural \( j \) to each identifier, we have that \( \text{inst'}(\{ v@id(\bar{S}_1) | \text{if } S_2 = \emptyset \}, j) = \{ v@id(\bar{S}_1^n) | \text{if } S_2^n = \emptyset \} \). Moreover, by definition of annotated rule \( id(T_v) \subseteq id(K, S_1, S_2) \) and \( \bar{Q} = (\bar{H}_1, H_3, \bar{Q}_1) \), where \( \bar{Q}_1 \) is obtained from \((K, S_1, \bar{P}_1)\) by adding the natural \( j \) to each identifier in \((K, S_1)\) and by adding the natural \( j + m \) to each identifier in \( \bar{P}_1 \). Then \( \text{clean}(Q, \text{inst'}(\text{clean}((K, S_1, T_r), j)) = \text{clean}(Q, \text{inst'}(T_r, j)) \) and then the thesis.

\[\square\]

We prove now the correctness of our unfolding rule.

**Proposition 4.9.** Let \( P \) be an annotated CHR program with \( r, v \in P \). Let \( r' \) be the result of the unfolding of \( r \) with respect to \( v \) and let \( P' \) be the program obtained from \( P \) by adding rule \( r' \). Then, for every goal \( G \), \( QA'_{P'}(G) = QA'_{P}(G) \) holds.

**Proof.** We prove the two inclusions separately.

\((QA'_{P'}(G) \subseteq QA'_{P}(G))\). The proof follows from Propositions 4.7 and 4.8 and by a straightforward inductive argument.

\((QA'_{P}(G) \subseteq QA'_{P'}(G))\). The proof is by contradiction. Assume that there exists \((K' \land d') \in QA'_{P'}(G) \setminus QA'_{P'}(G) \). By definition there exists a derivation
\[
\delta = \langle I_0^n(G), \text{true}, \emptyset \rangle_m \rightarrow^{\omega_1} (K, d, T) \rightarrow^{\omega_1} (K, d, T)_{n}
\]
in \( P \), such that \((K' \land d') = \exists_F v(G)(\text{chr}(\bar{K}) \land d) \). Since \( P \subseteq P' \), we have that there exists the derivation \((I_0^n(G), \text{true}, \emptyset)_m \rightarrow^{\omega_1} (K, d, T)_{n} \) in \( P' \). Moreover, since \( P' = P \cup \{ r' \} \) and by hypothesis \((K' \land d') \notin QA'_{P'}(G) \), we have that there exists a derivation step \((K, d, T)_{n} \rightarrow^{\omega_1} (K_1, d_1, T_1)_{n_1} \) by using the clause \( r' \). Then, by definition of unfolding there exists a derivation step \((K, d, T)_{n} \rightarrow^{\omega_1} (K_2, d_2, T_2)_{n_2} \) in \( P \), by using the clause \( r \) and then we have a contradiction.

\[\square\]

5. SAFE RULE REPLACEMENT

Previous corollary shows that we can safely add to a program \( P \) a rule resulting from the unfolding, while preserving the semantics of \( P \) (in terms of qualified answers). However, when a rule \( r \) in program \( P \) has been unfolded producing the new rule \( r' \), in some cases we would like also to replace \( r \) by \( r' \) in \( P \), since this could improve the efficiency of the resulting program. Performing such a replacement while preserving the semantics is in general a very difficult task for three reasons.

First of all, anticipating the guard of \( v \) in the guard of \( r \) (as we do in the unfold operation) could lead to some computations when the unfolded rule \( r' \) is used rather than the original rule \( r \). This is shown by the following example.
Example 5.1. Let us consider the program

\[ P = \{ \begin{array}{l} r@p(Y) \Leftrightarrow q(Y). \\ r'@q(Z) \Leftrightarrow Z = a | . \end{array} \} \]

where we do not consider the identifiers (and the local token store) in the body of rules, because we do not have propagation rules in \( P \).

The unfolding of \( r \) by using the rule \( r' \) returns the new rule \( r@p(Y) \Leftrightarrow Y = a | Y = Z \). The program

\[ P' = \{ \begin{array}{l} r@p(Y) \Leftrightarrow Y = a | Y = Z. \\ r'@q(Z) \Leftrightarrow Z = a | . \end{array} \} \]

is not semantically equivalent to \( P \) in terms of qualified answers. In fact, given the goal \( G = p(X) \) we have \( q(X) \in QA'P(G) \), while \( q(X) \notin QA'P'(G) \).

The second problem is related to multiple heads. In fact, the unfolding that we have defined assume that the head of a rule matches completely with the body of another one, while in general, during a CHR computation, a rule can match with constraints produced by more than one rule and/or introduced by the initial goal. The following example illustrates this point.

Example 5.2. Let us consider the program

\[ P = \{ \begin{array}{l} r@p(Y) \Leftrightarrow q(Y), h(b). \\ r'@q(Z), h(V) \Leftrightarrow Z = V. \end{array} \} \]

where we do not consider the identifiers and the token store in the body of rules, because we do not have propagation rules in \( P \).

The unfolding of \( r \) by using \( r' \) returns the new rule

\[ r@p(Y) \Leftrightarrow Y = Z, V = b, Z = V. \]

Now the the program

\[ P' = \{ \begin{array}{l} r@p(Y) \Leftrightarrow Y = Z, V = b, Z = V. \\ r'@q(Z), h(V) \Leftrightarrow Z = V. \end{array} \} \]

where we substitute the original rule by its unfolded version is not semantically equivalent to \( P \). In fact, given the goal \( G = p(X) \) we have \( q(X) \in QA'(r)P(G) \), while \( q(X) \notin QA'(r)P'(G) \).

The final problem is related to the matching substitution. In fact, following Definition 4.1 there are some matching that could become possible only at run time, and not at compile time, because a more powerful built-in constraint store is needed. Also in this case, a rule elimination could lead to lose possible answers as illustrated in the following example.

Example 5.3. Let \( P \) be a program

\[ P = \{ \begin{array}{l} r_1@g(X, Y) \Leftrightarrow f(X, Z) \\ r_2@f(a, W) \Leftrightarrow W = b. \\ r_3@f(T, J) \Leftrightarrow J = d. \end{array} \} \]

where we do not consider the identifiers and the token store in the body of rules, because we do not have propagation rules in \( P \). Let \( P' \) be the program where the
rule $r_1$, that is unfolded using $r_3$ in $P$, substitutes the original $r_1$ (note that other unfolding are not possible, in particular the rule $r_2$ can not be used to unfold $r_1$)

$$
\begin{align*}
P' &= \{ \ r_1@g(X,Y) \iff X = T, Z = J, J = d. \\
r_2@f(a,W) &\iff W = b. \\
r_3@f(T,J) &\iff J = d. \}
\end{align*}
$$

Let be $G = g(a,R)$ the goal, we can see that $(R = b) \in \mathcal{QA}_{P'}(G)$ and $(R = b) \not\in \mathcal{QA}_P(G)$ because, with the considered goal (and consequently the considered built-in constraint store) $r_2$ can fire in $P$ but can not fire in $P'$.

We have individuated a case in which we can safely replace the original rule $r$ by its unfolded version while maintaining the qualified answers semantics. Intuitively, this holds when: 1) the constraints of the body of $r$ can be rewritten only by CHR rules with a single-head, 2) there exists no rule $v$ which has a multiple head $H$ such that a part of $H$ can match with a part of the constraints introduced in the body of $r$ (that is, there exists no rule $v$ which can be fired by using a part of constraints introduced in the body of $r$ plus some other constraints) and 3) all the rules, that can be applied at run time to the body of the original rule $r$, can also be applied at transformation time (so unfolding avoidance for built-in constraint store and guard-anticipation problems are solved).

Before defining formally these conditions we need some further notations. First of all, given a rule $r@H_1\backslash H_2 \iff D \mid \hat{A};T$, we define two sets. The first one contains a set of pairs, whose first component is a rule that can be used to unfold $r@H_1\backslash H_2 \iff D \mid \hat{A};T$, while the second one is the sequence of the identifiers of the atoms in the body of $r$, which are used in the unfolding.

The second set contains all the rules that can be used for the partial unfolding of $r@H_1\backslash H_2 \iff D \mid \hat{A};T$, namely is the set of rules that can fire by using at least an atom in the body $\hat{A}$ of the rule and some others CHR and built-in constraints. It moreover contains the rules that can fire if an opportune built-in constraint store is given by the computation but that can not be unfolded following Definition 4.1

**Definition 5.4.** Let $P$ be an annotated CHR program and let

$$
\begin{align*}
r@H_1\backslash H_2 &\iff D \mid \hat{A};T \\
r'@H_1'\backslash H_2' &\iff D' \mid \hat{B};T'
\end{align*}
$$

be two annotated rules, such that $r, r' \in P$ and $r'$ is renamed apart with respect to $r$. We define $U^+$ and $U^\#$ as follows:

1. $(r@H_1\backslash H_2 \iff D \mid \hat{A};T, (i_1, \ldots, i_n)) \in U^+_P(r@H_1\backslash H_2 \iff D \mid \hat{A};T)$ if and only if $r@H_1\backslash H_2 \iff D \mid \hat{A};T$ can be unfolded with $r'@H_1'\backslash H_2' \iff D' \mid \hat{B};T'$ (by Definition 4.1) by using the sequence of the identified atoms in $\hat{A}$ with identifiers $(i_1, \ldots, i_n)$.

2. $(r'@H_1'\backslash H_2' \iff D' \mid \hat{B};T' \in U^\#_P(r@H_1\backslash H_2 \iff D \mid \hat{A};T)$ if and only if one of the following holds:

   a. either there exist $\hat{A}' = (\hat{A}_1', \hat{A}_2) \subseteq \hat{A}$ and a built in constraint $C'$ such that $Fv(C') \cap Fv(r') = \emptyset$, the constraint $D \land C'$ is satisfiable, $CT \models (D \land C') \rightarrow \exists_x((chr(\hat{A}_1, \hat{A}_2) = (H_1', H_2')) \land D')$, $r'@id(\hat{A}_1', \hat{A}_2) \not\in T$ and
(r'@H_1 \backslash H_2 \leftrightarrow D' | \tilde{B}; T', id(\tilde{A}_1, \tilde{A}_2)) \notin U^+_P(r@H_1 \backslash H_2 \leftrightarrow D | \tilde{A}; T)

(b) or there exist \tilde{A}' \subseteq \tilde{A}, a multiset of CHR constraints \(H' \neq \emptyset\) and a built-in constraint \(C'\) such that \(\tilde{A}' \neq \emptyset\), \(Fv(C') \cap Fv(r') = \emptyset\), the constraint \(D \land C'\) is satisfiable, \(\{\text{chr}(A'), H'\} = \{K_1, K_2\}\) and \(CT \models (D \land C') \rightarrow \exists_x(((A_1, A_2) = (H'_1, H'_2)) \land D')\).

Some explanations are in order here.

The set \(U^+\) contains all the couples composed by rules, that can be used to unfold a fixed rule \(r\), and the identifiers of the constraints considered in the unfolding, introduced in Definition 1.1.

Let us consider now the set \(U^\#\). The conjunction of built-in constraints \(C'\) represents a generic set of built-in constraints (said set naturally can be equal to every possible built-in constraint store that can be generated by a real computation before the application of rule \(r'\)); the condition \(Fv(C') \cap Fv(r') = \emptyset\) is required to avoid free variable capture, it represents the fresh variable rename of a rule \(r'\) with respect to the computation before the use of the \(r'\) itself in an \textit{Apply} transition; the condition \(r'@id(A_1, A_2) \notin T\) grants the propagation rules trivial non-termination avoidance; the conditions \(CT \models (D \land C') \rightarrow \exists_x((\text{chr}(A_1, A_2) = (H'_1, H'_2)) \land D')\) and \(CT \models (D \land C') \rightarrow \exists_x(((A_1, A_2) = (H'_1, H'_2)) \land D')\) secure that a strong enough built-in constraint is possessed by the computation, before the application of rule \(r'\); the conditions \(A_1' \neq \emptyset\) and \(H' \neq \emptyset\) assure respectively that at least one constraint in the body of rule \(r\) and that at least one constraint form the initial goal or introduced by the body of other rules are unfolded; finally the following condition \((r'@H_1 \backslash H_2 \leftrightarrow D' | \tilde{B}; T', id(\tilde{A}_1, \tilde{A}_2)) \notin U^+_P(r@H_1 \backslash H_2 \leftrightarrow D | \tilde{A}; T)\) is required to avoid the consideration of the rules that can be correctly unfolded in the body of \(r\). There are two kinds of rules that are added to \(U^\#\). The first one, introduced by the Example 5.3, points out the matching substitution problem (Condition 2a of Definition 5.4). The second kind, introduced by the Example 5.2, points out the multiple heads problem: the rule \(r'\) can match with the body of \(r\) but can also match with other constraints introduced by the initial goal or generated by other rules (Condition 2b of Definition 5.4).

Note also that if \(U^+_P(r@H_1 \backslash H_2 \leftrightarrow D | \tilde{A}; T)\) contains a pair, whose first component is not a rule with a single atom in the head, then by definition, \(U^+_P(r@H_1 \backslash H_2 \leftrightarrow D | \tilde{A}; T) \neq \emptyset\).

Finally, given an annotated CHR program \(P\) and an annotated rule \(r@H_1 \backslash H_2 \leftrightarrow D | \tilde{A}; T\), we define

\[\text{Unf}_P(r@H_1 \backslash H_2 \leftrightarrow D | \tilde{A}; T)\]

as the set of all annotated rules obtained by unfolding the rule \(r@H_1 \backslash H_2 \leftrightarrow D | \tilde{A}; T\) with a rule in \(P\), by using Definition 1.1.

We can now give the central definition of this section.

\textbf{Definition 5.5. (Safe Rule Replacement)} Let \(P\) be an annotated CHR program and let \(r@H_1 \backslash H_2 \leftrightarrow D | \tilde{A}; T \in P\), such that the following holds

i) \(U^\#_P((r@H_1 \backslash H_2 \leftrightarrow D | \tilde{A}; T) = \emptyset\) and
Then we say that the rule $r$ unfolded version) in

$$\text{iii) for each}$$

$$r@H_1 \setminus H_2 \Leftrightarrow D' \upharpoonright \tilde{A}; T' \in Unf_P(r@H_1 \setminus H_2 \Leftrightarrow D \upharpoonright \tilde{A}; T)$$

we have that $CT \models D \leftrightarrow D'$.

Then we say that the rule $r@H_1 \setminus H_2 \Leftrightarrow D \upharpoonright \tilde{A}; T$ can be safely replaced (by its unfolded version) in $P$.

Some explanations are in order here.

Condition i) of previous definition implies that $r@H_1 \setminus H_2 \Leftrightarrow D \upharpoonright \tilde{A}; T$ can be safely deleted from $P$ only if:

$- U^+_P(r@H_1 \setminus H_2 \Leftrightarrow D | \tilde{A}; T)$ contains only pairs, whose first component is a rule with a single atom in the head.

$- a$ sequence of identified atoms of body of the rule $r$ can be used to fire a rule $r'$ only if $r$ can be unfolded with $r'$ by using the same sequence of the identified atoms.

Condition ii) states that exist at least one rule that unfold the rule $r@H_1 \setminus H_2 \Leftrightarrow D | \tilde{A}$.

Condition iii) states that each annotated clause obtained by the unfolding of $r$ in $P$ must have guard equivalent to that of $r$: in fact the condition $CT \models D \leftrightarrow D'$ in iii) avoids the problems discussed in Example 5.1, thus allows the anticipation of the guard in the unfolded rule.

We can now provide the result which shows the correctness of the safe rule replacement condition.

**Proposition 5.6.** Let $r@H'_1 \setminus H'_2 \Leftrightarrow D_r \upharpoonright \tilde{K}_r; T_r$ and $v$ be annotated CHR rules such that the following holds

$- v$ is a rule with a single atom in the head

$- (r'@H'_1 \setminus H'_2 \Leftrightarrow D_{r'}, \upharpoonright \tilde{K}_{r'}; T_{r'}, i) \in U^+_v(r@H'_1 \setminus H'_2 \Leftrightarrow D_r | \tilde{K}_r; T_r)$ is the result of the unfolding of $r$ with respect to $v$, $CT \models D_r \leftrightarrow D_{r'}$ and the identified atom $\tilde{k} = k#i \in \tilde{K}_r$.

Moreover, let $\sigma$ be a generic built-in free state such that we can construct a derivation $\delta$ from $\sigma$ such that

$- \delta$ uses at most the clauses $r$ and $v$ in the order,

$- obtain a built-in free state $\sigma^f$ and

$- if v$ is used, then $v$ rewrites the atom $k#i'$ corresponding to $k#i \in \tilde{K}_r$.

Then we can use the transition $\text{Apply'}$ with the clause $r'$ obtaining the state $\sigma_{r'}$, and then the built-in free state $\sigma^f_{r'}$ such that $\sigma^f_{r'} \simeq \sigma^f$.

**Proof.** Assume that

$$\sigma \xrightarrow{r} \sigma_r \xrightarrow{\text{Solve}^*} \sigma^f_r (\xrightarrow{v} \sigma_v \xrightarrow{\text{Solve}^*} \sigma^f_v)$$

The labeled arrow $\xrightarrow{\text{Solve}^*}$ means that only solve transitions are applied. Moreover
— if \( \sigma_f \) has the form \( \langle \bar{G}, \text{false}, T \rangle \) then the derivation between the parenthesis is not present and \( \sigma_f = \sigma_f' \).
— the derivation between the parenthesis is present and \( \sigma_f = \sigma_f' \), otherwise.

We have two cases since the clause \( v \) is either of the form \( v@k' \) \( \iff \) \( D_v \mid \bar{P}, C_v; T_v \) or of the form \( v@k' \) \( \iff \) \( D_v \mid \bar{P}, C_v; T_v \). We consider only the first case. The other one is analogous and hence it is omitted.

**Preliminaries:** Let \( \sigma = \langle \langle \bar{H}_1, \bar{H}_2, \bar{H}_3 \rangle, C, T \rangle_j \) be a built-in free state and let \( r@H'_1 \backslash H'_2 \iff D_r \mid \bar{K}, k, C_r; T_r \) and \( v@k' \) \( \iff \) \( D_v \mid \bar{P}, C_v; T_v \) where \( k = k\#i \), \( C_r \) is the conjunction of all the built-in constraints in the body of \( r \) and

\[
CT \models (D_r \land C_r) \rightarrow chr(\bar{k}) = k' \theta. \tag{5}
\]

Furthermore assume that \( m \) is the greatest identifier which appears in the rule \( r \) and that \( \text{inst}(\bar{P}, T_v, m) = (\bar{P}_1, T_1, m_1) \). Then the unfolded rule is:

\[
r'@H'_1 \backslash H'_2 \iff D_r, (D'_r(\theta)) \mid \bar{K}, k, \bar{P}_1, C_r, \text{chr}(\bar{k}) = k'; T_r,
\]

where \( v@id(\bar{k}) \notin T_r, V \subseteq D_v \) is the greatest set of built-in constraints \( c \), such that \( CT \models (D_r \land C_r) \rightarrow c \theta \), \( D'_r = D_r \backslash V \), the constraint \( (D_r, (D'_r(\theta))) \) is satisfiable and then \( T_r' = \text{clean}((\bar{K}, k), T_r) \cup T_1 \cup \{v@id(\bar{k})\} \). Since by hypothesis, \( CT \models (D_r, (D'_r(\theta))) \iff D_r \), we have that

\[
CT \models (D_r \land C_r) \rightarrow D_r \theta \quad \text{and} \quad D'_r \theta = \emptyset. \tag{6}
\]

**The proof:** By definition of the transition **Apply**\(^*\), we have that

\[
CT \models C \rightarrow \exists_x ((chr(\bar{H}_1, \bar{H}_2) = (H'_1, H'_2)) \land D_r), \tag{7}
\]

where \( x = Fv(H'_1, H'_2) \) and

\[
\sigma_r = \langle \langle \bar{Q}_2, C_r \rangle, chr(\bar{H}_1, \bar{H}_2) = (H'_1, H'_2) \land C, T_4 \rangle_{j + m},
\]

where \( \bar{Q}_2 = (H_1, \bar{H}_3, \bar{K}', k') \), \( ((K''', k'''), T_2, j + m) = \text{inst}((\bar{K}, k), T_r, j) \) and

— if \( H'_2 = \emptyset \) then \( T_4 = T \cup T_2 \cup \{r@id(\bar{H}_1)\} \)
— if \( H'_2 \neq \emptyset \) then \( T_4 = T \cup T_2 \).

Therefore, by definition

\[
\sigma_r' = \langle \bar{Q}_2, C_r', T_4 \rangle_{j + m}.
\]

where

\[
CT \models C_r' \iff C_r \land chr(\bar{H}_1, \bar{H}_2) = (H'_1, H'_2) \land C. \tag{8}
\]

On the other hand, by \( \square_1 \), \( \square_2 \) and by definition of the transition **Apply**\(^*\), we have that

\[
\sigma_r' = \langle \langle \bar{Q}, C_r, C_v, chr(\bar{k}) = k' \rangle, chr(\bar{H}_1, \bar{H}_2) = (H'_1, H'_2) \land C, T_3 \rangle_{j + m_1},
\]

where \( \bar{Q} = (\bar{H}_1, \bar{H}_5, \bar{Q}_1) \), with \( \text{inst}((\bar{K}, k), T_r, j) = (\bar{Q}_1, T_r', j + m_1) \) and

— if \( H'_2 = \emptyset \) then \( T_3 = T \cup T_r' \cup \{r@id(\bar{H}_1)\} \)
— if \( H'_2 \neq \emptyset \) then \( T_3 = T \cup T_r' \).
Therefore, by definition
\[ \sigma_v^f = (\tilde{Q}, C_v^f, T_3)_{j+m_1}. \]
where
\[ CT \models C_v^f \iff C_v \land \sigma(\tilde{k}) = k' \land \operatorname{chr}(\tilde{H}_1, \tilde{H}_2) = (\tilde{H}_1', \tilde{H}_2') \land C. \]

Now, we have two possibilities

1. \( (C_v^f = \text{false}) \). In this case, by construction we have that \( C_v^f = \text{false} \). Therefore \( \sigma_v^f \simeq \sigma_v^f \) and then the thesis.

2. \( (C_v^f \neq \text{false}) \). By definition, since \( \operatorname{chr}(\tilde{k}) = \operatorname{chr}(\tilde{k}'') \), by (5), (6) and (7), we have that
\[ CT \models (C_v \land \operatorname{chr}(\tilde{H}_1, \tilde{H}_2) = (\tilde{H}_1', \tilde{H}_2') \land C) \rightarrow \exists_y((\operatorname{chr}(\tilde{k}'') = k') \land D_v), \]
where \( y = Fv(k) \). Therefore by (3)
\[ CT \models C_v^f \rightarrow (\exists_y((\operatorname{chr}(\tilde{k}'') = k') \land D_v)) \]
and since by hypothesis \( v \) rewrites the atom \( \tilde{k}'' \) corresponding to \( \tilde{k} \in \tilde{K}_r \), we have that
\[ \sigma_v = ((Q_3, C_v), \operatorname{chr}(\tilde{k}'') = k' \land C_v \land \operatorname{chr}(\tilde{H}_1, \tilde{H}_2) = (\tilde{H}_1', \tilde{H}_2') \land C, T_5)_{m_1}, \]
where \( Q_3 = (\tilde{H}_1, \tilde{H}_3, \tilde{k}'', \tilde{P}_2), \) with \( \operatorname{inst}(\tilde{P}, T_v, j + m) = (\tilde{P}_2, T_v', m_1) \) and \( T_5 = T_4 \cup T_v' \cup \{v@\operatorname{id}(\tilde{k}'')\} \).

Finally by definition, we have that
\[ \sigma_v^f = (Q_3, C_v^f, T_5)_{m_1}, \]
where
\[ CT \models C_v^f \iff C_v \land \operatorname{chr}(\tilde{k}'') = k' \land C_v \land \operatorname{chr}(\tilde{H}_1, \tilde{H}_2) = (\tilde{H}_1', \tilde{H}_2') \land C. \]

If \( C_v^f = \text{false} \) then the proof is analogous to the previous case and hence it is omitted.

Otherwise, the proof is analogous to that given for Proposition 4.8 and hence it is omitted.

\( \square \)

**Theorem 5.7.** Let \( P \) be an annotated program, \( r@H_1 \setminus H_2 \Leftrightarrow D | \tilde{A}; T \) be a rule in \( P \) such that \( r@H_1 \setminus H_2 \Leftrightarrow D | \tilde{A}; T \) can be safely replaced in \( P \) according to Definition 4.6. Assume also that
\[ P' = (P \setminus \{r@H_1 \setminus H_2 \Leftrightarrow D | \tilde{A}; T\}) \cup \operatorname{Unf}_P(r@H_1 \setminus H_2 \Leftrightarrow D | \tilde{A}; T). \]
Then \( QA'_{P'}(G) = QA'_{P'}(G) \) for any arbitrary goal \( G \).

**Proof.** By using a straightforward inductive argument and by Proposition 4.9 we have that
\[ QA'_{P'}(G) = QA'_{P'}(G) \]
where
\[ P'' = P \cup \operatorname{Unf}_P(r@H_1 \setminus H_2 \Leftrightarrow D | \tilde{A}; T), \]
for any arbitrary goal \( G \).
Then to prove the thesis, we have only to prove that
\[ QA'_{P'}(G) = QA'_{P''}(G). \]
We prove the two inclusions separately.

\( \{ QA'_{P'}(G) \subseteq QA'_{P''}(G) \} \). The proof is by contradiction. Assume that there exists \((K' \land d') \in QA'_{P'}(G) \setminus QA'_{P''}(G) \). By definition there exists a derivation
\[ \delta = (I_0^n(G), true, \emptyset)_m \rightarrow^*_{\omega_1} (K', d, T)_n \not\rightarrow^*_{\omega_1} \]
in \( P' \), such that \((K' \land d') = \exists_{F_{n(G)}}(chr(\bar{K}) \land d) \). Since \( P' \subseteq P'' \), we have that there exists a derivation
\[ (I_0^n(G), true, \emptyset)_m \rightarrow^*_{\omega_1} (\bar{K}, d, T)_n \]
in \( P'' \). Moreover, since \( P'' = P' \cup \{(r@H_1 \setminus H_2 \Leftrightarrow D | \bar{A}; T)\} \) and \((K' \land d') \not\in QA'_{P''}(G) \), we have that there exists a derivation step \((\bar{K}, d, T)_n \rightarrow^*_{\omega_1} (\bar{K}_1, d_1, T_1)_n \) by using the clause \( r@H_1 \setminus H_2 \Leftrightarrow D | \bar{A}; T \).

Since \( r@H_1 \setminus H_2 \Leftrightarrow D | \bar{A}; T \) can be safely replaced in \( P \), we have that there exists
\[ r@H_1 \setminus H_2 \Leftrightarrow D' | \bar{A}; T' \in Unf_P(r@H_1 \setminus H_2 \Leftrightarrow D | \bar{A}; T) \]
such that \( CT \models D \Leftrightarrow D' \).

Then there exists a derivation step \((\bar{K}, d, T)_n \rightarrow^*_{\omega_1} (\bar{K}_2, d_2, T_2)_n \) in \( P' \) (by using the clause \( r@H_1 \setminus H_2 \Leftrightarrow D' | \bar{A}; T' \in P'' \) and then we have a contradiction.

\( \{ QA'_{P''}(G) \subseteq QA'_{P'}(G) \} \). First of all, observe that by Proposition 4.7, \( QA'(P'') \) can be calculated by considering only normal terminating derivations.

Moreover, since by hypothesis \( r@H_1 \setminus H_2 \Leftrightarrow D | \bar{A}; T \) can be safely replaced in \( P \), following Definition 5.6 (Safe rule replacement), we have that
\[ Unf_P(r@H_1 \setminus H_2 \Leftrightarrow D | \bar{A}; T) \neq \emptyset \]
and
\[ r@H_1 \setminus H_2 \Leftrightarrow D' | \bar{B}; T', i \in Unf_P(r@H_1 \setminus H_2 \Leftrightarrow D | \bar{A}; T) \]
if and only if there exists a rule \( v \in P \) with a single atom in the head such that
\[ (r@H_1 \setminus H_2 \Leftrightarrow D' | \bar{B}; T', i) \in U^+_v (r@H_1 \setminus H_2 \Leftrightarrow D | \bar{A}; T), \]
and \( CT \models D \Leftrightarrow D' \).

Then for each normal terminating derivation \( \delta \), which uses the clause \( r@H_1 \setminus H_2 \Leftrightarrow D | \bar{A}; T \) after the application of \( r@H_1 \setminus H_2 \Leftrightarrow D | \bar{A}; T \), we obtain the state \( \sigma_r \) and then the built-in free state \( \sigma^f_r = (K, C, T'' \mid m). \) Now, we have two cases
—either \( CT \models C \not\models false \)
—or \( CT \models C \models false \). In this case, since by hypothesis \( r@H_1 \setminus H_2 \Leftrightarrow D | \bar{A}; T \) can be safely replaced in \( P \), following Definition 5.5, we have there exists an atom \( \bar{k} \in \bar{A} \), such that \( \bar{k} \) is rewritten in \( \delta \) by using a clause \( v \in P \), \( (r@H_1 \setminus H_2 \Leftrightarrow D' | \bar{B}; T', id(\bar{k})) \in U^+_v (r@H_1 \setminus H_2 \Leftrightarrow D | \bar{A}; T) \) and \( CT \models D \Leftrightarrow D' \). Without loss of generality we can assume that in the derivation \( \delta \), the clause \( v \) is applied to the considered state \( \sigma^f_r = (K, C, T'' \mid m) \) (in order to rewrite the atom \( \bar{k}' \) corresponding to \( \bar{k} \in \bar{A} \).
In both the cases, the proof is straightforward, by using previous observations and by Proposition 5.6.

Of course, previous result can be applied to a sequence of program transformations. Let us define such a sequence as follows.

**Definition** U-sequence. Let $P$ be an annotated CHR program. An U-sequence of programs starting from $P$ is a sequence of annotated CHR programs $P_0, \ldots, P_n$, such that

$$
P_0 = P \quad \text{and} \quad P_{i+1} = P_i \setminus \{(r \overrightarrow{H_1} \backslash H_2 \Leftrightarrow D | \tilde{A}; T)\} \cup \text{Unf}_{P_i}(r \overrightarrow{H_1} \backslash H_2 \Leftrightarrow D | \tilde{A}; T),$$

where $i \in [0, n - 1]$, $(r \overrightarrow{H_1} \backslash H_2 \Leftrightarrow D | \tilde{A}; T) \in P_i$ and $(r \overrightarrow{H_1} \backslash H_2 \Leftrightarrow D | \tilde{A}; T)$ is safety deleting from $P_i$.

Then from Theorem 5.7 and Proposition 3.6 we have immediately the following.

**Corollary 5.9.** Let $P$ be a program and let $P_0, \ldots, P_n$ be an U-sequence starting from $\text{Ann}(P)$. Then $\mathcal{QA}_P(G) = \mathcal{QA}_P(G)$ for any arbitrary goal $G$.

**Proof.** Proposition 3.6 proves that $\mathcal{QA}_P(G) = \mathcal{QA}_P(G)$, for every goal $G$, where $P_0 = \text{Ann}(P)$. Theorem 5.7 proves that, for every goal $G$ and for $i \in [1, n - 1]$, $\mathcal{QA}_P(G) = \mathcal{QA}_P(G)$. Then the proof follows by a straightforward inductive argument.

\[\square\]

### 6. CONFLUENCE AND TERMINATION

It is also possible to prove that our unfolding preserves normal termination and normal confluence.

The formal definition of termination from [Frühwirth 2004] is introduced and adapted to our $\omega'$ semantics.

**Definition** Termination. A CHR program $P$ is called terminating, if there are no infinite computations.

**Definition** Normal Termination. A (possibly annotated) CHR program $P$ is called normal terminating, if there are no infinite normal computations.

**Proposition** Normal Termination. Let $P$ be a CHR program and let $P_0, \ldots, P_n$ be an U-sequence starting from $\text{Ann}(P)$. $P$ satisfies normal termination if and only if $P_n$ satisfies normal termination.

**Proof.** By Lemma 3.3 we have that $P$ is normal terminating if and only if $\text{Ann}(P)$ is normal terminating. Moreover from Proposition 4.8 and Proposition 5.6 and by using a straightforward inductive argument, we have that for each $i = 0, \ldots, n - 1$, if $P_i$ satisfies normal termination if and only if $P_{i+1}$ satisfies the normal termination too and then the thesis.

\[\square\]
When (standard) termination is considered instead of normal termination, program transformation, defined in Definition 5.8 (U-sequence), can introduce problems connected to the guard elimination process of Definition 4.1 (Unfold) as showed in the following example.

**Example 6.4.** Let us consider the following program:

\[
P = \{ \begin{array}{l}
  r_1 @ p(X) \Leftrightarrow X = a, q(X). \\
  r_2 @ q(Y) \Leftrightarrow Y = a \mid r(Y). \\
  r_3 @ r(Z) \Leftrightarrow Z = d \mid p(Z). 
\end{array} \}
\]

where we do not consider the identifiers and the token store in the body of rules, because we do not have propagation rules in \(P\). Then the following possible unfolded program \(P'\) is given:

\[
P' = \{ \begin{array}{l}
  r_1 @ p(X) \Leftrightarrow X = a, X = Y, r(Y). \\
  r_2 @ q(Y) \Leftrightarrow Y = a \mid r(Y). \\
  r_3 @ r(Z) \Leftrightarrow Z = d \mid p(Z). 
\end{array} \}
\]

It is easy to check that the program \(P\) satisfies the (standard) termination. If instead the program \(P'\) and the start goal \((V = d, p(V))\) are considered, the following state can be reached

\[((X = a, p(Z) \neq 3), (V = d, V = X, X = Y, Y = Z), \emptyset)\]

where \(r_1, r_3\) (in the order) can be applied infinite times if the built-in constraint \(X = a\) is not moved by Solve' rule into the built-in store, where it would be evaluated.

This can happen because of the non determinism in rule application of \(\omega'\) semantics.

The confluence property guarantees that any computation for a goal results in the same final state, no matter which of the applicable rules are applied [Abdennadher and Frühwirth 2003].

This means that \(\mathcal{QA}_P(G)\) has cardinality at the most one for each goal \(G\). The formal definition of confluence from [Frühwirth 2004] is introduced and adapted to our \(\omega'\) semantics. Confluence is considered only for normal terminating programs and in this case \(\mathcal{QA}_P(G)\) has cardinality exactly one for each goal \(G\). In the following \(\rightarrow^*\) means either \(\rightarrow_{\omega'}\) or \(\rightarrow_{\omega'}^*\).

**Definition Confluence.** A CHR [annotated] program is confluent if for all states \(\sigma, \sigma_1, \sigma_2\): if \(\sigma \rightarrow^* \sigma_1\) and \(\sigma \rightarrow^* \sigma_2\) then exist states \(\sigma'_f\) and \(\sigma''_f\) such that \(\sigma_1 \rightarrow^* \sigma'_f\) and \(\sigma_2 \rightarrow^* \sigma''_f\) and \(\sigma'_f\) and \(\sigma''_f\) are identical up to renaming of local variables, identifiers and logical equivalence of built-in constraints.

We now introduce the concept of normal confluence.

**Definition 6.6.** Let \(\sigma_1, \sigma_2 \in \text{Conf}_f(\text{Conf}'_f)\) and let \(V\) be a set of variables. \(\sigma_1 \simeq \sigma_2\) if the following holds:

- either \(\sigma_1\) and \(\sigma_2\) are both failed configurations
- or \(\sigma_1\) and \(\sigma_2\) are identical up to renaming of variables not in \(V\), identifiers, up to cleaning the token store (namely, up to deleting from the token store all the tokens for which at least one identifier is not present in the set of identified CHR constraints) and logical equivalence of built-in constraints.
Definition Normal Confluence. A CHR [annotated] program is normal confluent if for all states \( \sigma, \sigma_1, \sigma_2 \): if there exist two normal derivations \( \sigma \rightarrow^* \sigma_1 \) and \( \sigma \rightarrow^* \sigma_2 \) then \( \sigma_1 \rightarrow^* \sigma_f' \) and \( \sigma_2 \rightarrow^* \sigma_f'' \), where \( \sigma_f' \equiv \langle \chi \rangle \sigma_f' \).

Observe that, by definition, if a CHR [annotated] program is confluent, then it is normal confluent.

Lemma 6.8. Let \( \sigma, \sigma' \) be final configurations in \( \text{Conf}_\chi \), \( \sigma_1, \sigma_2, \sigma'_1, \sigma'_2 \in \text{Conf}_\chi \) and let \( V \) be a set of variables.

- If \( \sigma \equiv \sigma, \sigma_1 \equiv \sigma' \) then \( \sigma \equiv \sigma', \sigma_1 \equiv \sigma_1' \) if and only if \( \sigma \equiv \sigma', \sigma_1 \equiv \sigma_1' \).
- If \( \sigma_1 \equiv \sigma_2, \sigma_1 \equiv \sigma_2 \) and \( \sigma_2 \equiv \sigma_2' \) then \( \sigma_2 \equiv \sigma_2' \).

Proof. The proof of the first statement follows by definition of \( \equiv \) and by observing that if \( \sigma \) is a final configuration in \( \text{Conf}_\chi \), then \( \sigma \) has either the form \( \langle G, \bar{S}, \text{false}, T \rangle \) or it has the form \( \langle \emptyset, \bar{S}, c, T \rangle \).

The proof of the second statement is straightforward, by observing that if \( \sigma_1 \equiv \sigma_2 \), then \( \sigma_1 \equiv \sigma_2 \) for each set of variables \( V \).

Lemma 6.9. Let \( P \) be a CHR [annotated] program. \( P \) is normal confluent if for all states \( \sigma, \sigma_1, \sigma_2 \): if there exist two normal derivations \( \sigma \rightarrow^* \sigma_1 \) and \( \sigma \rightarrow^* \sigma_2 \) then there exists two normal derivations \( \sigma_1 \rightarrow^* \sigma_f' \) and \( \sigma_2 \rightarrow^* \sigma_f'' \) such that \( \sigma_f' \equiv \sigma_f'' \).

Proof. In the following we assume that \( P \) is a CHR annotated program. If \( P \) is a standard CHR program, the proof is analogous and hence it is omitted.

The proof is by contradiction. Assume that \( P \) is normal confluent and there exists the states \( \sigma, \sigma_1, \sigma_2 \) such that there exists two normal derivations \( \sigma \rightarrow^* \sigma_1 \) and \( \sigma \rightarrow^* \sigma_2 \) such that there are no two normal derivations \( \sigma_1 \rightarrow^* \sigma_f' \) and \( \sigma_2 \rightarrow^* \sigma_f'' \) such that \( \sigma_f' \equiv \sigma_f'' \).

Let \( \sigma_f' = \langle K_1, D_1, T_1 \rangle \) and \( \sigma_f'' = \langle K_2, D_2, T_2 \rangle \) be the built-in free state obtained from \( \sigma_1' \) (\( \sigma_2' \)) by evaluating all the built-in constraints in \( \sigma_1' \) (\( \sigma_2' \)). Since \( \sigma_1' \equiv \sigma_f' \) \( \sigma_2' \), it is easy to check that \( \sigma_1' \equiv \sigma_f' \).

Now, we have two possibilities

- \( D_1 \neq \text{false} \) and \( D_2 \neq \text{false} \). In this case, it is easy to check that there exists two normal derivation \( \sigma_1 \rightarrow^* \sigma_f' \) and \( \sigma_2 \rightarrow^* \sigma_f'' \) obtained form \( \sigma_1 \rightarrow^* \sigma_1' \) and \( \sigma_2 \rightarrow^* \sigma_2' \) by evaluating the built-in constraints as soon as possible.

- \( D_1 = \text{false} \) and \( D_2 = \text{false} \). In this case, we that there exists two normal derivations, such that \( \sigma_1 \rightarrow^* \sigma_f' \) and \( \sigma_2 \rightarrow^* \sigma_f'' \), where

\[
\sigma_f' = \langle K_1', \text{false}, T_1' \rangle \quad \text{and} \quad \sigma_f'' = \langle K_2', \text{false}, T_2' \rangle.
\]

In both the case, by definition of \( \equiv \), we have a contradiction to the hypothesis that there are two normal derivations \( \sigma_1 \rightarrow^* \sigma_f' \) and \( \sigma_2 \rightarrow^* \sigma_f'' \) such that \( \sigma_f' \equiv \sigma_f'' \).

\( \square \)

The following Lemma is a straightforward consequence of the previous one.
LEMMA 6.10. Let $P$ be a CHR [annotated] normal terminating program. If $P$ is not normal confluent there exist a state $\sigma$ and two normal derivations $\sigma \rightarrow^* \sigma_1^f \not\rightarrow^* \sigma_2^f$ and $\sigma \rightarrow^* \sigma_2^f \not\rightarrow^* \sigma_1^f$ such that $\sigma_1^f \not\equiv_{F_v(\sigma)} \sigma_2^f$.

Proof. Assume that $P$ is not normal confluent. By Lemma 6.9 there exist the states $\sigma, \sigma_1, \sigma_2$ such that there exist two normal derivations $\sigma \rightarrow^* \sigma_1$ and $\sigma \rightarrow^* \sigma_2$ and there are no two normal derivations $\sigma_1 \rightarrow^* \sigma_1^f$ and $\sigma_2 \rightarrow^* \sigma_2^f$ in $P$ such that $\sigma_1^f \not\equiv_{F_v(\sigma)} \sigma_2^f$.

Since $P$ is normal terminating, there are two normal derivations $\sigma \rightarrow^* \sigma_1 \rightarrow^* \sigma_1^f \not\rightarrow^* \sigma_2^f$ and $\sigma \rightarrow^* \sigma_2 \rightarrow^* \sigma_2^f \not\rightarrow^* \sigma_1^f$ in $P$. By previous observation, we have that $\sigma_1^f \not\equiv_{F_v(\sigma)} \sigma_2^f$ and then the thesis.

COROLLARY Normal Confluence. Let $P$ be a normal terminating CHR program and let $P_0, \ldots, P_n$ be an U-sequence starting from Ann($P$). $P$ satisfies normal confluence if and only if $P_n$ satisfies normal confluence too.

Proof. —Assume that $P$ is a normal terminating CHR program and that $P$ satisfies normal confluence. We prove that $P_n$ satisfies normal confluence too. First of all, observe, that by hypothesis and by Proposition 6.3 we have that $P_n$ is normal terminating. Let us assume by contrary that $P_n$ does not satisfy normal confluence. By Lemma 6.10 there exists a state $\sigma = (\langle K, D, C, T \rangle_o, 2)$ and two normal derivations $\sigma \rightarrow^* \omega_i$, $\sigma_1^f \not\rightarrow^*_{\omega_i} \omega_i$ and $\sigma \rightarrow^*_{\omega_i} \sigma_2^f \not\rightarrow^*_{\omega_i} \omega_i$ in $P_n$ such that $\sigma_1^f \not\equiv_{F_v(\sigma)} \sigma_2^f$.

Then, by using arguments similar to that given in Proposition 4.8 we have that there exist two normal derivations $\sigma \rightarrow^*_{\omega_i} \sigma_1^f \not\rightarrow^*_{\omega_i} \omega_i$ and $\sigma \rightarrow^*_{\omega_i} \sigma_2^f \not\rightarrow^*_{\omega_i} \omega_i$ in $P_0$, where $\sigma_1^f \not\equiv \sigma_2^f$ and $\sigma_1^f \not\equiv \sigma_2^f$.

Therefore, by Proposition 5.6 there exist two normal derivations $\sigma' \rightarrow^*_{\omega_i} \sigma_1^f \not\rightarrow^*_{\omega_i} \omega_i$ and $\sigma' \rightarrow^*_{\omega_i} \sigma_2^f \not\rightarrow^*_{\omega_i} \omega_i$ in $P$, where $\sigma' = (\langle D, K, C, T \rangle_{o+1}, \sigma_1^f \equiv \sigma_1^f$ and $\sigma_2^f \equiv \sigma_2^f$. Since by hypothesis $P$ is normal confluent, we have that $\sigma_1^f \not\equiv_{F_v(\sigma)} \sigma_2^f$ and therefore, by Lemma 6.8 we have a contradiction to the fact that $\sigma_1^f \not\equiv_{F_v(\sigma)} \sigma_2^f$ and then the thesis.

—Assume that $P$ is a normal terminating CHR program and that $P_n$ satisfies normal confluence. The proof that $P$ satisfies normal confluence is analogous to the previous one, by using Proposition 5.6 instead of Proposition 4.8.

\[ \square \]

7. WEAK SAFE RULE REPLACEMENT

In this subsection we consider only normal terminating and normal confluent programs and we give a weaker condition in order to safely replace the original rule $r$ by its unfolded version while maintaining the qualified answers semantics. Intuitively this holds when there exists a rule obtained by the unfolding of $r$ in $P$ whose guard is equivalent to that of $r$. 

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Definition 7.1. (Weak safe rule replacement) Let \( P \) be an annotated CHR program and let \( r @ H_1 \backslash H_2 \Leftrightarrow D \mid \hat{A}; T \in P \), such that there exists
\[
r @ H_1 \backslash H_2 \Leftrightarrow D' \mid \hat{A}; T' \in Unf_P(r @ H_1 \backslash H_2 \Leftrightarrow D \mid \hat{A}; T)
\]
with \( CT \models D \leftrightarrow D' \).

Then we say that the rule \( r @ H_1 \backslash H_2 \Leftrightarrow D \mid \hat{A}; T \) can be weakly safe replaced (by its unfolded version) in \( P \).

Definition WU-sequence. Let \( P \) be an annotated CHR program. An WU-sequence of programs starting from \( P \) is a sequence of annotated CHR programs \( P_0, \ldots, P_n \), such that
\[
P_0 = P
\]
\[
P_{i+1} = P_i \backslash \{(r @ H_1 \backslash H_2 \Leftrightarrow D \mid \hat{A}; T)\} \cup Unf_P(r @ H_1 \backslash H_2 \Leftrightarrow D \mid \hat{A}; T),
\]
where \( i \in [0, n - 1] \), \( (r @ H_1 \backslash H_2 \Leftrightarrow D \mid \hat{A}; T) \in P_i \) and \( (r @ H_1 \backslash H_2 \Leftrightarrow D \mid \hat{A}; T) \) is weakly safety deleting from \( P_i \).

Proposition 7.3. Let \( P \) be an annotated CHR program and let \( r @ H_1 \backslash H_2 \Leftrightarrow D \mid \hat{A}; T \in P \) such that \( r @ H_1 \backslash H_2 \Leftrightarrow D \mid \hat{A}; T \) can be weakly safe replaced (by its unfolded version) in \( P \). Moreover let
\[
P' = (P \backslash \{(r @ H_1 \backslash H_2 \Leftrightarrow D \mid \hat{A}; T)\}) \cup Unf_P(r @ H_1 \backslash H_2 \Leftrightarrow D \mid \hat{A}; T)
\]
If \( P \) is normal terminating and normal confluent then \( P' \) is normal terminating and normal confluent too.

Proof. First, we prove that if \( P \) is normal terminating and normal confluent then \( P'' \) is normal terminating and normal confluent too, where
\[
P'' = P \cup Unf_P(r @ H_1 \backslash H_2 \Leftrightarrow D \mid \hat{A}; T).
\]
Then we prove that if \( P'' \) is normal terminating and normal confluent then \( P' \) is normal terminating and normal confluent and then the thesis.

—Assume that \( P \) is normal terminating. The proof of the normal termination of \( P'' \) follows by Proposition 4.8.

—Now, assume that \( P \) is normal terminating and normal confluent and by the contrary that \( P'' \) does not satisfy normal confluence.

By Lemma 6.10 and since by previous result \( P'' \) is normal terminating, there exist a state \( \sigma \) and two normal derivations
\[
\sigma \mathop{\rightarrow^*_{\omega_i}} \sigma' \mathop{\not\rightarrow_{\omega_i}} \sigma'' \mathop{\not\rightarrow_{\omega_i}} \sigma'\prime
\]
in \( P'' \) such that \( \sigma' \not\in \text{Unf}(\sigma) \sigma'' \).

Then, by using arguments similar to that given in Proposition 4.8 and since \( P \subseteq P'' \), we have that there exist two normal derivations
\[
\sigma \mathop{\rightarrow^*_{\omega_i}} \sigma_1 \mathop{\not\rightarrow_{\omega_i}} \sigma_2 \mathop{\not\rightarrow_{\omega_i}} \sigma'_1
\]
in \( P \), where \( \sigma' \simeq \sigma_1' \) and \( \sigma'' \simeq \sigma_2'' \). Since by hypothesis \( P \) is normal confluent, we have that \( \sigma_1' \simeq \text{Unf}(\sigma) \sigma_2' \). Therefore, by Lemma 6.10 we have a contradiction to the assumption that there exist two states \( \sigma'_1 \) and \( \sigma''_2 \) as previously defined.
Now, we prove that if $P''$ is normal terminating and normal confluent then $P'$ is normal terminating and normal confluent too and then the thesis.

—If $P''$ is normal terminating then, since $P' \subseteq P''$, we have that $P'$ is normal terminating too.

—Now, assume that $P''$ is normal terminating and normal confluent and by the contrary that $P'$ does not satisfy normal confluence. By Lemma 5.7 and since by previous result $P'$ is normal terminating, there exist a state $\sigma$ and two normal derivations

$$\sigma \xrightarrow{\omega_i} \sigma_1^f \xrightarrow{\omega_i} \sigma_2^f$$

in $P'$ such that $\sigma_1^f \not\equiv_{Fv(\sigma)} \sigma_2^f$.

Since $P' \subseteq P''$, we have that there exist two normal derivations

$$\sigma \xrightarrow{\omega_i} \sigma_1^f \text{ and } \sigma \xrightarrow{\omega_i} \sigma_2^f$$

in $P''$. Then, since $P''$ is normal confluent and $P'' = P' \cup \{r \in H_1 \mid H_2 \not\Rightarrow D \mid \hat{A}; T\}$ there exists $i \in [1, 2]$ such that $\sigma_i^f \not\xrightarrow{\omega_i} \sigma_i'^f$ in $P''$ by using the clause $r \in H_1 \mid H_2 \not\Rightarrow D \mid \hat{A}; T \in (P'' \setminus P')$. In this case, by definition of weakly safe replacement, there exists

$$r \in H_1 \mid H_2 \not\Rightarrow D' \mid \hat{A}; T'; D \not\Rightarrow D \mid \hat{A}; T$$

with $CT \models D \iff D'$. Therefore $\sigma_i^f \not\xrightarrow{\omega_i} \sigma_i'''$ in $P'$ by using the clause $r \in H_1 \mid H_2 \not\Rightarrow D' \mid \hat{A}; T'$ and then we have a contradiction.

\[ \Box \]

\textbf{Theorem 7.4.} Let $P$ be a normal terminating and normal confluent annotated program and let $r \in H_1 \mid H_2 \not\Rightarrow D \mid \hat{A}; T$ be a rule in $P$ such that $r \in H_1 \mid H_2 \not\Rightarrow D \mid \hat{A}; T$ can be weakly safely replaced in $P$ according to Definition 7.1. Assume also that

$$P' = (P \setminus \{r \in H_1 \mid H_2 \not\Rightarrow D \mid \hat{A}; T\}) \cup Unf_P(r \in H_1 \mid H_2 \not\Rightarrow D \mid \hat{A}; T).$$

Then $QA'(P) = QA'(P')$ for any arbitrary goal $G$.

\textbf{Proof.} Analogously to Theorem 5.7, we can prove that $QA'(P) = QA'(P')$ where

$$P' = P \cup Unf_P(r \in H_1 \mid H_2 \not\Rightarrow D \mid \hat{A}; T),$$

for any arbitrary goal $G$.

Then to prove the thesis, we have only to prove that

$$QA'(P) = QA'(P').$$

We prove the two inclusions separately.

$(QA'(P) \subseteq QA'(P'))$. The proof is the same of the case $QA'(P') \subseteq QA'(P')$ of Theorem 5.7 and hence it is omitted.

$(QA'(P') \subseteq QA'(P'))$. The proof is by contradiction. Assume that there exists $(P' \land d') \in QA'(P') \setminus QA'(P')$. Since $P''$ is normal terminating and normal confluent and since by previous point $QA'(P') \subseteq QA'(P')$, we have that $QA'(P') = \emptyset$. This means that each normal derivation in $P'$ is not terminating and hence, by using Proposition 7.3 we have a contradiction.
COROLLARY 7.5. Let $P$ be a normal terminating and normal confluent program and let $P_0, \ldots, P_n$ be an WU-sequence starting from $Ann(P)$. Then $QA_P(G) = QA'_{P_n}(G)$ for any arbitrary goal $G$.

PROOF. We prove by induction on $i$, that for each $i \in [1, n]$, $P_i$ is a normal terminating and normal confluent program and that $QA_P(G) = QA'_{P_n}(G)$ for any arbitrary goal $G$.

$i = 0$. Proposition 3.6 proves that the qualified answer for a program $P$ and its annotated version $P_0 = Ann(P)$, fixed a start goal, is the same. Moreover, by using Proposition 3.6 it is easy to check that if $P$ is normal terminating and normal confluent, then $P_0$ is normal terminating and normal confluent.

$i > 0$. Assume that the thesis holds for $i-1$, namely $P_{i-1}$ is a normal terminating and normal confluent program and that $QA_P(G) = QA'_{P_{i-1}}(G)$ for any arbitrary goal $G$. Then, by using Proposition 7.3 we have that $P_i$ is a normal terminating and normal confluent program. Moreover by Theorem 7.4 we have that $QA'_{P_i}(G) = QA'_{P_{i-1}}(G)$ Therefore by inductive hypothesis $QA_P(G) = QA'_{P_{i-1}}(G)$ and then the thesis.

8. CONCLUSIONS

In this paper we have defined an unfold operation for CHR which preserves the qualified answers of a program.

This was obtained by transforming a CHR program into an annotated one which is then unfolded. The equivalence of the unfolded program and the original (non annotated) one is proven (Proposition 3.6), by using a slightly modified operational semantics for annotated programs (as defined in Section 3). We then provided a condition that could be used to safely replace a rule with its unfolded version, whilst simultaneously preserving qualified answers, for a restricted class of rules. Confluence and termination maintenance of the program modified in the previous way are proven.

There are only few other papers that consider source to source transformation of CHR programs. [Frühwirth 2004], rather than considering a generic transformation system focuses on the specialization of rules regarding a specific goal, analogously to what happens in partial evaluation. In [Frühwirth and Holzbaur 2003], CHR rules are transformed in a relational normal form, over which a source to source transformation is performed. However, the correctness of such a transformation was not proven. Some form of transformation for probabilistic CHR is considered in [Frühwirth et al. 2002], while guard optimization was studied in [Sneyers et al. 2005].

Both the general and the goal specific approaches are important in order to define practical transformation systems for CHR. In fact, on the one hand of course one needs some general unfold rule, on the other hand, given the difficulties in removing rules from the transformed program, some goal specific techniques can help to improve the efficiency of the transformed program for specific classes of goals. A method for deleting redundant CHR rules is considered in [Abdenmadher and Frühwirth 2003]. However it is based on a semantic check and
it is not clear whether it can be transformed into a specific syntactic program transformation rule.

When considering more generally the field of concurrent logic languages, we find a few papers which address the issue of program transformation. Notable examples include [Etalle et al. 2001] that deals with the transformation of concurrent constraint programming (ccp) and [Ueda and Furukawa 1988] that considers Guarded Horn Clauses (GHC). The results in these papers are not directly applicable to CHR because neither ccp nor GHC allow rules with multiple heads.

The third section of this paper can be considered as a first step in the direction of defining a transformation system for CHR programs, based on unfolding. This step could be improved in several directions. First of all, the unfolding operation could be extended to also take into consideration the constraints in the propagation part of the head of a rule instead of only the body ones. In addition, the condition that we have provided for safely replacing a rule could be generalized to include more cases. Also, we could extend to CHR some of the other transformations, notably folding, which have been defined in [Etalle et al. 2001] for ccp. Finally, we would like to investigate from a practical perspective to what extent program transformation can improve the performances of the CHR solver. Clearly the application of an unfolded rule avoids some computational steps assuming of course that unfolding is done at the time of compilation, even though the increase in the number of rules could eliminate this improvement when the original rule cannot be removed. Here it would probably be important to consider some unfolding strategy, in order to decide which rules have to be unfolded.

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