Executable Transitive Closures of Finite Relations*

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Abstract

We provide a generic work-list algorithm to compute the transitive closure of finite relations where only successors of newly detected states are generated. This algorithm is then instantiated for lists over arbitrary carriers and red black trees [1] (which are faster but require a linear order on the carrier), respectively.

Our formalization was performed as part of the IsaFoR/CeTA project¹ [2], where reflexive transitive closures of large tree automata have to be computed.

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 $^{^{1}}http://cl-informatik.uibk.ac.at/software/ceta$

1 A Generic Work-List Algorithm

theory Transitive-Closure-Impl imports Main begin

Let R be some finite relation. We start to present a standard worklist algorithm to compute all elements that are reachable from some initial set by at most n R-steps. Then, we obtain algorithms for the (reflexive) transitive closure from a given starting set by exploiting the fact that for finite relations we have to iterate at most *card* R times. The presented algorithms are generic in the sense that the underlying data structure can freely be chosen, you just have to provide certain operations like union, membership, etc.

1.1 Bounded Reachability

We provide an algorithm relpow-impl that computes all states that are reachable from an initial set of states new by at most n steps. The algorithm also stores a set of states that have already been visited have, and then show, do not have to be expanded a second time. The algorithm is parametric in the underlying data structure, it just requires operations for union and membership as well as a function to compute the successors of a list.

fun

 $\begin{array}{l} relpow-impl :: \\ ('a\ list \Rightarrow 'a\ list) \Rightarrow \\ ('a\ list \Rightarrow 'b\ \Rightarrow 'b) \Rightarrow ('a \Rightarrow 'b \Rightarrow bool) \Rightarrow 'a\ list \Rightarrow 'b \Rightarrow nat \Rightarrow 'b \\ \hline \textbf{where} \\ relpow-impl\ succ\ un\ memb\ new\ have\ 0 = un\ new\ have\ | \\ relpow-impl\ succ\ un\ memb\ new\ have\ (Suc\ m) = \\ (if\ new\ = \ []\ then\ have \\ else \\ let \\ maybe\ = \ succ\ new; \\ have'\ = \ un\ new\ have; \\ new'\ = \ filter\ (\lambda\ n.\ \neg\ memb\ n\ have')\ maybe \\ in\ relpow-impl\ succ\ un\ memb\ new'\ have'\ m) \end{array}$

We need to know that the provided operations behave correctly.

locale set-access =
fixes un :: 'a list \Rightarrow 'b \Rightarrow 'b
and set-of :: 'b \Rightarrow 'a set
and memb :: 'a \Rightarrow 'b \Rightarrow bool
and empty :: 'b
assumes un: set-of (un as bs) = set as \cup set-of bs
and memb: memb a bs \longleftrightarrow (a \in set-of bs)
and empty: set-of empty = {}

locale set-access-succ = set-access un for $un :: 'a \ list \Rightarrow 'b \Rightarrow 'b +$ fixes $succ :: 'a \ list \Rightarrow 'a \ list$ $and <math>rel :: ('a \times 'a) \ set$ assumes $succ: set \ (succ \ as) = \{b. \exists a \in set \ as. \ (a, b) \in rel\}$ begin

abbreviation relpow- $i \equiv relpow$ -impl succ un memb

What follows is the main technical result of the *relpow-impl* algorithm: what it computes for arbitrary values of *new* and *have*.

```
lemma relpow-impl-main:
  set-of (relpow-i new have n) =
   \{b \mid a \ b \ m. \ a \in set \ new \land m \le n \land (a, b) \in (rel \cap \{(a, b). \ b \notin set \text{-of have}\})\}
\sim m 
   set	ext{-}of\ have
  (is ?! new have n = ?r new have n)
proof (induction n arbitrary: have new)
 case (Suc n hhave nnew)
 show ?case
 proof (cases nnew = [])
   case True
   then show ?thesis by auto
 next
   {\bf case} \ {\it False}
   let ?have = set - of hhave
   let ?new = set nnew
   obtain have new where hav: have = ?have and new: new = ?new by auto
   let ?reln = \lambda m. (rel \cap \{(a, b). b \notin new \land b \notin have\}) \frown m
   let ?rel = \lambda m. (rel \cap \{(a, b), b \notin have\}) \frown m
   have idl: ?l nnew hhave (Suc \ n) =
      {uu. \exists a. (\exists aa \in new. (aa,a) \in rel) \land a \notin new \land a \notin have \land (\exists m \leq n. (a, a))
uu) \in ?reln m) \} \cup
     (new \cup have)
     (is - ?l1 \cup (?l2 \cup ?l3))
     by (simp add: hav new False Let-def Suc, simp add: memb un succ)
   let ?l = ?l1 \cup (?l2 \cup ?l3)
   have idr: ?r nnew hhave (Suc n) = {b. \exists a m. a \in new \land m \leq Suc n \land (a, b)
\in ?rel m} \cup have
     (is - = (?r1 \cup ?r2)) by (simp add: hav new)
   let ?r = ?r1 \cup ?r2
    {
     fix b
     assume b: b \in ?l
     have b \in ?r
     proof (cases b \in new \lor b \in have)
       case True then show ?thesis
       proof
```

```
assume b \in have then show ?thesis by auto
      next
        assume b: b \in new
        have b \in ?r1
         by (intro CollectI, rule exI, rule exI [of - 0], intro conjI, rule b, auto)
        then show ?thesis by auto
      qed
     \mathbf{next}
      case False
      with b have b \in ?l1 by auto
      then obtain a2 a1 m where a2n: a2 \notin new and a2h: a2 \notin have and a1:
a1 \in new
         and a1a2: (a1,a2) \in rel and m: m \leq n and a2b: (a2,b) \in ?reln m by
auto
      have b \in ?r1
       by (rule CollectI, rule exI, rule exI [of - Suc m], intro conjI, rule a1, simp
add: m, rule relpow-Suc-I2, rule, rule a1a2, simp add: a2h, insert a2b, induct m
arbitrary: a2 b, auto)
      then show ?thesis by auto
    qed
   }
   moreover
   {
     fix b
    assume b: b \in ?r
     then have b \in ?l
     proof (cases b \in have)
      case True then show ?thesis by auto
     next
      case False
      with b have b \in ?r1 by auto
      then obtain a m where a: a \in new and m: m \leq Suc n and ab: (a, b) \in
?rel m by auto
      have seq: \exists a \in new. (a, b) \in ?rel m
        using a ab by auto
      obtain l where l: l = (LEAST m. (\exists a \in new. (a, b) \in ?rel m)) by auto
      have least: (\exists a \in new. (a, b) \in ?rel l)
        by (unfold l, rule LeastI, rule seq)
      have lm: l \leq m unfolding l
        by (rule Least-le, rule seq)
      with m have ln: l \leq Suc \ n by auto
      from least obtain a where a: a \in new
        and ab: (a, b) \in ?rel l by auto
      from ab [unfolded relpow-fun-conv]
      obtain f where fa: f \ 0 = a and fb: b = f \ l
        and steps: \bigwedge i. i < l \Longrightarrow (f i, f (Suc i)) \in ?rel 1 by auto
       {
        fix i
        assume i: i < l
```

```
have main: f (Suc i) \notin new
        proof
          assume new: f (Suc i) \in new
          let ?f = \lambda j. f (Suc i + j)
          have seq: (f (Suc i), b) \in ?rel (l - Suc i)
           unfolding relpow-fun-conv
          proof (rule exI[of - ?f], intro conjI allI impI)
           from i show f(Suc \ i + (l - Suc \ i)) = b
             unfolding fb by auto
          \mathbf{next}
           fix j
           assume j < l - Suc i
           then have small: Suc i + j < l by auto
             show (?f j, ?f (Suc j)) \in rel \cap \{(a, b), b \notin have\} using steps [OF]
small] by auto
          qed simp
          from i have small: l - Suc \ i < l by auto
          from seq new have \exists a \in new. (a, b) \in ?rel (l - Suc i) by auto
          with not-less-Least [OF small [unfolded l]]
          show False unfolding l by auto
        qed
        then have (f i, f (Suc i)) \in ?reln 1
          using steps [OF i] by auto
       } note steps = this
      have ab: (a, b) \in ?reln \ l \ unfolding \ relpow-fun-conv
        by (intro exI conjI, insert fa fb steps, auto)
      have b \in ?l1 \cup ?l2
      proof (cases l)
        case \theta
        with ab a show ?thesis by auto
      \mathbf{next}
        case (Suc ll)
        from relpow-Suc-D2 [OF ab [unfolded Suc]] a ln Suc
        show ?thesis by auto
      qed
      then show ?thesis by auto
     qed
   }
   ultimately show ?thesis
     unfolding idl idr by blast
 \mathbf{qed}
qed (simp add: un)
```

From the previous lemma we can directly derive that *relpow-impl* works correctly if *have* is initially set to *empty*

lemma relpow-impl:

set-of (relpow-i new empty n) = {b | a b m. $a \in set new \land m \le n \land (a, b) \in rel \ \ \ \ m$ } **proof** – have *id*: $rel \cap \{(a, b). True\} = rel by auto$ show ?thesis unfolding relpow-impl-main empty by (simp add: *id*) qed

end

1.2 Reflexive Transitive Closure and Transitive closure

Using *relpow-impl* it is now easy to obtain algorithms for the reflexive transitive closure and the transitive closure by restricting the number of steps to the size of the finite relation. Note that *relpow-impl* will abort the computation as soon as no new states are detected. Hence, there is no penalty in using this large bound.

definition

rtrancl-impl ::

 $\begin{array}{l} (('a \times 'a) \ list \Rightarrow 'a \ list \Rightarrow 'a \ list) \Rightarrow \\ ('a \ list \Rightarrow 'b \Rightarrow 'b) \Rightarrow ('a \Rightarrow 'b \Rightarrow bool) \Rightarrow 'b \Rightarrow ('a \times 'a) \ list \Rightarrow 'a \ list \Rightarrow 'b \end{array}$

where

rtrancl-impl gen-succ un memb emp rel =

(let

 $succ = gen-succ \ rel;$ $n = length \ rel$

in $(\lambda \text{ as. relpow-impl succ un memb as emp } n))$

definition

 $\begin{aligned} trancl-impl :: \\ (('a \times 'a) \ list \Rightarrow 'a \ list \Rightarrow 'a \ list) \Rightarrow \\ ('a \ list \Rightarrow 'b \Rightarrow 'b) \Rightarrow ('a \Rightarrow 'b \Rightarrow bool) \Rightarrow 'b \Rightarrow ('a \times 'a) \ list \Rightarrow 'a \ list \Rightarrow 'b \end{aligned}$ $\begin{aligned} \textbf{where} \\ trancl-impl \ gen-succ \ un \ memb \ emp \ rel = \\ (let \\ succ = \ gen-succ \ rel; \\ n = \ length \ rel \end{aligned}$

in (λ as. relpow-impl succ un memb (succ as) emp n))

The soundness of both *rtrancl-impl* and *trancl-impl* follows from the soundness of *relpow-impl* and the fact that for finite relations, we can limit the number of steps to explore all elements in the reflexive transitive closure.

lemma *rtrancl-finite-relpow*:

 $(a, b) \in (set rel)^* \longleftrightarrow (\exists n \leq length rel. (a, b) \in set rel \frown n)$ (is ?l = ?r) proof assume ?rthen show ?l unfolding rtrancl-power by auto next assume ?l from this [unfolded rtrancl-power] obtain n where $ab: (a,b) \in set rel \frown n ...$

obtain l where l: $l = (LEAST n. (a,b) \in set rel \frown n)$ by auto have ab: $(a, b) \in set rel \frown l$ unfolding lby (intro LeastI, rule ab) **from** this [unfolded relpow-fun-conv] **obtain** f where a: f 0 = a and b: f l = band steps: $\bigwedge i$. $i < l \implies (f i, f (Suc i)) \in set rel by auto$ let ?hits = map (λ i. f (Suc i)) [θ ..< l] **from** steps **have** subset: set ?hits \subseteq snd ' set rel by force have $l \leq length rel$ **proof** (cases distinct ?hits) case True have l = length?hits by simp also have $\dots = card$ (set ?hits) unfolding distinct-card [OF True] \dots also have $\dots \leq card$ (snd 'set rel) by (rule card-mono [OF - subset], auto) also have $\dots = card (set (map \ snd \ rel))$ by auto also have $\dots < length$ (map snd rel) by (rule card-length) finally show ?thesis by simp next case False **from** this [unfolded distinct-conv-nth] obtain *i j* where *i*: i < l and *j*: j < l and *ij*: $i \neq j$ and *fij*: f (Suc *i*) = f(Suc j) by *auto* let $?i = min \ i \ j$ let $?j = max \ i \ j$ have i: ?i < l and j: ?j < l and fij: f (Suc ?i) = f (Suc ?j) and *ij*: ?i < ?jusing *i j ij fij* unfolding *min-def* max-def by (cases $i \leq j$, auto) from i j f i j i j obtain i j where i: i < l and j: j < l and i j: i < j and f i j: f $(Suc \ i) = f \ (Suc \ j)$ by blast let $?g = \lambda$ n. if $n \leq i$ then f n else f (n + (j - i))let $\tilde{?l} = l - (j - i)$ have $abl: (a,b) \in set rel \frown ?l$ unfolding *relpow-fun-conv* **proof** (rule exI [of - ?g], intro conjI impI allI) show ?g ?l = b unfolding b [symmetric] using j ij by auto \mathbf{next} fix kassume k: k < ?l**show** $(?g k, ?g (Suc k)) \in set rel$ **proof** (cases k < i) case True with *i* have k < l by *auto* from steps [OF this] show ?thesis using True by simp next $\mathbf{case} \ \mathit{False}$ then have *ik*: $i \leq k$ by *auto* show ?thesis **proof** (cases k = i) case True

```
then show ?thesis using ij fij steps [OF i] by simp
      next
        case False
        with ik have ik: i < k by auto
        then have small: k + (j - i) < l using k by auto
        show ?thesis using steps[OF small] ik by auto
      qed
    qed
   \mathbf{qed} \ (simp \ add: \ a)
   from ij i have ll: ?l < l by auto
   have l \leq ?l unfolding l
    by (rule Least-le, rule abl [unfolded l])
   with ll have False by simp
   then show ?thesis by simp
 qed
 with ab show ?r by auto
qed
```

```
locale set-access-gen = set-access un
for un :: 'a \ list \Rightarrow 'b \Rightarrow 'b +
fixes gen-succ :: ('a \times 'a) \ list \Rightarrow 'a \ list \Rightarrow 'a \ list
assumes gen-succ: set (gen-succ rel as) = {b. \exists a \in set \ as. (a, b) \in set \ rel}
begin
```

abbreviation $rtrancl-i \equiv rtrancl-impl gen-succ$ un memb empty **abbreviation** $trancl-i \equiv trancl-impl gen-succ$ un memb empty

```
lemma rtrancl-impl:
  set-of (rtrancl-i rel as) = {b. (\exists a \in set as. (a, b) \in (set rel)^*)}
  proof -
    interpret set-access-succ set-of memb empty un gen-succ rel set rel
    by (unfold-locales, insert gen-succ, auto)
    show ?thesis unfolding rtrancl-impl-def Let-def relpow-impl
    by (auto simp: rtrancl-finite-relpow)
  qed
lemma trancl-impl:
    set-of (trancl-i rel as) = {b. (\exists a \in set as. (a, b) \in (set rel)^+)}
  proof -
    interpret set-access-succ set-of memb empty un gen-succ rel set rel
    by (unfold-locales, insert gen-succ, auto)
```

show ?thesis

unfolding trancl-impl-def Let-def relpow-impl trancl-unfold-left relcomp-unfold rtrancl-finite-relpow succ by auto

 \mathbf{qed}

end

end

2 Closure Computation using Lists

theory Transitive-Closure-List-Impl imports Transitive-Closure-Impl begin

We provide two algorithms for the computation of the reflexive transitive closure which internally work on lists. The first one (*rtrancl-list-impl*) computes the closure on demand for a given set of initial states. The second one (*memo-list-rtrancl*) precomputes the closure for each individual state, stores the result, and then only does a look-up.

For the transitive closure there are the corresponding algorithms *trancl-list-impl* and *memo-list-trancl*.

2.1 Computing Closures from Sets On-The-Fly

The algorithms are based on the generic algorithms *rtrancl-impl* and *trancl-impl* instantiated by list operations. Here, after computing the successors in a straightforward way, we use *remdups* to not have duplicates in the results. Moreover, also in the union operation we filter to those elements that have not yet been seen. The use of *filter* in the union operation is preferred over *remdups* since by construction the latter set will not contain duplicates.

definition rtrancl-list-impl :: $('a \times 'a)$ list \Rightarrow 'a list \Rightarrow 'a list **where** rtrancl-list-impl = rtrancl-impl $(\lambda \ r \ as. \ remdups \ (map \ snd \ (filter \ (\lambda \ (a, \ b). \ a \in set \ as) \ r))))$ $(\lambda \ xs \ ys. \ (filter \ (\lambda \ x. \ x \notin set \ ys) \ xs) \ @ \ ys)$ $(\lambda \ x \ xs. \ x \in set \ xs)$ []

definition trancl-list-impl :: $(a \times a)$ list $\Rightarrow a$ list $\Rightarrow a$ list where trancl-list-impl = trancl-impl $(\lambda \ r \ as. \ remdups \ (map \ snd \ (filter \ (\lambda \ (a, \ b). \ a \in set \ as) \ r)))$ $(\lambda \ xs \ ys. \ (filter \ (\lambda \ x. \ x \notin set \ ys) \ xs) \ @ \ ys)$

```
(\lambda \ x \ xs. \ x \in set \ xs)
```

lemma *rtrancl-list-impl*:

set $(rtrancl-list-impl \ r \ as) = \{b. \exists a \in set \ as. (a, b) \in (set \ r)^*\}$ unfolding rtrancl-list-impl-defby $(rule \ set-access-gen.rtrancl-impl, \ unfold-locales, \ force+)$

lemma trancl-list-impl:

set $(trancl-list-impl \ r \ as) = \{b. \exists a \in set as. (a, b) \in (set \ r)^+\}$ unfolding trancl-list-impl-defby $(rule \ set-access-gen.trancl-impl, \ unfold-locales, \ force+)$

2.2 Precomputing Closures for Single States

Storing all relevant entries is done by mapping all left-hand sides of the relation to their closure. To avoid redundant entries, *remdups* is used.

```
definition memo-list-rtrancl :: ('a \times 'a) list \Rightarrow ('a \Rightarrow 'a list)
where
  memo-list-rtrancl r =
   (let
     tr = rtrancl-list-impl r;
     rm = map \ (\lambda a. \ (a, \ tr \ [a])) \ ((remdups \circ map \ fst) \ r)
   in
     (\lambda a. \ case \ map-of \ rm \ a \ of
       None \Rightarrow [a]
     | Some as \Rightarrow as))
lemma memo-list-rtrancl:
  set (memo-list-rtrancl r a) = {b. (a, b) \in (set r)^*} (is ?l = ?r)
proof –
 let ?rm = map (\lambda \ a. (a, rtrancl-list-impl r [a])) ((remdups \circ map fst) r)
 show ?thesis
 proof (cases map-of ?rm a)
   case None
   have one: ?l = \{a\}
     unfolding memo-list-rtrancl-def Let-def None
     by auto
   from None [unfolded map-of-eq-None-iff]
   have a: a \notin fst 'set r by force
    ł
     fix b
     assume b \in ?r
     from this [unfolded rtrancl-power relpow-fun-conv] obtain n f where
       ab: f \ 0 = a \land f \ n = b and steps: \bigwedge i. i < n \Longrightarrow (f \ i, f \ (Suc \ i)) \in set \ r by
auto
     from ab steps [of 0] a have a = b
       by (cases n, force+)
   then have ?r = \{a\} by auto
   then show ?thesis unfolding one by simp
  next
   case (Some as)
   have as: set as = \{b. (a, b) \in (set r)^*\}
     using map-of-SomeD [OF Some]
       rtrancl-list-impl [of r [a]] by force
   {\bf then \ show} \ ? thesis \ {\bf unfolding} \ memo-list-rtrancl-def \ Let-def \ Some \ {\bf by} \ simp
 qed
qed
definition memo-list-trancl :: ('a \times 'a) list \Rightarrow ('a \Rightarrow 'a list)
```

where

```
\begin{array}{l} memo-list-trancl \ r = \\ (let \\ tr = trancl-list-impl \ r; \\ rm = map \ (\lambda a. \ (a, \ tr \ [a])) \ ((remdups \circ map \ fst) \ r) \\ in \\ (\lambda a. \ case \ map-of \ rm \ a \ of \\ None \Rightarrow \ [] \\ | \ Some \ as \Rightarrow \ as)) \end{array}
```

```
lemma memo-list-trancl:
 set (memo-list-trancl r a) = {b. (a, b) \in (set r)^+} (is ?l = ?r)
proof –
 let ?rm = map (\lambda \ a. (a, trancl-list-impl \ r \ [a])) ((remdups \circ map \ fst) \ r)
 show ?thesis
 proof (cases map-of ?rm a)
   case None
   have one: ?l = \{\}
    unfolding memo-list-trancl-def Let-def None
    by auto
   from None [unfolded map-of-eq-None-iff]
     have a: a \notin fst 'set r by force
   {
    fix b
    assume b \in ?r
    from this [unfolded trancl-unfold-left] a have False by force
   }
   then have ?r = \{\} by auto
   then show ?thesis unfolding one by simp
 next
   case (Some as)
   have as: set as = \{b. (a, b) \in (set r)^+\}
     using map-of-SomeD [OF Some]
      trancl-list-impl[of r [a]] by force
   then show ?thesis unfolding memo-list-trancl-def Let-def Some by simp
 qed
\mathbf{qed}
```

end

3 Accessing Values via Keys

```
theory RBT-Map-Set-Extension
imports
Collections.RBTMapImpl
Collections.RBTSetImpl
Matrix.Utility
begin
```

We provide two extensions of the red black tree implementation.

The first extension provides two convenience methods on sets which are represented by red black trees: a check on subsets and the big union operator.

The second extension is to provide two operations *elem-list-to-rm* and *rm-set-lookup* which can be used to index a set of values via keys. More precisely, given a list of values of type 'v and a key function of type 'v \Rightarrow 'k, *elem-list-to-rm* will generate a map of type 'k \Rightarrow 'v set. Then with *rs-set-lookup* we can efficiently access all values which match a given key.

3.1 Subset and Union

For the subset operation $r \subseteq s$ we provide two implementations. The first one (*rs-subset*) traverses over r and then performs membership tests $\in s$. Its complexity is $\mathcal{O}(|r| \cdot log(|s|))$. The second one (*rs-subset-list*) generates sorted lists for both r and s and then linearly checks the subset condition. Its complexity is $\mathcal{O}(|r| + |s|)$.

As union operator we use the standard fold function. Note that the order of the union is important so that new sets are added to the big union.

```
definition rs-subset :: ('a :: linorder) rs \Rightarrow 'a rs \Rightarrow 'a option
where
  rs-subset as bs = rs.iteratei
    as
    (\lambda \text{ maybe. case maybe of None} \Rightarrow \text{True} \mid \text{Some} \rightarrow \text{False})
    (\lambda \ a \ -. \ if \ rs.memb \ a \ bs \ then \ None \ else \ Some \ a)
    None
lemma rs-subset [simp]:
  rs-subset as bs = None \leftrightarrow rs.\alpha as \subseteq rs.\alpha bs
proof -
  let ?abort = \lambda maybe. case maybe of None \Rightarrow True | Some - \Rightarrow False
 let ?I = \lambda aas maybe. maybe = None \longleftrightarrow (\forall a. a \in rs.\alpha \ as - aas \longrightarrow a \in rs.\alpha)
bs)
  let ?it = rs-subset as bs
  have ?I {} ?it \lor (\exists it \subseteq rs.\alpha as. it \neq {} \land \neg ?abort ?it \land ?I it ?it)
    unfolding rs-subset-def
    by (rule rs.iteratei-rule-P [where I = ?I]) (auto simp: rs.correct)
  then show ?thesis by auto
qed
definition rs-subset-list :: ('a :: linorder) rs \Rightarrow 'a rs \Rightarrow 'a option
where
  rs-subset-list as bs = sorted-list-subset (rs.to-sorted-list as) (rs.to-sorted-list bs)
lemma rs-subset-list [simp]:
  rs-subset-list as bs = None \leftrightarrow rs.\alpha as \subseteq rs.\alpha bs
  unfolding rs-subset-list-def
```

```
sorted-list-subset[OF rs.to-sorted-list-correct(3)[OF rs.invar, of as]
rs.to-sorted-list-correct(3)[OF rs.invar, of bs]]
```

by (*simp add: rs.to-sorted-list-correct*)

```
definition rs-Union :: ('q :: linorder) rs list \Rightarrow 'q rs

where

rs-Union = foldl rs.union (rs.empty ())

lemma rs-Union [simp]:

rs.\alpha (rs-Union qs) = \bigcup (rs.\alpha ' set qs)

proof –

{

fix start

have rs.\alpha (foldl rs.union start qs) = rs.\alpha start \cup \bigcup (rs.\alpha ' set qs)

by (induct qs arbitrary: start, auto simp: rs.correct)

} from this[of rs.empty ()]

show ?thesis unfolding rs-Union-def

by (auto simp: rs.correct)

qed
```

3.2 Grouping Values via Keys

The functions to produce the index (elem-list-to-rm) and the lookup function (rm-set-lookup) are straight-forward, however it requires some tedious reasoning that they perform as they should.

```
fun elem-list-to-rm :: ('d \Rightarrow 'k :: linorder) \Rightarrow 'd \ list \Rightarrow ('k, \ 'd \ list) \ rm

where

elem-list-to-rm key [] = rm.empty () |

elem-list-to-rm key (d # ds) =

(let

rm = elem-list-to-rm key ds;

k = key d

in

(case rm.\alpha rm k of

None \Rightarrow rm.update-dj k [d] rm

| Some data \Rightarrow rm.update k (d # data) rm))
```

definition rm-set-lookup $rm = (\lambda \ a. \ (case \ rm.\alpha \ rm \ a \ of \ None \Rightarrow [] | Some \ rules \Rightarrow rules))$

locale rm-set =

```
fixes rm :: ('k :: linorder, 'd list) rm
   and key :: 'd \Rightarrow 'k
   and data :: 'd set
 assumes rm-set-lookup: \bigwedge k. set (rm-set-lookup rm k) = {d \in data. key d = k}
begin
lemma data-lookup:
  data = \bigcup \{set (rm-set-lookup rm k) \mid k. True\} (is - = ?R)
proof -
 {
   fix d
   assume d: d \in data
   then have d: d \in \{d' \in data. key d' = key d\} by auto
   have d \in ?R
   by (rule UnionI[OF - d], rule CollectI, rule exI[of - key d], unfold rm-set-lookup[of
key d], simp)
 }
 moreover
  {
   fix d
   assume d \in ?R
   from this[unfolded rm-set-lookup]
   have d \in data by auto
  }
 ultimately show ?thesis by blast
qed
lemma finite-data:
 finite data
 unfolding data-lookup
proof
 show finite {set (rm\text{-set-lookup } rm \ k) \mid k. True} (is finite ?L)
 proof -
   let ?rmset = rm.\alpha \ rm
   let ?M = ?rmset ' Map.dom ?rmset
   let ?N = ((\lambda \ e. \ set \ (case \ e \ of \ None \ \Rightarrow [] \ | \ Some \ ds \ \Rightarrow \ ds)) '?M)
   let ?K = ?N \cup \{\{\}\}
   from rm.finite[of rm] have fin: finite ?K by auto
   show ?thesis
   proof (rule finite-subset[OF - fin], rule)
     fix ds
     assume ds \in ?L
     from this [unfolded rm-set-lookup-def]
     obtain fn where ds: ds = set (case rm.\alpha rm fn of None \Rightarrow []
        | Some ds \Rightarrow ds) by auto
     show ds \in ?K
     proof (cases rm.\alpha rm fn)
       case None
       then show ?thesis unfolding ds by auto
```

```
\begin{array}{c} \mathbf{next} \\ \mathbf{case} \ (Some \ rules) \\ \mathbf{from} \ Some \ \mathbf{have} \ fn: \ fn \in Map. \ dom \ ?rmset \ \mathbf{by} \ auto \\ \mathbf{have} \ ds \in \ ?N \\ \mathbf{unfolding} \ ds \\ \mathbf{by} \ (rule, \ rule \ refl, \ rule, \ rule \ refl, \ rule \ fn) \\ \mathbf{then \ show} \ ?thesis \ \mathbf{by} \ auto \\ \mathbf{qed} \\ \mathbf{qed} \\ \mathbf{qed} \\ \mathbf{qed} \\ \mathbf{qed} \ (force \ simp: \ rm-set-lookup-def) \end{array}
```

\mathbf{end}

interpretation elem-list-to-rm: rm-set elem-list-to-rm key ds key set ds proof fix k**show** set (*rm*-set-lookup (elem-list-to-*rm* key ds) k) = { $d \in set ds. key d = k$ } **proof** (*induct* ds *arbitrary*: k) case Nil then show ?case unfolding rm-set-lookup-def **by** (*simp add: rm.correct*) \mathbf{next} **case** (Cons d ds k) let ?el = elem-list-to-rm keylet $?l = \lambda k \, ds. \, set \, (rm\text{-set-lookup} \, (?el \, ds) \, k)$ let $?r = \lambda k \, ds. \{ d \in set \, ds. \, key \, d = k \}$ from Cons have ind: $\bigwedge k$. ?l k ds = ?r k ds by auto show ?l k (d # ds) = ?r k (d # ds)**proof** (cases $rm.\alpha$ (?el ds) (key d)) case None **from** None ind[of key d] have $r: \{ da \in set \ ds. \ key \ da = key \ d \} = \{ \}$ unfolding *rm-set-lookup-def* by *auto* from None have el: ?el (d # ds) = rm.update-dj (key d) [d] (?el ds) by simp **from** None have ndom: key $d \notin Map.dom (rm.\alpha (?el ds))$ by auto have $r: ?r k (d \# ds) = ?r k ds \cap \{da. key da \neq key d\} \cup \{da. key da = k$ $\wedge da = d$ (is $- = ?r1 \cup ?r2$) using r by auto from ndom have l: ?l k (d # ds) =set (case ((rm. α (elem-list-to-rm key ds))(key $d \mapsto [d]$)) k of None \Rightarrow [] | Some rules \Rightarrow rules) (is - = ?l) unfolding el rm-set-lookup-def by (simp add: rm.correct) { $\mathbf{fix} \ da$ assume $da \in ?r1 \cup ?r2$ then have $da \in ?l$ proof assume $da \in ?r2$

```
then have da: da = d and k: key d = k by auto
        show ?thesis unfolding da k by auto
       next
        assume da \in ?r1
        from this [unfolded ind[symmetric] rm-set-lookup-def]
        obtain das where rm: rm.\alpha (?el ds) k = Some das and da: da \in set das
and k: key da \neq key d by (cases rm.\alpha (?el ds) k, auto)
        from ind[of k, unfolded rm-set-lookup-def] rm da k have k: key d \neq k by
auto
        have rm: ((rm.\alpha \ (elem-list-to-rm \ key \ ds))(key \ d \mapsto [d])) \ k = Some \ das
          unfolding rm[symmetric] using k by auto
        show ?thesis unfolding rm using da by auto
      qed
     }
     moreover
     ł
      fix da
      assume l: da \in ?l
      let ?rm = ((rm.\alpha \ (elem-list-to-rm \ key \ ds))(key \ d \mapsto [d])) \ k
      from l obtain das where rm: ?rm = Some \ das \ and \ da: da \in set \ das
        by (cases ?rm, auto)
      have da \in ?r1 \cup ?r2
      proof (cases k = key d)
        case True
        with rm \ da have da: \ da = d by auto
        then show ?thesis using True by auto
       \mathbf{next}
        case False
        with rm have rm.\alpha (?el ds) k = Some \ das \ by \ auto
        from ind[of k, unfolded rm-set-lookup-def this] da False
        show ?thesis by auto
      qed
     }
     ultimately have ?l = ?r1 \cup ?r2 by blast
     then show ? thesis unfolding l r.
   \mathbf{next}
     case (Some das)
     from Some ind [of key d] have das: \{da \in set \ ds. \ key \ da = key \ d\} = set \ das
       unfolding rm-set-lookup-def by auto
     from Some have el: ?el (d \# ds) = rm.update (key d) (d \# das) (?el ds)
      by simp
     from Some have dom: key d \in Map.dom (rm.\alpha (?el ds)) by auto
     from dom have l: ?l k (d \# ds) =
       set (case ((rm.\alpha (elem-list-to-rm key ds))(key d \mapsto (d \# das))) k of None
\Rightarrow []
       | Some rules \Rightarrow rules) (is - = ?l) unfolding el rm-set-lookup-def
      by (simp add: rm.correct)
     have r: ?r k (d \# ds) = ?r k ds \cup \{da. key da = k \land da = d\} (is - = ?r1 \cup
(?r2) by auto
```

```
{
                fix da
                assume da \in ?r1 \cup ?r2
                then have da \in ?l
                proof
                     assume da \in ?r2
                     then have da: da = d and k: key d = k by auto
                     show ?thesis unfolding da k by auto
                next
                     assume da \in ?r1
                     from this[unfolded ind[symmetric] rm-set-lookup-def]
                      obtain das' where rm: rm.\alpha (?el ds) k = Some \ das' \ and \ da: \ da \in set
das' by (cases rm.\alpha (?el ds) k, auto)
                    from ind[of k, unfolded rm-set-lookup-def rm] have das': set das' = \{d \in das' = da
set ds. key d = k by auto
                     show ?thesis
                     proof (cases k = key d)
                         case True
                         show ?thesis using das' das da unfolding True by simp
                     \mathbf{next}
                         case False
                        then show ?thesis using das' da rm by auto
                     qed
                \mathbf{qed}
            }
            moreover
            {
                fix da
                assume l: da \in ?l
                let ?rm = ((rm.\alpha \ (elem-list-to-rm \ key \ ds))(key \ d \mapsto d \ \# \ das)) \ k
                from l obtain das' where rm: ?rm = Some \ das' and da: da \in set \ das'
                     by (cases ?rm, auto)
                have da \in ?r1 \cup ?r2
                proof (cases k = key d)
                     case True
                     with rm da das have da: da \in set (d \# das) by auto
                     then have da = d \lor da \in set \ das \ by \ auto
                     then have k: key da = k
                     proof
                         assume da = d
                         then show ?thesis using True by simp
                     \mathbf{next}
                         assume da \in set das
                         with das True show ?thesis by auto
                     qed
                     from da k show ?thesis using das by auto
                 next
                     case False
                     with rm have rm.\alpha (?el ds) k = Some \ das' by auto
```

```
from ind[of k, unfolded rm-set-lookup-def this] da False
show ?thesis by auto
qed
}
ultimately have ?l = ?r1 \cup ?r2 by blast
then show ?thesis unfolding l r.
qed
qed
```

end

4 Closure Computation via Red Black Trees

theory Transitive-Closure-RBT-Impl imports Transitive-Closure-Impl

RBT-Map-Set-Extension begin

We provide two algorithms to compute the reflexive transitive closure which internally work on red black trees. Therefore, the carrier has to be linear ordered. The first one (*rtrancl-rbt-impl*) computes the closure on demand for a given set of initial states. The second one (*memo-rbt-rtrancl*) precomputes the closure for each individual state, stores the results, and then only does a look-up.

For the transitive closure there are the corresponding algorithms trancl-rbt-impl and memo-rbt-trancl

4.1 Computing Closures from Sets On-The-Fly

The algorithms are based on the generic algorithms *rtrancl-impl* and *trancl-impl* using red black trees. To compute the successors efficiently, all successors of a state are collected and stored in a red black tree map by using *elem-list-to-rm*. Then, to lift the successor relation for single states to lists of states, all results are united using *rs-Union*. The rest is standard.

interpretation set-access λ as bs. rs.union bs (rs.from-list as) rs. α rs.memb rs.empty ()

by (unfold-locales, auto simp: rs.correct)

abbreviation *rm-succ* :: ('*a* :: *linorder* \times '*a*) *list* \Rightarrow '*a list* \Rightarrow '*a list* **where**

rm-succ $\equiv (\lambda \ r. \ let \ rm = \ elem$ -list-to- $rm \ fst \ r \ in$

 $(\lambda \ as. \ rs.to-list \ (rs-Union \ (map \ (\lambda \ a. \ rs.from-list \ (map \ snd \ (rm-set-lookup \ rm \ a))) \ as))))$

definition *rtrancl-rbt-impl* :: ('a :: *linorder* \times 'a) *list* \Rightarrow 'a *list* \Rightarrow 'a *rs*

where

```
\begin{aligned} rtrancl-rbt-impl &= rtrancl-impl \ rm-succ \\ (\lambda \ as \ bs. \ rs.union \ bs \ (rs.from-list \ as)) \ rs.memb \ (rs.empty \ ()) \end{aligned}
```

definition trancl-rbt-impl :: ('a :: linorder \times 'a) list \Rightarrow 'a list \Rightarrow 'a rs where

trancl-rbt-impl = trancl-impl rm-succ

 $(\lambda \ as \ bs. \ rs.union \ bs \ (rs.from-list \ as)) \ rs.memb \ (rs.empty \ ())$

```
lemma rtrancl-rbt-impl:
```

 $rs.\alpha \ (rtrancl-rbt-impl \ r \ as) = \{b. \exists \ a \in set \ as. \ (a,b) \in (set \ r)^*\}$ unfolding rtrancl-rbt-impl-def

by (*rule set-access-gen.rtrancl-impl, unfold-locales, unfold Let-def, simp add: rs.correct elem-list-to-rm.rm-set-lookup, force*)

```
lemma trancl-rbt-impl:

rs.\alpha (trancl-rbt-impl r as) = {b. \exists a \in set as. (a,b) \in (set r)^+}

unfolding trancl-rbt-impl-def

by (rule set-access-gen.trancl-impl, unfold-locales, unfold Let-def, simp add: rs.correct

elem-list-to-rm.rm-set-lookup, force)
```

4.2 Precomputing Closures for Single States

Storing all relevant entries is done by mapping all left-hand sides of the relation to their closure. Since we assume a linear order on the carrier, for the lookup we can use maps that are implemented as red black trees.

```
definition memo-rbt-rtrancl :: ('a :: linorder \times 'a) list \Rightarrow ('a \Rightarrow 'a rs)
where
  memo-rbt-rtrancl r =
   (let
     tr = rtrancl-rbt-impl r;
      rm = rm.to-map \ (map \ (\lambda \ a. \ (a, \ tr \ [a])) \ ((rs.to-list \circ rs.from-list \circ map \ fst))
r))
   in
     (\lambda a. \ case \ rm.lookup \ a \ rm \ of
       None \Rightarrow rs.from-list [a]
     | Some as \Rightarrow as))
lemma memo-rbt-rtrancl:
  rs.\alpha (memo-rbt-rtrancl r a) = {b. (a, b) \in (set r)^*} (is ?l = ?r)
proof -
  let ?rm = rm.to-map
    (map (\lambda a. (a, rtrancl-rbt-impl r [a])) ((rs.to-list \circ rs.from-list \circ map fst) r))
  show ?thesis
  proof (cases rm.lookup a ?rm)
   case None
   have one: ?l = \{a\}
     unfolding memo-rbt-rtrancl-def Let-def None
     by (simp add: rs.correct)
```

```
from None [unfolded rm.lookup-correct [OF rm.invar], simplified rm.correct
map-of-eq-None-iff]
   have a: a \notin fst 'set r by (simp add: rs.correct, force)
    {
     fix b
     assume b \in ?r
     from this [unfolded rtrancl-power relpow-fun-conv] obtain n f where
       ab: f \ 0 = a \land f \ n = b and steps: \bigwedge i. i < n \Longrightarrow (f \ i, f \ (Suc \ i)) \in set \ r by
auto
     from ab steps [of 0] a have b = a
       by (cases n, force+)
   }
   then have ?r = \{a\} by auto
   then show ?thesis unfolding one by simp
 next
   case (Some as)
   have as: rs.\alpha as = {b. (a,b) \in (set \ r)^*}
     using map-of-SomeD [OF Some [unfolded rm.lookup-correct [OF rm.invar],
simplified rm.correct]
       rtrancl-rbt-impl [of r [a]] by force
   \textbf{then show ?thesis unfolding } \textit{memo-rbt-rtrancl-def Let-def Some by simp}
 qed
qed
definition memo-rbt-trancl :: ('a :: linorder \times 'a) list \Rightarrow ('a \Rightarrow 'a rs)
where
  memo-rbt-trancl r =
   (let
     tr = trancl-rbt-impl r;
     rm = rm.to-map \ (map \ (\lambda \ a. \ (a, \ tr \ [a])) \ ((rs.to-list \circ rs.from-list \circ map \ fst))
r))
    in (\lambda \ a.
     (case rm.lookup a rm of
       None \Rightarrow rs.empty ()
     | Some as \Rightarrow as)))
lemma memo-rbt-trancl:
  rs.\alpha (memo-rbt-trancl r a) = {b. (a, b) \in (set r)^+} (is ?l = ?r)
proof –
 let ?rm = rm.to-map
   (map \ (\lambda \ a. \ (a, \ trancl-rbt-impl \ r \ [a])) \ ((rs.to-list \circ \ rs.from-list \circ \ map \ fst) \ r))
 show ?thesis
 proof (cases rm.lookup a ?rm)
   case None
   have one: ?l = \{\}
     unfolding memo-rbt-trancl-def Let-def None
     by (simp add: rs.correct)
    from None [unfolded rm.lookup-correct [OF rm.invar], simplified rm.correct
map-of-eq-None-iff]
```

```
have a: a \notin fst 'set r by (simp add: rs.correct, force)
   {
    fix b
    assume b \in ?r
    from this [unfolded trancl-unfold-left] a have False by force
   }
   then have ?r = \{\} by auto
   then show ?thesis unfolding one by simp
 next
   case (Some as)
   have as: rs.\alpha as = {b. (a,b) \in (set r)^+}
     using map-of-SomeD [OF Some [unfolded rm.lookup-correct [OF rm.invar],
simplified rm.correct]]
      trancl-rbt-impl [of r [a]] by force
   then show ?thesis unfolding memo-rbt-trancl-def Let-def Some by simp
 qed
qed
```

 \mathbf{end}

5 Computing Images of Finite Transitive Closures

theory Finite-Transitive-Closure-Simprocs imports Transitive-Closure-List-Impl begin

lemma rtrancl-Image-eq: **assumes** r = set r' and x = set x' **shows** r^* "x = set (rtrancl-list-impl r' x') **using** assms **by** (auto simp: rtrancl-list-impl)

lemma trancl-Image-eq: **assumes** r = set r' and x = set x' **shows** r^+ "x = set (trancl-list-impl r' x') **using** assms by (auto simp: trancl-list-impl)

5.1 A Simproc for Computing the Images of Finite Transitive Closures

ML < signature FINITE-TRANCL-IMAGE = sig val trancl-simproc : Proof.context -> cterm -> thm option val rtrancl-simproc : Proof.context -> cterm -> thm option end

 $structure \ Finite-Trancl-Image: FINITE-TRANCL-IMAGE = struct$

 $\begin{array}{l} fun \ eval-tac \ ctxt = \\ let \ val \ conv = \ Code-Runtime.dynamic-holds-conv \ ctxt \\ in \ CONVERSION \ (Conv.params-conv \ \sim 1 \ (K \ (Conv.concl-conv \ \sim 1 \ conv)) \ ctxt) \\ THEN' \ resolve-tac \ ctxt \ [TrueI] \ end \end{array}$

fun mk-rtrancl $T = Const (@{const-name rtrancl-list-impl}, T);$

fun mk-trancl $T = Const (@{const-name trancl-list-impl}, T);$

fun dest-rtrancl-Image

 $\begin{array}{l} (Const \ (@\{ const-name \ Image \}, \ T) \ \$ \ (Const \ (@\{ const-name \ rtrancl \}, \ -) \ \$ \ r) \\ \$ \ x) = (T, \ r, \ x) \\ | \ dest-rtrancl-Image \ - = \ raise \ Match \end{array}$

fun dest-trancl-Image

 $\begin{array}{l} (Const \ (@ \{ const-name \ Image \}, \ T) \ \$ \ (Const \ (@ \{ const-name \ trancl \}, \ -) \ \$ \ r) \ \$ \\ x) = (T, \ r, \ x) \\ | \ dest-trancl-Image \ - = \ raise \ Match \end{array}$

fun gen-simproc dest mk-const eq-thm ctxt ct =letval t = Thm.term-of ct;val $(T, r, x) = t \mid > dest;$ in(*make sure that the relation as well as the given domain are finite sets*) (case (try HOLogic.dest-set r, try HOLogic.dest-set x) of(SOME xs, SOME ys) =>let(*types*) $val \ set T = T \mid > dest-fun T \mid > snd \mid > dest-fun T \mid > fst;$ $val \ eltT = setT \mid > HOLogic.dest-setT;$ $val \ prodT = HOLogic.mk-prodT \ (eltT, \ eltT);$ val prod-listT = HOLogic.listT prodT; $val \ listT = HOLogic.listT \ eltT;$ (*terms*) $val \ set = Const \ (@{const-name \ List.set}, \ listT \ --> \ setT);$ $val \ const = mk - const \ (prod-listT - -> listT);$ val r' = HOLogic.mk-list prodT xs; $val x' = HOLogic.mk-list \ eltT \ ys;$ val t' = set (const r' x') $val \ u = Value$ -Command. $value \ ctxt \ t';$ $val eval = (t', u) \mid > HOLogic.mk-eq \mid > HOLogic.mk-Trueprop;$ val maybe-rule =try (Goal.prove ctxt [] [] eval) (fn {context, ...} => eval-tac context 1); in(case maybe-rule of $SOME \ rule =>$

```
\begin{array}{l} let \\ val\ conv = (t,\ t') \mid > HOLogic.mk-eq \mid > HOLogic.mk-Trueprop; \\ val\ eq-thm' = Goal.prove\ ctxt \ [] \ []\ conv\ (fn\ \{context = ctxt',\ ...\} => \\ resolve-tac\ ctxt'\ [eq-thm]\ 1\ THEN\ REPEAT\ (simp-tac\ ctxt'\ 1)); \\ in \\ SOME\ (@\{thm\ HOL.trans\}\ OF\ [eq-thm',\ rule]\ RS\ @\{thm\ eq-reflection\}) \\ end \\ \mid NONE =>\ NONE) \\ end \\ \mid - =>\ NONE) \\ end \end{array}
```

 $val \ rtrancl-simproc = gen-simproc \ dest-rtrancl-Image \ mk-rtrancl \ @\{thm \ rtrancl-Image-eq\} \\ val \ trancl-simproc = gen-simproc \ dest-trancl-Image \ mk-trancl \ @\{thm \ trancl-Image-eq\} \\ \end{cases}$

end

>

simproc-setup *rtrancl-Image* $(r^* "x) = \langle K \ Finite-Trancl-Image.rtrancl-simproc \rangle$ **simproc-setup** *trancl-Image* $(r^+ "x) = \langle K \ Finite-Trancl-Image.rtrancl-simproc \rangle$

5.2 Example

The images of (reflexive) transitive closures are computed by evaluation.

lemma

```
 \{(1::nat, 2), (2, 3), (3, 4), (4, 5)\}^* ``\{1\} = \{1, 2, 3, 4, 5\} \\ \{(1::nat, 2), (2, 3), (3, 4), (4, 5)\}^+ ``\{1\} = \{2, 3, 4, 5\} \\ \textbf{apply simp-all} \\ \textbf{apply auto} \\ \textbf{done}
```

Evaluation does not allow for free variables and thus fails in their presence.

lemma

 ${(x, y)}^* `` {x} = {x, y}$ oops

end

References

- P. Lammich and A. Lochbihler. The Isabelle collections framework. In Proc. ITP'10, volume 6172 of LNCS, pages 339–354, 2010.
- [2] R. Thiemann and C. Sternagel. Certification of termination proofs using CeTA. In Proc. TPHOLs'09, volume 5674 of LNCS, pages 452–468, 2009.