

Executable Transitive Closures of Finite Relations*

Christian Sternagel and René Thiemann

April 20, 2020

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.

Contents

1	A Generic Work-List Algorithm	2
1.1	Bounded Reachability	2
1.2	Reflexive Transitive Closure and Transitive closure	6
2	Closure Computation using Lists	9
2.1	Computing Closures from Sets On-The-Fly	9
2.2	Precomputing Closures for Single States	10
3	Accessing Values via Keys	11
3.1	Subset and Union	12
3.2	Grouping Values via Keys	13
4	Closure Computation via Red Black Trees	18
4.1	Computing Closures from Sets On-The-Fly	18
4.2	Precomputing Closures for Single States	19
5	Computing Images of Finite Transitive Closures	21
5.1	A Simproc for Computing the Images of Finite Transitive Closures	21
5.2	Example	23

*Supported by FWF (Austrian Science Fund) project P22767-N13.

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 work-list 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 $\text{card } R$ 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
  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
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 ( $\lambda n. \neg \text{memb } n \text{ have}'$ ) maybe
      in relpow-impl succ un memb new' have' m)
```

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  $\longleftrightarrow$  ( $a \in \text{set-of } bs$ )
and empty: set-of empty = {}
```

```

locale set-access-succ = set-access un
  for un :: 'a list ⇒ 'b ⇒ 'b +
  fixes succ :: 'a list ⇒ 'a list
  and rel :: ('a × 'a) set
  assumes succ: set (succ as) = {b. ∃ a ∈ set as. (a, b) ∈ rel}
begin

```

```

abbreviation relpow-i ≡ 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 | a b m. a ∈ set new ∧ m ≤ n ∧ (a, b) ∈ (rel ∩ {(a, b). b ∉ set-of have})
  ^^ m} ∪
  set-of have

```

```

  (is ?l 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

```

```

    case 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 = λ m. (rel ∩ {(a, b). b ∉ new ∧ b ∉ have}) ^^ m

```

```

    let ?rel = λ m. (rel ∩ {(a, b). b ∉ have}) ^^ m

```

```

    have idl: ?l nnew hhave (Suc n) =

```

```

    {uu. ∃ a. (∃ aa ∈ new. (aa, a) ∈ rel) ∧ a ∉ new ∧ a ∉ have ∧ (∃ m ≤ n. (a,
    uu) ∈ ?reln m)} ∪
    (new ∪ have)

```

```

    (is - = ?l1 ∪ (?l2 ∪ ?l3))

```

```

    by (simp add: hav new False Let-def Suc, simp add: memb un succ)

```

```

    let ?l = ?l1 ∪ (?l2 ∪ ?l3)

```

```

    have idr: ?r nnew hhave (Suc n) = {b. ∃ a m. a ∈ new ∧ m ≤ Suc n ∧ (a,
    b) ∈ ?rel m} ∪ have

```

```

    (is - = (?r1 ∪ ?r2)) by (simp add: hav new)

```

```

    let ?r = ?r1 ∪ ?r2

```

```

    {

```

```

      fix b

```

```

      assume b: b ∈ ?l

```

```

      have b ∈ ?r

```

```

      proof (cases b ∈ new ∨ b ∈ have)

```

```

        case True then show ?thesis

```

```

        proof

```

```

    assume b ∈ have then show ?thesis by auto
  next
    assume b: b ∈ new
    have b ∈ ?r1
      by (intro CollectI, rule exI, rule exI [of - 0], intro conjI, rule b, auto)
    then show ?thesis by auto
  qed
next
case False
with b have b ∈ ?l1 by auto
then obtain a2 a1 m where a2n: a2 ∉ new and a2h: a2 ∉ have and a1:
a1 ∈ new
and a1a2: (a1,a2) ∈ rel and m: m ≤ n and a2b: (a2,b) ∈ ?reln m by
auto
have b ∈ ?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 ∈ ?r
  then have b ∈ ?l
  proof (cases b ∈ have)
    case True then show ?thesis by auto
  next
    case False
    with b have b ∈ ?r1 by auto
    then obtain a m where a: a ∈ new and m: m ≤ Suc n and ab: (a, b) ∈
?rel m by auto
    have seq: ∃ a ∈ new. (a, b) ∈ ?rel m
      using a ab by auto
    obtain l where l: l = (LEAST m. (∃ a ∈ new. (a, b) ∈ ?rel m)) by auto
    have least: (∃ a ∈ new. (a, b) ∈ ?rel l)
      by (unfold l, rule LeastI, rule seq)
    have lm: l ≤ m unfolding l
      by (rule Least-le, rule seq)
    with m have ln: l ≤ Suc n by auto
    from least obtain a where a: a ∈ new
      and ab: (a, b) ∈ ?rel l by auto
    from ab [unfolded relpow-fun-conv]
    obtain f where fa: f 0 = a and fb: b = f l
      and steps: ∧ i. i < l ⇒ (f i, f (Suc i)) ∈ ?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
  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 0
    with ab a show ?thesis by auto
  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
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) = $\{b \mid a\ b\ m. a \in set\ new \wedge m \leq n \wedge (a, b) \in rel\ \hat{\wedge}\ m\}$

proof –

```

have id: rel ∩ {(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 ::
  (('a × 'a) list ⇒ 'a list ⇒ 'a list) ⇒
  ('a list ⇒ 'b ⇒ 'b) ⇒ ('a ⇒ 'b ⇒ bool) ⇒ 'b ⇒ ('a × 'a) list ⇒ 'a list ⇒ 'b
where
  rtrancl-impl gen-succ un memb emp rel =
    (let
      succ = gen-succ rel;
      n = length rel
    in (λ as. relpow-impl succ un memb as emp n))

```

definition

```

trancl-impl ::
  (('a × 'a) list ⇒ 'a list ⇒ 'a list) ⇒
  ('a list ⇒ 'b ⇒ 'b) ⇒ ('a ⇒ 'b ⇒ bool) ⇒ 'b ⇒ ('a × 'a) list ⇒ 'a list ⇒ 'b
where
  trancl-impl gen-succ un memb emp rel =
    (let
      succ = gen-succ rel;
      n = length rel
    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*:

$(a, b) \in (\text{set rel})^* \iff (\exists n \leq \text{length rel}. (a, b) \in \text{set rel}^{\wedge n})$ (**is** ?l = ?r)

proof

```

assume ?r
then show ?l
  unfolding rtrancl-power by auto
next
assume ?l
from this [unfolded rtrancl-power]
obtain n where ab: (a,b) ∈ set rel ^ n ..

```

```

obtain  $l$  where  $l: l = (LEAST\ n.\ (a,b) \in set\ rel\ \wedge\wedge\ n)$  by auto
have  $ab: (a, b) \in set\ rel\ \wedge\wedge\ l$  unfolding  $l$ 
  by (intro LeastI, rule ab)
from this [unfolded relpow-fun-conv]
obtain  $f$  where  $a: f\ 0 = a$  and  $b: f\ l = b$ 
  and steps:  $\bigwedge\ i.\ i < l \implies (f\ i, f\ (Suc\ i)) \in set\ rel$  by auto
let  $?hits = map\ (\lambda\ i.\ f\ (Suc\ i))\ [0\ ..<\ l]$ 
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] ..
    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  $\dots \leq length\ (map\ snd\ rel)$  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  $ij: ?i < ?j$ 
        using  $i\ j\ fij\ fij$  unfolding min-def max-def by (cases i ≤ j, auto)
      from  $i\ j\ fij\ ij$  obtain  $i\ j$  where  $i: i < l$  and  $j: j < l$  and  $ij: i < j$  and  $fij: f\ (Suc\ i) = f\ (Suc\ j)$  by blast
      let  $?g = \lambda\ n.\ if\ n \leq i\ then\ f\ n\ else\ f\ (n + (j - i))$ 
      let  $?l = l - (j - i)$ 
      have  $abl: (a,b) \in set\ rel\ \wedge\wedge\ ?l$ 
        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
      next
        fix  $k$ 
        assume  $k: k < ?l$ 
        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
            case 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
qed (simp add: a)
from ij i have ll: ?l < l by auto
have l ≤ ?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 ⇒ 'b ⇒ 'b +
  fixes gen-succ :: ('a × 'a) list ⇒ 'a list ⇒ 'a list
  assumes gen-succ: set (gen-succ rel as) = {b. ∃ a ∈ set as. (a, b) ∈ set rel}
begin

abbreviation rtrancl-i ≡ rtrancl-impl gen-succ un memb empty
abbreviation trancl-i ≡ trancl-impl gen-succ un memb empty

lemma rtrancl-impl:
  set-of (rtrancl-i rel as) = {b. (∃ a ∈ set as. (a, b) ∈ (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. (∃ a ∈ set as. (a, b) ∈ (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
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 × 'a) list ⇒ 'a list ⇒ 'a list
where
  rtrancl-list-impl = rtrancl-impl
    (λ r as. remdups (map snd (filter (λ (a, b). a ∈ set as) r)))
    (λ xs ys. (filter (λ x. x ∉ set ys) xs) @ ys)
    (λ x xs. x ∈ set xs)
  []
```

```
definition trancl-list-impl :: ('a × 'a) list ⇒ 'a list ⇒ 'a list
where
  trancl-list-impl = trancl-impl
    (λ r as. remdups (map snd (filter (λ (a, b). a ∈ set as) r)))
    (λ xs ys. (filter (λ x. x ∉ set ys) xs) @ ys)
    (λ x xs. x ∈ set xs)
  []
```

```
lemma rtrancl-list-impl:
  set (rtrancl-list-impl r as) = {b. ∃ a ∈ set as. (a, b) ∈ (set r)*}
unfolding rtrancl-list-impl-def
by (rule set-access-gen.rtrancl-impl, unfold-locales, force+)
```

```
lemma trancl-list-impl:
  set (trancl-list-impl r as) = {b. ∃ a ∈ set as. (a, b) ∈ (set r)+}
unfolding trancl-list-impl-def
by (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 × 'a) list ⇒ ('a ⇒ 'a list)

where

```

memo-list-rtrancl r =
  (let
    tr = rtrancl-list-impl r;
    rm = map (λa. (a, tr [a])) ((remdups ∘ map fst) r)
  in
    (λa. case map-of rm a of
      None ⇒ [a]
    | Some as ⇒ as))

```

lemma *memo-list-rtrancl*:

```

set (memo-list-rtrancl r a) = {b. (a, b) ∈ (set r)*} (is ?l = ?r)

```

proof –

```

let ?rm = map (λ a. (a, rtrancl-list-impl r [a])) ((remdups ∘ 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 ∉ fst ‘ set r by *force*

{

fix *b*

assume *b* ∈ ?r

from *this [unfolded rtrancl-power relpow-fun-conv]* obtain *n f* where

ab: f 0 = a ∧ f n = b and *steps*: ∧ i. i < n ⇒ (f i, f (Suc i)) ∈ 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) ∈ (set r)*}

using *map-of-SomeD [OF Some]*

rtrancl-list-impl [of r [a]] by *force*

then show *?thesis* unfolding *memo-list-rtrancl-def Let-def Some* by *simp*

qed

qed

definition *memo-list-trancl* :: ('a × 'a) list ⇒ ('a ⇒ 'a list)

where

```

memo-list-trancl r =
  (let
    tr = trancl-list-impl r;
    rm = map (λa. (a, tr [a])) ((remdups ∘ map fst) r)
  in
    (λa. case map-of rm a of
      None ⇒ []
    | Some as ⇒ as))

```

lemma *memo-list-trancl*:

```

set (memo-list-trancl r a) = {b. (a, b) ∈ (set r)+} (is ?l = ?r)

```

proof –

```

let ?rm = map (λ a. (a, trancl-list-impl r [a])) ((remdups ∘ 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* ∉ *fst* ‘*set r* **by** *force*

{

fix *b*

assume *b* ∈ *?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*) ∈ (*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

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* :: ($'a :: \text{linorder}$) $rs \Rightarrow 'a$ $rs \Rightarrow 'a$ option

where

```

rs-subset as bs = rs.iteratei
  as
  ( $\lambda$  maybe. case maybe of None  $\Rightarrow$  True | Some -  $\Rightarrow$  False)
  ( $\lambda$  a -. if rs.memb a bs then None else Some a)
  None

```

lemma *rs-subset* [*simp*]:

```

rs-subset as bs = None  $\longleftrightarrow$   $rs.\alpha$  as  $\subseteq$   $rs.\alpha$  bs

```

proof –

```

let ?abort =  $\lambda$  maybe. case maybe of None  $\Rightarrow$  True | Some -  $\Rightarrow$  False
let ?I =  $\lambda$  a as maybe. maybe = None  $\longleftrightarrow$  ( $\forall$  a. a  $\in$   $rs.\alpha$  as  $\rightarrow$  a  $\in$ 
rs. $\alpha$  bs)
let ?it = rs-subset as bs
have ?I {} ?it  $\vee$  ( $\exists$  it  $\subseteq$   $rs.\alpha$  as. it  $\neq$  {}  $\wedge$   $\neg$  ?abort ?it  $\wedge$  ?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* :: ($'a :: \text{linorder}$) $rs \Rightarrow 'a$ $rs \Rightarrow 'a$ 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  $\longleftrightarrow$   $rs.\alpha$  as  $\subseteq$   $rs.\alpha$  bs

```

unfolding *rs-subset-list-def*

```

sorted-list-subset[OF rs.to-sorted-list-correct( $\mathcal{P}$ )] [OF rs.invar, of as]
rs.to-sorted-list-correct( $\mathcal{P}$ ) [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. α ' set qs)

proof –

{

 fix start

 have $rs.\alpha$ (foldl rs.union start qs) = $rs.\alpha$ start \cup \bigcup (rs. α ' 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. α 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 = (λ a. (case rm. α rm a of None \Rightarrow [] | Some rules \Rightarrow rules))

lemma *rm-to-list-empty* [simp]:

rm.to-list (rm.empty ()) = []

proof –

have map-of (*rm.to-list* (rm.empty ())) = Map.empty

 by (simp add: rm.correct)

moreover have map-of-empty-iff: $\bigwedge l$. map-of l = Map.empty \longleftrightarrow l = []

 by (case-tac l) auto

ultimately show ?thesis by metis

qed

locale *rm-set* =

```

fixes rm :: ('k :: linorder, 'd list) rm
  and key :: 'd ⇒ 'k
  and data :: 'd set
assumes rm-set-lookup: ∧ k. set (rm-set-lookup rm k) = {d ∈ data. key d = k}
begin

lemma data-lookup:
  data = ∪ {set (rm-set-lookup rm k) | k. True} (is - = ?R)
proof -
  {
    fix d
    assume d: d ∈ data
    then have d: d ∈ {d' ∈ data. key d' = key d} by auto
    have d ∈ ?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 ∈ ?R
    from this[unfolded rm-set-lookup]
    have d ∈ data by auto
  }
  ultimately show ?thesis by blast
qed

```

```

lemma finite-data:
  finite data
  unfolding data-lookup
proof
show finite {set (rm-set-lookup rm k) | k. True} (is finite ?L)
proof -
  let ?rmset = rm.α rm
  let ?M = ?rmset ' Map.dom ?rmset
  let ?N = ((λ e. set (case e of None ⇒ [] | Some ds ⇒ ds)) ' ?M)
  let ?K = ?N ∪ {{}}
  from rm.finite[of rm] have fin: finite ?K by auto
  show ?thesis
  proof (rule finite-subset[OF - fin], rule)
    fix ds
    assume ds ∈ ?L
    from this[unfolded rm-set-lookup-def]
    obtain fn where ds: ds = set (case rm.α rm fn of None ⇒ []
      | Some ds ⇒ ds) by auto
    show ds ∈ ?K
    proof (cases rm.α rm fn)
      case None
      then show ?thesis unfolding ds by auto

```

```

next
  case (Some rules)
  from Some have fn: fn ∈ Map.dom ?rmset by auto
  have ds ∈ ?N
  unfolding ds
  by (rule, rule refl, rule, rule refl, rule fn)
  then show ?thesis by auto
qed
qed
qed
qed (force simp: rm-set-lookup-def)

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 ∈ 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)
next
  case (Cons d ds k)
  let ?el = elem-list-to-rm key
  let ?l = λk ds. set (rm-set-lookup (?el ds) k)
  let ?r = λk ds. {d ∈ set ds. key d = k}
  from Cons have ind:
    ∧ k. ?l k ds = ?r k ds by auto
  show ?l k (d # ds) = ?r k (d # ds)
  proof (cases rm.α (?el ds) (key d))
    case None
    from None ind[of key d] have r: {da ∈ 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 ∉ Map.dom (rm.α (?el ds)) by auto
    have r: ?r k (d # ds) = ?r k ds ∩ {da. key da ≠ key d} ∪ {da . key da = k
  ∧ da = d} (is - = ?r1 ∪ ?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 ↦ [d])) k of None ⇒ []
    | Some rules ⇒ rules) (is - = ?l) unfolding el rm-set-lookup-def
    by (simp add: rm.correct)
  {
    fix da
    assume da ∈ ?r1 ∪ ?r2
    then have da ∈ ?l
    proof
      assume da ∈ ?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
{
  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
    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  $l\ r$  .
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  $el: ?el\ (d \# ds) = rm.update\ (key\ d)\ (d \# ds)\ (?el\ ds)$ 
  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  $(rm.\alpha\ (elem-list-to-rm\ key\ ds)(key\ d \mapsto (d \# ds)))\ k$  of None  $\Rightarrow$ 
  []
  | Some  $rules \Rightarrow rules$ ) (is - = ? $l$ ) unfolding  $el\ rm-set-lookup-def$ 
  by (simp add:  $rm.correct$ )
have  $r: ?r\ k\ (d \# ds) = ?r\ k\ ds \cup \{da. key\ da = k \wedge da = d\}$  (is - = ? $r1$ 
 $\cup\ ?r2$ ) by auto

```



```

{
  fix da
  assume da ∈ ?r1 ∪ ?r2
  then have da ∈ ?l
  proof
    assume da ∈ ?r2
    then have da: da = d and k: key d = k by auto
    show ?thesis unfolding da k by auto
  next
    assume da ∈ ?r1
    from this[unfolded ind[symmetric] rm-set-lookup-def]
    obtain das' where rm: rm.α (?el ds) k = Some das' and da: da ∈ set
das' by (cases rm.α (?el ds) k, auto)
    from ind[of k, unfolded rm-set-lookup-def rm] have das': set das' = {d ∈
set ds. key d = k} by auto
    show ?thesis
    proof (cases k = key d)
      case True
        show ?thesis using das' da unfolding True by simp
      next
        case False
          then show ?thesis using das' da rm by auto
    qed
  qed
}
moreover
{
  fix da
  assume l: da ∈ ?l
  let ?rm = ((rm.α (elem-list-to-rm key ds))(key d ↦ d # das)) k
  from l obtain das' where rm: ?rm = Some das' and da: da ∈ set das'
  by (cases ?rm, auto)
  have da ∈ ?r1 ∪ ?r2
  proof (cases k = key d)
    case True
      with rm da das have da: da ∈ set (d # das) by auto
      then have da = d ∨ da ∈ set das by auto
      then have k: key da = k
      proof
        assume da = d
          then show ?thesis using True by simp
      next
        assume da ∈ 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.α (?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 ∪ ?r2 by blast
  then show ?thesis unfolding l r .
    qed
  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.membr
rs.empty ()
  by (unfold-locales, auto simp: rs.correct)

```

```

abbreviation rm-succ :: ('a :: linorder × 'a) list ⇒ 'a list ⇒ 'a list
where

```

```

  rm-succ ≡ (λ r. let rm = elem-list-to-rm fst r in
    (λ as. rs.to-list (rs-Union (map (λ a. rs.from-list (map snd (rm-set-lookup rm
a)))) as))))

```

```

definition rtrancl-rbt-impl :: ('a :: linorder × 'a) list ⇒ 'a list ⇒ 'a rs

```

where

$rtrancl-rbt-impl = rtrancl-impl\ rm-succ$
 $(\lambda\ as\ bs.\ rs.union\ bs\ (rs.from-list\ as))\ rs.memb\ (rs.empty\ ())$

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 ∉ fst ‘ set r by (simp add: rs.correct, force)
{
  fix b
  assume b ∈ ?r
  from this [unfolded rtrancl-power relpow-fun-conv] obtain n f where
    ab: f 0 = a ∧ f n = b and steps: ∧ i. i < n ⇒ (f i, f (Suc i)) ∈ 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.α as = {b. (a,b) ∈ (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
  then show ?thesis unfolding memo-rbt-rtrancl-def Let-def Some by simp
qed
qed

```

definition memo-rbt-trancl :: ('a :: linorder × 'a) list ⇒ ('a ⇒ 'a rs)
where

```

memo-rbt-trancl r =
  (let
    tr = trancl-rbt-impl r;
    rm = rm.to-map (map (λ a. (a, tr [a])) ((rs.to-list ∘ rs.from-list ∘ map fst)
r))
  in (λ a.
    (case rm.lookup a rm of
      None ⇒ rs.empty ()
    | Some as ⇒ as)))

```

lemma memo-rbt-trancl:

rs.α (memo-rbt-trancl r a) = {b. (a, b) ∈ (set r)⁺} (is ?l = ?r)

proof –

let ?rm = rm.to-map

(map (λ a. (a, trancl-rbt-impl r [a])) ((rs.to-list ∘ rs.from-list ∘ 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 ∉ fst ` set r by (simp add: rs.correct, force)
{
  fix b
  assume b ∈ ?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.α as = {b. (a,b) ∈ (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
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

```

```

fun eval-tac ctxt =
  let val conv = Code-Runtime.dynamic-holds-conv ctxt
  in CONVERSION (Conv.params-conv ~1 (K (Conv.concl-conv ~1 conv)) ctxt)
  THEN' resolve-tac ctxt [TrueI] end

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

fun dest-trancl-Image
  (Const (@{const-name Image}, T) $ (Const (@{const-name trancl}, -) $ r)
  $ x) = (T, r, x)
  | dest-trancl-Image - = raise Match

fun gen-simproc dest mk-const eq-thm ctxt ct =
  let
    val t = Thm.term-of ct;
    val (T, r, x) = t |> 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 setT = T |> dest-funT |> snd |> dest-funT |> fst;
          val eltT = setT |> 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 --> 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) |> HOLogic.mk-eq |> HOLogic.mk-Trueprop;

          val maybe-rule =
            try (Goal.prove ctxt [] [] eval) (fn {context, ...} => eval-tac context 1);
        in
          (case maybe-rule of
            SOME rule =>

```

```

let
  val conv = (t, t') |> HOLogic.mk-eq |> 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
| NONE => NONE)
end
| - => NONE)
end

```

```

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
)

```

```

simproc-setup rtrancl-Image (r* “x) = ⟨K Finite-Trancl-Image.rtrancl-simproc⟩
simproc-setup trancl-Image (r+ “x) = ⟨K Finite-Trancl-Image.trancl-simproc⟩

```

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}

```

apply simp-all

apply auto

done

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

lemma

```

{(x, y)}* “ {x} = {x, y}

```

oops

end

References

- [1] 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.