

TECHNICAL UNIVERSITY OF MUNICH

Bachelor's Thesis in Informatics

Formalisation of a Congruence Closure Algorithm in Isabelle/HOL

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Formalisierung eines Kongruenzhüllen-Algorithmus in Isabelle/HOL

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I confirm that this bachelor's thesis is mented all sources and material used	in informatics is my own work and I have docu- l.
Munich, 15.09.2022	Rebecca Ghidini

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Abstract

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1 Introduction

I use Isabelle [NPW02]

1.1 Outline

Citation test [Lam94].

apply(simp)
apply(auto)
done

2 Preliminaries

- 2.1 Isabelle/HOL
- 2.2 Union Find with Explain Operation
- 2.2.1 Union Find in Isabelle
- 2.3 Congruence Closure with Explain Operation
- 2.4 Notation

3 Explain Operation for Union Find

3.1 The Union Find Data Structure

The section below describes the implementation of the modified Union Find data structure, as well as the *Explain* operation and its correctness proof, as described in [NO05].

The data structure for the Union, Find and Explain operations consists of the following three lists:

- uf_list: This is the usual union-find list, which contains the parent node of each element in the forest data structure. It is the one described in Section TODO.
- unions: This list simply contains all the pairs of input elements in chronological order.
- au: This is the *associated unions* list, it contains for each edge in the union-find forest a label with the union that corresponds to this edge. Similarly to the uf_list, it is indexed by the element, and for each element *e* which has a parent in the uf_list, au contains the input equation which caused the creation of this edge between *e* and its parent. The equations are represented as indexes in the unions list. The type of the entries is nat option, so that for elements without a parent, the au entry is None.

Example 1. For a union-find algorithm with 4 variables, the initial empty union find looks as follows:

```
(uf_list = [0, 1, 2, 3], unions = [], au = [None, None, None, None])
```

Each element is its own parent in the uf_list, which means that it is a root, the unions list is empty because no unions were made yet, and there are no edges in the tree, therefore there are no labels in au.

In order to reason about paths in the union-find forest, we define the following path predicate.

```
inductive path :: "nat list \Rightarrow nat \Rightarrow nat list \Rightarrow nat \Rightarrow bool" where single: "n < length l \Longrightarrow path l n [n] n" | step: "r < length l \Longrightarrow l ! u = r \Longrightarrow l ! u \neq u \Longrightarrow path l u p v \Longrightarrow path l r (r # p) v"
```

path l r p v defines a path from r to v, where r is an ancestor of v, which means that it is closer to the root, and p contains all the nodes visited on the path from r to v. This definition proved to be very useful for many proofs, as will become clearer later in this thesis.

The theory Path contains many lemmas about paths, including lemmas about concatenation of adjacent paths, and splitting of one path into two subpaths, and that the length of a path is at least 1, as well as others, many of which could be proven by rule induction on path. The most interesting and useful lemma was about the unicity of paths between two nodes:

```
theorem path_unique: "ufa_invar l \Longrightarrow path l u p1 v \Longrightarrow path l u p2 v \Longrightarrow p1 = p2"
```

Proof. The lemma is proven by induction on the length of *p*1.

For the base case we assume that the length of p1 is 1. There is only one node in the path, therefore v = u. Then I proved a lemma which showed that if the ufa_invar holds, each path from v to v has length 1, or, in other words, there are no cycles in the graph. For this I showed that if there was a cycle, the function rep_of would not terminate, because there would be an infinite loop.

For the induction step, we assume that the length of p1 is greater than 1. Therefore, we can remove the last node from p1 and the last node from p2 to get two paths from p1 to the parent of p1, where the first one is shorter that p1, and we can apply the induction hypothesis, which tells us that the two paths are equal. Adding the node p1 to those two paths gives us back the original paths p1 and p1, therefore we conclude that p1 = p2.

3.2 Implementation

3.2.1 **Union**

The *union* operation was already implemented for the uf_list in the theory Union_Find [LM12] (chapter 18, Union-Find Data-Structure), it only needed to be extended in order to appropriately update the other two lists:

The algorithm only modifies the data structure if the parameters are not already in the same equivalence class. The union find tree is modified with the ufa_union from the theory Union_Find[LM12]. The current union (x, y) is added at the end of the

unions list. au is updated such that the new edge between rep_of 1 x and rep_of 1 y is labeled with the last index of unions, which contains the current pair of elements (x,y).

```
fun ufe_union :: "ufe_data_structure \Rightarrow nat \Rightarrow nat \Rightarrow ufe_data_structure"
where
"ufe_union (uf_list = l, unions = u, au = a) x y = (
if (rep_of l x \neq rep_of l y) then
(uf_list = ufa_union l x y,
unions = u @ [(x,y)],
au = a[rep_of l x := Some (length u)])
else (uf_list = l, unions = u, au = a))"
```

Example 2. After a union of 0 and 1, the data structure from Example 1 looks as follows:

```
\{uf_{list} = [1, 1, 2, 3], unions = [(0, 1)], au = [Some 0, None, None, None]\}
```

This means that there is an edge between 1 and 0, labeled with the union at index 0, which is (0,1).

Next, we define a function which takes a list of unions as parameter and simply applies each of those unions to the data structure. This will be needed for the invariant and the correctness proof in the next sections.

```
fun apply_unions::"(nat * nat) list ⇒ ufe_data_structure ⇒
    ufe_data_structure"
where
"apply_unions [] p = p" |
"apply_unions ((x, y) # u) p = apply_unions u (ufe_union p x y)"
```

3.2.2 Helper Functions for Explain

The explain function is based on other functions, which will be described in the following pages.

path_to_root

The function $path_to_root \ 1 \ x$ computes the path from the root of x to the node x in the union-find forest 1. It simply starts at x and continues to add the parent of the current node to the path, until it reaches the root.

```
function path_to_root :: "nat list \Rightarrow nat \Rightarrow nat list" where
```

```
"path_to_root l x = (if l ! x = x then [x] else path_to_root l (l ! x) @ [x])
by pat_completeness auto
```

It was easy to show that it has the same domain as the rep_of function, as it has the same recursive calls.

```
\textbf{lemma} \hspace{0.1cm} \textbf{path\_to\_root\_domain: "rep\_of\_dom (l, i)} \longleftrightarrow \textbf{path\_to\_root\_dom (l, i)"}
```

The correctness of the function follows easily by induction.

```
theorem path_to_root_correct:
assumes "ufa_invar l"
shows "path l (rep of l x) (path to root l x) x"
```

lowest_common_ancestor

The function lowest_common_ancestor $l \times y$ finds the lowest common ancestor of x and y in the union-find forest l.

Definition. A *common ancestor* of two nodes x and y is a node which has a path to x and a path to y. The *lowest common ancestor* of two nodes x and y is a node common ancestor where its path to the root has maximal length.

The function will only be used for two nodes which have the same root, otherwise there is no common ancestor. It first computes the paths from x and y to their root, and then returns the last element which the two paths have in common. For this it uses the function longest_common_prefix from HOL-Library.Sublist[NW].

```
fun lowest_common_ancestor :: "nat list ⇒ nat ⇒ nat ⇒ nat"
where
"lowest_common_ancestor l x y =
last (longest common prefix (path to root l x) (path to root l y))"
```

Regarding the correctness proof, there were two aspects to prove: the most useful result is that lowest_common_ancestor $l \times y$ is a common ancestor of x and y. The second aspect stated that any other common ancestor of x and y has a shorter distance from the root. The proof assumes that that x and y have the same root.

Proof. Let $lca = lowest_common_ancestor l x y$. We previously proved that path_to_root computes a path p_x from the root to x and p_y from the root to y. Evidently, lca lies on both paths, because it is part of their common prefix. Splitting the paths, we get a path from the root to lca and one from lca to x, and the same for y. This shows that lca is a common ancestor.

To prove that it is the *lowest* common ancestor, we can prove it by contradiction. If there was a common ancestor lca_2 with a longer path from the root than lca, then we

can show that there is a path from the root to x passing through lca_2 , and the same for y. Because of the uniqueness of paths, these paths are equal to path_to_root l x and path_to_root l y, respectively. That means, that there is a prefix of path_to_root l x and path_to_root l y which is longer than the one calculated by the function longest_common_prefix. The theory Sublist[NW] contains a correctness proof for longest_common_prefix, which we can use to show the contradiction.

find_newest_on_path

The function find_newest_on_path finds the newest edge on the path from y to x. It is assumed that y is an ancestor of x. The function simply checks all the elements on the path from y to x and returns the one with the largest index in a, which represents the associated unions list.

```
function (domintros) find_newest_on_path :: "nat list ⇒ nat option list ⇒
    nat ⇒ nat ⇒ nat option"
where
"find_newest_on_path l a x y =
(if x = y then None
else max (a ! x) (find_newest_on_path l a (l ! x) y))"
by pat completeness auto
```

If there is a path *p* from *y* to *x*, it is easily shown by induction that the function terminates.

```
lemma find_newest_on_path_domain:
assumes "ufa_invar l"
and "path l y p x"
shows "find newest on path dom (l, a, x, y)"
```

For the correctness proof we define an abstract definition of the newest element on the path: Newest_on_path is the maximal value in the associated unions list for indexes in p.

```
abbreviation "Newest_on_path l a x y newest \equiv \exists p . path l y p x \land newest = (MAX i \in set [1..<length p]. a ! (p ! i))"
```

Then it can easily be shown by computation induction on find_newest_on_path that our function is correct.

```
theorem find_newest_on_path_correct: assumes "path l y p x" and "ufa_invar l" and "x \neq y" shows "Newest_on_path l a x y (find_newest_on_path l a x y)"
```

3.2.3 Explain

We implement the explain function following the description of the first version of the union-find algorithm in the paper[NO05].

The explain function takes as parameter two elements x and y and calculates a subset of the input unions which explain why the two given variables are in the same equivalence class. If we consider the graph which has as nodes the elements and as edges the input unions, then the output of explain would be all the unions on the path from x to y. However, the union-find forest in our data structure does not have as edges the unions, but only edges between representatives of the elements of the unions.

From this graph, we can calculate the desired output in the following way: first add the last union (a, b) made between the equivalence class of x and the one of y, then recursively call the explain operation with the new parameters (x, a) and (b, y) (or (x, b) and (a, y), depending on which branch a and b are on). The newst union is the label of the newest edge in the union-find forest.

(a,b) is calculated by finding the lowest common ancestor lca of x and y, and then finding the newest union on the path from x to lca and from y to lca. There is a case distinction at the end to account for the cases that the newest union is on same branch as x or as y.

TODO example

```
function (domintros) explain :: "ufe data structure \Rightarrow nat \Rightarrow nat \Rightarrow (nat *
    nat) set"
where
"explain (uf list = l, unions = u, au = a) x y =
(if x = y \lor rep of l x \neq rep of l y then {}
(let lca = lowest common ancestor l x y;
newest index x = find newest on path l a x lca;
newest index y = find newest on path l a y lca;
(ax, bx) = u ! the (newest index x);
(ay, by) = u ! the (newest_index_y)
in
(if newest index x \ge newest index y then
\{(ax, bx)\} \cup explain (uf_list = l, unions = u, au = a) x ax
∪ explain (uf_list = l, unions = u, au = a) bx y
\{(ay, by)\} \cup explain (uf list = l, unions = u, au = a) \times by
∪ explain (uf_list = l, unions = u, au = a) ay y)
by pat completeness auto
```

3.3 Proofs

This section introduces an invariant for the union find data structure and proves that the .explain function terminates and is correct, when invoked with valid parameters.

3.3.1 Invariant and Induction Rule

The validity invariant of the data structure expresses that the data structure derived from subsequent unions with ufe_union, starting from the initial empty data structure. It also states that the unions were made with valid variables, i.e. varibles which are in bounds.

```
abbreviation "ufe_invar ufe ≡
valid_unions (unions ufe) (length (uf_list ufe)) ∧
apply unions (unions ufe) (initial ufe (length (uf list ufe))) = ufe"
```

With this definition, it is easy to show that the invariant holds after a union.

```
lemma union_ufe_invar:
assumes "ufe_invar ufe"
shows "ufe_invar (ufe_union ufe x y)"
```

It is also useful to prove that the old invariant, ufa_invar, is implied by the new invariant, so that we can use all the previously proved lemmas about ufa_invar. This is easily shown by computation induction on the function apply_unions, and by using the lemma from the Theory Union Find[LM12], which states that ufa_invar holds after having applied ufa_union, and proving that it holds for the initial ufe.

```
theorem ufe_invar_imp_ufa_invar: "ufe_invar ufe ⇒ ufa_invar (uf_list ufe)"
```

With this definition of the invariant, we can prove a new induction rule, which will be very useful for proving many properties of a union find data structure. The induction rule, called apply_unions_induct, has as an assumption that the invariant holds for the given data structure ufe, and shows that a certain predicate holds for ufe. The base case that needs to be proven is that it holds for the initial data structure, and the induction step is that the property remains invariant after applying a union.

```
lemma apply_unions_induct[consumes 1, case_names initial union]:
assumes "ufe_invar ufe"
assumes "P (initial_ufe (length (uf_list ufe)))"
assumes "∧pufe x y. ufe_invar pufe ⇒ x < length (uf_list pufe) ⇒ y <
   length (uf_list pufe) ⇒ P pufe ⇒ P (ufe_union pufe x y)"
shows "P ufe"</pre>
```

This induction rule can be used for most of the proofs about explain.

3.3.2 Termination Proof

An important result was to show that the function always terminates if ufe_invar holds.

```
theorem explain_domain:
assumes "ufe_invar ufe"
shows "explain_dom (ufe, x, y)"
```

Proof. For the base case, we consider the empty data structure. There are no different variables with the same representative, therefore the algorithm terminates immediately.

For the induction step we need to show that if the function terminates for a data structure ufe, then it also terminates for ufe_union ufe x y. The lowest common ancestor and the newest index on path do not change after a union was applied. Therefore the entire algorithm is executed with exactly the same results at each intermediate step, therefore the recursive calls are equal, and they terminate by induction hypothesis. TODO

3.3.3 Correctness Proof

TODO There are two properties which define the correctness of explain: foremost, the equivalence closure of explain x y should contain the pair (x,y) (we shall refer to this property as "correctness"), additionally, the elements in the output should only be equations which are part of the input (we shall refer to this property as "validity"). The proposition about the validity of explain looks as follows:

```
theorem explain_valid:
assumes "ufe_invar ufe"
and "xy ∈ (explain ufe x y)"
shows "xy ∈ set (unions ufe)"
```

We know from Subsection 3.3.2 that when the invariant holds, the function terminates. Therefore we can use the partial induction rule that Isabelle automatically generates for partial functions. We can prove that (a,b) is a valid union, given that it is in the unions list, for that we need to prove that the index found by find_nearest_on_path is in bounds.

```
lemma find_newest_on_path_Some: assumes "path l y p x" and "ufe_invar (uf_list = l, unions = u, au = a)" and "x \neq y" obtains k where "find newest on path l a x y = Some k \wedge k < length u"
```

which follows from the following lemma, that shows that the entries in the associated union list are valid, aka less than the length of u

```
lemma au_valid:
assumes "ufe_invar ufe"
and "i < length (au ufe)"
shows "au ufe ! i < Some (length (unions ufe))"</pre>
```

It is easily proven, given that all the values that are added to au are valid.

Thus we have shown the validity of the explain function. It remains to show the correctness.

```
theorem explain_correct:
assumes "ufe_invar ufe"
and "rep_of (uf_list ufe) x = rep_of (uf_list ufe) y"
shows "(x, y) \in (symcl (explain ufe x y))*"
```

This was shown by computation induction on explain. For example for case x: $(x,ax) \in (\exp \| x \| x \|)^*$ and $(bx,y) \in (\exp \| x \| y \|)^*$ and $(ax,bx) \in (\exp \| x \| y \|)^*$

4 Congruence Closure with Explain Operation

4.1 Implementation

For the implementation of the congruence closure algorithm, we follow the description in the paper. [NO05]

4.1.1 Modified Union Find Algorithm

In order to implement an explain operation with a reasonable runtime for the congruence closure data structure, the paper [NO05] introduces an alternative union-find algorithm. We will not discuss in detail the runtimes of the functions, since the main objective of this thesis is to prove the correctness of the algorithms, and for this purpose we disregared sThe find function remains the same, but for union and explain a new data structure is introduced, the *proof forest*, i.e. a forest which has as nodes the variables, and as edges the unions that were made. The forest structure is preserved by union, because redundant unions are ignored.

add_edge

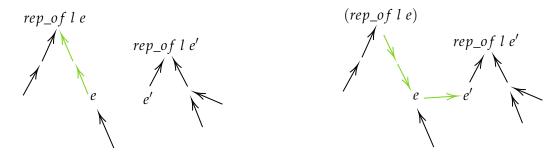
The proof forest has directed edges, and for each equivalence class there is a representative node, where all the edges are directed towards. To keep this invariant, each time and edge from e to e' is added, all the edges on the path from the root of e to e' are reversed. In the implementation, the proof forest is represented by a list which stores the parent of each node, exactly as in the union-find list. My implementation for adding an edge, which corresponds to the union operation, is the following:

We can show that add_edge e e' terminates, if the invariant ufa_invar holds for the proof forest and e and e' do not belong to the same equivalence class.

```
lemma add_edge_domain:
  assumes "ufa_invar l" "rep_of l e ≠ rep_of l e'"
  shows "add edge dom (l, e, e')"
```

Proof. It can be proven by induction on the length of the path p from the root of e to e. In the base case there is only one node in the path, therefore e must be equal to its root, therefore pf!e=e, and the algorithm terminates immediately.

In the other case e is not a root, then there is a path p' from the root to the parent of e which is shorter than the path from the root to e. The path p' is also present in the pf[e:=e'], because the path does not contain e. Also, the representative of e in pf[e:=e'] is equal to the representative of e', and the representative of the parent of e is still the old representative of e, therefore they are not in the same representative class, and we can apply the induction hypothesis and conclude that the recursive call terminates, therefore the function terminates.



add_label

Additionally, each edge is labeled with the input equation or the input equations which caused the adding of this edge. This is not necessary for the union-find algorithm by itself, but it will be needed by the explain operation for congruence closure. There are two possible types of labels: either an equation a = b was input, or two equations of the type $F(a_1, a_2) = a$ and $F(b_1, b_2) = b$, where a_1 and b_1 were already in the same equivalence class before this union, as well as a_2 and b_2 . In both theses cases a union between the equivalence classes of a and b must be made. The labeling is implemented by using an additional list, which at each index contains the label of the outgoing edge, or None if there is no outgoing edge. It is similar to the associated unions list of union-find, but it contains directly the labels instead of an index to another list.

We define a new datatype for the equations used in the algorithm. Equations of the type a=b will be written as a \approx b, and equations of the type F(a,b)=c are written as F a b \approx c

```
datatype equation = Constants nat nat ("_ \approx _")
    | Function nat nat nat ("F _ _ \approx _")
```

The labels have the type pending equation, which can be either one or two equations.

The name pending_equation derives from the fact that it is also the type of the elements of the pending list, which will be described in the next section. Theoretically this allows also for invalid equations for example two equations of the type a = b and c = d, but we will prove in the next sections that the equations in the labels list are always either One (a = b) or Two $(F(a_1, a_2) = a)$ $(F(b_1, b_2) = b)$.

Each time an edge gets added to the proof forest, the labels need to be updated as well. The function add_label adds a label to the new edge, and modifies the labels for the edges which are modified by add_edge:

```
function (domintros) add_label :: "pending_equation option list ⇒ nat list
    ⇒ nat ⇒ pending_equation ⇒ pending_equation option list"
    where
"add_label pfl pf e lbl =
    (if pf ! e = e
        then (pfl[e := Some lbl])
        else add_label (pfl[e := Some lbl]) pf (pf ! e) (the (pfl ! e)))"
    by pat_completeness auto
```

Similarly to the path_to_root function, add_label has the same recursive calls as rep of, therefore it has the same domain.

```
lemma rep_of_dom_iff_add_label_dom:
   "rep_of_dom (pf, y) ←→ add_label_dom (pfl, pf, y, y')"
```

4.1.2 Congruence Closure Data Structure

For the congruence closure algorithm there are five important data structures, which are described in the following. More details on this topic can be found in [NO05].

- cc_list: the union-find list, corresponds to the uf_list.
- use_list: a two-dimensional list which contains for each representative a a list of input equations $F(b_1, b_2) = b$ where the representative of b_1 or b_2 is a.

- lookup: a lookup table indexed by pairs of representatives b and c, which stores an input equation $F(a_1, a_2) = a$ such that b is the representative of a_1 and c is the representative of a_2 , or None if no such equation exists.
- pending: equations of the type 0ne (a = b) or Two $(F(a_1, a_2) = a)$ $(F(b_1, b_2) = b)$ where a and b need to be merged, and a_1 and b_1 are already in the same congruence class, as well as a_2 and b_2 .
- proof_forest: the proof forest as described in the previous subsection.
- pf_labels: the labels of the proof forest as described in the previous subsection
- input: a set of the input equation, which will be useful for some proofs in the next sections.

In the following, we shall sometimes refer to cc_list as l, the use list as u, the lookup table as t, the pending list as pe, the proof forest as pf, the labels list for the proof forest as pfl and the input as ip.

4.1.3 Congruence Closure Algorithm

With this data structure we can implement the merge function as described in [NO05]. The merge function adds the equation to pending, and then calls propagate. If the input equation is of the type $F(a_1, a_2) = a$, then there are two possibilities: if there is already an equation $F(b_1, b_2) = b$ in the lookup table at the $(rep_of(a_1), rep_of(a_2))$, then we know that $a_1 = b_1$ and $a_2 = b_2$, and we add $F(b_1, b_2) = b$ and $F(a_1, a_2) = a$ to pending. On the other hand, if the respective lookup entry is None, then the equation is added to the lookup table, at the index $(rep_of(a_1), rep_of(a_2))$ so that the next time an equation with congruent parameters is input, they will be added together to pending.

For this case distinction there is a function lookup_Some, which returns True if there is an entry in lookup at the index $(rep_of(a_1), rep_of(a_2))$ and False otherwise, and a function update_lookup, which adds the equation to lookup at the index $(rep_of(a_1), rep_of(a_2))$.

```
| "merge (cc_list = l, use_list = u, lookup = t, pending = pe, proof_forest = pf, pf_labels = pfl, input = ip)  
(F a_1 \ a_2 \approx a) = (if (lookup_Some t l (F a_1 \ a_2 \approx a))  
then propagate (cc_list = l, use_list = u, lookup = t, pending = link_to_lookup t l (F a_1 \ a_2 \approx a)#pe, proof_forest = pf, pf_labels = pfl, input = insert (F a_1 \ a_2 \approx a) ip) else (cc_list = l, use_list = (u[rep_of l a_1 := (F a_1 \ a_2 \approx a)#(u ! rep_of l a_1)])[rep_of l a_2 := (F a_1 \ a_2 \approx a)#(u ! rep_of l a_2)], lookup = update_lookup t l (F a_1 \ a_2 \approx a), pending = pe, proof_forest = pf, pf_labels = pfl, input = insert (F a_1 \ a_2 \approx a) ip)
```

The main part of the algorithm is executed in propagate, which recursively takes one item from pending and performs the union of the representative classes. As previously mentioned, the pending item could be either an equation of the type a = b, or two equations of the type $F(a_1, a_2) = a$ and $F(b_1, b_2) = b$, where a_1 and a_2 are already in the same representative class as b_1 and b_2 respectively. In both cases the representative classes of a and b need to be merged. The functions left and right simply retrieve a and b from either of the two types of pending equations. If a and b are already in the same representative class, nothing needs to be done, otherwise the union is performed. For more clarity, I defined the union separately as $propagate_step$.

Concerning the union, we disregard some optimisations, namely the path compression and the optimisation which considers the size of the representative classes in order to choose in which direction to add the union edge. These optimisations are

not relevant for the correctness of the algorithm, and they could later be added to a refinement of the algorithm.

The union consists of the previously discussed ufa_union, add_edge and add_label, as well as a loop which moves all elements from the use list of the representative of a to either the representative of b, or to pending. This is necessary, because the old representative of a is not a representative any more, and its new representative is $rep_of(l,b)$.

The loop is defined as a recursive function, which considers each element of the use list of $rep_of(l,a)$, and either adds it to the use list and the lookup table, or if there is already an entry in lookup, then that entry together with the current equation are added to pending.

```
fun propagate_loop
 where
"propagate loop rep b (u1 # urest)
(cc_list = l, use_list = u, lookup = t, pending = pe, proof_forest = pf,
   pf labels = pfl, input = ip)
 propagate loop rep b urest (
  if (lookup Some t l u1)
  then
    (cc list = l, use list = u, lookup = t,
         pending = link to lookup t l u1#pe,
         proof_forest = pf, pf_labels = pfl, input = ip)
  else
    (cc list = l,
         use list = u[rep b := u1 # (u ! rep b)],
         lookup = update lookup t l u1,
         pending = pe, proof forest = pf, pf labels = pfl, input = ip)
| "propagate loop [] cc = cc"
```

The function are_congruent returns True if an equation is in the congruence closure of all the input equations so far. It simply checks if the elements have the same

representative or if they have the same representative as the correspondent entry in lookup.

```
fun are_congruent :: "congruence_closure ⇒ equation ⇒ bool"
  where
"are_congruent (cc_list = l, use_list = u, lookup = t, pending = pe,
    proof_forest = pf, pf_labels = pfl, input = ip) (a ≈ b) =
    (rep_of l a = rep_of l b)"
| "are_congruent (cc_list = l, use_list = u, lookup = t, pending = pe,
    proof_forest = pf, pf_labels = pfl, input = ip) (F a₁ a₂ ≈ a) =
    (case lookup_entry t l a₁ a₂ of
    Some (F b₁ b₂ ≈ b) ⇒ (rep_of l a = rep_of l b)
    | None ⇒ False
)"
```

4.2 Correctness Proof

4.2.1 Invariants

At this point we can already prove some properties of the congruence closure data structure. Our approach this time is different than the one for the union-find algorithm. Instead of defining an induction rule like in the union find section and then prove the properties through the induction rule, we define the properties as invariants and then prove that they remain invariant after applying merge. For each invariant, we need to follow the same steps:

- 1. Prove that the invariant holds for the initial empty congruence closure.
- 2. Prove that if the invariant holds before the merge operation, it also holds after the merge operation. Below is a list of what needs to be proven:
 - a) The invariant holds after one step in the propagate_loop. We shall refer to the two possible cases as loop1 and loop2.
 - b) The invariant holds after the entire propagate loop.
 - c) The invariant holds for the parameters of propagate_loop in propagate_step. We shall refer to the this case as mini step.
 - d) It holds after propagate_step.
 - e) It holds after propagate.
 - f) And finally, it holds after merge.

After having defined all the invariants and proven the above properties, we can put all the invariants together in the invariant cc_invar and prove the following two theorems, which state exactly the two properties described above for the invariant cc_invar:

```
theorem cc_invar_initial_cc: "cc_invar (initial_cc n)"
theorem cc_invar_merge:
   assumes "cc_invar cc" "valid_vars eq (nr_vars cc)"
   shows "cc invar (merge cc eq)"
```

Let us now look at the concrete invariants. Each list in the data structure has an invariant which states that all the elements which are in the list are in bounds. This is easy to prove if we assume that all the input equations contain only valid elements.

One of the invariants is the usual ufa_invar that we know from the union-find algorithm. The ufa_invar holds for the cc_list and the proof_forest. These two are only modified before entering the in the mini_step, and we already proved previously that the ufa_invar holds after ufa_union (section union find from AFP TODO) and after add_edge (Subsection 4.1.1). Therefore it also holds after merge.

We define a new invariant inv_same_rep_classes, which states, as the name suggests, that the union-find forest and the proof forest represent the same equivalence classes:

```
rep_of l i = rep_of l j ←→ rep_of pf i = rep_of pf j
```

In order to prove this, given that the two lists are only modified during the $mini_step$, it is sufficient to show that $ufa_union\ l\ x\ y$ and $add_edge\ pf\ x\ y$ have the same behaviour. The theory $Union_Find$ from the AFP[LM12] already provides the following lemma for ufa_union :

```
lemma ufa_union_aux:
    "rep_of (ufa_union l x y) i =
        (if rep_of l i = rep_of l x then rep_of l y else rep_of l i)"

We can show a similar lemma for add_edge:
lemma rep_of_add_edge_aux:
    assumes "rep_of l x ≠ rep_of l y"
    shows "rep_of (add_edge l x y) i =
         (if rep_of l i = rep_of l x then rep_of l y else rep_of l i)"
```

The additional assumption "rep_of l x \neq rep_of l y" does not cause problems, because add_edge is only used within propagate_step, and propagate_step is only executed if "rep of l x \neq rep of l y".

Proof. We already showed that the function terminates in Subsection 4.1.1, therefore we can prove it by induction on add_edge.

TODO describe the proof.

Additionally, for each data structure there is an invariant which states the properties which were informally described in Subsection 4.1.2.

For the use list, the invariant states that for each representative a, its use list only contains equations of the type $F(b_1, b_2) = b$, where a is the representative of either b_1 or b_2 .

Proof. In order to prove the use list invariant, we can follow the steps described earlier. For the correctness proof after the propagate_loop, I needed to add an additional assumption that the second parameter only contains equations of the type $F(a_1, a_2) = a$ and the representative of either a_1 or a_2 is $rep_of(l,b)$ (where b is the right side of the equation which is being propagated). This follows from the facts that the parameter of propagate_loop was $(u!rep_of(l,a))$, and the new representative of a after the union is b.

With this assumption I could show that each time an equation gets added to the use list in the propagate_loop, it is a valid equation.

In the proof after the merge operation, the use list is only modified in the third case, and only equations of a valid form are added to $rep_of(l, a_1)$ and $rrep_of(l, a_2)$. Therefore all the necessary properties hold for these new equations.

For the remaining cases, use list is either unchanged, or something is removed from it, therefore the invariant trivially holds. \Box

The invariant for lookup is similar, it states that each entry in the lookup table at index (i, j), for representatives i and j, is either None or is an equation of the form $F(a_1, a_2) = a$ where the representative of a_1 is i and the representative of a_2 is j.

Proof. Each time an equation is added to lookup, it has the desired form and it is added to the index $(rep_of(l, a_1), rep_of(l, a_2))$. This happens in the propagate_loop and in merge. In the propagate_loop, the added equation derives from the use list, for which we proved with the previous invariant that its equations have the desired form. In merge, only the equations of the type $F(a_1, a_2) = a$ are added to lookup.

For pending, the invariant states that the equations are either of the form 0ne (a = b) or Two $(F(a_1, a_2) = a)$ $(F(b_1, b_2) = b)$ where $rep_of(l, a_1) = rep_of(l, b_1)$ and $rep_of(l, a_2) = rep_of(l, b_2)$: It is important to know that they are in the same representative class, because TODO

Proof. We need to show that in the propagate_loop the equation u1 we add to pending has a valid format. We know that u1 derives from the use list, therefore it is of the form $F(a_1,a_2)=a$. Then we link to it the lookup entry at the index $(rep_of(l,a_1),rep_of(l,a_2))$. From the lookup invariant we know that there is an

```
entry of the form F(b_1, b_2) = b at this index where rep\_of(l, a_1) = rep\_of(l, b_1) and rep\_of(l, a_2) = rep\_of(l, b_2). This shows that they are valid equations for pending. The same holds for the equations added to pending in merge.
```

There is also an invariant which states that the cc_list, the first dimension of the use list, both dimensions of lookup, the proof forest and the pf_labels have the same length. This was trivial to prove, given that the algorithm never changes the length of the lists, and initially the lists have the same length.

All the above-mentioned invariants hold trivially for the initial case, given that all the data structures are empty or contain only None in the beginning.

The remaining invariants will be described later on, when they become relevant.

4.2.2 Abstract Formalisation of Congruence Closure

In order to prove the correctness of the algorithm, we define an abstraction of congruence closure. We cannot use any previouly defined definitions, because the data structure that we use can only represent a subset of all possible equations, for example it cannot represent equations of the type a = F(b,c) or F(F(a,b),c) = d. For this reason, we define an inductive set which represents the congruence closure of a set of equations and only uses the our restricted definition of equation.

```
inductive_set Congruence_Closure :: "equation set ⇒ equation set" for S
    base: "eqt \in S \Longrightarrow eqt \in Congruence Closure S"
  | reflexive: "(a pprox a) \in Congruence_Closure S"
    symmetric: "(a \approx b) \in Congruence Closure S \Longrightarrow (b \approx a) \in
       Congruence Closure S"
  | transitivel: "(a \approx b) \in Congruence Closure S \Longrightarrow (b \approx c) \in
       Congruence Closure S
\implies (a \approx c) \in Congruence Closure S"
  | transitive2: "(F a_1 a_2 \approx b) \in Congruence_Closure S \Longrightarrow (b \approx c) \in
       Congruence Closure S
\Longrightarrow (F \mathsf{a}_1\ \mathsf{a}_2\ pprox c) \in Congruence_Closure S"
  | transitive3: "(F a_1 a_2 \approx a) \in Congruence_Closure S
\Longrightarrow (a_1 pprox \mathsf{b}_1) \in Congruence Closure S \Longrightarrow (a_2 pprox \mathsf{b}_2) \in Congruence Closure S
\implies (F b_1 b_2 \approx a) \in Congruence_Closure S"
  | monotonic: "(F a_1 a_2 \approx a) \in Congruence_Closure S \Longrightarrow (F a_1 a_2 \approx b) \in
       Congruence Closure S
\implies (a \approx b) \in Congruence Closure S"
```

The following proof rule follows directly from the definition of Congruence Closure, and proved to be very useful for multiple proofs:

```
lemma Congruence_Closure_eq[case_names left right]:
   assumes "∧ a. a ∈ A ⇒ a ∈ Congruence Closure B"
```

```
"\land b. b \in B \Longrightarrow b \in Congruence_Closure A" shows "Congruence Closure A = Congruence Closure B"
```

It is used to prove equality between congruence closures of *A* and *B*. It states that it is sufficient to prove that all elements of set *A* are in the congruence closure of *B* and vice versa, instead of having to prove that all elements of the congruence closure of *A* are in the congruence closure of *B*.

4.2.3 Correctness

To prove the correctness of the congruence closure implementation, we need to show that the invariants imply that are_congruent cc eq returns True if and only if the equation *eq* lies in the congruence closure of the input equations.

```
theorem are_congruenct_correct:
    assumes "cc_invar cc" "pending cc = []"
    shows "eq ∈ Congruence Closure ((input cc)) ←→ are congruent cc eq"
```

The paper [NO05] proves this by stating athe following invariant which holds throughout the algorithm,

```
Congruence_Closure(representativeE ∪ pending) = Congruence_Closure (input)
```

where representative E can be seen as the set of equations derived from our union-find list and the equations in lookup. It is the union of the following two sets:

- representative_set is defined such that its congruence closure contains all the equations between two elements which have the same representative.
- lookup_entries_set is the set of all the entries in lookup at indexes which are representatives.

```
abbreviation representatives_set :: "nat list \Rightarrow equation set" where "representatives_set l \equiv \{a \approx rep\_of \ l \ a \mid a. \ l \mid a \neq a\}" abbreviation lookup_entries_set :: "congruence_closure \Rightarrow equation set" where "lookup_entries_set cc \equiv \{F \ a' \ b' \approx rep\_of \ (cc\_list \ cc) \ c \mid a' \ b' \ c \ c_1 \ c_2 \ .  cc\_list \ cc \mid a' = a' \land cc\_list \ cc \mid b' = b' \land lookup \ cc \mid a' \mid b' = Some \ (F \ c_1 \ c_2 \approx c)\}"  definition \ representativeE \ :: "congruence\_closure \Rightarrow equation \ set" where "representativeE \ cc = representatives_set \ (cc\_list \ cc) \ \cup lookup\_entries\_set \ cc"
```

The formal definition of the aforementioned invariant is the following, where pending_set converts the pending list to a set of equations of the type a = b:

```
definition inv2 :: "congruence_closure ⇒ bool"
  where
    "inv2 cc ≡
Congruence_Closure (representativeE cc ∪ pending_set (pending cc)) =
    Congruence Closure (input cc)"
```

The set of input equations is only modified by the merge function, but remains constant throughout the propagate function, therefore for the proof we just need to show that the congruence closure of the representative E set and pending remain unchanged after the propagate function.

The main challenge is to prove that the invariant holds after the mini_step. We will show that Congruence Closure (representativeE \cup pending) before the propagate_step is equal to Congruence Closure (representativeE \cup pending \cup (u ! rep_of l a)) after the mini_step. Then we prove that Congruence Closure (representativeE \cup pending \cup (u ! rep_of l a)) is equal to Congruence Closure (representativeE \cup pending) after the propagate_loop. These two lemmas imply that the congruence closure of the representativeE set and pending remain unchanged after the propagate function.

We will first prove the second statement, given that it is much easer to show.

Proof. We need to shhow that Congruence Closure (representativeE \cup pending \cup (u ! rep_of l a)) is equal to Congruence Closure (representativeE \cup pending) after the propagate_loop. In each step of the loop, one element from $(u!rep_of(l,a))$ is moved either to pending or to lookup. Therefore after the loop each element of $(u!rep_of(l,a))$ is either in pending or in representativeE.

The first lemma is more difficult to prove. The following is the statement of the lemma:

```
lemma inv2_mini_step:
    assumes "a = left eq" "b = right eq"
    "cc_invar (cc_list = l, use_list = u, lookup = t, pending = (eq # pe),
    proof_forest = pf, pf_labels = pfl, input = ip)"
        shows "Congruence_Closure
(representativeE
(cc_list = l, use_list = u, lookup = t, pending = (eq # pe),
    proof_forest = pf, pf_labels = pfl, input = ip)
    U pending_set (eq # pe))
=
Congruence_Closure (representativeE
(cc_list = ufa_union l a b,
        use_list = u[rep_of l a := []],
```

```
lookup = t,
  pending = pe,
  proof_forest = add_edge pf a b,
  pf_labels = add_label pfl pf a eq,
  input = ip)
U pending_set pe
U set (u ! rep_of l a))"
```

Proof. There are two inclusions which need to be shown. We can use the rule Congruence_Closure_eq from Subsection 4.2.2, which means that it is sufficient to show that each equation in the set on the left hand side is in the congruence closure of the right hand side and vice versa.

"⊆" It needs to be shown that the equations of the representatives_set, in lookup and in pending are in the Congruence Closure of the right-hand side.

Regarding the representatives_set, all the elements which had the same representative before a union also have the same representative after a union.

For the pending set, we need to prove that the equation that is removed from pending is still in the congruence closure after the mini_step. This holds, because the equation which is removed is a = b, and a and b are in the same equivalence class after the ufe union.

The problematic case are the equations in lookup. Given that after the union there is one element $c = rep_of(l,a)$ which is not a representative any more, the entries in lookup which have as first or second index c are not in lookup anymore after the union. The goal is to prove that these equations are exactly the equations which are present in $(u!rep_of(l,a))$, but until now it was only proven that the equations in the use list are valid, not that they are exhaustive. A new invariant use_list_inv2 is needed which states that all elements which are present in the lookup table at index (i,j) are also in the corresponding use lists of i and j. I will introduce this invariant later.

" \supseteq " We need to show that the equations of the representatives_set, lookup_entries_set , pending set and of $(u!rep_of(l,a))$ on the right-hand side are in the congruence closure of the left-hand side.

The representatives_set, contains equations of the type $c = rep_of(ufa_union(l,a,b),c)$. If the representative after the union is the same before the union, the same equation is in the representatives_set of the left hand side. The only representative that is different than before the union is the representative of a, which has as new representative $rep_of(l,b)$. The left-hand side contains the equations $b = rep_of(l,b)$ and a = b (which is in pending). By transitivity, the congruence closure also contains $a = rep_of(l,b)$ and $rep_of(l,b)$ is exactly the same as $rep_of(ufa_union(l,a,b),a)$.

Regarding lookup, all the elements which are roots after the union, are also roots before the union, therefore all elements in the lookup entry set of the right-hand side

are also in the left-hand side.

It is evident that the equations in pending on the right-hand side are also in pending in the left-hand side.

It is more difficult to show that the equations in $(u!rep_of(l,a))$ are also present in the lookup table of the left-hand side. Like before, we need a new invariant lookup_invar2, which I will describe below.

Thus we need two new invariants of this form:

- lookup_invar2: The elements in the lookup table are also present in the use list.
- use list invar2: The elements in the use list are also present in the lookup table.

Unfortunately, these two invariants are not exactly true, because if there are two different equations where the elements have the same representatives, then they can't both be present in the lookup table, because it only stores one equation for each pair of representatives. In fact, the set of equations in lookup and in the use list are not exactly the same, but for each equation in one of them, there is a "similar" equation in the other one.

The difficulty was to find a suitable definition of 'similar" which is not too strong, otherwise it wouldn't be true, but also not too weak, otherwise it is not possible to prove the invariant inv2.

The right definition of similar turned out to be the following:

Definition. Two equations $F(a_1, a_2) = a$ and $F(b_1, b_2) = b$ are similar, if $rep_of(l, a_1) = rep_of(l, b_1)$, $rep_of(a_2) = rep_of(b_2)$ and $(a = b) \in Congruence_Closure(representatives_set \cup pending)$.

Simply stating that a and b have the same representative would be too strong, because during the propagate function, they are added to pending in order to be merged later, and are not merged yet. If we use representativeE instead of representatives_set, the inariant is not strong enough in order to prove inv2 mini step.

Here follows the proof for lookup invar2:

Proof. We need to show that if before the merge the invariant holds, then it also holds after the merge. The invariant states that for each equation in lookup at the index (i, j) (where i and j are representatives) there is a similar equation in use list i and one in use list j.

The main aim is to show that it holds after propagate. We assume that before propagate the invariant holds. In particular, each equation $F(c_1, c_2) = c$ in $u_a = (u!rep_of(l,a))$ there is a similar equation in $(u!rep_of(l,c_1))$ and in $(u!rep_of(l,c_2))$.

In the propagate_loop u_a is emptied, while the other use lists are not modified, and u_a is handed over as a parameter to the propagate_loop.

From now on let l be the cc_list after the ufe_union.

In propagate_loop1 the lookup table and the use lists are not modified, thus there is nothing to show.

In propagate_loop2 we take an equation u1 of the form $F(c_1, c_2) = c$ from u_a .

u1 is then added to lookup at the index $(rep_of(l,c_1), rep_of(l,c_2))$. We need to show that after this step, an equation similar to u1 is present both in the use list of $rep_of(l,c_1)$ and the use list of $rep_of(l,c_2)$. This holds if one (or both) of them is equal to $rep_of(l,b)$, because u1 is also added to $u!rep_of(l,b)$ by the function.

If they are not equal to $rep_of(l,b)$, there is a similar equation in the corresponding use list, because the use list has not been changed.

Here follows the proof for use_list_invar2:

Proof. We need to show that if before the merge the invariant holds, then it also holds after the merge. The invariant states that for each equation $F(c_1, c_2) = c$ in use list at the index i (where i is a representative) there is a similar equation in lookup($rep_of(l, c_1)$, $rep_of(l, c_2)$).

The difficulty in this proof was when after the mini_step, because of the union, $rep_of(l,a)$ is not a root any more, therefore the lookup entries at the indexes of $rep_of(l,a)$ are not valid anymore. However, there could be equations in a use list at an index which is not $rep_of(l,a)$, which contains equations where the second parameter has the same representative of a. These equations do not have a similar equation in lookup at this moment in the algorithm, they have only a similar equation in $u_a = u!rep_ofla$, therefore the invariant does not hold for these equations. Nevertheless, we will show that it holds after the propagate_loop was executed.

From now on let l be the cc list after the ufe union.

The propagate_loop removes an equation $F(c_1,c_2)=c$ from u_a , and it enters propagate_loop1 when lookup contains an equation $F(d_1,d_2)=d$ at the index $(rep_of(l,c_1),rep_of(l,c_2))$. Then the equation c=d is added to pending. Note that $F(c_1,c_2)=c$ and $F(d_1,d_2)=d$ are similar at this point, because $rep_of(l,c_1)=rep_of(l,d_1)$ and $rep_of(l,c_2)=rep_of(l,d_2)$ follows from the lookup_invar.

We know that for all the equations in the use list, there is a similar equation in lookup or u_a . For those equations where the similar equation is exactly the one that we are removing from u_a , know that that there is another equation $F(d_1, d_2) = d$ in lookup which is similar to $F(c_1, c_2) = c$.

This case is exactly the reason why we can only prove that there is a "similar" equation in lookup, and not exactly the same.

The propagate_loop2 is entered, when lookup contains None at the index $(rep_of(l, c_1), rep_of(l, c_2))$. $F(c_1, c_2) = c$ is added to $(u!rep_of(l, b))$ and lookup. Each equation which was in use list has a similar equation in lookup or u_a . For those equations where the similar equation is exactly the one that we are removing from u_a , we know that it was also added to lookup.

There is also a new element in the use list, which is $F(c_1, c_2) = c$, and it has a similar

There is also a new element in the use list, which is $F(c_1, c_2) = c$, and it has a similar equation in lookup, which is $F(c_1, c_2) = c$ itself.

With these two invariants the proof for inv2 is completed.

Given that the pending list is always empty after the termination of propagate, the correctness proof are_congruent_correct follows directly from this invariant.

To completely finish the proof, one would need to prove that propagate terminates, which is currently left open for future work.

4.3 Implementation of the Explain Operation

I implemented the explain operation for congruence closure, leaving the proof of termination and correctness open for future work. Nevertheless I would like to dedicate this section on the description of the implementation and a proposal of how the correctness could be proven.

TODO

5 Conclusion

5.1 Future work

List of Figures

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