Formal Proofs of Tarjan's Strongly Connected Components Algorithm in Why3, Coq and Isabelle

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18 — Abstract -

 $_{19}$ $\,$ Comparing provers on a formalization of the same problem is always a valuable exercise. In this

²⁰ paper, we present the formal proof of correctness of a non-trivial algorithm from graph theory that

 $_{\rm 21}$ $\,$ was carried out in three proof assistants: Why3, Coq, and Isabelle.

22 2012 ACM Subject Classification Logic and verification, Automated reasoning, Higher order logic

23 Keywords and phrases Mathematical logic, Formal proof, Graph algorithm, Program verification

²⁴ **1** Introduction

Graph algorithms are notoriously obscure in the sense that it is hard to grasp why exactly they work. Therefore proof of correctness are more than welcome in this domain. In this paper, we consider Tarjan's algorithm [28] for discovering the strongly connected components in a directed graph and present a formal proof of its correctness in three different systems: Why3, COQ and Isabelle/HOL. The algorithm is treated at an abstract level with a functional programming style manipulating finite sets, stacks and mappings, but it respects the linear time behaviour of the original presentation.

To our knowledge this is the first time that the formal correctness proof of a non-trivial 32 program is carried out in three very different proof assistants: Why3 is based on a first-order 33 logic with inductive predicates and automatic provers, CoQ on an expressive theory of 34 higher-order logic and dependent types, and Isabelle/HOL combines higher-order logic with 35 automatic provers. We claim that our proof is direct, readable, elegant, and follows Tarjan's 36 presentation. Crucially for our comparison, the algorithm is defined at the same level of 37 abstraction in all three systems, and the proof relies on the same arguments in the three 38 formal systems. Note that a similar exercise but for a much more elementary proof (the 39 irrationality of square root of 2) and using many more proof assistants (17) was presented 40 in [32]. 41

Formal and informal proofs of algorithms about graphs were already performed in [24, 30, 25, 13, 17, 29, 19, 27, 26, 15, 8]. Some of them are part of a larger library, others focus on the treatment of pointers or on concurrent algorithms. In particular, only Lammich and

⁴⁵ Neumann [17] gave an alternative formal proof of Tarjan's algorithm within their framework
⁴⁶ for verifying graph algorithms in Isabelle/HOL.

We expose here the key parts of the proofs. The interested reader can access the details of the proofs and run them on the web [7, 9, 20]. In this paper, we recall the principles of the algorithm in section 2; we describe the proofs in the three systems in sections 3, 4, and 5 by emphasizing the differences induced by the logics which are used; we conclude in sections 6

 $_{^{51}}$ $\,$ and 7 by commenting the developments and advantages of each proof system.

⁵² **2** The algorithm

In a directed graph, two vertices x and y are strongly connected if there exists a path from x to y and a path from y to x. A strongly connected component (scc) is a maximal set of vertices where all pairs of vertices are strongly connected. A fundamental property relates sccs and depth-first search (DFS) traversal in a directed graph: each scc is a prefix of a single subtree in the corresponding spanning forest (see figure 1c). Its root is named the base of the scc. Tarjan's algorithm [28] relies on the detection of these bases and collects the sccs in a pushdown stack. It performs a single DFS traversal of the graph assigning a serial number num[x] to any vertex x in the order of the visit. It computes the following function for every vertex x:

 $LOWLINK(x) = \min\{num[y] \mid x \Longrightarrow^* z \hookrightarrow y \land x \text{ and } y \text{ are in the same scc}\}$

The relation $x \Longrightarrow z$ means that z is a son of x in the spanning forest, the relation $\stackrel{*}{\Longrightarrow}$ is its transitive and reflexive closure, and $z \hookrightarrow y$ means that there is a cross-edge from z to y in the spanning forest (a cross-edge is an edge of the graph which is not an edge in the spanning forest). In figure 1c, \Longrightarrow is drawn in thick lines and \hookrightarrow in dotted lines; in figure 1b the table of the values of the *LOWLINK* function is shown. The minimum of the empty set is assumed to be $+\infty$ (this is a slight simplification w.r.t. the original algorithm).

The base x of an scc is found when $LOWLINK(x) \ge num[x]$, and the component is formed by the nodes of the subtree rooted at x and pruned of the sccs already discovered in that subtree. Notice that LOWLINK(x) need neither be the lowest serial number of a vertex accessible from x, nor of an ancestor of x in the spanning forest. Take for instance, vertices 8 or 9 in figure 1c. Moreover, the DFS traversal sets to $+\infty$ the serial numbers of vertices in already discovered sccs. The definition of LOWLINK can therefore be written as:

 $LOWLINK(x) = \min\{num[y] \mid x \Longrightarrow^* z \hookrightarrow y\}$

⁵⁹ Our implementation of graphs uses an abstract type *vertex* for vertices, a constant *vertices* ⁶⁰ for the finite set of all vertices in the graph, and a *successors* function from vertices to their ⁶¹ adjacency set. The algorithm maintains an environment *e* implemented as a record of type ⁶² *env* with four fields: a stack *e.stack*, a set *e.sccs* of strongly connected components, a fresh ⁶³ serial number *e.sn*, and a function *e.num* from vertices to serial numbers.

```
64
65 type vertex
```

```
66 constant vertices: set vertex
```

```
67 function successors vertex : set vertex
```

```
gg type env = {stack: list vertex; sccs: set (set vertex); sn: int; num: map vertex int}
```

The DFS traversal is organized by two mutually recursive functions dfs1 and dfs. The function dfs1 visits a new vertex x and computes LOWLINK(x). Furthermore it adds a new scc when x is the base of a new scc. The function dfs takes as argument a set r of roots and



Figure 1 The vertices are numbered and pushed onto the stack in the order of their visit by the recursive function dfs1. When the first component $\{0\}$ is discovered, vertex 0 is popped; similarly when the second component $\{5, 6, 7\}$ is found, its vertices are popped; finally all vertices are popped when the third component $\{1, 2, 3, 4, 8, 9\}$ is found. Notice that there is no cross-edge to a vertex with a number less than 5 when the second component is discovered. Similarly in the first component, there is no edge to a vertex with a number less than 0. In the third component, there is no edge to a vertex less than 1 since we have set the serial number of vertex 0 to $+\infty$ when 0 was popped.

⁷³ an environment *e*. It calls dfs1 on non-visited vertices in *r* and returns a pair consisting of an ⁷⁴ integer and the modified environment. The integer is the minimum of the values computed ⁷⁵ by dfs1 on non-visited vertices in *r* and the serial numbers of already visited vertices in *r*. If ⁷⁶ the set of roots is empty, the returned integer is $+\infty$.

The main procedure *tarjan* initializes the environment with an empty stack, an empty set of sccs, the fresh serial number 0 and the constant function giving the number -1 to each vertex. The result is the set of components returned by the function *dfs* called on all vertices in the graph.

```
81
    let rec dfs1 x e =
82
      let n0 = e.sn in
83
      let (n1, e1) = dfs (successors x) (add_stack_incr x e) in
84
       if n1 < n0 then (n1, e1) else
85
86
         let (s2, s3) = split x e1.stack in
87
         (+\infty, \{\text{stack} = s3; \text{ sccs} = \text{add} \text{ (elements s2) e1.sccs}; 
            sn = e1.sn; num = set_infty s2 e1.num})
88
89
90
    with dfs r e = if is_empty r then (+\infty, e) else
      let x = choose r in let r' = remove x r in
91
      let (n1, e1) = if e.num[x] \neq -1 then (e.num[x], e) else dfs1 x e in
92
      let (n2, e2) = dfs r' e1 in (min n1 n2, e2)
93
94
    let tarjan () =
95
      let e = {stack = Nil; sccs = empty; sn = 0; num = const (-1)} in
96
      let (_, e') = dfs vertices e in e'.sccs
88
```

In the body of dfs1, the auxiliary function add_stack_incr updates the environment by 99 pushing x on the stack, assigning it the current fresh serial number, and incrementing that 100 number in view of future calls. The function dfs1 performs a recursive call to dfs for the 101 adjacent vertices of x as roots and the updated environment. If the returned integer value n1102 is less than the number $n\theta$ assigned to x, the function simply returns n1 and the current 103 environment. Otherwise, the function declares that a new scc has been found, consisting of 104 all vertices that are contained on top of x in the current stack. Therefore the stack is popped 105 until x; the popped vertices are stored as a new set in *e.sccs*; and their serial numbers are all 106 set to $+\infty$, ensuring that they do not interfere with future calculations of min values. The 107 auxiliary functions *split* and *set_infty* are used to carry out these updates. 108

```
let add_stack_incr x e = let n = e.sn in
{stack = Cons x e.stack; sccs = e.sccs; sn = n+1; num = e.num[x 	leftarrow n]}
```

109

Figure 1 illustrates the behavior of the algorithm by an example. We presented the 118 algorithm as a functional program, using data structures available in the Why3 standard 119 library [3]. For lists we have the constructors Nil and Cons; the function elements returns 120 the set of elements of a list. For finite sets, we have the empty set *empty*, and the functions 121 add to add an element to a set, remove to remove an element from a set, choose to pick an 122 arbitrary element in a (non-empty) set, and *is_empty* to test for emptiness. We also use 123 maps with functions *const* denoting the constant function, _[_] to access the value of an 124 element, and $[[\leftarrow]]$ for creating a map obtained from an existing map by setting an 125 element to a given value. 126

For a correspondence between our presentation and the imperative programs used in standard textbooks, the reader is referred to [8]. The present version can be directly translated into CoQ or Isabelle functions, and it respects the linear running time behaviour of the algorithm, since vertices could be easily implemented by integers, $+\infty$ by the cardinal of *vertices*, finite sets by lists of integers and mappings by mutable arrays (see for instance [7]).

Thus for each environment *e* in the algorithm, the working stack *e.stack* corresponds to a cut of the spanning forest where strongly connected components to its left are pruned and stored in *e.sccs*. In this stack, any vertex can reach any vertex higher in the stack. And if a vertex is a base of an scc, no cross-edge can reach some vertex lower than this base in the stack, otherwise that last vertex would be in the same scc with a strictly lower serial number.

We therefore have to organize the proofs of the algorithm around these arguments. To maintain these invariants we will distinguish, as is common for DFS algorithms, three sets of vertices: white vertices are the non-visited ones, black vertices are those that are already fully visited, and gray vertices are those that are still being visited. Clearly, these sets are disjoint and white vertices can be considered as forming the complement in *vertices* of the union of the gray and black ones.

The previously mentioned invariant properties can now be expressed for vertices in the stack: no such vertex is white, any vertex can reach all vertices higher in the stack, any vertex can reach some gray vertex lower in the stack. Moreover, vertices in the stack respect the numbering order, i.e. a vertex x is lower than y in the stack if and only if the number assigned to x is strictly less than the number assigned to y.

¹⁴⁸ **3** The proof in Why3

The Why3 system comprises the programming language WhyML used in previous section and a many sorted first-order logic with inductive data types and inductive predicates to express the logical assertions. The system generates proof obligations w.r.t. the assertions, pre- and post-conditions and lemmas inserted in the WhyML program. The system is interfaced with off-the-shelf automatic provers and interactive proof assistants.

From the Why3 library, we use pre-defined theories for integer arithmetic, polymorphic lists, finite sets and mappings. There is also a small theory for paths in graphs. Here we define graphs, paths and sccs as follows.

```
axiom successors_vertices: \forall x. mem x vertices \rightarrow subset (successors x) vertices
predicate edge (x y: vertex) = mem x vertices \land mem y (successors x)
inductive path vertex (list vertex) vertex =
```

```
| Path_empty: \forall x: vertex. path x Nil x
161
         | Path_cons: ∀x y z: vertex, 1: list vertex.
162
              edge x y \rightarrow path y l z \rightarrow path x (Cons x l) z
163
164
      predicate reachable (x y: vertex) = ∃1. path x l y
165
      predicate in_same_scc (x y: vertex) = reachable x y \lambda reachable y x
166
      predicate is_subscc (s: set vertex) = \forall x \ y. mem x s \rightarrow mem y s \rightarrow in_same_scc x y
167
      predicate is_scc (s: set vertex) = not is_empty s
168
         \wedge is_subscc s \wedge (\forall \texttt{s'. subset s s'} \rightarrow \texttt{is\_subscc s'} \rightarrow \texttt{s == s'})
<del>1</del>98
```

¹⁷¹ where *mem* and *subset* denote membership and the subset relation for finite sets.

We add two ghost fields in environments for the black and gray sets of vertices. These fields are used in the proofs but not used in the calculation of the sccs, which is checked by the type-checker of the language.¹

```
175
176 type env = {ghost black: set vertex; ghost gray: set vertex;
177 stack: list vertex; sccs: set (set vertex); sn: int; num: map vertex int}
```

¹⁷⁹ The functions now become:

196

205

```
180
     let rec dfs1 x e =
181
182
       let n0 = e.sn in
       let (n1, e1) = dfs (successors x) (add_stack_incr x e) in
183
       if n1 < n0 then (n1, add_black x e1) else
184
         let (s2, s3) = split x e1.stack in
185
         (+\infty, {black = add x e1.black; gray = e.gray; stack = s3;
186
187
            sccs = add (elements s2) e1.sccs; sn = e1.sn; num = set_infty s2 e1.num})
     with dfs r e = ... (* unmodified *)
188
     let tarjan () =
189
       let e = {black = empty; gray = empty;
190
         stack = Nil; sccs = empty; sn = 0; num = const (-1)} in
191
       let (_, e') = dfs vertices e in e'.sccs
183
```

¹⁹⁴ with a new function *add_black* turning a vertex from gray to black and the modified ¹⁹⁵ *add_stack_incr* adding a new gray vertex with a fresh serial number to the current stack.

```
197 let add_black x e =
198 {black = add x e.black; gray = remove x e.gray;
199 stack = e.stack; sccs = e.sccs; sn = e.sn; num = e.num}
200 let add_stack_incr x e =
201 let n = e.sn in
202 {black = e.black; gray = add x e.gray;
203 stack = Cons x e.stack; sccs = e.sccs; sn = n+1; num = e.num[x 	leftarrow n]}
```

The main invariant (\mathcal{I}) of our program states that the environment is well-formed:

```
206
207 predicate wf_env (e: env) =
208 let {stack = s; black = b; gray = g} = e in
209 wf_color e \land wf_num e \land simplelist s \land no_black_to_white b g \land
210 (\forall x y. lmem x s \rightarrow lmem y s \rightarrow e.num[x] \leq e.num[y] \rightarrow reachable x y) \land
211 (\forall y. lmem y s \rightarrow \exists x. mem x g \land e.num[x] \leq e.num[y] \land reachable y x) \land
212 (\forall cc. mem cc e.sccs \leftrightarrow subset cc b \land is_scc cc)
```

where *lmem* stands for membership in a list. The well-formedness property is the conjunction of seven clauses. The two first clauses express elementary conditions about the colored sets of vertices and the numbering function (see [7, 8] for a detailed description). The third clause states that there are no repetitions in the stack, and the fourth that there is no edge from a

¹ In Why3-1.2.0, this check is performed differently

²¹⁸ black vertex to a white vertex. The next two clauses formally express the property already ²¹⁹ stated above: any vertex in the stack reaches all higher vertices and any vertex in the stack ²²⁰ can reach a lower gray vertex. The last clause states that the *sccs* field is the set of all sccs ²²¹ all of whose vertices are black.

Since at the end of the *tarjan* function, all vertices are black, the *sccs* field will contain exactly the set of all strongly connected components.

```
224
225 let tarjan () = returns {r \rightarrow \forall cc. mem cc r \leftrightarrow subset cc vertices \land is_scc cc}
226 let e = {black = empty; gray = empty;
227 stack = Nil; sccs = empty; sn = 0; num = const (-1)} in
228 let (_, e') = dfs vertices e in assert {subset vertices e'.black};
229 e'.sccs
```

Our functions *dfs1* and *dfs* modify the environment in a monotonic way. Namely they augment the set of visited vertices (the black ones); they keep invariant the set of the ones currently under visit (the gray set); they increase the stack with new black vertices; they also discover new sccs and they keep invariant the serial numbers of vertices in the stack,

Once these invariants are expressed, it remains to locate them in the program text and 241 to add assertions which help to prove them. The pre-conditions of dfs1 are quite natural: 242 the vertex x must be a white vertex of the graph, and it must be reachable from all gray 243 vertices. Moreover invariant (\mathcal{I}) must hold. The post-conditions of dfs1 are of three kinds. 244 Firstly (\mathcal{I}) and the monotony property subenv hold in the resulting environment. Vertex 245 x is black at the end of dfs1. Finally we express properties of the integer value n returned 246 by this function which should be LOWLINK(x) as noted previously. In this proof, we give 247 three implicit properties for characterizing n. First, the returned value is never higher than 248 the number of x in the final environment. Secondly, the returned value is either $+\infty$ or the 249 number of a vertex in the stack reachable from x. Finally, if there is an edge from a vertex y'250 in the new part of the stack to a vertex y in its old part, the resulting value n must be lower 251 or equal to the serial number of y. 252

```
253
      let rec dfs1 x e
254
       (* pre-condition *)
255
       requires {mem x vertices \lambda not mem x (union e.black e.gray)}
256
257
       requires {\forall y. mem y e.gray \rightarrow reachable y x}
258
       requires{wf_env e} (* I *)
       (* post-condition *)
259
       \mathsf{returns}\{(\_, e') \rightarrow \mathsf{wf\_env} e' \land \mathsf{subenv} e e'\}
260
       \operatorname{returns}\{(\_, e') \rightarrow \operatorname{mem} x e'.black\}
261
       returns{(n, e') \rightarrow n \leq e'.num[x]}
262
       returns {(n, e') \rightarrow n = +\infty \lor num_of_reachable_in_stack n x e'}
263
      returns {(n, e') \rightarrow \forall y. xedge_to e'.stack e.stack y \rightarrow n \leq e'.num[y]}
264
```

²⁶⁶ The auxiliary predicates used above are formally defined in the following way.

Notice that the definition of $xedge_to$ fits the definition of LOWLINK when the cross edge ends at a vertex residing in the stack before the call of dfs1. The pre- and post-conditions for the function dfs are quite similar up to a generalization to sets of vertices considered as the roots of the algorithm (see [7]).

We now add seven assertions in the body of the dfs1 function to help the automatic 277 provers. In contrast, the function dfs needs no extra assertions in its body. In dfs1, when the 278 number $n\theta$ of x is strictly greater than the number n1 resulting from the call to its successors, 279 the first assertion states that n1 cannot be $+\infty$; it helps proving the next assertion. The 280 second assertion states that a lower gray vertex is reachable from x and that thus the scc of 281 x is not fully black at end of dfs1. In that assertion the inequality $y \neq x$ is redundant, but 282 helps showing the sccs constraint at the end of dfs1. When $n1 \ge n0$, the next four assertions 283 show that the strongly connected component *elements s2* of x is on top of x in the current 284 stack and that then x is the base of that scc. The seventh assertion helps proving that the 285 coloring constraint is preserved at the end of dfs1. 286

```
287
288
      let n0 = e.sn in
289
      let (n1, e1) = dfs (successors x) (add_stack_incr x e) in
      if n1 < n0 then begin
290
         assert {n1 \neq +\infty};
291
        \texttt{assert} \{\exists y. y \neq x \land \texttt{mem y e1.gray} \land \texttt{e1.num}[y] < \texttt{e1.num}[x] \land \texttt{in\_same\_scc x y};
292
293
        (n1, add_black x e1) end
      else
294
        let (s2, s3) = split x e1.stack in
295
296
        assert{is_last x s2 \land s3 = e.stack \land subset (elements s2) (add x e1.black)};
        assert { is_subscc (elements s2) };
297
        assert {\forall y. in_same_scc y x \rightarrow lmem y s2};
298
        assert{is_scc (elements s2)};
299
        assert { inter e.gray (elements s2) == empty};
300
        (+\infty, \{b | ack = add x e1.b | ack; gray = e.gray; stack = s3;
301
            sccs = add (elements s2) e1.sccs; sn = e1.sn; num = set_infty s2 e1.num})
383
```

³⁰⁴ where *inter* is set intersection, and *is_last* is defined below.

305

predicate is_last (x: α) (s: list α) = \exists s'. s = s' ++ Cons x Nil

All proofs are discovered by the automatic provers except for two proofs carried out 308 interactively in Coq. One is the proof of the black extension of the stack in case n1 < n0. 309 The provers could not work with the existential quantifier, although the Coq proof is quite 310 short. The second Coq proof is the fifth assertion in the body of dfs1, which asserts that any 311 y in the scc of x belongs to s^2 . It is a maximality assertion which states that the set *elements* 312 s2 is a complete scc. The proof of that assertion is by contradiction. If y is not in s2, there 313 must be an edge from x' in s2 to some y' not in s2 such that x reaches x' and y' reaches y. 314 There are three cases, depending on the position of y'. Case 1 is when y is in sccs: this is 315 not possible since x would then be in sccs which contradicts x being gray. Case 2 is when y' 316 is an element of s3: the serial number of y' is strictly less than the one of x which is n0. If 317 $x' \neq x$, the cross-edge from x' to y' contradicts $n1 \geq n0$ (post-condition 5); if x' = x, then y' 318 is a successor of x and again it contradicts $n1 \ge n\theta$ (post-condition 3). Case 3 is when y' 319 is white, then $x' \neq x$ is impossible since x' is then black in s2 and would be the origin of a 320 black-to-white edge to y'; if x' = x, then y' is not white by post-condition 2 of dfs. 321

Some quantitative information about the Why3 proof is listed in table 1. Alt-Ergo 2.3 and CVC4 1.5 proved the bulk of the proof obligations.² The proof uses 49 lemmas that were all proved automatically, but with an interactive interface providing hints to apply inlining, splitting, or induction strategies. This includes 13 lemmas on sets, 16 on lists, 5 on lists

 $^{^{2}}$ In addition to the results reported in the table, Spass was used to discharge one proof obligation.

provers	Alt-Ergo	CVC4	E-prover	Z3	#VC	#PO
49 lemmas	1.91	26.11	3.33		70	49
split	0.09	0.16			6	6
add_stack_incr	0.01				1	1
add_black	0.02				1	1
set_infty	0.03				1	1
dfs1	77.89	150.2	19.99	13.67	79	20
dfs	4.71	3.52		0.26	58	25
tarjan	0.85				15	5
total	85.51	179.99	23.32	13.93	231	108

Table 1 Performance results with provers in Why3-0.88.3 (in seconds, on a 3.3 GHz Intel Core i5 processor). Total time is 341.15 seconds. The two last columns contain the numbers of verification conditions and proof obligations. Notice that there may be several VCs per proof obligation.

without repetitions, 3 on paths, 5 on sccs and 7 very specialized lemmas directly involved 326 in the proof obligations of the algorithm. Among the lemmas, a critical one is the lemma 327 *xpath_xedge* on paths which reduces a predicate on paths to a predicate on edges. In fact, 328 most of the Why3 proof works on edges which are handled more robustly by the automatic 329 provers than paths. Another important lemma is *subscc_after_last_gray* which shows that 330 the stack elements on top of the last gray vertex form a subset of an scc. This means that 331 another program with the *split* call before the if-statement would make a simpler proof, but 332 it would be a non-linear-time program. The two CoQ proofs are only 9 and 81 lines long (the 333 Coq files of 677 and 680 lines include preambles that are automatically generated during 334 the translation from Why3 to Coq). The interested reader is referred to [7] where the full 335 proof is available. 336

The proof explained so far only showed the partial correctness of the algorithm. But after adding two lemmas about union and difference for finite sets, termination is automatically proved by the following lexicographic ordering on the number of white vertices and roots.

- 340 341
- let rec dfs1 x e = variant{cardinal (diff vertices (union e.black e.gray)), 0}
- with dfs r e = variant{cardinal (diff vertices (union e.black e.gray)), 1, cardinal r}

4 The proof in Coq

Coq is based on type theory and the calculus of constructions, a higher order lambda-calculus, 345 for expressing formulae and proofs. Some basic notions of graph theory are provided by 346 the Mathematical Components Library [18]. Our formalization is parameterized by a finite 347 type V for the vertices and the function successors such that successors x is the adjacency 348 set of any vertex x. The boolean g connect x y indicates that a path connects the vertex 349 x to the vertex y. It is straightforward to define the set gsccs of the sccs using gconnect. 350 Components are represented as sets of sets ($\{set \{set V\}\}$). We use library operations for 351 creating singletons ([set x]), taking unions $(S_1 \cup S_2)$, differences $(S_1 \setminus S_2)$, complements 352 $(\sim: S)$, and unions of all sets of a set of sets (cover S). 353

COQ proposes several mechanisms to put together properties (boolean conjunction, propositional conjunction, record, inductive family) that have their own specificities. In order to make the presentation more readable for a non-COQ expert, we write them all with the propositional conjunction $[\land P_1, \ldots \& P_n]$. We refer to [9] for the actual code.

The CoQ proof differs from the one in Why3: it uses natural numbers only and does not mention colors (white, gray and black). In particular, the number ∞ is defined as the cardinality of V, vertices with ∞ .+1 as serial number correspond to the white vertices of the previous section and the environment is defined as a record with only two fields, a set of sccs and the mapping assigning serial numbers to vertices:

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373

387

Given an environment e, the set of visited vertices is *visited* e (the vertices with serial number less or equal to ∞), the current fresh serial number is sn e (the cardinal of visited vertices), and the stack is *stack* e (the list of elements x which satisfy *num* e x < sn e, sorted by increasing serial number).

Another difference with the Why3 algorithm is the disentanglement of the mutually recursive function *tarjan* into two separate functions The first one *dfs1* treats a vertex x and the second one *dfs* a set of vertices *roots* in an environment *e*.

where $visit \ x \ e$ produces the environment where x gets the next serial number, *store* stores a new strongly connected component.

Then, the two functions are glued together in a recursive function rec where the parameter k controls the maximal recursive height.

Fixpoint rec k r e := if k is k'.+1 then dfs (dfs1 (rec k')) (rec k') r e else (∞, e) .

If k is not zero (i.e. it is a successor of some k'), rec calls dfs taking care that its parameters can only use recursive calls to rec with a smaller recursive height, here k'. This ensures termination. A dummy value is returned in the case where k is zero. Finally, the top level tarjan calls rec with the proper initial arguments.

```
Definition <u>tarjan</u> := let: (_, e) := rec (\infty * \infty.+2) V (Env \emptyset [ffun \Rightarrow \infty.+1]) in esccs e.
```

Initially, the roots are all the vertices (V) and the environment has no component and all vertices are not visited (their number is ∞ .+1). As both *dfs* and *dfs1* cannot be applied more than the number of vertices, the value $\infty * \infty$.+2 encodes the lexicographic product of the two maximal heights. It gives *rec* enough fuel to never encounter the dummy value so *tarjan* correctly terminates the computation. This allows us to separate the proof of the termination from the algorithm itself, and this last statement is of course proved formally later and named *rec_terminates*.

The invariants of the Coq proof are usually shorter than in the Why3 proof since they do not mention colors. We first define well-formed environments and their valid extension:

Then we state that new visited vertices are the ones reachable by paths accessible from roots with non-visited vertices (i.e. by white paths in the colored setting). The function *nexts* such that *nexts* D X returns the set of vertices reachable from the set X by a path which only contains vertices in D except maybe the last one.

419

```
Definition <u>outenv</u> (roots : {set V}) (e e' : env) := [\land

\forall x y, x \in \text{stack e'} \setminus \text{stack e} \rightarrow y \in \text{stack e'} \setminus \text{stack e} \rightarrow \text{gconnect } x y,

\forall x, x \in \text{stack e'} \setminus \text{stack e} \rightarrow \exists y, y \in \text{stack e} \land \text{gconnect } x y \&

\forall x \text{ isited e'} = \text{visited e} \cup \text{nexts} (\sim: \text{visited e}) \text{ roots }].
```

The post-condition is the conjunction of these three properties and the characterization of the output rank:

Here, the argument ne' is the result of a dfs. The output rank n is the minimum of the serial numbers of the vertices which can be reached from the roots through a path where all the vertices except maybe the last one were not already visited. Note that this characterization differs from the notion of LOWLINK which requires that the last vertex was visited.

⁴³⁶ Finally, we express correctness as the implication between pre- and post-conditions:

These invariants are expressed differently from the formulation in Why3, but they reflect essentially the same ideas. Rephrasing the invariants made it possible to reduce by approximately 50% the size of the Coq proofs. The two central theorems are:

They state that *dfs* and *dfs1* are correct if their respective recursive calls are correct. The proof of the first lemma is straightforward since *dfs* simply iterates on a list. It mostly requires book-keeping between what is known and what needs to be proved. This is done in about 54 lines. The second one is more intricate and requires 124 lines. Gluing these two theorems together and proving termination gives us an extra 12 lines to prove the theorem

```
459
460 Theorem <u>rec_terminates</u> k (roots : {set V}) e :
```

```
\texttt{k} \geq \#| \sim: \texttt{visited e}| \, \ast \, \infty \, \texttt{.+1} \, + \, \#|\texttt{roots}| \, \rightarrow \, \texttt{dfs\_correct} \, (\texttt{rec k}) \, \texttt{roots e}.
```

⁴⁶³ The correctness of *tarjan* follows directly in 19 lines of straightforward proof.

Theorem <u>tarjan_correct</u> : tarjan = gsccs.

464

We now provide some quantitative information. The Coq contribution is composed of 467 two files. The *extra_nocolors* file defines the *bigmin* operator and some notions of graph 468 theory that we intend to add to Mathematical Components. This file is 294 lines long. The 469 main file is tarjan_nocolors and is 605 lines long. It is compiled in 12 seconds with a memory 470 footprint of 800 Mb (3/4 of which is resident) on a Intel[®] i7 2.60GHz quad-core laptop 471 running Linux. The proofs are performed in the SSREFLECT proof language [14] with very 472 little automation. The proof script is mostly procedural, alternating book-keeping tactics 473 (move) with transformational ones (mostly rewrite and apply), but often intermediate steps 474

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Number of lines	1	2	3	4	5	6	11	12	16	19	54	124
Number of proofs	19	7	5	2	1	2	2	1	1	1	1	1

Table 2 Distribution of the numbers of lines of the 43 proofs in the file *tarjan_nocolors*.

are explicitly declared with the *have* tactic. There are more than fifty of such intermediate
steps in the 320 lines of proof of the file *tarjan_nocolors*. Table 2 gives the distribution of
the numbers of lines of these proofs. Most of them are very short (26 are less than 2 lines)
and the only complicated proof is the one corresponding to the lemma *dfs1P*.

5 The proof in Isabelle/HOL

Isabelle/HOL [21] is the encoding of simply typed higher-order logic in the logical framework 480 Isabelle [23]. Unlike Why3, it is not primarily intended as an environment for program 481 verification and does not contain specific syntax for stating pre- and post-conditions or 482 intermediate assertions in function definitions. Logics and formalisms for program verification 483 have been developed within Isabelle/HOL (e.g., [16]), but they target imperative rather 484 than functional programming, so we simply formalize the algorithm as an Isabelle function. 485 Isabelle/HOL provides an extensive library of data structures and proofs. In this development 486 we mainly rely on the set and list libraries. We start by introducing a *locale*, fixing parameters 487 and assumptions for the remainder of the proof. We explicitly assume that the set of vertices 488 is finite. 489

We introduce reachability in graphs using an inductive predicate definition, rather than via an explicit reference to paths as in the Why3 definition. Isabelle then generates appropriate induction theorems for use in proofs.

The definition of strongly connected components mirrors that used in Why3. The following lemma states that SCCs are disjoint; its one-line proof is found automatically using *Sledgehammer* [2], which heuristically selects suitable lemmas from the set of available facts (including Isabelle's library), invokes several automatic provers, and finally reconstructs a proof that is checked by the Isabelle kernel.

Environments are represented by records, similar to the formalization in Why3, except
that there is no distinction between regular and "ghost" fields. Also, the definition of the
well-formedness predicate closely mirrors that used in Why3.³

³ We use the infix operator \leq to denote precedence in lists.

528

The definition of the two mutually recursive functions dfs1 and dfs again closely follows their representation in Why3.

```
function (domintros) dfs1 and dfs where
529
       dfs1 x e =
530
531
        (let (n1,e1) = dfs (successors x) (add_stack_incr x e) in
          if n1 < int (sn e) then (n1, add_black x e1)
532
          else (let (l,r) = split_list x (stack e1) in
533
             (+\infty, (| black = insert x (black e1), gray = gray e,
534
               stack = r, sn = sn e1, sccs = insert (set 1) (sccs e1),
535
               num = set_infty 1 (num e1) ))) and
536
       dfs roots e
537
        (if roots = {} then (+\infty, e)
538
         else (let x = SOME x. x \in roots;
539
             res1 = (if num e x \neq -1 then (num e x, e) else dfs1 x e);
540
             res2 = dfs (roots - {x}) (snd res1)
541
             in (min (fst res1) (fst res2), snd res2) ))
543
```

The **function** keyword introduces the definition of a recursive function. Isabelle checks that 544 the definition is well-formed and generates appropriate simplification and induction theorems. 545 Because HOL is a logic of total functions, it introduces two proof obligations: the first one 546 requires the user to prove that the cases in the function definitions cover all type-correct 547 arguments; this holds trivially for the above definitions. The second obligation requires 548 exhibiting a well-founded ordering on the function parameters that ensures the termination 549 of recursive function invocations, and Isabelle provides a number of heuristics that work in 550 many cases. However, the functions defined above will in fact not terminate for arbitrary 551 calls, in particular for environments that assign sequence number -1 to non-white vertices. 552 The *domintros* attribute instructs Isabelle to consider these functions as "partial". More 553 precisely, it introduces an explicit predicate representing the domains for which the functions 554 are defined. This "domain condition" appears as a hypothesis in the simplification rules 555 that mirror the function definitions so that the user can assert the equality of the left- and 556 right-hand sides of the definitions only if the domain predicate holds. Isabelle also proves 557 (mutually inductive) rules for proving when the domain condition is guaranteed to hold. Our 558 first objective is therefore to establish sufficient conditions that ensure the termination of the 559 two functions. Assuming the domain condition, we prove that the functions never decrease 560 the set of colored vertices and that vertices are never explicitly assigned the number -1 by 561 our functions. Denoting the union of gray and black vertices as *colored*, we introduce the 562 predicate 563

and show that this predicate is an invariant of the functions. We then prove that the triple defined as

```
570
(vertices - colored e, {x}, 1)
573
(vertices - colored e, roots, 2)
```

for the arguments of dfs1 and dfs, respectively, decreases w.r.t. lexicographical ordering on finite subset inclusion and < on natural numbers across recursive function calls, provided that *colored_num* holds when the function is called and x is a white vertex. These conditions ⁵⁷⁷ are therefore sufficient to ensure that the domain condition holds:⁴

The proof of partial correctness follows the same ideas as the proof presented for Why3. We define the pre- and post-conditions of the two functions as predicates in Isabelle. For example, the predicates for *dfs1* are defined as follows:

⁵⁹⁵ We now show the following theorems:

The pre-condition of each function establishes the pre-condition of every recursive call appearing in the body of that function. For the second recursive call in the body of dfs we also assume the post-condition of the first recursive call.

⁵⁹⁹ The pre-condition of each function, plus the post-conditions of each recursive call in the ⁶⁰⁰ body of that function, establishes the post-condition of the function.

J J I

601 Combining these results, we establish partial correctness:

⁶⁰⁷ We define the initial environment and the overall function.

⁶¹⁴ It is trivial to show that the arguments to the call of *dfs* in the definition of *tarjan* satisfy ⁶¹⁵ the pre-condition of *dfs*. Putting together the theorems establishing termination and partial ⁶¹⁶ correctness, we obtain the desired total correctness results.

The intermediate assertions appearing in the Why3 code guided the overall proof: they are established either as separate lemmas or as intermediate steps within the proofs of the above theorems. Similarly to the CoQ proof, the overall induction proof was explicitly decomposed into individual lemmas as laid out above. In particular, whereas Why3 identifies the predicates that can be used from the function code and its annotation with pre- and post-conditions, these assertions appear explicitly in the intermediate lemmas used in the

⁴ Observe that Isabelle introduces a single operator corresponding to the two mutually recursive functions whose domain is the disjoint sum of the domains of both functions.

28 8 4 1 2 1 1 1	ſ	i = 1	$i \leq 5$	$i \leq 10$	$i \leq 20$	$i \leq 30$	i = 35	i = 43	i = 48
	[28	8	4	1	2	1	1	1

Table 3 Distribution of interactions in the Isabelle proofs.

⁶³⁰ proof of theorem *dfs_partial_correct*. The induction rules that Isabelle generated from the ⁶³¹ function definitions were helpful for finding the appropriate decomposition of the overall ⁶³² correctness proof.

Despite the extensive use of *Sledgehammer* for invoking automatic back-end provers, 633 including the SMT solvers CVC4 and Z3, from Isabelle, we found that in comparison to Why3, 634 significantly more user interactions were necessary in order to guide the proof. Although 635 many of those were straightforward, a few required thinking about how a given assertion 636 could be derived from the facts available in the context. Table 3 indicates the distribution 637 of the number of interactions used for the proofs of the 46 lemmas the theory contains. 638 These numbers cannot be compared directly to those shown in Table 2 for the Coq proof 639 because an Isabelle interaction is typically much coarser-grained than a line in a CoQ proof. 640 As in the case of Why3 and Coq, the proofs of partial correctness of dfs1 (split into two 641 lemmas following the case distinction) and of dfs required the most effort. It took about one 642 person-month to carry out the case study, starting from an initial version of the Why3 proof. 643 Processing the entire Isabelle theory on a laptop with a 2.7 GHz Intel[®] Core i5 (dual-core) 644 processor and 8 GB of RAM takes 35 seconds of CPU time. 645

646 **General comments about the proof**

⁶⁴⁷ Our formal proofs refer to colors, finite sets, and the stack, although the informal correctness ⁶⁴⁸ argument is about properties of strongly connected components in spanning trees. The ⁶⁴⁹ algorithmician would explain the algorithm with spanning trees as in Tarjan's article. It ⁶⁵⁰ would be nice to extract a program from such a proof, but programmers like to understand ⁶⁵¹ the proof in terms of variables and data that their program is using.

A first version of the formal proof used *ranks* in the working stack and a flat representation 652 of environments by adding extra arguments to functions for the black, gray, scc sets and the 653 stack. That was perfect for the automatic provers of Why3. But after remodelling the proof 654 in CoQ and Isabelle/HOL, it was simpler to gather these extra arguments in records and 655 have a single extra argument for environments. Also ranks disappeared in favor of the num 656 function and the precedence relation, which are easier to understand. The automatic provers 657 have more difficulties with the inlining of environments, but with a few hints they could still 658 succeed. 659

Our proof is mainly about the correctness of Tarjan's algorithm. It relies on surprisingly few and elementary concepts of finite graphs. With the exception of the use of the Mathematical Components library for CoQ, we therefore did not use existing libraries formalizing advanced concepts of graph theory [11, 22].

Finally, coloring of vertices is usual for graph algorithms. The stack used in our algorithm is also not necessary since it is just used to efficiently output new strongly connected components. The CoQ formalization actually shows that proof can be done with just serial numbers and the store of connected components. The stack and current serial number could be added back using a program refinement, in order to recover a linear time computation.

There is always a tension between the concision of the proof, its clarity and its relation to the real program. In our presentation, we have allowed for a few redundancies.

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	Why3	Coq	Isabelle/HOL
expressivity	-	+	+
readability	+	-	+
stability	-	+	+
ease of use	-	-	-
automation	+	-	+
ignore termination	+	-	-
trusted base	-	+	+
automatic proof line-count	395	0	314 ui
manual proof line-count	90	898	1690

Table 4 Compared usage of the three formal systems in the case of our three proofs

671 **7** Conclusion

The formal proof expressed in this article was initially designed and implemented in Why3 [8] as the result of a long process, nearly a 2-year half-time work with many attempts of proofs about various graph algorithms (depth first search, Kosaraju strong connectivity, bi-connectivity, articulation points, minimum spanning tree). Why3 has a clear separation between programs and the logic. It makes the correctness proof quite readable for a programmer. Also first-order logic is easy to understand. Moreover, one can prove partial correctness without caring about termination.

Another important feature of Why3 is its interface with various off-the-shelf theorem 679 provers (mainly SMT provers). Thus the system benefits from the current technology in 680 theorem provers and clerical sub-goals can be delegated to these provers, which makes the 681 overall proof shorter and easier to understand. Although the proof must be split in more 682 elementary pieces, this has the benefit of improving its readability. Several hints about 683 inlining or induction reasoning are still needed and two Coq proofs were used. The system 684 records sessions and facilitates incremental proofs. However, the automatic provers are 685 sometimes no longer able to handle a proof obligation after seemingly minor modifications to 686 the formulation of the algorithm or the predicates, making the proof somewhat unstable. 687

The COQ and Isabelle proofs were inspired by the Why3 proof. Their development therefore required much less time although their text is longer. The COQ proof uses SSREFLECT and the Mathematical Components library, which helps reduce the size of the proof compared to classical COQ. The proof also uses the bigops library and several other higher-order features which makes it more abstract and closer to Tarjan's original proof.

In Coq, one could prove termination using well-foundedness [1, 4], but because of nested recursion the Function command fails, and both Equations and Program Fixpoint require the addition of an extra proof argument to the function. Instead, we define the functionals dfs1and dfs and recombine them in *rec* and *tarjan* by recursion on a natural number used as fuel. We prove partial correctness on functionals and postpone termination on *rec*.

Our CoQ proof does not use significant automation.⁵ All details are explicitly expressed, but many of them were already present in the Mathematical Components library. Moreover, a proof certificate is produced and a functional program could in principle be extracted. The absence of automation makes the system very stable to use since the proof script is explicit, but it requires a higher degree of expertise from the user.

The Isabelle/HOL proof can be seen as a mid-point between the Why3 and Coq proofs. Tot It uses higher order logic and the level of abstraction is close to the one of the Coq proof,

⁵ Hammers exist for Coq [10, 12] but unfortunately they currently perform badly when used in conjunction with the Mathematical Components library.

although more readable in this case study. The proof makes use of Isabelle's extensive support 705 for automation. In particular, *Sledgehammer* [2] was very useful for finding individual proof 706 steps. It heuristically selects lemmas and facts available in the context and then calls 707 automatic provers (SMT solvers and superposition-based provers for first-order logic). When 708 one of these provers finds a proof, Sledgehammer attempts to find a proof that can be 709 certified by the Isabelle kernel, using various proof methods such as combinations of rewriting 710 and first-order reasoning (blast, fastforce etc.), calls to the *metis* prover or reconstruction of 711 SMT proofs through the *smt* proof method. Unlike in Why3, the automatic provers used to 712 find the initial proof are not part of the trusted code base because ultimately the proof is 713 checked by the kernel. The price to pay is that the degree of automation in Isabelle is still 714 significantly lower compared to Why3. Adapting the proof to modified definitions was fast: 715 the Isabelle/jEdit GUI eagerly processes the proof script and quickly indicates those steps 716 that require attention. 717

The Isabelle proof also faces the termination problem to achieve general consistency. 718 We chose to delay handling termination, using the *domintros* attribute. The proofs of 719 termination and of partial correctness are independent; in particular, we obtain a weaker 720 predicate ensuring termination than the one used for partial correctness. Although the basic 721 principle of the termination proof is very similar to the Coq proof and relies on considering 722 functionals of which the recursive functions are fixpoints, the technical formulation is more 723 flexible because we rely on proving well-foundedness of an appropriate relation rather than 724 computing an explicit upper bound on the number of recursive calls. 725

One strong point of Isabelle/HOL is its nice IATEX output and the flexibility of its parser, supporting mathematical symbols. Combined with the hierarchical Isar proof language [31], the proof is in principle understandable without actually running the system, although some familiarity with the system is still required.

In the end, the three systems Why3, Coq, and Isabelle/HOL are mature, and each one 730 has its own advantages w.r.t. readability, expressivity, stability, ease of use, automation, 731 partial-correctness, code extraction, trusted base and length of proof (see table 4). Coming 732 up with invariants that are both strong enough and understandable was by far the hardest 733 part in this work. This effort requires creativity and understanding, although proof assistants 734 provide some help: missing predicates can be discovered by understanding which parts of 735 the proof fail. We think that formalizing the proof in all three systems was very rewarding 736 and helped us better understand the state of the art in computer-aided deductive program 737 verification. It could be also interesting to implement this proof in other formal systems and 738 establish comparisons based on this quite challenging example.⁶ 739

Another interesting work would be to verify an implementation of this algorithm with imperative programs and concrete data structures. This will make the proof more complex, since mutable variables and mutable data structures have to be considered. There is support for verifying imperative programs in general-purpose proof assistants [5, 6, 16], and it would be interesting to also develop them simultaneously in various formal systems and to understand how these proofs can be derived from ours.

A final and totally different remark is about teaching of algorithms. Do we want students to
formally prove algorithms, or to present algorithms with assertions, pre- and post-conditions,
and make them prove these assertions informally as exercises? In both cases, we believe that
our work could make a useful contribution.

⁶ We have set up a Web page http://www-sop.inria.fr/marelle/Tarjan/contributions.html in order to collect formalizations.

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