Towards the formally validated crystallographic software

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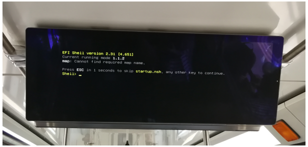
Software is ubiquitous...

... and so, it seems, are software bugs ...



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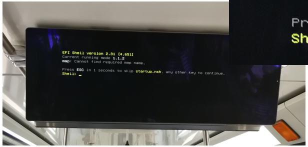

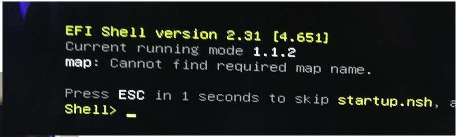

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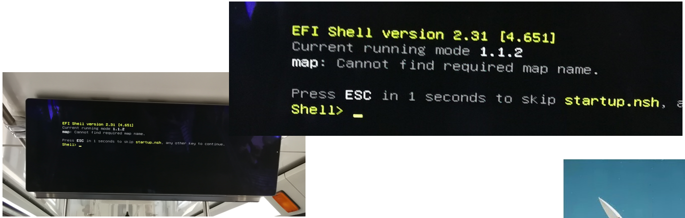
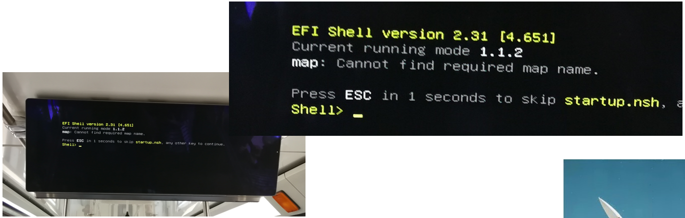


Accumulating 0.1 s intervals for 100 h (in 24 bit binary) resulted in missing the target by 0.3 s...



*"/The/ program, which was not part of a conventional data processing package, converted the anomalous pairs (**I+** and I–) to (**F–** and F+), thereby introducing a sign change. /As a result/ the structures reported had the wrong hand."*

Accumulating 0.1 s intervals for 100 h (in 24 bit binary) resulted in missing the target by 0.3 s...

Understandable software

We want our source code to be readable! Not like this:

```
$s=2;
$d=500;
$w="A";$_='ZIsHPX=$s-Z*Z;$|C;J"sH=\nZ.";O!XNJ"0"x$d,"\n";exit}QZNpush
(F,Z%10PZIZD)}QXNpush(@W,X%10PXIXD)}subT{GMw>MW)OMw!=MWPZ=Mw;QE1NGZV>B)
OZV!=BPZK}1}subY{my(FPZ=0;X=Mw+1;QX>ZNXV+=ZV*S;X[E1]IXVDPXV%C0;E+}MYKO!X
[MY]PF}Q$dKNLF;S=2;@T=Y;@W=(0,0,@WPSC;QSNAOTNF=(KS,FPlast}S++}AZ[0]K;Z=0;S
=MW+1;QZ-SNB+=9-ZV;OB>CONB-C0;Z[E1]K}E+}Q!U[MW]NMWK};JX[0]}J"\n";
';foreach$s(qw/ L(S,@TPLY; UV =1*.1 Z+ @Y return( qrt($s) =R(
prR -- @w= $# )
{ if( ); Te( int Ul Wl Xi [Z] Yi Zh wh $w
/){s;$w;$s;g;$w++}eval;
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(F,Z%10PZIZD)}QXNpush(@W,X%10PXIXD)}subT{GMw>MW)OMw!=MWPZ=Mw;QE1NGZV>B)
OZV!=BPZK}1}subY{my(FPZ=0;X=Mw+1;QX>ZNXV+=ZV*S;X[E1]IXVDPXV%C0;E+}MYKO!X
[MY]PF}Q$dKNLF;S=2;@T=Y;@W=(0,0,@WPSC;QSNAOTNF=(KS,FPlast}S++}AZ[0]K;Z=0;S
=MW+1;QZ-SNB+=9-ZV;OB>CONB-CO;Z[E1]K}E+}Q!U[MW]NMWK};JX[0]}J"\n";
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```

Daniel Rinehart, a self-uncompressing square root finder and custom bignum library.

http://www.foo.be/docs/tpj/issues/vol2_3/tpj0203-0012.html

Formal specifications

Formal methods:

1. Allow to *specify* software behaviour formally;
2. Allow to *prove* that software conforms to specification;
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function Belongs_To (E : Element; G : Group) return Boolean
is (for some F of G => (E = F))
```

Formal systems for software development

A non-exhaustive list of tools:

1. Proof assistants
   - Isabelle/HOL;
   - Coq/Gallina;
2. Software development systems (proovers)
   - Ada/SPARK
   - C#/Spec#;
   - C/Frama-C;
   - Daphny/Boogie;
   - Java/KeY;
   - Java/JML;
   - Java/EST;
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Why Ada/SPARK?

1. Durable design – first designed in 1983!
2. Modern language – latest standard is Ada 2022;
3. Mostly backwards compatible;
4. Good F/LOSS compiler available – GNAT;
5. Ada is statically very strictly typed;
6. Programs are easy to read (Level (Ada) > Level (C));
7. Ada & SPARK has a rich type system;
8. Language level concurrent programming;
9. Produces fast optimised native code, links with any language;
10. SPARK subset takes computer arithmetic into account;
11. Not controlled by any private company;

Why is Ada not popular (yet)?

1. The language is complex and difficult to implement;
2. No good compilers in the 1990's;
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The algorithm to work with

The group reconstruction algorithm: generate, when presented with a subset of elements from some existing finite group G, a (smallest) subgroup $H \leq G$ containing those elements:

$$\{g_1, ..., g_n\}, \forall g_i : g_i \in G \to H \leq G : \text{Is\_Group}(H) \wedge \forall g_i : g_i \in H$$

Uses of this algorithm:

- check symmetry operators of a CIF file (for the COD);
- determine symmetry of special position;
- check whether an atom is on a sp. pos.;
- constrain an atom to a sp. pos. for refinement (PD?);
- analyse disorder around a special position;

(Grosse-Kunstleve 1999)

Formal proofs of the the algorithms in use

Require: H – a subgroup of a finite group G
Require: g – an element of the finite group G, $g \in G$
Ensure: The list L of the operators of a subgroup $L \leq G$ without duplicates
Ensure: L contains both g and the elements of H

```
procedure SimpleBuilder(H, g)
    ▷ Build a space group generated by H and g
    L ← [e, h_1, h_2, ..., h_n], where ∀i. h_i ∈ H
    L_new ← [g]
    while L_new is not empty do
        g' ← head(L_new)
        L_new ← tail(L_new)
        L ← append(L, g')
        for all h' ∈ L do
            g'' ← h' ⊗ g'
            if g'' ∉ L ∪ L_new then
                L_new ← append(L_new, g'')
            end if
        end for
    end while
    return L
end procedure
```

Figure 2
The optimized simple space-group-builder (core) algorithm.

```
have "subgroup R G"
proof -
    have R_subset: "R ⊆ carrier G" sorry
    moreover have R_m_closed: "⋀x y. ⟦x ∈ R; y ∈ R⟧ ⟹ x ⊗ y ∈ R" sorry
    moreover have R_one_closed: "1 ∈ R" sorry
    moreover have R_m_inv_closed: "⋀x. x ∈ R ⟹ inv x ∈ R" sorry
    ultimately show "subgroup R G" by (simp add: subgroup_def)
qed
```

```
for my $group_symop (@{$self->{symops}}) {
    do {
        my $product =
            snap_to_crystallographic(
                symop_modulo_1(
                    symop_mul( $group_symop, $test_symop )
                )
            );
        my $product_key = string_from_symop( $product );
        if( !exists $self->{symop_hash}{$product_key} ) {
```

(Petrauskas et al. 2022)

Group theory in Ada/SPARK

examples/group_theory.ads

```
pragma Spark_Mode (On);

generic
   type Element is private;
   Identity : Element;
   with function "*" (E, F: Element) return Element is <>;
```

```
   function Is_Closed_On_Multiplication (G : Group) return Boolean
   is (for all E of G =>
         (for all F of G => (Belongs_To (E*F, G))))
     with Ghost;

   function All_Elements_Have_Inverses (G : Group) return Boolean
   is (for all E of G => Has_Inverse (E, G))
     with Ghost;

   function Is_Group (G : Group) return Boolean
   is (Has_Identity (G) and then
         All_Elements_Have_Inverses (G) and then
         Is_Closed_On_Multiplication (G)
      )
     with Ghost;
```

examples/make_group.ads

```
8   type Ring_Element is mod 37;
```

```
29  function Build_Group (E : Ring_Element) return Group
30    with
31    Post => Is_Group (Build_Group'Result);
```

gnatprove -P main.gpr --report=all make_group.adb

```
make_group.ads:23:14: info: postcondition proved
make_group.ads:27:14: info: postcondition proved
make_group.ads:31:14: info: postcondition proved
group_theory.ads:16:15: info: postcondition proved, in instantiation at make_group.ads:16
```

```
saulius@tasmanijos-velnias spacegroups/ $ ./run_make_group 8
(1, 8, 27, 31, 26, 23, 36, 29, 10, 6, 11, 14)

saulius@tasmanijos-velnias spacegroups/ $ ./run_make_group 7
(1, 7, 12, 10, 33, 9, 26, 34, 16)
```

Current assumptions

... need to be made

```
function Build_Group (G : Group; E : Ring_Element) return Group
```

```
for I in N'First .. NN loop
   declare
      H : Ring_Element := N (I) * T;
   begin
      if not Contains (N (N'First..NN), H) then
         Add_Element (N, NN, H); -- Add the element to the growing group
         Add_Element (L, NL, H); -- Add the element to the candidate list
      end if;
   end;
end loop;
```

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```

```
   pragma Assume (All_Elements_Have_Inverses (Group (N (N'First .. NN))));
   pragma Assume (Is_Closed_On_Multiplication (Group (N (N'First .. NN))));

   return Group (N (N'First .. NN));
end Build_Group;
```

Conclusions

- Ada/SPARK provide production-ready F/LOSS dev. environment;
- Software functions (Pre/Post) can be formally specified in SPARK;
- Certain properties can be proved automatically; others – with explicit assumptions;
- More properties will be possible to prove in the future;
- Working (library) code can be generated from the verified source;

Vision for the future

- A reusable F/LOSS library of *verified* crystallographic algorithms;
- Stable and future-proof;
- Compatible with any languages and platforms (Ada, C(++), Go, Julia, Rust, Perl, Python, WebAssembly, etc.);
- Make software *readable* and *understandable*;
- Make software a part of documentation for *scientifc inferences* along with human readable texts (papers, presentations, etc.) and databases (COD, etc.)

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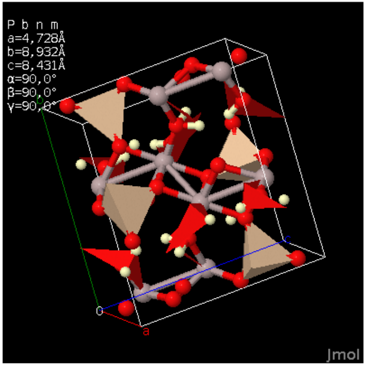
[1] Co-authors of this work

Thank you!



Coordinates 2207377.cif
Original IUCr paper HTML

http://en.wikipedia.org/wiki/Topaz

http://www.crystallography.net/2207377.html

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Petrauskas, Karolis et al. (May 2022). “Proving the correctness of the algorithm for building a crystallographic space group”. In: *Journal of Applied Crystallography* 55.3, pp. 515–525. DOI: 10.1107/s1600576722003107.