

# Formalization of Incremental Simplex Algorithm by Stepwise Refinement

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# Overview

- 1 Introduction
- 2 Approach and Techniques
- 3 Linear Arithmetic, Incremental Simplex
- 4 Evaluation
- 5 Conclusions

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  - Formal Verification of SMT solvers?
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# SMT solvers

- SMT solvers are very important tools in formal hardware and software verification.
- *Quis custodiet ipsos custodes?* — who will guard the guards?
- How to trust SMT solvers results, having in mind their complexity?
- Several approaches:
  - formal verification of solvers (and their underlying algorithms),
  - generating and checking certificates.
- Certificate checking shows very good results in practice and therefore it has been the dominant approach in industry (e.g., Böhme and Weber 2010., Armand et al. 2011.).

# Why formal verification?

Still, we advocate that formal verification of SMT solving algorithms within a proof assistant may have its own merits.

- Mathematical proofs have two main components: **justification** (certification) and **explanation** (message).
- Approach to formalization may be more important than the final result itself.
- Apart from giving assurance that a procedure is correct, formalization effort should carry important messages for the reader.
- Formalization offers clear explanations for subtle details.
- The formalization is a contribution to the growing body of verified theorem proving algorithms.

# Overview

- 1 Introduction
- 2 Approach and Techniques
  - Approach
  - Refinement
  - Refinement in Isabelle/HOL
- 3 Linear Arithmetic, Incremental Simplex
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# Approach to verification

- **Shallow embedding** in the proof assistant Isabelle/HOL.
  - HOL treated as a functional programming language.
  - Functional model of the procedure implemented in HOL and verified.
  - Executable **code can be extracted** (in SML, Haskell, Scala, OCaml, ...).
  - By means of **reflection**, the procedure can be used within the proof assistant.

# Approach to verification — refinement

- Procedure is developed through a long series of small **refinement** steps.
- **Refinement** is a verifiable transformation of abstract formal (high-level) specification into a concrete executable (low-level) program.
- **Stepwise refinement** assumes that the refinement process is performed through a series of simple steps.



# Refinement

- Top-down approach.
- Correct-by-construction.
- Each step reduces the amount of non-determinism in a program.
- Rich history (systematically explored by E. W. Dijkstra and N. Wirth in 1960s, formal treatment given by R. J. Back in 1970s).

# Data vs Algorithm refinement

- **Data refinement** assumes replacing abstract data structures by concrete ones.
- **Algorithm (program) refinement** assumes replacing abstract algorithms (operations) by concrete ones.

# Benefits of using refinement in our formalization

- The procedure can be analyzed and understood on different levels of abstraction.
- Abstract layers in the formalization allow easy porting of the formalization to other systems.
- Makes the formalization suitable for teaching formal methods.
- Makes the correctness proofs significantly simpler.

# Code generation as a refinement framework of Isabelle/HOL

- Haftmann and Nipkow, 2010.
- No axiomatic specification is used.
- Specification is done in terms of a reference implementation (usually simple and abstract).
- Correctness proofs for the system rely only on the reference implementation, while concrete representations are used only during code generation.

# Code generation as a refinement framework of Isabelle/HOL

- Algorithm refinement:
  - Give a new (better) implementation of a function.
  - Prove the equivalence with the reference implementation.
  - Instruct the code generator to use the new implementation.
- Data refinement:
  - Define an abstract data type representation and functions operating on this representation.
  - Define a concrete data type representation, functions operating on this representation and the conversion from the concrete to the abstract representation.
  - Prove the equivalence.
  - Instruct the code generator to use the concrete representation.

# Program refinement in Isabelle/HOL by using locales

- **Locales** — Isabelle's version of parametrized theories.
- A locale is a named context of functions  $f_1, \dots, f_n$  and assumptions  $P_1, \dots, P_m$ :  
**locale**  $loc = \mathbf{fixes}$   $f_1, \dots, f_n$  **assumes**  $P_1, \dots, P_m$
- Locales can be hierarchical as in:  
**locale**  $loc = loc_1 + loc_2 + \mathbf{fixes}$  ...
- Locales are ideal for giving axiomatic function specifications:

## Example

```

locale sorting =
  fixes sort :: "'a list  $\Rightarrow$  'a list"
  assumes
    sorted : let  $l' = \mathit{sort} \ l$  in  $\forall i < \mathit{length} \ l' - 1. l'_{[i]} \leq l'_{[i+1]}$ 
    elems :  $\mathit{multiset\_of} (\mathit{sort} \ l) = \mathit{multiset\_of} \ l$ 

```

# Program refinement by using locales

- In the context of a locale, definitions can be made and theorems can be proved.
- Locales can be *interpreted* by concrete instances of  $f_1, \dots, f_n$ , and then it must be shown that these satisfy assumptions  $P_1, \dots, P_m$ .
- Locales are naturally combined with the code generation.

# Program refinement by using locales

- A locale  $l$  is a **sublocale** of a locale  $l'$  if all functions of  $loc'$  can be defined using the functions of  $l$  and all assumptions of  $l'$  can be proved using the assumptions of  $l$ .
- Then every interpretation for  $loc$  can be automatically converted to an interpretation of  $loc'$ .



# Program refinement by using locales

## Example

```

locale min_selection =
  fixes min :: "'a list ⇒ 'a × 'a list"
  assumes
    "let (m, l') = min l in multiset_of (m#l') = multiset_of l"
    "let (m, l') = min l in ∀x ∈ set l'. m ≤ x"
begin
  function ssort where
    "ssort l = (if l = [] then [] else let (m, l') = min l in m#ssort l)"
end

sublocale min_selection < sort ssort
proof
  ...
qed

```

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- 2 Approach and Techniques
- 3 Linear Arithmetic, Incremental Simplex**
  - Linear Arithmetic
  - Incremental Simplex for SMT
  - Some fragments of our formalization
- 4 Evaluation
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# Linear arithmetic

- A first order theory (usually semantically specified).
- Atomic formulae of the form  $c_1x_1 + \dots c_nx_n \bowtie c$ , where  $\bowtie \in \{<, >, \leq, \geq, =, \neq\}$ , and  $c_1, \dots, c_n, \dots c$  are integer (or rational) constants.
- Usually, only universally quantified fragment is assumed (i.e., satisfiability of ground formulae is checked).
- Several variants:
  - LRA — satisfiability over  $\mathbb{Q}$
  - LIA — satisfiability over  $\mathbb{Z}$

## Example

Are there rational constants  $x$  and  $y$  such that

$$x \leq -4 \wedge x > -8 \wedge y - x < 1 \wedge x + y \geq 2?$$

# SMT solvers

- Formulae encountered in verification practice are not only conjunctions of literals and have rich propositional structure. E.g.,  $(3x + 4y > 0 \vee x + y < 3) \Rightarrow (2x - 3y \geq 5 \wedge x < 0)$ .
- **SMT** solvers combine powerful SAT solvers for propositional reasoning with decision procedures for conjunctions of literals in concrete theories.
- Maximal efficiency requires modification of both SAT solvers and decision procedures.

# Decision procedures for linear arithmetic

- Decidable theory.
- Different decision procedures. Most popular are based on:
  - Fourier-Motzkin elimination (in some aspects similar to Gaussian elimination for equality systems),
  - Simplex algorithm (Dantzig, 1947, linear programming and elimination algorithm).

# Incremental Simplex for SMT

- Duterte and de Moura, 2006.
- Yices solver.
- Adopted by many state-of-the-art SMT solvers.
- Dual-simplex with Bland's rule for ensuring termination.
- Basic solver for LRA with extensions for LIA (branch-and-bound, Gomory's cuts).
- Only proof sketch of termination (partial correctness not proved).

# Polynomials

- Polynomials are of the form  $a_1 \cdot x_1 + \dots + a_n \cdot x_n$ .
- Abstract representation:
  - Functions mapping variables  $x_i$  into coefficients  $a_i$ , such that only finitely many variables have a non-zero coefficient.
  - The sum of  $p_1$  and  $p_2$  is the polynomial  $\lambda x. p_1 x + p_2 x$ .
  - The value of the polynomial  $p$  for the valuation  $v$ , denoted by  $p\{v\}$  is  $\sum_{x \in \{x. p x \neq 0\}} p x \cdot v x$
- Concrete representations:
  - Lists of coefficients.
  - Red-black tree implemented mappings.

# Linear constraints

Linear constraints are of the form  $p \bowtie c$  or  $p_1 \bowtie p_2$ :

- $p, p_1$  i  $p_2$  su linearni polinomi,
- $c$  is a rational constant,
- $\bowtie \in \{<, >, \leq, \geq, =\}$ .

**datatype** constraint =

LT linear\_poly rat |

GT linear\_poly rat | ...



# Semantics of linear constraints

- $v \models_c c$  — valuation  $v$  satisfies the constraint  $c$ 
  - $v \models_c \text{LT } l \ r \iff |v| < r$
  - $v \models_c \text{GT } l \ r \iff |v| > r$
- $v \models_{cs} cs$  — valuation  $v$  satisfies the list of constraints  $cs$ 
  - $v \models_{cs} cs \equiv \forall c \in \text{set } cs. v \models_c c$

# Procedure specification

**locale** Solve =

— Decide if the given list of constraints is satisfiable. Return the satisfiability status and, in the satisfiable case, one satisfying valuation.

**fixes** solve :: "constraint list  $\Rightarrow$  bool  $\times$  rat valuation option"

— If the status *True* is returned, then returned valuation satisfies all constraints.

**assumes** "let (sat, v) = solve cs in sat  $\longrightarrow$  v  $\models_{cs}$  cs"

— If the status *False* is returned, then constraints are unsatisfiable.

**assumes** "let (sat, \_) = solve cs in  $\neg$  sat  $\longrightarrow$   $\neg$  ( $\exists$  v. v  $\models_{cs}$  cs)"

# Eliminating non-strict inequalities

- $p < c$  can be replaced by  $p \leq c - \delta$ ,
- $p > c$  can be replaced by  $p \geq c + \delta$
- All further computations are done in the structure  $\mathbb{Q}_\delta$  (ordered vector space over  $\mathbb{Q}$ )
  - elements are of the form  $a + b \cdot \delta$ ,  $a, b \in \mathbb{Q}$ ,
  - $(a_1 + b_1 \cdot \delta) + (a_2 + b_2 \cdot \delta) = (a_1 + a_2) + (b_1 + b_2) \cdot \delta$ ,
  - $c \cdot (a + b \cdot \delta) = c \cdot a + c \cdot b \cdot \delta$ ,
  - $(a_1 + b_1 \cdot \delta) < (a_2 + b_2 \cdot \delta) \iff a_1 < a_2 \vee (a_1 = a_2 \wedge b_1 < b_2)$ .

# Specification of eliminating strict constraints

**locale** To\_ns =

— Convert a constraint list to an equisatisfiable non-strict constraint list.

**fixes** to\_ns :: "constraint list  $\Rightarrow$  'a::lrv ns\_constraint list"

**assumes** "v  $\models_{cs}$  cs  $\Longrightarrow$   $\exists$  v'. v'  $\models_{nss}$  to\_ns cs"

— Convert the valuation that satisfies all non-strict constraints to the valuation that satisfies all initial constraints.

**fixes** from\_ns :: "(var  $\Rightarrow$  'a)  $\Rightarrow$  'a ns\_constraint list  $\Rightarrow$  (var  $\Rightarrow$  rat)"

**assumes** " $\langle$ v' $\rangle \models_{nss}$  to\_ns cs  $\Longrightarrow$   $\langle$ from\_ns v' (to\_ns cs) $\rangle \models_{cs}$  cs"

# Implementation of the solve function

Assuming that there is a function `solve_ns` solving the non-strict constraints (with a specification analogous to the one for the function `solve`), the `solve` function can be implemented simply:

```
solve cs ≡ let cs' = to_ns cs; (sat, v) = solve_ns cs' in  
  if sat then (True, Some (from_ns v cs')) else (False, None)
```

# Preprocessing

In the next step, the list of non-strict constraints is transformed into:

- a **tableau** — list of linear equalities
- list of atoms **atom** of the form  $x_i \bowtie b_i$ , such that  $x_i$  is a variable, and  $b_i$  is a constant from  $\mathbb{Q}_\delta$

For example,  $[x_1 + x_2 \leq b_1, x_1 + x_2 \geq b_2, x_2 \geq b_3]$  is transformed into  $[x_3 = x_1 + x_2]$  and atoms  $[x_3 \leq b_1, x_3 \geq b_2, x_2 \geq b_3]$

# Formalization of tableau and atoms

**type** eq = var × linear\_poly

$v \models_e (x, p) \equiv v x = p \{ \{ v \} \}$

**type** tableau = eq list

Tableau is normalized (denoted by  $\Delta t$ ) if variables on the left sides are all different and do not occur on the right side.

**datatype** 'a atom = Leq var 'a | Geq var 'a

" $v \models_a \text{Leq } x \ c \longleftrightarrow v x \leq c$ " | " $v \models_a \text{Geq } x \ c \longleftrightarrow v x \geq c$ "

" $v \models_{as} a_s \equiv \forall a \in as. v \models_a a$ "

# Preprocessing specification

**locale** Preprocess = **fixes** preprocess: "'a::lrv ns\_constraint list  $\Rightarrow$  tableau  $\times$  'a atom list"

**assumes**

— The returned tableau is always normalized.

"let (t, as) = preprocess cs in  $\Delta$  t"

— Tableau and atoms are equisatisfiable with starting non-strict constraints.

"let (t, as) = preprocess cs in  $v \models_{as}$  set as  $\wedge v \models_t t \longrightarrow v \models_{nss}$  cs"

"let (t, as) = preprocess cs in  $v \models_{nss}$  cs  $\longrightarrow (\exists v'. v' \models_{as}$  set as  $\wedge v' \models_t t)$ "



# Implementation of solve\_ns

Assuming that the `assert_all` function, which has the precondition that the tableau is normalized, and the effect similar to the function `solve`, the function `solve_ns` can be easily implemented:

```
solve_ns s ≡ let (t, as) = preprocess s in assert_all t as
```



# Proof metrics

- Around 8K lines of proof (3K devoted to termination).
- A previous „monolithic” attempt was abandoned when it went over 25K lines of proofs.
- Crucial aspects for proof simplification: refinement approach and treatment of symmetric cases.

# Run-time comparison with other implementations

- Verified (Chaieb and Nipkow — Isabelle/HOL)
- Semi-verified (Spasić and Marić — C++)
- Unverified (SMT solvers Z3 and OpenSMT)

# Choice of benchmarks

- We are handling only conjunctions of constraints.
- Benchmarks contain many conjuncts with many variables (up to  $100 \times 50$ ).
- Randomly generated.
- Dense — non realistic for the SMT applications.

# What did the experiments show?

- Simplex was several orders of magnitude faster than previously verified algorithms in Isabelle/HOL.
- Much slower than its counterpart C++ implementation and Z3.
- C++ not always much slower than Z3 (different variable orderings).

# Surprising profiling results

- The cause of inefficiency: functional (non-destructive) data structures vs imperative data-structures?
- No!
- Reference C++ used exact rationals of the GMP library, while the extracted code reduces everything to ML native integers (also backed up by GMP).
- Manually changed the generated code to use native rationals (this time in Haskell since ML does not support rationals natively).
- The tweaked Haskell code slightly outperformed the C++ implementation!
- More than 80% of the times is spend doing rational arithmetic, so in this scenario it does not matter whether imperative or functional data structures are used.





# Conclusions

- Verified incremental Simplex algorithm in Isabelle/HOL.
- In some scenarios, generated code is competitive with state-of-the art solvers.
- Much more important than the result itself is the approach to the formalization.
- Refinement — many layers of abstraction give strength to a formalization attempt.