Sulfur: a Reflective Tactic for Substitution Simplification

Mathis Bouverot-Dupuis
Inria Paris, ENS Paris
Paris, France
mathis.bouverot-dupuis@inria.fr

Théo Winterhalter
Inria Saclay, ENS Paris-Saclay
Gif-sur-Yvette, France
theo.winterhalter@inria.fr

Kathrin Stark
Heriot-Watt University
Edinburgh, United Kingdom
K.Stark@hw.ac.uk

Kenji Maillard
Inria Rennes
Nantes, France
kenji@maillard.blue

1 Introduction

When formalizing the meta-theory of programming languages or type systems in proof assistants such as Rocq [23], a key design decision is the choice of variable representation (see e.g. the PoplMark challenge [4]). De Bruijn indices [7] are a popular option because they make α-equivalence coincide with syntactic equality. However, de Bruijn indices also introduce significant overhead in the form of lift and renaming operations, which require many technical lemmas and can make proofs tedious.

To address this, many libraries attempt to automate repetitive aspects of dealing with de Bruijn indices and substitution, both in programming languages (e.g. Rebound [8] or BindLib [14]) and in proof assistants (e.g. Autosubst [19, 22], Tealeaves [9], DBGen [16], Fiore and Szamozvancev [10], and Allais et al. [3]). In particular, while Autosubst has been successfully used in many formalizations [2, 6, 11, 12, 21, 24, 25], its simplification tactic `asimpl` suffers from significant performance issues when used in large developments. In this talk, we present Sulfur[1] (Substitution logical framework using reflection), a Rocq plugin that attempts to solve the performance issues of Autosubst's `asimpl` tactic by implementing it as a *reflective tactic* [5, 13, 15]. For now, Sulfur supports single-sorted, extrinsic syntax: extensions to more complex signatures are discussed in Section 4.

2 Using Sulfur

Sulfur provides a similar interface to Autosubst: given a user-specified language signature (Figure 1a), Sulfur automatically generates Rocq code (Figure 1b) implementing an inductive type `term` representing terms with variables encoded as de Bruijn indices, and a parallel substitution function.

Most importantly, Sulfur automates reasoning about substitution: like Autosubst, it provides a tactic `asimpl` which simplifies terms and substitutions according to the rules of σ-calculus [1]. For instance consider the technical lemma

```
Sulfur Generate {{
  term : Type
  app : term → term → term
  lam : (bind term in term) → term
}}.
```

(a) User-specified signature.

```
Inductive term :=
| var (i : nat)
| app (t u : term)
| lam (t : term).

Definition substitute : (nat → term) → term → term.
(** substitute s t is abbreviated as t[s]. *)
```

(b) Code generated by Sulfur.

```
Lemma technical_lemma (t1 t2 : term) (s : nat → term) :
  t1[0 . (s >> shift)][t2[s] . id] = t1[t2 . id][s].
```

(c) Example substitution-heavy lemma.

Figure 1. Untyped λ-calculus, using Sulfur. The code in Figure 1b is automatically generated by Sulfur.

in Figure 1c, which is needed when proving standard properties of λ-calculus. In this lemma, `id` is the identity substitution, `shift` is the substitution which adds 1 to every de Bruijn index, `t . s` is a substitution which maps index `0` to `t` and index `i+1` to `s i`, and `s1 >> s2` is the composition of `s1` followed by `s2`. Proving this equality by hand requires significantly more effort than one might expect, using many auxiliary lemmas. However, `asimpl` simplifies both sides of the equation to `t1[t2[s] . s]`, trivializing the proof.

3 Key ideas

While Sulfur provides, by design, the same user interface as Autosubst, its implementation diverges significantly. In particular, Autosubst's `asimpl` tactic relies on Rocq's *setoid rewrite* facilities [20], and has significant performance issues when used in large developments. Sulfur aims to improve performance by using a logical framework approach: we define a generic notion of syntax with explicit substitutions

[1] Our development is available at https://github.com/MathisBD/rocq-sulfur.

within Rocq, and implement `asimpl` as a plain Rocq function over this generic syntax.

Signatures. We encode the *signature* of a language as a set of constructors (`ctor`) along with information about the arity and binding structure of each constructor (`ctor_args`):

```
Inductive arg :=
| arg_term
| arg_bind (x : arg).

Record signature := {
  ctor : Type ;
  ctor_args : ctor -> list arg }.
```

As an example we give the signature for the untyped lambda-calculus of Figure 1:

```
Inductive ctor := App | Lam.
ctor_args App = [ arg_term ; arg_term ]
ctor_args Lam = [ (arg_bind arg_term) ]
```

Generic syntax. Inspired by σ-calculus, we define a notion of syntax with explicit substitutions, which is moreover *generic*, i.e. parameterized over a signature. We give a simplified version of generic syntax:

```
Inductive g_term {s : signature} :=
| g_var (i : nat)
| g_ctor (c : ctor s) (args : list g_term)
| g_substitute (s : g_subst) (t : g_term)
| g_term_mvar (m : mvar)
with g_subst {s : signature} :=
| g_id
| g_shift
| g_cons (t : g_term) (s : g_subst)
| g_comp (s1 s2 : g_subst)
| g_subst_mvar (m : mvar).
```

Substitutions are not arbitrary functions of type `nat → g_term` but are instead built using a set of constructors `gid`, `gshift`, `gcons`, and `gcomp`, which correspond to the substitution primitives `id`, `shift`, `_ . _`, and `_ >> _` of the σ-calculus. Substitutions can be explicitly applied to terms using `g_substitute`.

Not all substitutions `nat → term` are representable using the constructors of σ-calculus. Substitutions which don't fit in the framework of σ-calculus are represented using *meta-variables* (constructor `g_subst_mvar`). Terms can similarly contain meta-variables (constructor `g_term_mvar`). Meta-variables `mvar` are drawn from an infinite set with decidable equality (in our development we define `mvar` as `nat`).

Generic syntax contains enough information to be able to implement a simplification function directly in Rocq:

```
Definition simplify sig : g_term sig → g_term sig.
```

Reification and denotation. Generic syntax is quite far from what we picture as the untyped λ-calculus, and we certainly do not want users to work with `g_term`. Thus, we still generate syntax specialized to the user's signature, as in Figure 1b.

The mapping between user syntax and generic syntax, i.e. between `term` and `g_term`, is fairly straightforward. A *denotation* function `denote : env → gterm sig → term` can be implemented directly within Rocq (for any signature `sig`) by simple structural recursion over the input term. The first argument of `denote` is an *environment*, which is a mapping from meta-variables to concrete terms and substitutions.

The other direction, *reification*, requires us to step outside Rocq. Leveraging Rocq's support for meta-programming, we can reify a term `t` into a generic term `t' : g_term sig` and an environment `e : env`, which are required to obey the invariant that `denote e t'` is convertible (i.e. definitionally equal) to `t`.

Implementing `asimpl` using reflection. In order to simplify terms in user syntax, we first establish the soundness of `simplify`:

```
Theorem soundness e t : denote e t = denote e (simplify t).
```

Using all these ingredients, we can implement `asimpl` as follows. To simplify a term `t : term` appearing in a goal:

1. Reify `t` into `t' : g_term sig` and `e : env`.
2. Because `t` is convertible to `denote e t'`, which itself is equal to `denote e (simplify t')`, we can replace all occurrences of `t` with `denote e (simplify t')` in the goal.
3. Use Rocq's evaluation mechanisms to reduce the expression `denote e (simplify t')`.

4 Future work

Benchmarking. Early experiments suggest that Sulfur's `asimpl` tactic is indeed faster than the equivalent Autosubst tactic. We plan on conducting detailed benchmarks to quantify the performance gain more precisely.

More complex signatures. Central future work is to extend Sulfur to accommodate more complex signatures, scaling up to the full generality of Autosubst. For instance, signatures with multiple sorts of terms (e.g. System F) and signatures including functors (e.g. using lists to represent n-ary applications) are not supported yet. Extending our generic syntax to handle multiple sorts requires encoding subtle invariants: for instance in System F, term variables cannot occur in types and thus parallel substitution in types only requires a substitution on type variables. We hope to benefit from related work on multi-sorted substitution [17].

Proving completeness. The following completeness theorem holds in simpler variants of σ-calculus [18]:

```
Theorem completeness (t t' : g_term sig) :
  (forall e, denote e t = denote e t') →
  simplify t = simplify t'
```

Intuitively this states that reification followed by simplification is enough to decide equality of concrete terms. Unfortunately, this completeness theorem does not hold on our version of generic syntax due to the presence of explicit renamings, however we conjecture that some weaker version of completeness still holds, and believe that proving such a result is an interesting direction for future work.

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