

# Substitution without copy and paste

Thorsten Altenkirch ✉

University of Nottingham, Nottingham, United Kingdom

Nathaniel Burke ✉

Imperial College London, London, United Kingdom

Philip Wadler ✉

University of Edinburgh, Edinburgh, United Kingdom

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## Abstract

When defining substitution recursively for a language with binders like the simply typed  $\lambda$ -calculus, we need to define substitution and renaming separately. When we want to verify the categorical properties of this calculus, we end up repeating the same argument many times. In this paper we present a lightweight method that avoids this repetition and is implemented in Agda.

We use our setup to also show that the recursive definition of substitution gives rise to a simply typed category with families (CwF) and indeed that it is isomorphic to the initial simply typed CwF.

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## 1 Introduction

Some half dozen persons have written technically on combinatory logic, and most of these, including ourselves, have published something erroneous. [9]

The first author was writing an introduction to category theory for functional programmers. One category is that of simply-typed  $\lambda$ -terms and substitutions; the text gives the definition and asks the reader to prove the category laws. Writing the answer was more difficult than expected, so to minimise mistakes we started to formalise the solution in Agda. The main setback is that the same proofs were repeated many times. One guideline of good software engineering is **do not write code by copy and paste**, and that applies doubly to formal proofs.

This paper is the result of our effort to refactor the proof. The method used also applies to other problems. In particular, we see the current construction as a warmup for the recursive definition of substitution for dependent type theory. This in turn may have interesting applications for coherence, i.e., interpreting dependent types in higher categories.

### 1.1 In a nutshell

When working with substitution for a calculus with binders, we find that you have to differentiate between renamings ( $\Delta \models_v \Gamma$ ) where variables are substituted only for variables ( $\Gamma \ni A$ ) and proper substitutions ( $\Delta \models \Gamma$ ) where variables are replaced with terms ( $\Gamma \vdash A$ ). This results in having to define several similar operations

$$\begin{array}{ll} \_v[_]_v : \Gamma \ni A \rightarrow \Delta \models_v \Gamma \rightarrow \Delta \ni A & \_[_]_v : \Gamma \vdash A \rightarrow \Delta \models_v \Gamma \rightarrow \Delta \vdash A \\ \_v[_] : \Gamma \ni A \rightarrow \Delta \models \Gamma \rightarrow \Delta \vdash A & \_[_] : \Gamma \vdash A \rightarrow \Delta \models \Gamma \rightarrow \Delta \vdash A \end{array}$$

And indeed the operations on terms depend on the operations on variables. This duplication gets worse when we prove properties of substitution, such as the functor law,  $x [ xs \circ ys ] \equiv x [ xs ] [ ys ]$ . Since all components  $x$ ,  $xs$ ,  $ys$  can be either variables/renamings



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or terms/substitutions, we seemingly need to prove eight possibilities (with the repetition extending also to the intermediary lemmas). Our solution is to introduce a type of sorts with  $V : \text{Sort}$  for variables/renamings and  $T : \text{Sort}$  for terms/substitutions, leading to a single substitution operation  $\_ \sqcup \_ : \Gamma \vdash [q] A \rightarrow \Delta \models [r] \Gamma \rightarrow \Delta \vdash [q \sqcup r] A$  where  $q, r : \text{Sort}$  and  $q \sqcup r$  is the least upper bound in the lattice of sorts ( $V \sqsubseteq T$ ). With this, we only need to prove one variant of the functor law, relying on the fact that  $\_ \sqcup \_$  is associative. We manage to convince Agda’s termination checker that  $V$  is structurally smaller than  $T$  (see section 3) and, indeed, our highly mutually recursive proof relying on this is accepted by Agda.

We also relate the recursive definition of substitution to a specification using a quotient-inductive-inductive type (QIIT) (a mutual inductive type with equations) where substitution is a term former (i.e. explicit substitutions). Specifically, our specification is such that the substitution laws correspond to the equations of a simply typed category with families (CwF) (a variant of a category with families where the types do not depend on a context). We show that our recursive definition of substitution leads to a simply typed CwF which is isomorphic to the specified initial one. This can be viewed as a normalisation result where the usual  $\lambda$ -terms without explicit substitutions are the *substitution normal forms*.

## 1.2 Related work

[10] introduces his eponymous indices and also the notion of simultaneous substitution. We are here using a typed version of de Bruijn indices, e.g. see [6] where the problem of showing termination of a simple definition of substitution (for the untyped  $\lambda$ -calculus) is addressed using a well-founded recursion. The present approach seems to be simpler and scales better, avoiding well-founded recursion. Andreas Abel used a very similar technique to ours in his unpublished Agda proof [1] for untyped  $\lambda$ -terms when implementing [6].

The monadic approach has been further investigated in [13]. The structure of the proofs is explained in [3] from a monadic perspective. Indeed this example is one of the motivations for relative monads [7].

In the monadic approach, we represent substitutions as functions, however it is not clear how to extend this to dependent types without “very dependent” types.

There are a number of publications on formalising substitution laws. Just to mention a few recent ones: [16] develops a Coq library which automatically derives substitution lemmas, but the proofs are repeated for renamings and substitutions. Their equational theory is similar to the simply typed CwFs we are using in section 5. [14] is also using Agda, but extrinsically (i.e. separating preterms and typed syntax). Here the approach from [3] is used to factor the construction using *kits*. [15] instead uses intrinsic syntax, but with renamings and substitutions defined separately, and relevant substitution lemmas repeated for all required combinations.

## 1.3 Using Agda

For the technical details of Agda we refer to the online documentation [17]. We only use plain Agda, inductive definitions and structurally recursive programs and proofs. Termination is checked by Agda’s termination checker [2] which uses a lexical combination of structural descent that is inferred by the termination checker by investigating all possible recursive paths. We will define mutually recursive proofs which heavily rely on each other.

The only recent feature we use, albeit sparingly, is the possibility to turn propositional equations into rewriting rules (i.e. definitional equalities). This makes the statement of some

theorems more readable because we can avoid using `subst`, but it is not essential.

We extensively use variable declarations to introduce implicit quantification (we summarize the variable conventions in passing in the text). We also use  $\forall$ -prefix so we can elide types of function parameters where they can be inferred, i.e. instead of  $\{\Gamma : \text{Con}\} \rightarrow \dots$  we just write  $\forall \{\Gamma\} \rightarrow \dots$ . Implicit variables, which are indicated by using  $\{.. \}$  instead of  $(..)$  in dependent function types, can be instantiated using the syntax  $a \{x = b\}$ .

Agda syntax is very flexible, allowing mixfix syntax declarations using `_` to indicate where the parameters go. In the proofs, we use the Agda standard library's definitions for equational derivations, which exploit this flexibility.

The source of this document contains the actual Agda code, i.e. it is a literate Agda file. Different chapters are in different modules to avoid name clashes, e.g. preliminary definitions from section 2 are redefined later.

## 2 The naive approach

Let us first review the naive approach which leads to the copy-and-paste proof. We define types  $(A, B, C)$  and contexts  $(\Gamma, \Delta, \Theta)$ :

**data Ty : Set where**

`o` : Ty

`_  $\Rightarrow$  _` : Ty  $\rightarrow$  Ty  $\rightarrow$  Ty

**data Con : Set where**

`•` : Con

`_  $\triangleright$  _` : Con  $\rightarrow$  Ty  $\rightarrow$  Con

Next we introduce intrinsically typed de Bruijn variables  $(i, j, k)$  and  $\lambda$ -terms  $(t, u, v)$ :

**data \_  $\ni$  \_ : Con  $\rightarrow$  Ty  $\rightarrow$  Set where**

`zero` :  $\Gamma \triangleright A \ni A$

`suc` :  $\Gamma \ni A \rightarrow (B : \text{Ty}) \rightarrow \Gamma \triangleright B \ni A$

**data \_  $\vdash$  \_ : Con  $\rightarrow$  Ty  $\rightarrow$  Set where**

``_` :  $\Gamma \ni A \rightarrow \Gamma \vdash A$

`·_` :  $\Gamma \vdash A \Rightarrow B \rightarrow \Gamma \vdash A \rightarrow \Gamma \vdash B$

`$\lambda$ _` :  $\Gamma \triangleright A \vdash B \rightarrow \Gamma \vdash A \Rightarrow B$

Here the constructor ``_` corresponds to *variables are  $\lambda$ -terms*. We write applications as `t · u`. Since we use de Bruijn variables, lambda abstraction  `$\lambda$ _` doesn't bind a name explicitly (instead, variables count the number of binders between them and their actual binding site). We also define substitutions as sequences of terms:

**data \_  $\models$  \_ : Con  $\rightarrow$  Con  $\rightarrow$  Set where**

`$\varepsilon$`  :  $\Gamma \models \bullet$

`_,_` :  $\Gamma \models \Delta \rightarrow \Gamma \vdash A \rightarrow \Gamma \models \Delta \triangleright A$

Now to define the categorical structure  $(\_ \circ \_, \text{id})$  we first need to define substitution for terms and variables:

`_v[_]` :  $\Gamma \ni A \rightarrow \Delta \models \Gamma \rightarrow \Delta \vdash A$

`zero` v[ts, t] = t

`(suc i _)` v[ts, t] = i v[ts]

`_[_]` :  $\Gamma \vdash A \rightarrow \Delta \models \Gamma \rightarrow \Delta \vdash A$

`(`i)` [ts] = i v[ts]

`(t · u)` [ts] = (t [ts]) · (u [ts])

`( $\lambda$  t)` [ts] =  $\lambda ?$

As usual, we encounter a problem with the case for binders  `$\lambda$ _`. We are given a substitution `ts :  $\Delta \models \Gamma$`  but the body `t` lives in the extended context `t :  $\Gamma, A \vdash B$` . We need to exploit the fact that context extension `_  $\triangleright$  _` is functorial: `_  $\uparrow$  _` :  $\Gamma \models \Delta \rightarrow (A : \text{Ty}) \rightarrow \Gamma \triangleright A \models \Delta \triangleright A$ . Using `_  $\uparrow$  _` we can complete `_[_]`: `( $\lambda$  t) [ts] =  $\lambda$  (t [ts  $\uparrow$  _])`.

However, now we have to define `_  $\uparrow$  _`. This is easy (isn't it?) but we need weakening on substitutions:

`ts  $\uparrow$  A = ts+ A, `zero`

`_+_` :  $\Gamma \models \Delta \rightarrow (A : \text{Ty}) \rightarrow \Gamma \triangleright A \models \Delta$

Now we need to define `_+_`, which is nothing but a fold of weakening of terms:

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```

123      ε      + A = ε
      (ts, t) + A = ts + A, suc-tm t A    suc-tm : Γ ⊢ B → (A : Ty) → Γ ▷ A ⊢ B

124 But how can we define suc-tm when we only have weakening for variables? If we already had
125 identity id : Γ ⊢ Γ and substitution we could write: suc-tm t A = t [ id + A ], but this is
126 certainly not structurally recursive (and hence rejected by Agda's termination checker).
127 Actually, we realise that id is a renaming, i.e. it is a substitution only containing variables,
128 and we can easily define  $\_+^v$  for renamings. This leads to a structurally recursive definition,
129 but we have to repeat the definition of substitutions for renamings.
130      data  $\_ \models_v \_$  : Con → Con → Set where
131      ε : Γ  $\models_v$  •
132       $\_ , \_$  : Γ  $\models_v$  Δ → Γ ∋ A → Γ  $\models_v$  Δ ▷ A

       $\_ v [ \_ ] v$  : Γ ∋ A → Δ  $\models_v$  Γ → Δ ∋ A       $\_ [ \_ ] v$  : Γ ⊢ A → Δ  $\models_v$  Γ → Δ ⊢ A
      zero      v [ is, i ] v = i                    (˘ i) [ is ] v      = ˘ (i v [ is ] v)
      (suc i  $\_$ ) v [ is, j ] v = i v [ is ] v          (t · u) [ is ] v      = (t [ is ] v) · (u [ is ] v)
       $\_ +^v \_$  : Γ  $\models_v$  Δ → ∀ A → Γ ▷ A  $\models_v$  Δ      (λ t) [ is ] v      = λ (t [ is ↑v  $\_$  ] v)

133      ε      +v A      = ε
      (is, i) +v A      = is +v A, suc i A
       $\_ \uparrow v \_$  : Γ  $\models_v$  Δ → ∀ A → Γ ▷ A  $\models_v$  Δ ▷ A
      is ↑v A      = is +v A, zero
      idv : Γ  $\models_v$  Γ
      idv {Γ = •}      = ε
      idv {Γ = Γ ▷ A} = idv ↑v A
      suc-tm t A      = t [ idv +v A ] v

```

134 This may not seem too bad: to obtain structural termination we just have to duplicate a few  
135 definitions, but it gets even worse when proving the laws. For example, to prove associativity,  
136 we first need to prove functoriality of substitution:  $[o] : t [ us \circ vs ] \equiv t [ us ] [ vs ]$ .  
137 Since  $t$ ,  $us$ ,  $vs$  can be variables/renamings or terms/substitutions, there are in principle eight  
138 combinations (though it turns out that four is enough). Each time, we must to prove a  
139 number of lemmas again in a different setting.

140 In the rest of the paper we describe a technique for factoring these definitions and  
141 the proofs, only relying on the Agda termination checker to validate that the recursion is  
142 structurally terminating.

### 3 Factorising with sorts

144 Our main idea is to turn the distinction between variables and terms into a parameter. The  
145 first approximation is to define a type `Sort (q, r, s)`:

```

146      data Sort : Set where
147      V T : Sort

```

148 but this is not exactly what we want; ideally, Agda should know that the sort of variables  $V$   
149 is *smaller* than the sort of terms  $T$  (following intuition that variable weakening is trivial, but  
150 to weaken a term we must construct a renaming). Agda's termination checker only knows  
151 about the structural orderings, but with the following definition, we can make  $V$  structurally  
152 smaller than  $T > V V$  isV, while maintaining that `Sort` has only two elements.

```

153      data Sort : Set where
      V      : Sort
      T > V : (s : Sort) → isV s → Sort
      data isV : Sort → Set where
      isV : isV V

```

154 Here the predicate `isV` only holds for  $V$ . This particular encoding makes use of Agda's  
155 support for inductive-inductive datatypes (IITs), but a pair of a natural number  $n$  and a  
156 proof  $n \leq 1$  would also work, i.e. `Sort = Σ ℕ (λ _ → 1)`.

157 We can now define  $T = T > V V$  isV : `Sort` but, even better, we can tell Agda that this  
158 is a derived pattern with `pattern T = T > V V isV`.

159 This means we can pattern match over `Sort` just with `V` and `T`, while ensuring `V` is visibly  
 160 (to Agda's termination checker) structurally smaller than `T`.

161 We can now define terms and variables in one go  $(x, y, z)$ :

```
162 data _ ⊢ [ ] _ : Con → Sort → Ty → Set where
163   zero : Γ ▷ A ⊢ [ V ] A
164   suc  : Γ ⊢ [ V ] A → (B : Ty) → Γ ▷ B ⊢ [ V ] A
165   ` _  : Γ ⊢ [ V ] A → Γ ⊢ [ T ] A
166   _ · _ : Γ ⊢ [ T ] A ⇒ B → Γ ⊢ [ T ] A → Γ ⊢ [ T ] B
167   λ _  : Γ ▷ A ⊢ [ T ] B → Γ ⊢ [ T ] A ⇒ B
```

168 While almost identical to the previous definition ( $\Gamma \vdash [V] A$  corresponds to  $\Gamma \ni A$  and  
 169  $\Gamma \vdash [T] A$  to  $\Gamma \vdash A$ ) we can now parametrize all definitions and theorems explicitly. As a  
 170 first step, we can generalize renamings and substitutions  $(xs, ys, zs)$ :

```
171 data _ ⊢ [ q ] _ : Con → Sort → Con → Set where
172   ε      : Γ ⊢ [ q ] •
173   _ , _ : Γ ⊢ [ q ] Δ → Γ ⊢ [ q ] A → Γ ⊢ [ q ] Δ ▷ A
```

174 To account for the non-uniform behaviour of substitution and composition (the result is  
 175 `V` only if both inputs are `V`) we define a least upper bound on `Sort`. We also need this order  
 176 as a relation.

```
177 _ ⊔ _ : Sort → Sort → Sort
178 V ⊔ r = r
179 T ⊔ r = T
180 data _ ⊑ _ : Sort → Sort → Set where
181   rfl : s ⊑ s
182   v ⊑ t : V ⊑ T
```

178 Yes, this is just boolean algebra. We need a number of laws:

```
179 ⊑ t : s ⊑ T
180 v ⊑ : V ⊑ s
181 ⊑ q ⊔ : q ⊑ (q ⊔ r)
182 ⊑ ⊔ r : r ⊑ (q ⊔ r)
183 ⊔ ⊔ : q ⊔ (r ⊔ s) ≡ (q ⊔ r) ⊔ s
184 ⊔ v : q ⊔ V ≡ q
```

180 which are easy to prove by case analysis, e.g.  $\sqsubseteq t \{V\} = v \sqsubseteq t$  and  $\sqsubseteq t \{T\} = \text{rfl}$ . To  
 181 improve readability we turn the equations  $(\sqcup \sqcup, \sqcup v)$  into rewrite rules.

182 This introduces new definitional equalities, i.e.  $q \sqcup (r \sqcup s) = (q \sqcup r) \sqcup s$  and  
 183  $q \sqcup V = q$  are now used by the type checker<sup>1</sup>. The order gives rise to a functor which is  
 184 witnessed by  $\text{tm} \sqsubseteq : q \sqsubseteq s \rightarrow \Gamma \vdash [q] A \rightarrow \Gamma \vdash [s] A$ , where  $\text{tm} \sqsubseteq \text{rfl } x = x$  and  
 185  $\text{tm} \sqsubseteq v \sqsubseteq t \text{ i} = ` \text{i}$ .

186 By making functoriality of context extension parameteric,  $\_ \uparrow \_ : \Gamma \vdash [q] \Delta \rightarrow$   
 187  $\forall A \rightarrow \Gamma \triangleright A \vdash [q] \Delta \triangleright A$ , we are ready to define substitution and renaming in one  
 188 operation:

```
189 _ [ ] : Γ ⊢ [ q ] A → Δ ⊢ [ r ] Γ → Δ ⊢ [ q ⊔ r ] A    ( ` i )  [ xs ] = tm ⊑ ⊑ t ( i [ xs ] )
190 zero [ xs , x ] = x                                     ( t · u ) [ xs ] = ( t [ xs ] ) · ( u [ xs ] )
191 (suc i ` ) [ xs , x ] = i [ xs ]                       ( λ t )  [ xs ] = λ ( t [ xs ↑ ` ] )
```

190 We use  $\_ \sqcup \_$  here to take care of the fact that substitution will only return a variable if  
 191 both inputs are variables / renamings. We need to use  $\text{tm} \sqsubseteq$  to take care of the two cases  
 192 when substituting for a variable.

193 We can also implement `id` using  $\_ \uparrow \_$  (by folding contexts), but to define  $\_ \uparrow \_$  itself,  
 194 we need parametric versions of `zero` and `suc`. `zero` is easy:

```
195 id : Γ ⊢ [ V ] Γ
196 id {Γ = •} = ε
197 id {Γ = Γ ▷ A} = id ↑ A
198 zero [ ] : ∀ q → Γ ▷ A ⊢ [ q ] A
199 zero [ V ] = zero
200 zero [ T ] = ` zero
```

<sup>1</sup> Effectively, this feature allows a selective use of extensional Type Theory.

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However, `suc` is more subtle since the case for `T` depends on its fold over substitutions ( $\_ \uparrow \_$ ):

$$\begin{array}{ll} \text{suc}[\_] : \forall q \rightarrow \Gamma \vdash [q] B \rightarrow \forall A & \_ \uparrow \_ : \Gamma \models [q] \Delta \rightarrow \forall A \\ \rightarrow \Gamma \triangleright A \vdash [q] B & \rightarrow \Gamma \triangleright A \models [q] \Delta \\ \text{suc}[V] i A = \text{suc } i A & \varepsilon \quad \uparrow A = \varepsilon \\ \text{suc}[T] t A = t [id \uparrow A] & (xs, x) \uparrow A = xs \uparrow A, \text{suc}[\_] \times A \end{array}$$

And now we can define  $xs \uparrow A = xs \uparrow A$ ,  $\text{zero}[\_] = \text{zero}[\_]$ .

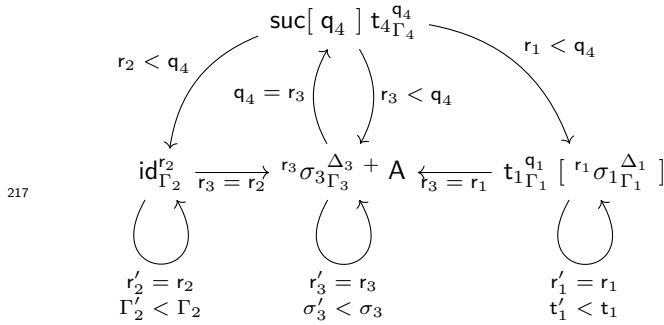
### 3.1 Termination

Unfortunately (as of Agda 2.7.0.1<sup>2</sup>), we now hit a termination error.

The cause turns out to be `id`. Termination here hinges on weakening for terms ( $\text{suc}[T] t A$ ) building and applying a renaming (i.e. a sequence of variables, for which weakening is trivial) rather than a full substitution. Note that if `id` produced  $\Gamma \models [T] \Gamma$ 's, or if we implemented weakening for variables ( $\text{suc}[V] i A$ ) with  $i [id \uparrow A]$ , our operations would still be type-correct, but would genuinely loop, so perhaps Agda is right to be careful.

Of course, we have specialised weakening for variables, so we now must ask why Agda still doesn't accept our program. The limitation is ultimately a technical one: Agda only looks at the direct arguments to function calls when building the call graph from which it identifies termination order [2]. Because `id` is not passed a sort, the sort cannot be considered as decreasing in the case of term weakening ( $\text{suc}[T] t A$ ).

Luckily, there is an easy solution here: making `id` `Sort`-polymorphic and instantiating with `V` at the call-sites adds new rows/columns (corresponding to the `Sort` argument) to the call matrices involving `id`, enabling the decrease to be tracked and termination to be correctly inferred by Agda. We present the call graph diagrammatically (inlining  $\_ \uparrow \_$ ), in the style of [12].



Function	Measure
$t_{1\Gamma_1}^{q_1} [r_1 \sigma_1^{\Delta_1}]$	$(r_1, t_1)$
$id_{\Gamma_2}^{r_2}$	$(r_2, \Gamma_2)$
$r_3 \sigma_3^{\Delta_3} + A$	$(r_3, \sigma_3)$
$\text{suc}[q_4] t_{4\Gamma_4}^{q_4}$	$(q_4)$

■ **Table 1** Per-function termination measures

■ **Figure 1** Call graph of substitution operations

To justify termination formally, we note that along all cycles in the graph, either the `Sort` strictly decreases in size, or the size of the `Sort` is preserved and some other argument (the context, substitution or term) gets smaller. Following this, we can assign lexicographically-decreasing measures to each of the functions (Table 1).

In practice, we will generally require identity renamings, rather than substitutions, and so we shall continue as if the original `id` definition worked (recovering `V`-only `id` from the

<sup>2</sup> One of the authors to this paper has submitted a PR (#7695) to Agda that extends the termination checking algorithm such that these definitions are accepted directly.

Sort-polymorphic one is easy after all: we merely need to instantiate the `Sort` argument with `V`).

Finally, we define composition,  $\_ \circ \_ : \Gamma \models [q] \Theta \rightarrow \Delta \models [r] \Gamma \rightarrow \Delta \models [q \sqcup r] \Theta$  by folding substitution.

## 4 Proving the laws

We now present a formal proof of the categorical laws, proving each lemma only once while only using structural induction. Indeed termination isn't completely trivial but is still inferred by the termination checker.

### 4.1 The right identity law

Let's get the easy case out of the way: the right-identity law ( $xs \circ id \equiv xs$ ). It is easy because it doesn't depend on any other categorical equations.

The main lemma is the identity law for the substitution functor  $[id] : x [id] \equiv x$ . To prove the successor case, we need naturality of  $suc [q]$  applied to a variable, which can be shown by simple induction over said variable:<sup>3</sup>

```

+nat[[v : i [ xs + A ] ≡ suc [ q ] (i [ xs ]) A
+nat[[v { i = zero } { xs = xs , x } = refl
+nat[[v { i = suc j A } { xs = xs , x } = +nat[[v { i = j }

```

The identity law is now easily provable by structural induction:

```

[id] {x = zero} = refl
[id] {x = suc i A} =
  i [ id + A ] ≡ ( +nat[[v { i = i } )
  suc (i [ id ]) A
  ≡ ( cong (λ j → suc j A) ([id] {x = i}) )
  suc i A ■
[id] {x = ` i } =
  cong ` _ ([id] {x = i})
[id] {x = t · u} =
  cong₂ _ · _ ([id] {x = t}) ([id] {x = u})
[id] {x = λ t } =
  cong λ _ ([id] {x = t})

```

Note that the  $\lambda\_$  case is easy here: we need the law to hold for  $t : \Gamma, A \vdash [T] B$ , but this is still covered by the inductive hypothesis because  $id \{ \Gamma = \Gamma, A \} = id \uparrow A$ .

Note also that is the first time we use Agda's syntax for equational derivations. This is just syntactic sugar for constructing an equational derivation using transitivity, exploiting Agda's flexible syntax. Here  $e \equiv \langle p \rangle e'$  means that  $p$  is a proof of  $e \equiv e'$ . Later we will also use the special case  $e \equiv \langle \rangle e'$  which means that  $e$  and  $e'$  are definitionally equal (this corresponds to  $e \equiv \langle refl \rangle e'$  and is just used to make the proof more readable). The proof is terminated with  $\blacksquare$  which inserts `refl`. We also make heavy use of congruence  $cong f : a \equiv b \rightarrow f a \equiv f b$  and a version for binary functions  $cong_2 g : a \equiv b \rightarrow c \equiv d \rightarrow g a c \equiv g b d$ .

The category law  $oid : xs \circ id \equiv xs$  is now simply a fold of the functor law  $[id]$ .

### 4.2 The left identity law

We need to prove the left identity law mutually with the second functor law for substitution. This is the main lemma for associativity.

Let's state the functor law but postpone the proof until the next section:  $[o] : x [ xs \circ ys ] \equiv x [ xs ] [ ys ]$ . This implicitly relies on the definitional equality<sup>4</sup>  $\sqcup : q \sqcup (r \sqcup s) = (q \sqcup r) \sqcup s$

<sup>3</sup> We are using the naming conventions introduced in sections 2 and 3, e.g.  $i : \Gamma \ni A$ .

<sup>4</sup> We rely on Agda's rewrite rules here. Alternatively we would have to insert a transport using `subst`.

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because the left hand side has the type  $\Delta \vdash [q \sqcup (r \sqcup s)] A$  while the right hand side has type  $\Delta \vdash ((q \sqcup r) \sqcup s) A$ .

Of course, we must also state the left-identity law  $\text{id} \circ : \text{id} \circ \text{xs} \equiv \text{xs}$ . Similarly to  $\text{id}$ , Agda will not accept a direct implementation of  $\text{id} \circ$  as structurally recursive. Unfortunately, adapting the law to deal with a **Sort**-polymorphic  $\text{id}$  complicates matters: when  $\text{xs}$  is a renaming (i.e. at sort **V**) composed with an identity substitution (i.e. at sort **T**), its sort must be lifted on the RHS (e.g. by extending the  $\text{tm} \sqsubseteq$  functor to lists of terms) to obey  $\_ \sqcup \_$ .

Accounting for this lifting is certainly do-able, but in keeping with the single-responsibility principle of software design, we argue it is neater to consider only **V**-sorted  $\text{id}$  here and worry about equations involving **Sort**-coercions later (in 5.2). Therefore, we instead add a “dummy” **Sort** argument (i.e.  $\text{id} \circ' : \text{Sort} \rightarrow \text{id} \circ \text{xs} \equiv \text{xs}$ ) to track the size decrease (such that we can eventually just use  $\text{id} \circ = \text{id} \circ' \text{V}$ ).<sup>5</sup>

To prove  $\text{id} \circ'$ , we need the  $\beta$ -law for  $\_ + \_$ ,  $+ \circ : \text{xs} + A \circ (\text{ys}, x) \equiv \text{xs} \circ \text{ys}$ , which can be shown with a fold over a corresponding property for  $\text{suc}[\_]$ ,  $\text{suc}[] : (\text{suc}[q] \times \_) [ \text{ys}, y ] \equiv x [ \text{ys} ]$ .

$$\begin{array}{ll}
 \text{suc}[] \{q = \text{V}\} = \text{refl} & + \circ \{ \text{xs} = \varepsilon \} = \text{refl} \\
 \text{suc}[] \{q = \text{T}\} \{x = x\} \{ \text{ys} = \text{ys} \} \{y = y\} = & + \circ \{ \text{xs} = \text{xs}, x \} = \\
 (\text{suc}[\text{T}] \times \_) [ \text{ys}, y ] \equiv \langle & \text{cong}_2 \_ \_ (+ \circ \{ \text{xs} = \text{xs} \}) (\text{suc}[] \{x = x\}) \\
 x [ \text{id}^+ \_ ] [ \text{ys}, y ] \equiv \langle \text{sym} ([\circ] \{x = x\}) \rangle & \text{id} \circ' \{ \text{xs} = \varepsilon \} \_ = \text{refl} \\
 x [ (\text{id}^+ \_) \circ (\text{ys}, y) ] & \text{id} \circ' \{ \text{xs} = \text{xs}, x \} \_ = \text{cong}_2 \_ \_ \\
 \equiv \langle \text{cong} (\lambda \rho \rightarrow x [ \rho ]) + \circ \rangle & (\text{id}^+ \_ \circ (\text{xs}, x)) \equiv \langle + \circ \{ \text{xs} = \text{id} \} \rangle \\
 x [ \text{id} \circ \text{ys} ] & \text{id} \circ \text{xs} \equiv \langle \text{id} \circ \rangle \\
 \equiv \langle \text{cong} (\lambda \rho \rightarrow x [ \rho ]) \text{id} \circ \rangle & \text{xs} \blacksquare \\
 x [ \text{ys} ] \blacksquare & \text{refl}
 \end{array}$$

One may note that  $+ \circ$  relies on itself indirectly via  $\text{suc}[]$ . Like with the substitution operations, termination is justified here by the **Sort** decreasing.

### 4.3 Associativity

We finally get to the proof of the second functor law  $([\circ] : x [ \text{xs} \circ \text{ys} ] \equiv x [ \text{xs} ] [ \text{ys} ])$ , the main lemma for associativity. The main obstacle is that for the  $\lambda \_$  case; we need the second functor law for context extension:  $\uparrow \circ : (\text{xs} \circ \text{ys}) \uparrow A \equiv (\text{xs} \uparrow A) \circ (\text{ys} \uparrow A)$ .

To verify the variable case we also need that  $\text{tm} \sqsubseteq$  commutes with substitution,  $\text{tm}[] : \text{tm} \sqsubseteq \sqsubseteq t (x [ \text{xs} ]) \equiv (\text{tm} \sqsubseteq \sqsubseteq t x) [ \text{xs} ]$ , which is easy to prove by case analysis.

We are now ready to prove  $[\circ]$  by structural induction:

<sup>5</sup> Perhaps surprisingly, this “dummy” argument does not even need to be of type **Sort** to satisfy Agda here. More discussion on this trick can be found at Agda issue #7693, but in summary:

- Agda considers all base constructors (constructors with no parameters) to be of minimal size structurally, so their presence can track size preservation of other base-constructor arguments across function calls.
- It turns out that a strict decrease in **Sort** is not necessary everywhere for termination: the context also gets structurally smaller in the call to  $\_ + \_$  from  $\text{id}$ .



$$\begin{array}{llll}
[o] \{x = \text{zero}\} \{xs = xs, x\} & = \text{refl} & [o] \{x = t \cdot u\} & = \\
[o] \{x = \text{suc } i \_ \} \{xs = xs, x\} & = & \text{cong}_2 \_ \cdot \_ ([o] \{x = t\}) ([o] \{x = u\}) & \\
[o] \{x = i\} & & [o] \{x = \lambda t\} \{xs = xs\} \{ys = ys\} = & \\
284 \quad [o] \{x = \_ x\} \{xs = xs\} \{ys = ys\} = & \text{cong } \lambda \_ ( & & \\
\quad \text{tm} \sqsubseteq \sqsubseteq t (x [xs \circ ys]) & \quad t [ (xs \circ ys) \uparrow \_ ] & & \\
\quad \equiv \langle \text{cong } (\text{tm} \sqsubseteq \sqsubseteq t) ([o] \{x = x\}) \rangle & \quad \equiv \langle \text{cong } (\lambda zs \rightarrow t [zs]) \uparrow \circ \rangle & & \\
\quad \text{tm} \sqsubseteq \sqsubseteq t (x [xs] [ys]) & \quad t [ (xs \uparrow \_) \circ (ys \uparrow \_) ] & & \\
\quad \equiv \langle \text{tm} [] \{x = x [xs]\} \rangle & \quad \equiv \langle [o] \{x = t\} \rangle & & \\
\quad (\text{tm} \sqsubseteq \sqsubseteq t (x [xs])) [ys] \blacksquare & \quad (t [xs \uparrow \_] [ys \uparrow \_]) \blacksquare & &
\end{array}$$

285 Associativity  $\circ \circ : xs \circ (ys \circ zs) \equiv (xs \circ ys) \circ zs$  can be proven merely by a fold of  $[o]$   
 286 over substitutions.

287 However, we need to prove the second functor law for  $\_ \uparrow \_$   
 288  $(\uparrow \circ)$ . It turns out that this depends on the naturality of weakening  $^+ \text{-nat} \circ : xs \circ (ys^+ A) \equiv$   
 289  $(xs \circ ys)^+ A$ , which unsurprisingly must be shown by establishing a corresponding property  
 290 for substitutions:  $^+ \text{-nat} [] : x [xs^+ A] \equiv \text{suc} [ \_ ] (x [xs]) A$ . The case  $q = V$  is just the  
 291 naturality for variables which we have already proven ( $^+ \text{-nat} [v]$ ). The case for  $q = T$  is  
 292 more interesting and relies again on  $[o]$  and  $\circ \text{id}$ :

$$\begin{array}{ll}
293 \quad ^+ \text{-nat} [] \{q = T\} \{A = A\} \{x = x\} \{xs = xs\} = & \\
294 \quad x [xs^+ A] & \equiv \langle \text{cong } (\lambda zs \rightarrow x [zs^+ A]) (\text{sym} \circ \text{id}) \rangle \\
295 \quad x [(xs \circ \text{id})^+ A] & \equiv \langle \text{cong } (\lambda zs \rightarrow x [zs]) (\text{sym } (^+ \text{-nat} \circ \{xs = xs\})) \rangle \\
296 \quad x [xs \circ (\text{id}^+ A)] & \equiv \langle [o] \{x = x\} \rangle \\
297 \quad x [xs] [ \text{id}^+ A ] \blacksquare &
\end{array}$$

298 It also turns out we need  $\text{zero} [] : \text{zero} [q] [xs, x] \equiv \text{tm} \sqsubseteq (\sqsubseteq \sqcup r \{q = q\}) x$ , the  
 299  $\beta$ -law for  $\text{zero} [ \_ ]$ , which holds definitionally in the case for either  $\text{Sort}$ .

300 Finally, we have all the ingredients to prove the second functor law  $\uparrow \circ$ :<sup>6</sup>

$$\begin{array}{ll}
301 \quad \uparrow \circ \{r = r\} \{s = s\} \{xs = xs\} \{ys = ys\} \{A = A\} = & \\
302 \quad (xs \circ ys) \uparrow A & \equiv \langle \rangle \\
303 \quad (xs \circ ys)^+ A, \text{zero} [r \sqcup s] & \equiv \langle \text{cong}_2 \_ \cdot \_ (\text{sym } (^+ \text{-nat} \circ \{xs = xs\})) \text{refl} \rangle \\
304 \quad xs \circ (ys^+ A), \text{zero} [r \sqcup s] & \\
305 \quad \equiv \langle \text{cong}_2 \_ \cdot \_ \text{refl } (\text{tm} \sqsubseteq \text{zero} (\sqsubseteq \sqcup r \{r = s\} \{q = r\})) \rangle & \\
306 \quad xs \circ (ys^+ A), \text{tm} \sqsubseteq (\sqsubseteq \sqcup r \{q = r\}) \text{zero} [s] & \\
307 \quad \equiv \langle \text{cong}_2 \_ \cdot \_ (\text{sym } (^+ \circ \{xs = xs\})) (\text{sym } (\text{zero} [] \{q = r\} \{x = \text{zero} [s]\})) \rangle & \\
308 \quad (xs^+ A) \circ (ys \uparrow A), \text{zero} [r] [ys \uparrow A] \equiv \langle \rangle & \\
309 \quad (xs \uparrow A) \circ (ys \uparrow A) \blacksquare &
\end{array}$$

## 310 5 Initiality

311 We can do more than just prove that we have a category. Indeed we can verify the laws of a  
 312 simply typed category with families (CwF). CwFs are mostly known as models of dependent  
 313 type theory, but they can be specialised to simple types [8]. We summarize the definition of  
 314 a simply typed CwF as follows:

- 315 ■ A category of contexts (Con) and substitutions ( $\_ \models \_$ ),
- 316 ■ A set of types  $\text{Ty}$ ,
- 317 ■ For every type  $A$  a presheaf of terms  $\_ \vdash A$  over the category of contexts (i.e. a  
 318 contravariant functor into the category of sets),

<sup>6</sup> Actually, we also need that  $\text{zero}$  commutes with  $\text{tm} \sqsubseteq$ : that is for any  $q \sqsubseteq r : q \sqsubseteq r$  we have that  $\text{tm} \sqsubseteq \text{zero } q \sqsubseteq r : \text{zero} [r] \equiv \text{tm} \sqsubseteq q \sqsubseteq r \text{zero} [q]$ .

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319 ■ A terminal object (the empty context) and a context extension operation  $\_ \triangleright \_$  such  
320 that  $\Gamma \models \Delta \triangleright A$  is naturally isomorphic to  $(\Gamma \models \Delta) \times (\Gamma \vdash A)$ .

321 I.e. a simply typed CwF is just a CwF where the presheaf of types is constant. We will  
322 give the precise definition in the next section, hence it isn't necessary to be familiar with the  
323 categorical terminology to follow the rest of the paper.

324 We can add further constructors like function types  $\_ \Rightarrow \_$ . These usually come with  
325 a natural isomorphisms, giving rise to  $\beta$  and  $\eta$  laws, but since we are only interested in  
326 substitutions, we don't assume these. Instead we add the term formers for application  $(\_ \cdot \_)$   
327 and lambda-abstraction  $\lambda$  as natural transformations.

328 We start with a precise definition of a simply typed CwF with the additional structure to  
329 model simply typed  $\lambda$ -calculus (section 5.1) and then we show that the recursive definition  
330 of substitution gives rise to a simply typed CwF (section 5.2). We can define the initial CwF  
331 as a quotient inductive-inductive type (QIIT). To simplify our development, rather than  
332 using a Cubical Agda HIT,<sup>7</sup> we just postulate the existence of this QIIT in Agda (with the  
333 associated  $\beta$ -laws as rewriting rules). By initiality, there is an evaluation functor from the  
334 initial CwF to the recursively defined CwF (defined in section 5.2). On the other hand, we  
335 can embed the recursive CwF into the initial CwF; this corresponds to the embedding of  
336 normal forms into  $\lambda$ -terms, only that here we talk about *substitution normal forms*. We then  
337 show that these two structure maps are inverse to each other and hence that the recursively  
338 defined CwF is indeed initial (section 5.3). The two identities correspond to completeness  
339 and stability in the language of normalisation functions.

### 340 5.1 Simply Typed CwFs

341 We define a record to capture simply typed CWFs: **record** CwF-simple : Set<sub>1</sub>.

342 For the contents, we begin with the category of contexts, using the same naming conven-  
343 tions as introduced previously:

Con	: Set	
$\_ \models \_$	: Con $\rightarrow$ Con $\rightarrow$ Set	$\text{id} \circ \_ : \text{id} \circ \delta \equiv \delta$
id	: $\Gamma \models \Gamma$	$\_ \circ \text{id} : \delta \circ \text{id} \equiv \delta$
$\_ \circ \_$	: $\Delta \models \Theta \rightarrow \Gamma \models \Delta \rightarrow \Gamma \models \Theta$	$\_ \circ \_ : (\xi \circ \theta) \circ \delta \equiv \xi \circ (\theta \circ \delta)$

345 We introduce the set of types and associate a presheaf with each type:

Ty	: Set	
$\_ \vdash \_$	: Con $\rightarrow$ Ty $\rightarrow$ Set	$[\text{id}] : (\text{t} [\text{id}]) \equiv \text{t}$
$\_ \llbracket \_ \rrbracket$	: $\Gamma \vdash A \rightarrow \Delta \models \Gamma \rightarrow \Delta \vdash A$	$[\_] : \text{t} [\theta] [\delta] \equiv \text{t} [\theta \circ \delta]$

347 The category of contexts has a terminal object (the empty context), and context extension  
348 resembles categorical products but mixing contexts and types:

$\bullet$	: Con	$\bullet \dashv \eta : \delta \equiv \varepsilon$
$\varepsilon$	: $\Gamma \models \bullet$	$\triangleright \dashv \beta_0 : \pi_0 (\delta, \text{t}) \equiv \delta$
$\_ \triangleright \_$	: Con $\rightarrow$ Ty $\rightarrow$ Con	$\triangleright \dashv \beta_1 : \pi_1 (\delta, \text{t}) \equiv \text{t}$
$\_ \cdot \_$	: $\Gamma \models \Delta \rightarrow \Gamma \vdash A \rightarrow \Gamma \models (\Delta \triangleright A)$	$\triangleright \dashv \eta : (\pi_0 \delta, \pi_1 \delta) \equiv \delta$
$\pi_0$	: $\Gamma \models (\Delta \triangleright A) \rightarrow \Gamma \models \Delta$	$\pi_0 \circ \_ : \pi_0 (\theta \circ \delta) \equiv \pi_0 \theta \circ \delta$
$\pi_1$	: $\Gamma \models (\Delta \triangleright A) \rightarrow \Gamma \vdash A$	$\pi_1 \circ \_ : \pi_1 (\theta \circ \delta) \equiv (\pi_1 \theta) [\delta]$

350 We can define the morphism part of the context extension functor as before:

<sup>7</sup> Cubical Agda still lacks some essential automation, e.g. integrating no-confusion properties into pattern matching.

351  $\_ \uparrow \_ : \Gamma \models \Delta \rightarrow \forall A \rightarrow \Gamma \triangleright A \models \Delta \triangleright A$   
 352  $\delta \uparrow A = (\delta \circ (\pi_0 \text{id})) , \pi_1 \text{id}$

353 We need to add the specific components for simply typed  $\lambda$ -calculus; we add the type  
 354 constructors, the term constructors and the corresponding naturality laws:

355  $\circ : \text{Ty} \rightarrow \text{Ty} \rightarrow \text{Ty} \quad \lambda \_ : \Gamma \triangleright A \vdash B \rightarrow \Gamma \vdash A \Rightarrow B$   
 $\_ \Rightarrow \_ : \text{Ty} \rightarrow \text{Ty} \rightarrow \text{Ty} \quad \cdot [] : (t \cdot u) [\delta] \equiv (t [\delta]) \cdot (u [\delta])$   
 $\_ \cdot \_ : \Gamma \vdash A \Rightarrow B \rightarrow \Gamma \vdash A \rightarrow \Gamma \vdash B \quad \lambda [] : (\lambda t) [\delta] \equiv \lambda (t [\delta \uparrow \_])$

## 356 5.2 The CwF of recursive substitutions

357 We are building towards a proof of initiality for our recursive substitution syntax, but  
 358 shall start by showing that our recursive substitution syntax obeys the specified CwF laws,  
 359 specifically that **CwF-simple** can be instantiated with  $\_ \vdash [\_] \_ / \_ \models [\_] \_$ . This will be more-  
 360 or-less enough to implement the “normalisation” direction of our initial  $\text{CwF} \simeq \text{recursive}$   
 361 sub syntax isomorphism.

362 Most of the work to prove these laws was already done in section 4 but there are a couple  
 363 tricky details with fitting into the exact structure the **CwF-simple** record requires.

364 Our first non-trivial decision is which type family to interpret substitutions into. In our  
 365 first attempt, we tried to pair renamings/substitutions with their sorts to stay polymorphic:  
 366  $\text{is-cwf} . \text{CwF} . \_ \models \_ = \Sigma \text{Sort} (\Delta \models [\_] \Gamma)$ . Unfortunately, this approach quickly breaks.  
 367 The  $\bullet - \eta$  CwF law forces us to provide a unique morphism to the terminal context (i.e. a  
 368 unique weakening from the empty context);  $\Sigma \text{Sort} (\Delta \models [\_] \Gamma)$  is simply too flexible here,  
 369 allowing both  $V, \varepsilon$  and  $T, \varepsilon$ .

370 Therefore, we instead fix the sort to  $T$ .

371  $\text{is-cwf} . \text{CwF} . \_ \models \_ = \_ \models [T] \_ \quad \text{is-cwf} . \text{CwF} . \bullet - \eta \{ \delta = \varepsilon \} = \text{refl}$   
 $\text{is-cwf} . \text{CwF} . \blacksquare = \bullet \quad \text{is-cwf} . \text{CwF} . \_ \circ \_ = \_ \circ \_$   
 $\text{is-cwf} . \text{CwF} . \varepsilon = \varepsilon \quad \text{is-cwf} . \text{CwF} . \circ \circ = \text{sym} \circ \circ$

372 The lack of flexibility over sorts when constructing substitutions does, however, make  
 373 identity a little trickier.  $\text{id}$  doesn't fit  $\text{CwF} . \text{id}$  directly as it produces a renaming  $\Gamma \models [V] \Gamma$ .  
 374 We need the equivalent substitution  $\Gamma \models [T] \Gamma$ .

375 We first extend  $\text{tm} \sqsubseteq$  to renamings/substitutions with a fold:  $\text{tm}^* \sqsubseteq : q \sqsubseteq s \rightarrow \Gamma \models$   
 376  $[q] \Delta \rightarrow \Gamma \models [s] \Delta$ , and  $\text{nd}$  prove various lemmas about how  $\text{tm}^* \sqsubseteq$  coercions can be  
 377 lifted outside of our substitution operators:

378  $\sqsubseteq \circ : \text{tm}^* \sqsubseteq v \sqsubseteq t \text{xs} \circ \text{ys} \equiv \text{xs} \circ \text{ys} \quad \sqsubseteq^+ : \text{tm}^* \sqsubseteq \sqsubseteq t \text{xs}^+ A \equiv \text{tm}^* \sqsubseteq v \sqsubseteq t (\text{xs}^+ A)$   
 $\circ \sqsubseteq : \text{xs} \circ \text{tm}^* \sqsubseteq v \sqsubseteq t \text{ys} \equiv \text{xs} \circ \text{ys} \quad \sqsubseteq \uparrow : \text{tm}^* \sqsubseteq v \sqsubseteq t \text{xs} \uparrow A \equiv \text{tm}^* \sqsubseteq v \sqsubseteq t (\text{xs} \uparrow A)$   
 $t[\sqsubseteq] : t [\text{tm}^* \sqsubseteq v \sqsubseteq t \text{ys}] \equiv t [\text{ys}] \quad v[\sqsubseteq] : i [\text{tm}^* \sqsubseteq v \sqsubseteq t \text{ys}] \equiv \text{tm} \sqsubseteq v \sqsubseteq t i [\text{ys}]$

379 Most of these are proofs come out easily by induction on terms and substitutions so we  
 380 skip over them. Perhaps worth noting though is that  $\sqsubseteq^+$  requires folding over substitutions  
 381 using one new law, relating our two ways of weakening variables.

382  $\text{suc}[\text{id}^+] : i [\text{id}^+ A] \equiv \text{suc} i A$   
 383  $\text{suc}[\text{id}^+] \{i = i\} \{A = A\} =$   
 384  $i [\text{id}^+ A] \equiv \langle ^+ \text{-nat} [\text{v} \{i = i\}] \rangle$   
 385  $\text{suc} (i [\text{id}]) A \equiv \langle \text{cong} (\lambda j \rightarrow \text{suc} j A) [\text{id}] \rangle$   
 386  $\text{suc} i A \blacksquare$

387 We can now build an identity substitution by applying this coercion to the identity  
 388 renaming:  $\text{is-cwf} . \text{CwF} . \text{id} = \text{tm}^* \sqsubseteq v \sqsubseteq t \text{id}$ . The left and right identity CwF laws take the

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form  $\text{tm}^* \sqsubseteq v \sqsubseteq t \text{ id} \circ \delta \equiv \delta$  and  $\delta \circ \text{tm}^* \sqsubseteq v \sqsubseteq t \text{ id} \equiv \delta$ . This is where we can take full advantage of the  $\text{tm}^* \sqsubseteq$  machinery; these lemmas let us reuse our existing  $\text{id} \circ$ / $\text{oid}$  proofs!

$$\begin{array}{ll} \text{is-cwf} . \text{CwF} . \text{id} \circ \{ \delta = \delta \} = & \text{is-cwf} . \text{CwF} . \circ \text{id} \{ \delta = \delta \} = \\ \text{tm}^* \sqsubseteq v \sqsubseteq t \text{ id} \circ \delta \equiv \langle \sqsubseteq \circ \rangle & \delta \circ \text{tm}^* \sqsubseteq v \sqsubseteq t \text{ id} \equiv \langle \circ \sqsubseteq \rangle \\ \text{id} \circ \delta \equiv \langle \text{id} \circ \rangle & \delta \circ \text{id} \equiv \langle \text{oid} \rangle \\ \delta \blacksquare & \delta \blacksquare \end{array}$$

Similarly to substitutions, we must fix the sort of our terms to  $\mathsf{T}$  (in this case, so we can prove the identity law - note that applying the identity substitution to a variable  $i$  produces the distinct term  $\text{`i}$ ).

$$\begin{array}{ll} \text{is-cwf} . \text{CwF} . [\text{id}] \{ t = t \} = & \\ t [ \text{tm}^* \sqsubseteq v \sqsubseteq t \text{ id} ] \equiv \langle t [\sqsubseteq] \{ t = t \} \rangle & \text{is-cwf} . \text{CwF} . \_ \vdash \_ = \_ \vdash [ \mathsf{T} ] \_ \\ t [ \text{id} ] \equiv \langle [\text{id}] \rangle & \text{is-cwf} . \text{CwF} . \_ [\_] = \_ [\_] \\ t \blacksquare & \end{array}$$

We now define projections  $\pi_0 (\delta, t) = \delta$  and  $\pi_1 (\delta, t) = t$  and  $\triangleright - \beta_0, \triangleright - \beta_1, \triangleright - \eta, \pi_0$  and  $\pi_1$  all hold by definition (though the latter three only after matching on the guaranteed-non-empty substitution).

Finally, we can deal with the cases specific to simply typed  $\lambda$ -calculus.  $\cdot \sqsubseteq$  holds by definition, but the  $\beta$ -rule for substitutions applied to lambdas requires a bit of equational reasoning due to differing implementations of  $\_ \uparrow \_$ .

$$\begin{array}{ll} \text{is-cwf} . \text{CwF} . \lambda \_ \{ A = A \} \{ t = x \} \{ \delta = ys \} = & \\ \lambda x [ ys \uparrow A ] \equiv \langle \text{cong} (\lambda \rho \rightarrow \lambda x [ \rho \uparrow A ]) (\text{sym} \circ \text{id}) \rangle & \\ \lambda x [ (ys \circ \text{id}) \uparrow A ] \equiv \langle \text{cong} (\lambda \rho \rightarrow \lambda x [ \rho, \text{`zero} ]) (\text{sym}^+ - \text{nat} \circ) \rangle & \\ \lambda x [ ys \circ \text{id}^+ A, \text{`zero} ] \equiv \langle \text{cong} (\lambda \rho \rightarrow \lambda x [ \rho, \text{`zero} ]) (\text{sym} (\circ \sqsubseteq \{ ys = \text{id}^+ \_ \})) \rangle & \\ \lambda x [ ys \circ \text{tm}^* \sqsubseteq v \sqsubseteq t (\text{id}^+ A), \text{`zero} ] \blacksquare & \end{array}$$

We have shown our recursive substitution syntax satisfies the CwF laws, but we want to go a step further and show initiality: that our syntax is isomorphic to the initial CwF.

An important first step is to actually define the initial CwF (and its eliminator). We use postulates and rewrite rules instead of a Cubical Agda higher inductive type (HIT) because of technical limitations mentioned previously. We also reuse our existing datatypes for contexts and types for convenience (note terms do not occur inside types in STLC).

To state the dependent equations between outputs of the eliminator, we need dependent identity types  $\_ \equiv [\_] \equiv \_ : \forall \{ A B : \text{Set } \ell \} \rightarrow A \rightarrow B \rightarrow B \rightarrow \text{Set } \ell$ . We can define these simply by matching on the identity between the LHS and RHS types  $x \equiv [\text{refl}] \equiv y = x \equiv y$ .

To avoid name clashes between our existing syntax and the initial CwF constructors, we annotate every  $\text{ICwF}$  constructor with  $^I$ . e.g.  $\_ \vdash^I \_ : \text{Con} \rightarrow \text{Ty} \rightarrow \text{Set}$ ,  $\text{id}^I : \Gamma \models^I \Gamma$  etc. Note we reuse the definitions of contexts and types as in STLC there are no non-trivial equations on these components.

We state the eliminator for the initial CwF in terms of  $\text{Motive} : \text{Set}_1$  and  $\text{Methods} : \text{Motive} \rightarrow \text{Set}_1$  records as in [4].

**module**  $\_ \{ \mathbb{M} \} (\mathbf{m} : \text{Methods } \mathbb{M}) \text{ where}$

$$\begin{array}{ll} \text{elim-con} : \forall \Gamma \rightarrow \text{Con}^{\mathbb{M}} \Gamma & \text{elim-cwf} : \forall t^I \rightarrow \text{Tm}^{\mathbb{M}} (\text{elim-con } \Gamma) (\text{elim-ty } A) t^I \\ \text{elim-ty} : \forall A \rightarrow \text{Ty}^{\mathbb{M}} A & \text{elim-cwf*} : \forall \delta^I \rightarrow \text{Tms}^{\mathbb{M}} (\text{elim-con } \Delta) (\text{elim-con } \Gamma) \delta^I \end{array}$$

Normalisation from the initial CwF into substitution normal forms now only needs a way to connect our notion of “being a CwF” with our initial CwF’s eliminator: specifically, that any set of type families satisfying the CwF laws gives rise to a  $\text{Motive}$  and associated set of  $\text{Methods}$ . To achieve this, we define  $\text{cwf-to-motive} : \text{CwF-simple} \rightarrow \text{Motive}$  and

429 `cwf-to-methods` : `CwF-simple`  $\rightarrow$  `Methods`, which simply project out the relevant fields, and  
 430 then implement e.g. `rec-cwf` = `elim-cwf cwf-to-methods`.

431 The one extra ingredient we need to make this work out neatly is to introduce a new  
 432 reduction for `cong`, `cong` ( $\lambda \_ \rightarrow x$ ) `p`  $\equiv$  `refl`<sup>8</sup>, via an Agda rewrite rule. This enables the  
 433 no-longer-dependent  $\_ \equiv [\_] \equiv \_$  to collapse to  $\_ \equiv \_$  automatically.

434 Normalisation into our substitution normal forms can now be achieved by with:

435 `norm` :  $\Gamma \vdash^I A \rightarrow \text{rec-con is-cwf } \Gamma \vdash [T] \text{ rec-ty is-cwf } A$   
 436 `norm` = `rec-cwf is-cwf`

437 Of course, normalisation shouldn't change the type of a term, or the context it is in, so  
 438 we might hope for a simpler signature  $\Gamma \vdash^I A \rightarrow \Gamma \vdash [T] A$  and, conveniently, rewrite  
 439 rules (`rec-con is-cwf`  $\Gamma \equiv \Gamma$ , `rec-ty is-cwf`  $A \equiv A$ ) can get us there!

440 `norm` :  $\Gamma \vdash^I A \rightarrow \Gamma \vdash [T] A$  `norm*` :  $\Delta \models^I \Gamma \rightarrow \Delta \models [T] \Gamma$   
`norm*` = `rec-cwf* is-cwf`  
 441 `norm` = `rec-cwf is-cwf`

442 The inverse operation to inject our syntax back into the initial CwF is easily implemented  
 by recursion on substitution normal forms.

443  $\ulcorner \_ \urcorner$  :  $\Gamma \vdash [q] A \rightarrow \Gamma \vdash^I A$   $\ulcorner t \cdot u \urcorner = \ulcorner t \urcorner \cdot^I \ulcorner u \urcorner$   
 $\ulcorner \lambda t \urcorner = \lambda^I \ulcorner t \urcorner$   
 $\ulcorner \varepsilon \urcorner_* = \varepsilon^I$   
 $\ulcorner \delta, x \urcorner_* = \ulcorner \delta \urcorner_*,^I \ulcorner x \urcorner$   
 $\ulcorner \_ \urcorner^*$  :  $\Delta \models [q] \Gamma \rightarrow \Delta \models^I \Gamma$   
 $\ulcorner \text{zero} \urcorner = \text{zero}^I$   
 $\ulcorner \text{suc } i \text{ B} \urcorner = \text{suc}^I \ulcorner i \urcorner \ulcorner B \urcorner$   
 $\ulcorner \_ \urcorner^i \ulcorner \_ \urcorner = \ulcorner i \urcorner$

### 444 5.3 Proving initiality

445 We have implemented both directions of the isomorphism. Now to show this truly is an  
 446 isomorphism and not just a pair of functions between two types, we must prove that `norm` and  
 447  $\ulcorner \_ \urcorner$  are mutual inverses - i.e. stability (`norm`  $\ulcorner t \urcorner \equiv t$ ) and completeness ( $\ulcorner \text{norm } t \urcorner \equiv t$ ).

448 We start with stability, as it is considerably easier. There are just a couple details worth  
 449 mentioning:

- 450 ■ To deal with variables in the  $\_$  case, we phrase the lemma in a slightly more general  
 451 way, taking expressions of any sort and coercing them up to sort `T` on the RHS.
- 452 ■ The case for variables relies on a bit of coercion manipulation and our earlier lemma  
 453 equating  $i [id^+ B]$  and `suc`  $i$  `B`.

454 `stab` : `norm`  $\ulcorner x \urcorner \equiv \text{tm} \sqsubseteq \ulcorner t \urcorner x$   
 455 `stab` {`x` = `zero`} = `refl`  
 456 `stab` {`x` = `suc`  $i$  `B`} =  
 457 `norm`  $\ulcorner i \urcorner [ \text{tm} \sqsubseteq v \sqsubseteq t (id^+ B) ] \equiv \langle t \sqsubseteq \{ t = \text{norm } \ulcorner i \urcorner \} \rangle$   
 458 `norm`  $\ulcorner i \urcorner [ id^+ B ] \equiv \langle \text{cong } (\lambda j \rightarrow \text{suc } [ \_ ] j B) (\text{stab } \{ x = i \}) \rangle$   
 459  $\ulcorner i [ id^+ B ] \equiv \langle \text{cong } \_ \text{suc} [id^+] \rangle$   
 460  $\ulcorner \text{suc } i \text{ B} \urcorner$  ■  
 461 `stab` {`x` =  $\ulcorner i \urcorner$ } = `stab` {`x` = `i`}  
 462 `stab` {`x` = `t`  $\cdot$  `u`} = `cong`<sub>2</sub>  $\_ \cdot \_$  (`stab` {`x` = `t`} (`stab` {`x` = `u`}))  
 463 `stab` {`x` =  $\lambda t$ } = `cong`  $\lambda \_$  (`stab` {`x` = `t`}))

464 To prove completeness, we must instead induct on the initial CwF itself, which means  
 465 there are many more cases. We start with the motive:

466 `compl-M` : `Motive`

<sup>8</sup> This definitional identity also holds natively in Cubical.

## XX:14 Substitution without copy and paste

$$\begin{aligned} \text{compl-}\mathbb{M}.\text{TM}^M \_ \_ t^I &= \ulcorner \text{norm } t^I \urcorner \equiv t^I & \text{compl-}\mathbb{M}.\text{Con}^M \_ &= \top \\ \text{compl-}\mathbb{M}.\text{Tms}^M \_ \_ \delta^I &= \ulcorner \text{norm}^* \delta^I \urcorner_* \equiv \delta^I & \text{compl-}\mathbb{M}.\text{Ty}^M \_ &= \top \end{aligned}$$

To show these identities, we need to prove that our various recursively defined syntax operations are preserved by  $\ulcorner \_ \urcorner$ .

Preservation of  $\text{zero}[\_]$ ,  $\ulcorner \text{zero} \urcorner : \ulcorner \text{zero}[q] \urcorner \equiv \text{zero}^I$  reduces to reflexivity after splitting on the sort.

Preservation of each of the projections out of sequences of terms (e.g.  $\ulcorner \pi_0 \delta \urcorner_* \equiv \pi_0^I \ulcorner \delta \urcorner_*$ ) reduce to the associated  $\beta$ -laws of the initial CwF (e.g.  $\triangleright - \beta_0^I$ ).

Preservation proofs for  $\ulcorner \_ \urcorner$ ,  $\ulcorner \_ \uparrow \_ \urcorner$ ,  $\ulcorner \_ + \_ \urcorner$ ,  $\text{id}$  and  $\text{suc}[\_]$  are all mutually inductive, mirroring their original recursive definitions. We must stay polymorphic over sorts and again use our dummy `Sort` argument trick when implementing  $\ulcorner \text{id} \urcorner$  to keep Agda's termination checker happy.

$$\begin{aligned} \ulcorner [] \urcorner : \ulcorner x[ys] \urcorner &\equiv \ulcorner x \urcorner [\ulcorner ys \urcorner_*]^I & \ulcorner \text{suc} \urcorner : \ulcorner \text{suc}[q] \urcorner \times B \urcorner &\equiv \ulcorner x \urcorner [\ulcorner \text{wk} \urcorner]^I \\ \ulcorner \uparrow \urcorner : \ulcorner xs \uparrow A \urcorner_* &\equiv \ulcorner xs \urcorner_* \uparrow^I A & \ulcorner \text{id}' \urcorner : \text{Sort} \rightarrow \ulcorner \text{id} \{ \Gamma = \Gamma \} \urcorner_* &\equiv \text{id}^I \\ \ulcorner + \urcorner : \ulcorner xs + A \urcorner_* &\equiv \ulcorner xs \urcorner_* \circ^I \text{wk}^I & \ulcorner \text{id} \urcorner &= \ulcorner \text{id}' \urcorner \vee \\ \ulcorner \text{id} \urcorner : \ulcorner \text{id} \{ \Gamma = \Gamma \} \urcorner_* &\equiv \text{id}^I \end{aligned}$$

To complete these proofs, we also need  $\beta$ -laws for our initial CwF substitutions, so we derive these now.

$$\begin{aligned} \text{zero}[]^I : \text{zero}^I [\delta^I, t^I]^I &\equiv t^I & \text{suc}[]^I : \text{suc}^I t^I B [\delta^I, u^I]^I &\equiv t^I [\delta^I]^I \\ \text{zero}[]^I \{ \delta^I = \delta^I \} \{ t^I = t^I \} &= & \text{suc}[]^I &= \dots \\ \text{zero}^I [\delta^I, t^I]^I &\equiv \langle \text{sym } \pi_1 \circ^I \rangle & , \circ^I : (\delta^I, t^I) \circ^I \sigma^I &\equiv (\delta^I \circ^I \sigma^I), t^I (\sigma^I)^I \\ \pi_1^I (\text{id}^I \circ^I (\delta^I, t^I)) &\equiv \langle \text{cong } \pi_1^I \text{id} \circ^I \rangle & , \circ^I &= \dots \\ \pi_1^I (\delta^I, t^I) &\equiv \langle \triangleright - \beta_1^I \rangle \end{aligned}$$

We also need a couple lemmas about how  $\ulcorner \_ \urcorner$  treats terms of different sorts identically:  $\ulcorner \sqsubseteq \urcorner : \forall \{x : \Gamma \vdash [q] A\} \rightarrow \ulcorner \text{tm} \sqsubseteq \sqsubseteq t x \urcorner \equiv \ulcorner x \urcorner$  and  $\ulcorner \sqsubseteq \urcorner_* : \ulcorner \text{tm} \sqsubseteq \sqsubseteq t xs \urcorner_* \equiv \ulcorner xs \urcorner_*$ .

We can now proceed with the preservation proofs. There are quite a few cases to cover, so for brevity we elide the proofs of  $\ulcorner [] \urcorner$  and  $\ulcorner \text{suc} \urcorner$ .

$$\ulcorner \uparrow \urcorner \{q = q\} = \text{cong}_2 \_ \_ \ulcorner + \urcorner (\ulcorner \text{zero} \urcorner \{q = q\})$$

$$\begin{aligned} \ulcorner + \urcorner \{xs = \varepsilon\} &= \text{sym} \bullet \neg \eta^I & \ulcorner \text{id}' \urcorner \{ \Gamma = \bullet \} &= \text{sym} \bullet \neg \eta^I \\ \ulcorner + \urcorner \{xs = xs, x\} \{A = A\} &= & \ulcorner \text{id}' \urcorner \{ \Gamma = \Gamma \triangleright A \} &= \\ \ulcorner xs + A \urcorner_*, \ulcorner \text{suc}[\_] \times A \urcorner & & \ulcorner \text{id} + A \urcorner_*, \ulcorner \text{zero} \urcorner^I &\equiv \langle \text{cong}(\_, \ulcorner \text{zero} \urcorner^I) \ulcorner + \urcorner \rangle \\ \equiv \langle \text{cong}_2 \_ \_ \ulcorner + \urcorner (\ulcorner \text{suc} \urcorner \{x = x\}) \rangle & & \ulcorner \text{id} \urcorner_* \uparrow^I A &\equiv \langle \text{cong}(\_, \ulcorner \uparrow \urcorner^I A) \ulcorner \text{id} \urcorner \rangle \\ (\ulcorner xs \urcorner_* \circ^I \text{wk}^I), \ulcorner \ulcorner x \urcorner [\ulcorner \text{wk} \urcorner]^I \rangle & & \text{id}^I \uparrow^I A &\equiv \langle \text{cong}(\_, \ulcorner \text{zero} \urcorner^I) \text{id} \circ^I \rangle \\ \equiv \langle \text{sym}, \circ^I \rangle & & \text{wk}^I, \ulcorner \text{zero} \urcorner^I &\equiv \langle \triangleright - \eta^I \rangle \\ (\ulcorner xs \urcorner_*, \ulcorner \ulcorner x \urcorner \rangle \circ^I \text{wk}^I) & & \text{id}^I & \blacksquare \end{aligned}$$

We also prove preservation of substitution composition  $\ulcorner \circ \urcorner : \ulcorner xs \circ ys \urcorner_* \equiv \ulcorner xs \urcorner_* \circ^I \ulcorner ys \urcorner_*$  in similar fashion, folding  $\ulcorner [] \urcorner$ .

The main cases of `Methods compl-M` can now be proved by just applying the preservation lemmas and inductive hypotheses, e.g:

$$\begin{aligned} \text{compl-m}.\text{id}^M &= & \text{compl-m}.\_ \circ^M \_ \{ \sigma^I = \sigma^I \} \{ \delta^I = \delta^I \} \sigma^M \delta^M &= \\ \ulcorner \text{tm} \sqsubseteq \sqsubseteq v \sqsubseteq t \text{id} \urcorner_* &\equiv \langle \ulcorner \sqsubseteq \urcorner_* \rangle & \ulcorner \text{norm}^* \sigma^I \circ \text{norm}^* \delta^I \urcorner_* &\equiv \langle \ulcorner \circ \urcorner \rangle \\ \ulcorner \text{id} \urcorner_* &\equiv \langle \ulcorner \text{id} \urcorner \rangle & \ulcorner \text{norm}^* \sigma^I \urcorner_* \circ^I \ulcorner \text{norm}^* \delta^I \urcorner_* &\equiv \langle \text{cong}_2 \_ \_ \sigma^M \delta^M \rangle \\ \text{id}^I &\blacksquare & \sigma^I \circ^I \delta^I &\blacksquare \end{aligned}$$

The remaining cases correspond to the CwF laws, which must hold for whatever type family we eliminate into in order to retain congruence of  $\_ \equiv \_$ . In our completeness

proof, we are eliminating into equations, and so all of these cases are higher identities (demanding we equate different proof trees for completeness, instantiated with the LHS/RHS terms/substitutions).

In a univalent type theory, we might try and carefully introduce additional coherences to our initial CwF to try and make these identities provable without the sledgehammer of set truncation (which prevents eliminating the initial CwF into any non-set).

As we are working in vanilla Agda, we'll take a simpler approach, and rely on UIP ( $\text{duip} : \forall \{x\ y\ z\ w\ r\} \{p : x \equiv y\} \{q : z \equiv w\} \rightarrow p \equiv [r] \equiv q^9$ ), enabling e.g.  $\text{compl-m} . \text{id}^M = \text{duip}$

And completeness is just one call to the eliminator away.

```
compl :  $\ulcorner$  norm  $t^I \urcorner \equiv t^I$ 
compl  $\{t^I = t^I\} = \text{elim-cwf compl-m } t^I$ 
```

## 6 Conclusions and further work

The subject of the paper is a problem which everybody (including ourselves) would have thought to be trivial.

It is perhaps worth mentioning that the convenience of our solution heavily relies on Agda's built-in support for lexicographic termination [2]. This is in contrast to Rocq and Lean; the former's `Fixpoint` command merely supports structural recursion on a single argument and the latter has only raw elimination principles as primitive. Luckily, both of these proof assistants layer on additional commands/tactics to support more natural use of non-primitive induction<sup>10</sup>.

One reviewer asked about another alternative: since we are merging  $\_ \ni \_$  and  $\_ \vdash \_$  why not go further and merge them entirely? Instead of a separate type for variables, one could have a term corresponding to de Bruijn index zero (written  $\bullet : \Gamma \triangleright A \vdash' A$  and an explicit weakening operator on terms (written  $\_ \uparrow : \Gamma \vdash' B \rightarrow \Gamma \triangleright A \vdash' B$ ). This has the unfortunate property that there is now more than one way to write terms that used to be identical. For instance, the terms  $\bullet \uparrow \uparrow \bullet$ ,  $\bullet \uparrow \bullet$  and  $(\bullet \uparrow \bullet) \uparrow \bullet$  are equivalent, where  $\bullet \uparrow \uparrow$  corresponds to the variable with de Bruijn index two. A development along these lines is explored in [18].

This paper can also be seen as a preparation for the harder problem to implement recursive substitution for dependent types. This is harder, because here the typing of the constructors actually depends on the substitution laws. While such a Mönchhausen [5] construction<sup>11</sup> should actually be possible in Agda, the theoretical underpinning of inductive-inductive-recursive definitions is mostly unexplored (with the exception of the proposal by [11]). However, there are potential interesting applications: strictifying substitution laws is essential to prove coherence of models of type theory in higher types, in the sense of HoTT.

Hence this paper has two aspects: it turns out that an apparently trivial problem isn't so easy after all, and it is a stepping stone to more exciting open questions. But before you can run you need to walk and we believe that the construction here can be useful to others.

<sup>9</sup> Note that proving this form of (dependent) UIP relies on type constructor injectivity (specifically, injectivity of  $\_ \equiv \_$ ). We could use a weaker version taking an additional proof of  $x \equiv z$ , but this would be clunkier to use; Agda has no hope of inferring such a proof by unification.

<sup>10</sup> Indeed, Lean can be convinced that our substitution operations terminate after specifying measures similar to those in section 3.1, via the `decreasing_by` tactic.

<sup>11</sup> The reference is to Baron Münchhausen, who allegedly pulled himself out of a swamp by his own hair.

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