A Sound and Complete Substitution Algorithm for Multimode Type Theory

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Abstract

Multimode Type Theory (MTT) is a generic type theory that can be instantiated with an arbitrary mode theory to model features like parametricity, cohesion and guarded recursion. However, the presence of modalities in MTT significantly complicates the substitution calculus of this system. Moreover, MTT's syntax has explicit substitutions with an axiomatic system – not an algorithm – governing the connection between an explicitly substituted term and the resulting term in which variables have actually been replaced. So far, the only results on eliminating explicit substitutions in MTT rely on normalisation by evaluation and hence also immediately normalise a term. In this paper, we present a substitution algorithm for MTT that is completely separated from normalisation. To this end, we introduce Substitution-Free Multimode Type Theory (SFMTT): a formulation of MTT without explicit substitutions, but for which we are able to give a structurally recursive substitution algorithm, suitable for implementation in a total programming language or proof assistant. On the usual formulation of MTT, we consider *σ-equality*, the congruence generated solely by equality rules for explicit substitutions. There is a trivial embedding from SFMTT to MTT, and a converse translation that eliminates the explicit substitutions. We prove soundness and completeness of our algorithm with respect to σ-equivalence and thus establish that MTT with σ-equality has computable σ-normal forms, given by the terms of SFMTT.

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1 Introduction

Substitution is the operation that replaces variables in a term with other terms. It is a key part in defining the semantics of many programming languages. In a dependent type system, it is even necessary in order to formulate the typing rules, such as the one for dependent function application. However, defining substitution is not as simple as it intuitively may seem.

1.1 Renaming and Substitution in the Simply Typed Lambda Calculus

For example, consider the well-known simply typed lambda calculus. We call $\mathsf{Tm}^{\text{STLC}}(\Gamma \vdash T)$ the set of terms of type T with free variables in context Γ and $\mathsf{Sub}^{\text{STLC}}(\Gamma \to \Delta)$ the set of well-formed (simultaneous) substitutions from Γ to Δ. These substitutions are lists of terms: they contain a term of type T in context Γ for every variable of type T in context Δ. In other words, STLC substitutions are constructed in two ways: $!_\Gamma \in \mathsf{Sub}^{\text{STLC}}(\Gamma \to \cdot)$ representing the empty list and $\sigma.t \in \mathsf{Sub}^{\text{STLC}}(\Gamma \to (\Delta, x : T))$ which substitutes variables in Δ according to $\sigma \in \mathsf{Sub}^{\text{STLC}}(\Gamma \to \Delta)$ and substitutes $t \in \mathsf{Tm}^{\text{STLC}}(\Gamma \vdash T)$ for the variable $x : T$.

Applying a substitution $\sigma \in \mathsf{Sub}^{\text{STLC}}(\Gamma \to \Delta)$ to a term $t \in \mathsf{Tm}^{\text{STLC}}(\Delta \vdash T)$ should produce a term $t\,[\,\sigma\,] \in \mathsf{Tm}^{\text{STLC}}(\Gamma \vdash T)$. This can be defined via recursion on the term t. Some cases are very simple: for variables x the corresponding term is found in σ and for applications $(fs)[\,\sigma\,]$ we recurse on the subterms $(f\,[\,\sigma\,])(s\,[\,\sigma\,])$. However, difficulty arises when binders are involved. For lambda terms $\lambda x.s \in \mathsf{Tm}^{\text{STLC}}(\Delta \vdash T \to S)$ with $s \in \mathsf{Tm}^{\text{STLC}}(\Delta, x : T \vdash S)$, the substitution $(\lambda x.s)[\,\sigma\,]$ is defined as $\lambda x.(s\,[\,\sigma^+\,])$ where $\sigma^+ \in \mathsf{Sub}^{\text{STLC}}((\Gamma, x : T) \to (\Delta, x : T))$ is a version of σ that is lifted to the contexts extended with x. We can construct σ^+ as $\mathsf{weaken}(\sigma).x$, where $\mathsf{weaken}(\sigma)$ contains the same terms as σ, but weakened to live in the extended context $\Gamma, x : T$. A naive definition might implement this weakening of terms $t \in \mathsf{Tm}^{\text{STLC}}(\Gamma \vdash A)$ to $\mathsf{Tm}^{\text{STLC}}(\Gamma, x : B \vdash A)$ by applying a substitution from $\Gamma, x : B$ to Γ, but this makes the story cyclic.

An elegant solution to avoid this cycle, standard in the literature, is to separately consider renamings and substitutions. Whereas a substitution maps variables to terms, a renaming from Γ to Δ maps every variable in Δ to a variable in Γ of the same type. Weakening, in particular, is a renaming.[1] Thus, the terms listed in a substitution can be weakened by applying a weakening *renaming*, and the variables listed in a renaming – represented as De Bruijn indices – can be weakened by incrementation. So we can break the cycle by defining first how to rename and then how to substitute in a term, each time by induction on the term. Going further, code duplication between the two term traversals can be avoided with a shared generic implementation [23, 4].

1.2 Multimode Type Theory

This paper is concerned with substitution in modal type theory, more specifically in the system MTT (Multimode Type Theory[2]) by Gratzer et al. [20]. MTT is a type theory that can be instantiated with a mode theory that specifies, among others, a collection of modes and modalities. Modes m index typing judgements and qualify their meaning: judgements in one mode may represent, for example, regular values, while judgements in other modes may represent time-indexed values or pairs of values satisfying a certain relation [12]. Modalities $\mu : m_1 \to m_2$ represent ways to transport terms and types from mode m_1 to mode m_2. We postpone a more extensive introduction to MTT to Section 2, but we will already explain why (algorithmic) substitution in modal type theory is significantly more complicated.

First, modes and modalities complicate the context structure in MTT. For every modality μ, MTT has a new primitive context operation $\_.\mathbf{🔒}_\mu$ which also extends to substitutions: if $\sigma \in \mathsf{Sub}^{\text{MTT}}(\Gamma \to \Delta)$, then we get a new substitution $\sigma\,.\mathbf{🔒}_\mu \in \mathsf{Sub}^{\text{MTT}}(\Gamma\,.\mathbf{🔒}_\mu \to \Delta\,.\mathbf{🔒}_\mu)$.[3] Furthermore, all variables in a context are annotated with a modality. This also impacts

[1] Note that our notion of renaming has little to do with α-conversion. Rather, a renaming will map free variables to possibly different free variables. It is also a useful concept in an unnamed setting.

[2] The names Multimode and Multimodal Type Theory are used interchangeably for the same system MTT which supports both multiple modes and multiple modalities.

[3] The operation $\_.\mathbf{🔒}_\mu$ can be seen as some sort of left adjoint to μ. See Section 2.1 for more details.

how substitutions are defined: to produce a substitution from Γ to $\Delta \,.\, (\mu \mid x : T)$ (i.e. Δ extended with a variable x of type T annotated with modality μ), we need to provide a $\sigma \in \mathsf{Sub}^{\mathrm{MTT}}(\Gamma \to \Delta)$ and a term $t \in \mathsf{Tm}^{\mathrm{MTT}}(\Gamma \,.\, 🔒_{\mu} \vdash T)$ in a locked context. Complicating things further, mode theories can define 2-cells $\alpha \in \mu \Rightarrow \rho$ between modalities μ and ρ. For every 2-cell $\alpha \in \mu \Rightarrow \rho$ from μ to ρ and every context Γ we get a new primitive *key substitution* $🗝^{\alpha}_{\Gamma}$ from $\Gamma \,.\, 🔒_{\rho}$ to $\Gamma \,.\, 🔒_{\mu}$ and we have to specify how these act on variables and terms. We conclude that MTT substitutions are not mere lists of terms and applying substitutions to variables is not just a lookup operation.

In the original presentation of MTT [20, 19], these difficulties are circumvented by using explicit substitutions [1]: the syntax for terms has a constructor for applying a substitution to a term. A system of judgemental equality axioms then allows us to rewrite the explicitly substituted terms. However, this axiom system does not provide an algorithm to compute substitutions away. A priori, it is not even clear if every MTT term is judgementally equal to a term in which no explicit substitutions occur.

In this paper we give a positive answer to the last question by constructing a substitution algorithm for MTT. Moreover, we want this algorithm to be structurally recursive so that it can be implemented in a proof assistant. This requirement makes the construction even more complicated: in a non-modal setting such as STLC, composition of substitutions can be a defined operation. However, in MTT the additional primitive substitutions make this impossible (we refer to Theorem 2 for more details). For that reason, MTT includes a primitive constructor $\tau \circ \sigma$ for substitution composition. However, in an algorithm for computing $t\,[\,\sigma\,]$ we first traverse t until we reach a variable. During this phase, the substitution σ can grow, for instance the lifting operation $^{+}$ is applied when going under a binder. To then compute $x\,[\,\sigma\,]$ for a variable x, we perform a case split and recursion on σ. In the case where σ is a composite of the form $\tau \circ \psi$, we would like to define $x\,[\,\tau \circ \psi\,]$ as $(x\,[\,\tau\,])[\,\psi\,]$. However, $x\,[\,\tau\,]$ is again an arbitrary term so that $(x\,[\,\tau\,])[\,\psi\,]$ may trigger another arbitrary term traversal. Thus, this naïve definition of the substitution algorithm is not structurally recursive, and restructuring the algorithm to restore structural recursion is one of the main contributions of the current paper (Section 3).

1.3 Contributions and Overview

In this paper, we define substitution for MTT, resolving the above problems by identifying the equivalent of renamings and substitutions in MTT and building a structurally recursive substitution algorithm in terms of them. Specifically, we contribute the following.

- We define WSMTT: an intrinsically and modally scoped untyped syntax for MTT. One can see MTT as an extrinsic typing discipline over WSMTT and as such, our substitution results for WSMTT carry over to MTT. Moreover, we define σ-equivalence for WSMTT: the congruence relation generated by substitution-related equality rules, but not β- and η-rules.
- We define SFMTT: a variant of WSMTT without explicit substitutions in terms or types. Moreover, we define a notion of SFMTT renamings and substitutions and implement a structurally recursive algorithm to apply those to types and terms.
- We provide a translation $[\![\_]\!]$ from WSMTT to SFMTT, which translates every WSMTT term and type to an expression without substitutions. In the other direction, there is an almost trivial embedding function $\mathsf{embed}(\_)$ from SFMTT to WSMTT.
- We prove the soundness and completeness of our algorithm. Soundness means that the substitution-free WSMTT term obtained as $\mathsf{embed}([\![t]\!])$ is σ-equivalent to the original term t. Completeness states that $[\![\_]\!]$ maps σ-equivalent WSMTT terms to equal SFMTT terms. Both results combined show that SFMTT terms are the σ-normal forms of WSMTT terms.

Section 2 will provide the necessary background and details about the multimode type theory MTT and introduce WSMTT. We continue in Section 3 to describe the SFMTT syntax and the algorithm for renaming and substitution in that setting. The translation $[\![\_]\!]$ from WSMTT to SFMTT is also discussed there. Section 4 then covers the soundness and completeness results. We conclude in Section 5 with related and future work. A technical report accompanying this paper contains all details of the soundness and completeness proofs, as well as full descriptions of the systems WSMTT and SFMTT [13].

2 Multimode Type Theory (MTT)

In this section we introduce the type system MTT as developed by Gratzer et al. [20]. We start in Section 2.1 with the necessary background and continue in Section 2.2 with our own presentation of MTT that we call WSMTT, including a discussion of the differences with the original formulation. In this section we also discuss (WS)MTT's substitution calculus. Section 2.3 concludes with a discussion on an equivalence relation on terms and substitutions called σ-equivalence.

2.1 Background on the MTT Type System

MTT can be seen as a *framework* for modal type theory: it is parametrised by a mode theory which specifies the modalities and how they interact. More concretely, a mode theory in MTT is a strict 2-category of which the 0-cells (objects) are called modes and the 1-cells (morphisms) are called modalities. This already makes it clear that we have a unit modality $\mathbb{1}_m$ for every mode m (sometimes just written $\mathbb{1}$ when the mode is clear) and that compatible modalities can be composed. Moreover, we also have a notion of 2-cells between modalities, which will be denoted as $\alpha \in \mu \Rightarrow \nu$ for a 2-cell α from μ to ν. Such 2-cells can be composed vertically (which we write as $\beta \circ \alpha$) and horizontally (written as $\beta \star \alpha$). For every modality $\mu : m \to n$ there is a unit 2-cell $1_\mu \in \mu \Rightarrow \mu$.

In MTT, every judgement (so every context, type and term) lives at a particular mode of the mode theory. This is made clear by adding $@\,m$ to a judgement at mode m. We can think of every mode as containing a copy of Martin-Löf Type Theory (MLTT [22]) with natural numbers, products, etc. As they are confined to a single mode and do not really interact with modalities, we will not discuss these rules in the paper (as an illustration we do include a type of Booleans in the technical report though [13]). The connection between the different modes is made via the modalities, as explained in the following paragraphs.

A selection of the rules for constructing contexts, types and terms in MTT can be found in Figure 1. Contexts consist of variables (CTX-EXTEND), each annotated with a modality, and locks (CTX-LOCK), which play an important role in determining when a variable can be used to construct a term. Note that a lock goes in the opposite direction of its modality: the lock operation for a modality $\mu : m \to n$ takes a context from mode n to mode m.

A variable can be used as a term whenever there is a 2-cell from its annotation to the composition of all locks to the right of that variable (TM-VAR). Note that the 2-cell α used to access a variable is an integral part of the term and consequently the terms x^α and x^β are not considered equal when the 2-cells α and β are distinct. Furthermore, an operation $\_^\alpha$ is applied to the type T of the variable in order to bridge the gap between the context in the conclusion of TM-VAR and $\Gamma\,.\,🔒_\mu$ (in which T is well-formed). We refer to [20] for more details about this operation.

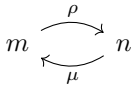
$$\textsc{ctx-empty}\ \frac{}{\cdot\ \mathsf{ctx} \mathbin{@} m} \qquad \textsc{ctx-lock}\ \frac{\Gamma\ \mathsf{ctx} \mathbin{@} n \qquad \mu : m \to n}{\Gamma \,.\, \mathbb{\color{black}🔒}_\mu\ \mathsf{ctx} \mathbin{@} m} \qquad \textsc{ctx-extend}\ \frac{\Gamma\ \mathsf{ctx} \mathbin{@} n \qquad \mu : m \to n \qquad \Gamma \,.\, \mathbb{\color{black}🔒}_\mu \vdash T\ \mathsf{ty} \mathbin{@} m}{\Gamma \,.\, (\mu \mid x : T)\ \mathsf{ctx} \mathbin{@} n}$$

$$\mathsf{locks}\,(\cdot) = \mathbb{1} \qquad \mathsf{locks}\,(\Gamma \,.\, \mathbb{\color{black}🔒}_\mu) = \mathsf{locks}\,(\Gamma) \circ \mu \qquad \mathsf{locks}\,(\Gamma \,.\, (\mu \mid x : T)) = \mathsf{locks}\,(\Gamma)$$

$$\textsc{ty-arrow}\ \frac{\mu : m \to n \qquad \Gamma \,.\, \mathbb{\color{black}🔒}_\mu \vdash T\ \mathsf{ty} \mathbin{@} m \qquad \Gamma \,.\, (\mu \mid x : T) \vdash S\ \mathsf{ty} \mathbin{@} n}{\Gamma \vdash (\mu \mid T) \to S\ \mathsf{ty} \mathbin{@} n} \qquad \textsc{tm-var}\ \frac{\mu : m \to n \qquad \alpha \in \mu \Rightarrow \mathsf{locks}\,(\Delta)}{\Gamma \,.\, (\mu \mid x : T) \,.\, \Delta \vdash x^\alpha : T^\alpha \mathbin{@} m} \qquad \textsc{tm-mod}\ \frac{\mu : m \to n \qquad \Gamma \,.\, \mathbb{\color{black}🔒}_\mu \vdash t : T \mathbin{@} m}{\Gamma \vdash \mathsf{mod}_\mu\,(t) : \langle \mu \mid T \rangle \mathbin{@} n}$$

$$\textsc{tm-lam}\ \frac{\mu : m \to n \qquad \Gamma \,.\, (\mu \mid x : T) \vdash s : S \mathbin{@} n}{\Gamma \vdash \lambda(\mu \mid x).s : (\mu \mid T) \to S \mathbin{@} n} \qquad \textsc{tm-app}\ \frac{\mu : m \to n \qquad \Gamma \vdash f : (\mu \mid T) \to S \mathbin{@} n \qquad \Gamma \,.\, \mathbb{\color{black}🔒}_\mu \vdash t : T \mathbin{@} m}{\Gamma \vdash \mathsf{app}_\mu\,(f; t) : S\ [\ \mathsf{id}.t\ ] \mathbin{@} n} \qquad \textsc{ty-mod}\ \frac{\mu : m \to n \qquad \Gamma \,.\, \mathbb{\color{black}🔒}_\mu \vdash T\ \mathsf{ty} \mathbin{@} m}{\Gamma \vdash \langle \mu \mid T \rangle\ \mathsf{ty} \mathbin{@} n}$$

Figure 1 Selection of rules that define MTT contexts, types, and terms.



$$\eta \in \mathbb{1}_n \Rightarrow \rho \circ \mu$$
$$\varepsilon \in \mu \circ \rho \Rightarrow \mathbb{1}_m$$

Figure 2 The mode theory for Examples 1 and 8 is the strict 2-category freely generated by the depicted modalities and 2-cells (triangle identities for η and ε have been omitted).

Every modality μ gives rise to a modal type former $\langle \mu \mid \_ \rangle$ which can be seen as a (weak) dependent right adjoint [10] to $\_ \,.\, \mathbb{\color{black}🔒}_\mu$ (TY-MOD). One direction of transposition for this dependent adjunction is given by TM-MOD: to construct a term of type $\langle \mu \mid T \rangle$, we must construct a term of type T after locking the context with μ. We do not discuss the MTT elimination principle for modal types here.

Finally, we can also consider modal function types (TY-ARROW). Their values can be constructed via lambda abstraction (TM-LAM), which adds an annotated variable to the context. Eliminating functions is done via application (TM-APP) where the argument should type check in a locked context. Note that we are using a substitution in this rule to accommodate for dependent types, but we postpone the discussion about substitution in MTT to Section 2.2.1.

▶ **Example 1.** To illustrate MTT, we look at an example program in a concrete mode theory as depicted in Figure 2. This mode theory consists of an adjunction of modalities $\mu \dashv \rho$, as witnessed by the unit 2-cell η and the counit 2-cell ε. For such a mode theory, Gratzer et al. [19, 20] already showed that the type formers $\langle \mu \mid \_ \rangle$ and $\langle \rho \mid \_ \rangle$ can also be seen as adjoint. For example, the unit function f of type $(\mathbb{1} \mid A) \to \langle \rho \mid \langle \mu \mid A^\eta \rangle \rangle$ can be constructed as follows: $f = \lambda(\mathbb{1} \mid x).\mathsf{mod}_\rho\,(\mathsf{mod}_\mu\,(x^\eta))$. The variable x gets bound under the unit modality $\mathbb{1}$ by lambda abstraction and subsequently the modal constructors mod_ρ and mod_μ add $\mathbb{\color{black}🔒}_\rho$ and $\mathbb{\color{black}🔒}_\mu$ to the context. In such a context, the variable x can be used, since the 2-cell η has the proper domain and codomain to access it according to the rule TM-VAR.

2.2 Alternative Presentation: Extrinsically Typed, Intrinsically Scoped

The way the MTT syntax is presented in the previous section, which is also how it is originally presented in [20], can be called *intrinsically typed*. This means that we see the typing rules from Figure 1 as the way types and terms are introduced. In other words, we cannot even talk about ill-typed terms or ill-formed types.

$$\textsc{sctx-empty}\ \frac{}{\cdot\ \mathsf{sctx}\ @\, m} \qquad \textsc{sctx-lock}\ \frac{\hat{\Gamma}\ \mathsf{sctx}\ @\, n \qquad \mu : m \to n}{\hat{\Gamma}\,.\,\mathbf{\Large 🔒}_{\mu}\ \mathsf{sctx}\ @\, m} \qquad \textsc{sctx-extend}\ \frac{\hat{\Gamma}\ \mathsf{sctx}\ @\, n \qquad \mu : m \to n}{\hat{\Gamma}\,.\,\mu\ \mathsf{sctx}\ @\, n}$$

$$\textsc{locktele-empty}\ \frac{}{\cdot : \mathsf{LockTele}(m \to m)} \qquad \textsc{locktele-lock}\ \frac{\Lambda : \mathsf{LockTele}(o \to n) \qquad \mu : m \to n}{\Lambda\,.\,\mathbf{\Large 🔒}_{\mu} : \mathsf{LockTele}(o \to m)}$$

$$\mathsf{locks}\,(\cdot) = \mathbb{1} \qquad \mathsf{locks}\,(\Lambda\,.\,\mathbf{\Large 🔒}_{\mu}) = \mathsf{locks}\,(\Lambda) \circ \mu$$

Figure 3 Definition of scoping contexts and lock telescopes.

For the purposes of this paper, it will be more useful to work with extrinsically typed (one could say raw) syntax. In that way, our substitution algorithm can work on pure syntax without having to take typing derivations into account. Moreover, substitution is necessary to formulate some typing rules (such as TM-APP). In MTT, this does not lead to circularity thanks to the use of explicit substitutions (see further) but it would make a substitution algorithm problematically cyclic if it works with intrinsically typed syntax.

However, in order to conveniently develop our substitution algorithm, we will use *intrinsically scoped* syntax, defined in this section. In order to distinguish between our system and the original presentation of MTT, we call the intrinsically scoped syntax WSMTT (for well-scoped MTT). Apart from the change from an intrinsically-typed to an extrinsically-typed presentation, this reformulation does not modify the MTT type theory. Specifically, it does not modify MTT's treatment of substitution; that will only happen in Section 3, in a different system called SFMTT.

For defining the intrinsically scoped syntax, we introduce scoping contexts in Figure 3. They are essentially MTT contexts from Figure 1 where all type information has been removed. We note that in the rule SCTX-EXTEND only the modality annotation of a variable is added to a scoping context. Indeed, in the rest of the paper we will not use named variables but a form of De Bruijn indices. This allows us to ignore α-equivalence and variable capture when implementing substitution.

The WSMTT syntax is now introduced via a judgement $\hat{\Gamma} \vdash_{\mathsf{ws}} t\ \mathsf{expr}\ @\, m$, meaning that t is a WSMTT expression in scoping context $\hat{\Gamma}$ at mode m. Intrinsic scoping means that the inference rules for such a judgement do not define a relation between scoping contexts and some predefined notion of raw syntax; they rather *construct* a WSMTT expression, which can not be seen outside of its scoping context. Put differently, in a proof assistant one would formalise WSMTT expressions as a dependent type indexed by scoping contexts. Note that since we are not specifying typing rules, the distinction between types and terms has disappeared and we talk about WSMTT *expressions*.

Some examples of rules that introduce WSMTT syntax (in other words, WSMTT constructors) can be found in the first two rows of Figure 4. In order to construct a modal function type in scoping context $\hat{\Gamma}$, we need a domain type in the locked scoping context $\hat{\Gamma}\,.\,\mathbf{\Large 🔒}_{\mu}$ and a codomain type where we extend the scoping context with a variable annotated with μ (WSMTT-EXPR-ARROW). The rule for introducing lambda abstraction is similar (WSMTT-EXPR-LAM). Note that we can obtain all these constructors by removing the typing information from the typing rules in Figure 1. The WSMTT variable rule WSMTT-EXPR-VAR has changed somewhat with respect to Figure 1: it only allows us to access the last variable added to a scoping context and only if it is locked behind the same modality as its annotation. It is standard, in formulations of type theory with explicit substitutions [1], to only allow access to the last variable which has De Bruijn index zero, since the De Bruijn index can then be

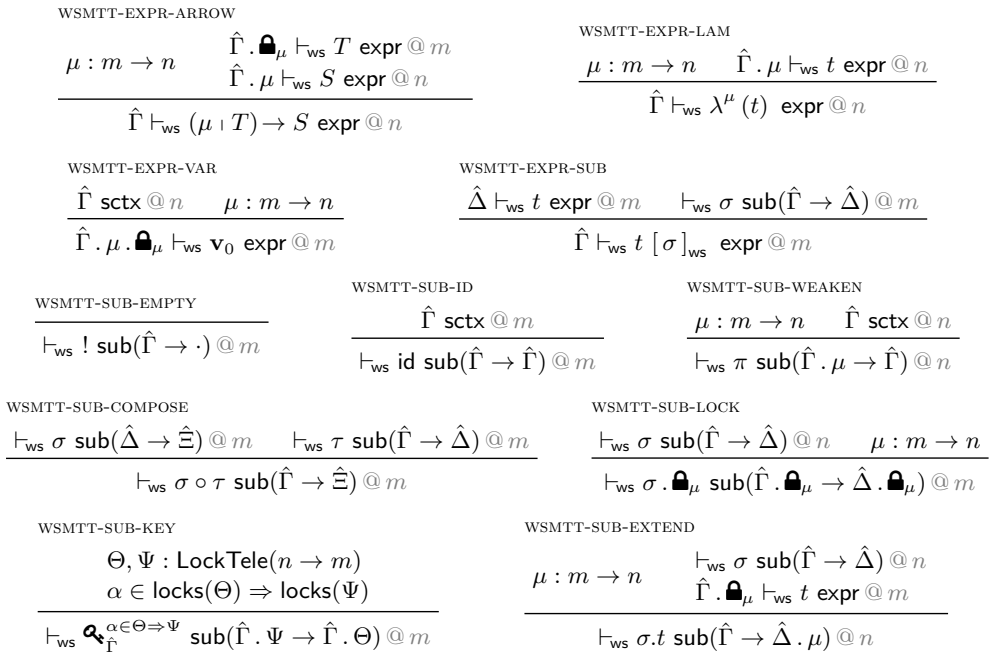


Figure 4 Constructors for intrinsically well-scoped WSMTT expressions (defined using the judgement $\hat{\Gamma} \vdash_{\mathsf{ws}} t \ \mathsf{expr} \mathbin{@} m$) and substitutions (defined using the judgement $\vdash_{\mathsf{ws}} \sigma \ \mathsf{sub}(\hat{\Gamma} \to \hat{\Delta}) \mathbin{@} m$).

incremented using a weakening substitution π (WSMTT-SUB-WEAKEN). This is similar to the representation of variables in a CwF. In the technical report on MTT [19], this standard practice is adapted to MTT with a variable rule that is a typed version of WSMTT-EXPR-VAR. The general variable rule TM-VAR (or its intrinsically scoped counterpart) remains derivable by explicitly substituting $\mathbf{v}_0$ with substitutions constructed via π, key^{α} (WSMTT-SUB-KEY) and $\_ \,.\, \mathbin{@}_{\mu}$ (WSMTT-SUB-LOCK).

2.2.1 Substitution Calculus

In both [20, 19] and our presentation, MTT is a system with explicit substitution: applying a substitution to an expression is viewed as a syntax constructor (WSMTT-EXPR-SUB). This also means that expressions are defined mutually inductively with substitutions. For the latter, we introduce a judgement form $\vdash_{\mathsf{ws}} \sigma \ \mathsf{sub}(\hat{\Gamma} \to \hat{\Delta}) \mathbin{@} m$ expressing that σ is a substitution from scoping context $\hat{\Gamma}$ to $\hat{\Delta}$ at mode m (again, the inference rules for this judgement *construct* WSMTT substitutions, rather than defining a well-scopedness relation over them).

Figure 4 shows all WSMTT substitution constructors. There is a unique substitution to the empty context (WSMTT-SUB-EMPTY) and identity (WSMTT-SUB-ID) and weakening (WSMTT-SUB-WEAKEN) substitutions. We can compose substitutions (WSMTT-SUB-COMPOSE, note that this is a constructor), lock them (WSMTT-SUB-LOCK) and extend them with a term to extend the codomain with a new variable (WSMTT-SUB-EXTEND). Note that this term has to live in a locked scoping context. Finally, every 2-cell in the mode theory gives rise to a key substitution (WSMTT-SUB-KEY). This last rule introduces the concept of lock telescopes: sequences of zero or more locks that have the right domain and codomain modes to be composed. A lock telescope $\Theta : \mathsf{LockTele}(n \to m)$ can be applied to a scoping context at mode n to obtain a scoping context at mode m; and similarly to a well-scoped substitution by iteratively applying WSMTT-SUB-LOCK. We can also compose all modalities in Θ to obtain a modality $\mathsf{locks}(\Theta) : m \to n$. Precise definitions are given in Figure 3.

$$\textsc{sctx-lock-id}\ \frac{\hat{\Gamma}\ \mathsf{sctx} \mathbin{@} m}{\hat{\Gamma} \,.\, \mathbb{1} = \hat{\Gamma}\ \mathsf{sctx} \mathbin{@} m} \qquad \textsc{sctx-lock-comp}\ \frac{\hat{\Gamma}\ \mathsf{sctx} \mathbin{@} o \qquad \mu : m \to n \qquad \nu : n \to o}{\hat{\Gamma} \,.\, \mu \circ \nu = \hat{\Gamma} \,.\, \nu \,.\, \mu\ \mathsf{sctx} \mathbin{@} m}$$

Figure 5 Strict functoriality of the lock operation on scoping contexts (optional).

2.2.2 Lock Telescopes vs. Strict Functoriality of Locks

The original presentation of MTT [20, 19] makes no mention of lock telescopes. Instead, it features strict functoriality rules for the lock operation on contexts, of which we give counterparts for scoping contexts in Figure 5. A consequence of these rules is that any lock telescope can be fused into a single lock.

It is however quite unusual to have a non-trivial equational theory on contexts and early explorations of a *lock calculus* for MTT [25] suggest that it may be advantageous to drop the functoriality rules; by WSMTT-SUB-KEY for the identity 2-cell, they automatically hold up to isomorphism. During the development of the current paper, we had a formulation of MTT in mind *without* these functoriality rules. However, nowhere in our constructions and proofs do we case distinguish on the number of locks in a given part of the context, or read off the modality annotation of a specific lock, so our results remain valid when we extend raw WSMTT with the rules in Figure 5.

▶ **Theorem 2** (Non-definability of composition). *Even with the rules in Figure 5, it is still* not *true that any WSMTT substitution can be alternatively constructed without using* WSMTT-SUB-COMPOSE *directly (i.e. not through a generalised rule). This remains impossible even if we use composition to generalise the rules* WSMTT-SUB-WEAKEN *and (jointly)* WSMTT-SUB-KEY *and* WSMTT-SUB-LOCK*, so that we would get* $\pi(\sigma) := \sigma \circ \pi$ *and* $\sigma \,.\, \mathsf{key}^{\alpha \in \Theta \Rightarrow \Psi} := \mathsf{key}_{\hat{\Gamma}}^{\alpha \in \Theta \Rightarrow \Psi} \circ (\sigma \,.\, \Psi)$ *each by a single rule.*

Proof. Consider a mode theory with three modes p, q, r, three modalities $p \xrightarrow{\nu} q \xrightarrow{\mu} r \xleftarrow{\rho} p$ and a 2-cell $\alpha \in \mu \circ \nu \Rightarrow \rho$. Then we can consider the key substitution $\vdash_{\mathsf{ws}} \mathsf{key}_{\hat{\Gamma}}^{\alpha \in \mathbb{1} \,.\, \mu \,.\, \nu \Rightarrow \rho}\ \mathsf{sub}(\hat{\Gamma} \,.\, \rho \to \hat{\Gamma} \,.\, \mu \,.\, \nu) \mathbin{@} p$. Furthermore, given an expression t (e.g. true) in $\hat{\Gamma} \,.\, \mu \,.\, \mathbb{1}$ we can construct $\vdash_{\mathsf{ws}} (\mathsf{id}.t) \,.\, \nu\ \mathsf{sub}(\hat{\Gamma} \,.\, \mu \,.\, \nu \to \hat{\Gamma} \,.\, \mu \,.\, \mathbb{1} \,.\, \nu) \mathbin{@} p$. The composite of these two is a substitution from $\hat{\Gamma} \,.\, \rho$ to $\hat{\Gamma} \,.\, \mu \,.\, \mathbb{1} \,.\, \nu$, which both splits ρ into $\mu \circ \nu$ and extends the codomain with a variable. Assume we have an alternative substitution τ of the same domain and codomain, constructed without using WSMTT-SUB-COMPOSE directly. Since all remaining substitution constructors cause domain and codomain to be extended with locks and variables, travelling the derivation tree of τ upwards (constructed using the possibly generalised rules in Figure 4), we somehow need to peel off ν from the codomain, using the operation $\sigma \,.\, \mathsf{key}^{\alpha \in \Theta \Rightarrow \Psi}$. This is impossible since $\rho : p \to r$ has no decomposition $p \to q \to r$.

An alternative proof can be given in the mode theory with α reversed, where the composite substitution combines α with a weakening in between the locks. ◀

2.3 σ-equivalence

Since substitution in WSMTT expressions is an explicit constructor, it does not compute (as will be the case in SFMTT in Section 3). This means that there are a lot of distinct WSMTT expressions that we would actually like to consider equivalent. For example, from the perspective of the rules in Figure 4 the expressions $t\ [\sigma]_{\mathsf{ws}}\ [\tau]_{\mathsf{ws}}$ and $t\ [\sigma \circ \tau]_{\mathsf{ws}}$ have nothing to do with each other. For this reason, we add an axiomatic system to the intrinsically

$$\frac{\hat{\Xi} \vdash_{\mathsf{ws}} t\ \mathsf{expr}\ @\, m \qquad \vdash_{\mathsf{ws}} \sigma\ \mathsf{sub}(\hat{\Delta} \to \hat{\Xi})\ @\, m \qquad \vdash_{\mathsf{ws}} \tau\ \mathsf{sub}(\hat{\Gamma} \to \hat{\Delta})\ @\, m}{\hat{\Gamma} \vdash_{\mathsf{ws}} t\ [\sigma \circ \tau]_{\mathsf{ws}} \equiv^{\sigma} t\ [\sigma]_{\mathsf{ws}}\ [\tau]_{\mathsf{ws}}\ \mathsf{expr}\ @\, m} \qquad \frac{\hat{\Delta} \vdash_{\mathsf{ws}} t \equiv^{\sigma} s\ \mathsf{expr}\ @\, m \qquad \vdash_{\mathsf{ws}} \tau \equiv^{\sigma} \sigma\ \mathsf{sub}(\hat{\Gamma} \to \hat{\Delta})\ @\, m}{\hat{\Gamma} \vdash_{\mathsf{ws}} t\ [\tau]_{\mathsf{ws}} \equiv^{\sigma} s\ [\sigma]_{\mathsf{ws}}\ \mathsf{expr}\ @\, m}$$

$$\frac{\mu : m \to n \qquad \hat{\Delta}\,.\,\mu \vdash_{\mathsf{ws}} t\ \mathsf{expr}\ @\, n \qquad \vdash_{\mathsf{ws}} \sigma\ \mathsf{sub}(\hat{\Gamma} \to \hat{\Delta})\ @\, n}{\hat{\Gamma} \vdash_{\mathsf{ws}} (\lambda^{\mu}\,(t))\ [\sigma]_{\mathsf{ws}} \equiv^{\sigma} \lambda^{\mu}\left(t\ \left[\sigma^{+}\right]_{\mathsf{ws}}\right)\ \mathsf{expr}\ @\, n} \quad \text{with } \sigma^{+} = (\sigma \circ \pi).\mathbf{v}_0$$

$$\frac{\vdash_{\mathsf{ws}} \sigma\ \mathsf{sub}(\hat{\Delta} \to \hat{\Xi})\ @\, m \qquad \vdash_{\mathsf{ws}} \tau\ \mathsf{sub}(\hat{\Gamma} \to \hat{\Delta})\ @\, m}{\vdash_{\mathsf{ws}} (\sigma \circ \tau)\,.\,🔒_{\mu} \equiv^{\sigma} (\sigma\,.\,🔒_{\mu}) \circ (\tau\,.\,🔒_{\mu})\ \mathsf{sub}(\hat{\Gamma}\,.\,🔒_{\mu} \to \hat{\Xi}\,.\,🔒_{\mu})\ @\, n}$$

$$\frac{\hat{\Gamma}\ \mathsf{sctx}\ @\, n \qquad \Lambda : \mathsf{LockTele}(n \to m)}{\vdash_{\mathsf{ws}} \mathsf{q}_{\hat{\Gamma}}^{1_{\mathsf{locks}(\Lambda)} \in \Lambda \Rightarrow \Lambda} \equiv^{\sigma} \mathsf{id}\ \mathsf{sub}(\hat{\Gamma}\,.\,\Lambda \to \hat{\Gamma}\,.\,\Lambda)\ @\, m}$$

$$\frac{\alpha \in \mathsf{locks}\,(\Lambda) \Rightarrow \mathsf{locks}\,(\Theta) \qquad \beta \in \mathsf{locks}\,(\Theta) \Rightarrow \mathsf{locks}\,(\Psi)}{\vdash_{\mathsf{ws}} \mathsf{q}_{\hat{\Gamma}}^{\beta \circ \alpha \in \Lambda \Rightarrow \Psi} \equiv^{\sigma} \mathsf{q}_{\hat{\Gamma}}^{\alpha \in \Lambda \Rightarrow \Theta} \circ \mathsf{q}_{\hat{\Gamma}}^{\beta \in \Theta \Rightarrow \Psi}\ \mathsf{sub}(\hat{\Gamma}\,.\,\Psi \to \hat{\Gamma}\,.\,\Lambda)\ @\, m}$$

$$\frac{\alpha \in \mathsf{locks}\,(\Lambda) \Rightarrow \mathsf{locks}\,(\Theta) \qquad \vdash_{\mathsf{ws}} \sigma\ \mathsf{sub}(\hat{\Gamma} \to \hat{\Delta})\ @\, n}{\vdash_{\mathsf{ws}} \mathsf{q}_{\hat{\Delta}}^{\alpha \in \Lambda \Rightarrow \Theta} \circ (\sigma\,.\,\Theta) \equiv^{\sigma} (\sigma\,.\,\Lambda) \circ \mathsf{q}_{\hat{\Gamma}}^{\alpha \in \Lambda \Rightarrow \Theta}\ \mathsf{sub}(\hat{\Gamma}\,.\,\Theta \to \hat{\Delta}\,.\,\Lambda)\ @\, m}$$

Figure 6 Selected rules for σ-equivalence in WSMTT.

scoped WSMTT syntax that specifies when two expressions or substitutions are σ-equivalent (note that we do not add β- or η-equivalence to this system yet, those should be covered in the type system that would be defined on top of the syntax described in this paper).

Some of the rules for σ-equivalence can be found in Figure 6. We make use of a judgement $\hat{\Gamma} \vdash_{\mathsf{ws}} t \equiv^{\sigma} s\ \mathsf{expr}\ @\, m$ for expressions and $\vdash_{\mathsf{ws}} \sigma \equiv^{\sigma} \tau\ \mathsf{sub}(\hat{\Gamma} \to \hat{\Delta})\ @\, m$ for substitutions. We find rules expressing the connection between applying a composed substitution and consecutively applying both substitutions, expressing how to push a substitution through expression constructors such as λ^{μ} (here σ^{+} is the lifting of σ defined as $\sigma^{+} = (\sigma \circ \pi).\mathbf{v}_0$) and expressing functoriality of locks on substitutions. There are also quite some rules that express properties of key substitutions: their naturality and their behaviour with respect to the unit 2-cell and composition of 2-cells. The full definition of σ-equivalence for WSMTT can be found in the technical report [13].

3 Substitution Algorithm

In this section we describe our substitution algorithm for MTT. For this purpose we introduce a new language called SFMTT (for substitution-free MTT), which has no expression constructor for substitutions like WSMTT-EXPR-SUB in Figure 4. We also introduce renamings and substitutions for SFMTT. All of this is included in Section 3.1. We then proceed in Section 3.2 to the core part of the substitution algorithm: applying SFMTT renamings and substitutions to SFMTT expressions. Finally, using this functionality we can translate WSMTT expressions to SFMTT expressions.

3.1 Substitution-free Multimode Type Theory (SFMTT)

3.1.1 SFMTT Expressions

Exactly like our presentation of WSMTT, the expressions in SFMTT will be extrinsically typed but intrinsically scoped. We can reuse the same notion of scoping context and lock telescope from Figure 3. However, as indicated in Section 2.2, the WSMTT representation

$$\textsc{sf-var-zero}\ \frac{\Theta : \mathsf{LockTele}(n \to m) \quad \mu : m \to n \quad \hat{\Gamma}\ \mathsf{sctx} \mathbin{@} n \quad \alpha \in \mu \Rightarrow \mathsf{locks}(\Theta)}{\hat{\Gamma} \mathbin{.} \mu \mathbin{.} \Theta \vdash_{\mathsf{sf}} \mathbf{v}_0^{\alpha}\ \mathsf{var} \mathbin{@} m}$$

$$\textsc{sf-var-suc}\ \frac{\Theta : \mathsf{LockTele}(n \to m) \quad \hat{\Gamma} \mathbin{.} \Theta \vdash_{\mathsf{sf}} v\ \mathsf{var} \mathbin{@} m \quad \mu : o \to n}{\hat{\Gamma} \mathbin{.} \mu \mathbin{.} \Theta \vdash_{\mathsf{sf}} \mathsf{suc}\,(v)\ \ \mathsf{var} \mathbin{@} m}$$

Figure 7 Constructors for well-scoped SFMTT variables.

of variables makes use of explicit substitutions, which we do not have in SFMTT. For this reason, SFMTT has a dedicated variable judgement $\hat{\Gamma} \vdash_{\mathsf{sf}} v\ \mathsf{var} \mathbin{@} m$ introducing the syntactic category of accessible variables v in scoping context $\hat{\Gamma}$ at mode m. The inference rules for this judgement can be found in Figure 7. Either we access the last variable in the scoping context, in which case we have to provide an appropriate 2-cell (SF-VAR-ZERO), or we skip the last variable in the scoping context, which may be located under a lock telescope (SF-VAR-SUC). As a conclusion, an SFMTT variable is of the form $\mathsf{suc}^n\,(\mathbf{v}_0^{\alpha})$, so it is just a De Bruijn index with a 2-cell annotation.

Similar to WSMTT, SFMTT expressions can now be introduced via a judgement $\hat{\Gamma} \vdash_{\mathsf{sf}} t\ \mathsf{expr} \mathbin{@} m$. The constructors are the same as those for WSMTT in Figure 4, except for WSMTT-EXPR-VAR and WSMTT-EXPR-SUB, which are not included. Instead, there is a constructor promoting any variable $\hat{\Gamma} \vdash_{\mathsf{sf}} v\ \mathsf{var} \mathbin{@} m$ to an SFMTT expression in $\hat{\Gamma}$. We emphasize that SFMTT expressions cannot contain substitutions.

3.1.2 SFMTT Renamings and Substitutions

We can also define substitutions for the SFMTT syntax, which will be required in the next section. As in our intrinsically scoped presentation of WSMTT, every SFMTT renaming and substitution has a domain and a codomain scoping context. This ensures that applying a renaming or substitution to an SFMTT expression is a total (always defined) operation.

Similar to McBride [23] and Allais et al. [4], we define an action of renaming on expressions before we discuss the action of substitutions. Such a renaming does not only allow us to lift a substitution when pushing it under a binder, but also to perform some modal operations. Of course, we have to take into account that we want a structurally recursive substitution algorithm, which is impossible when substitution composition is added as a constructor. We solve this problem by first defining atomic renamings and substitutions, which are not closed under composition but which can be applied to SFMTT expressions in a structurally recursive way. Regular renamings and substitutions (from now on also referred to as rensubs) will be defined in terms of these atomic rensubs.

Just like substitutions in WSMTT, atomic renamings and substitutions are defined using a judgement $\vdash_{\mathsf{sf}} \sigma\ \mathsf{aren/asub}(\hat{\Gamma} \to \hat{\Delta}) \mathbin{@} m$ (much of the structure between renamings and substitutions is shared). There is a similar judgement $\vdash_{\mathsf{sf}} \sigma\ \mathsf{ren/sub}(\hat{\Gamma} \to \hat{\Delta}) \mathbin{@} m$ for regular rensubs. The constructors for atomic rensubs can be found in Figure 8. Many of them are similar to the ones for WSMTT substitutions, such as the empty atomic rensub (SF-ARENSUB-EMPTY), locking (SF-ARENSUB-LOCK) and keys (SF-ARENSUB-KEY). As explained, we purposely omit a constructor for composition of atomic rensubs. As a consequence, we need a constructor for weakening rensubs (SF-ARENSUB-WEAKEN) which in WSMTT would have been accomplished by precomposing with π. Also note that we have an atomic identity rensub id^{a} (SF-ARENSUB-ID). We could have alternatively implemented id^{a} in terms of the other constructors but taking it as a constructor will make the rest of the paper easier because we can *define* its action on expressions to be trivial, whereas otherwise that would require a

$$\textsc{sf-arensub-empty}\ \frac{}{\vdash_{\mathsf{sf}} !\ \mathsf{aren/asub}(\hat{\Gamma} \to \cdot)\ @\, m}$$

$$\textsc{sf-arensub-id}\ \frac{\hat{\Gamma}\ \mathsf{sctx} @\, m}{\vdash_{\mathsf{sf}} \mathsf{id}^{\mathsf{a}}\ \mathsf{aren/asub}(\hat{\Gamma} \to \hat{\Gamma})\ @\, m}$$

$$\textsc{sf-arensub-weaken}\ \frac{\vdash_{\mathsf{sf}} \sigma\ \mathsf{aren/asub}(\hat{\Gamma} \to \hat{\Delta})\ @\, m}{\vdash_{\mathsf{sf}} \mathsf{weaken}(\sigma)\ \mathsf{aren/asub}(\hat{\Gamma} \,.\, \mu \to \hat{\Delta})\ @\, m}$$

$$\textsc{sf-arensub-lock}\ \frac{\vdash_{\mathsf{sf}} \sigma\ \mathsf{aren/asub}(\hat{\Gamma} \to \hat{\Delta})\ @\, n \qquad \mu : m \to n}{\vdash_{\mathsf{sf}} \sigma \,.\, \mathsf{lock}_{\mu}\ \mathsf{aren/asub}(\hat{\Gamma} \,.\, \mathsf{lock}_{\mu} \to \hat{\Delta} \,.\, \mathsf{lock}_{\mu})\ @\, m}$$

$$\textsc{sf-arensub-key}\ \frac{\Theta, \Psi : \mathsf{LockTele}(n \to m) \qquad \alpha \in \mathsf{locks}(\Theta) \Rightarrow \mathsf{locks}(\Psi)}{\vdash_{\mathsf{sf}} \mathsf{key}_{\hat{\Gamma}}^{\alpha \in \Theta \Rightarrow \Psi}\ \mathsf{aren/asub}(\hat{\Gamma} \,.\, \Psi \to \hat{\Gamma} \,.\, \Theta)\ @\, m}$$

$$\textsc{sf-aren-extend}\ \frac{\mu : m \to n \qquad \vdash_{\mathsf{sf}} \sigma\ \mathsf{aren}(\hat{\Gamma} \to \hat{\Delta})\ @\, n \qquad \hat{\Gamma} \,.\, \mathsf{lock}_{\mu} \vdash_{\mathsf{sf}} v\ \mathsf{var}\ @\, m}{\vdash_{\mathsf{sf}} \sigma.v\ \mathsf{aren}(\hat{\Gamma} \to \hat{\Delta} \,.\, \mu)\ @\, n}$$

$$\textsc{sf-asub-extend}\ \frac{\mu : m \to n \qquad \vdash_{\mathsf{sf}} \sigma\ \mathsf{asub}(\hat{\Gamma} \to \hat{\Delta})\ @\, n \qquad \hat{\Gamma} \,.\, \mathsf{lock}_{\mu} \vdash_{\mathsf{sf}} t\ \mathsf{expr}\ @\, m}{\vdash_{\mathsf{sf}} \sigma.t\ \mathsf{asub}(\hat{\Gamma} \to \hat{\Delta} \,.\, \mu)\ @\, n}$$

Figure 8 Constructors for atomic SFMTT renamings and substitutions.

$$\textsc{sf-rensub-id}\ \frac{\hat{\Gamma}\ \mathsf{sctx} @\, m}{\vdash_{\mathsf{sf}} \mathsf{id}\ \mathsf{ren/sub}(\hat{\Gamma} \to \hat{\Gamma})\ @\, m}$$

$$\textsc{sf-rensub-snoc}\ \frac{\vdash_{\mathsf{sf}} \sigma\ \mathsf{ren/sub}(\hat{\Delta} \to \hat{\Xi})\ @\, m \qquad \vdash_{\mathsf{sf}} \tau\ \mathsf{aren/asub}(\hat{\Gamma} \to \hat{\Delta})\ @\, m}{\vdash_{\mathsf{sf}} \sigma \fatsemi \tau\ \mathsf{ren/sub}(\hat{\Gamma} \to \hat{\Xi})\ @\, m}$$

Figure 9 Constructors for regular SFMTT renamings and substitutions.

non-trivial proof. The only difference between atomic renamings and substitutions is the way they can be extended: a renaming is extended with a variable (SF-AREN-EXTEND) whereas a substitution can be extended with an arbitrary SFMTT expression (SF-ASUB-EXTEND).

Figure 9 shows the full definition of regular rensubs. In essence, a rensub is well-scoped snoc-lists of atomic substitutions. It can be empty, so it is actually the identity (SF-RENSUB-ID), or it consists of an atomic rensub postcomposed with a regular rensub (SF-RENSUB-SNOC).

One operation that we will need in the next section, is the lifting of atomic rensubs. Given an atomic rensub σ from $\hat{\Gamma}$ to $\hat{\Delta}$, we can construct a new, lifted atomic rensub $\sigma^+ := \mathsf{weaken}(\sigma).\mathbf{v}_0^{1\mu}$ from $\hat{\Gamma} \,.\, \mu$ to $\hat{\Delta} \,.\, \mu$ (here $\mathbf{v}_0^{1\mu}$ is interpreted as a variable in the case of renamings and as an expression in the case of substitutions).[4] Moreover, for any scoping context $\hat{\Gamma}$ and modality μ, we have a weakening atomic rensub $\pi := \mathsf{weaken}(\mathsf{id}^{\mathsf{a}})$ from $\hat{\Gamma} \,.\, \mu$ to $\hat{\Gamma}$. The lift and lock operations can be extended to regular rensubs by applying those operations to all constituent atomic rensubs. In other words, we have $\mathsf{id}^+ = \mathsf{id}$, $(\sigma \fatsemi \tau)^+ = \sigma^+ \fatsemi \tau^+$, $\mathsf{id} \,.\, \mathsf{lock}_{\mu} = \mathsf{id}$ and $(\sigma \fatsemi \tau) \,.\, \mathsf{lock}_{\mu} = (\sigma \,.\, \mathsf{lock}_{\mu}) \fatsemi (\tau \,.\, \mathsf{lock}_{\mu})$.

3.2 Renaming and Substitution Algorithm for SFMTT

We are now ready to describe one of the core parts of the paper: the algorithm for applying an SFMTT substitution to an SFMTT expression. The definition is built up in 4 steps, each defining the action of another class of syntactic objects on SFMTT expressions: 1. atomic renamings, 2. regular renamings, 3. atomic substitutions, and 4. regular substitutions.

[4] It might be surprising that this works for substitutions too, since we explained in the introduction for STLC that defining weakening for substitutions requires recursively applying a subtitution (or renaming) to terms in the context. However, substituting a variable with $\mathsf{weaken}(\sigma)$ will involve the application of a renaming, as we will see in the next section.

However, there is considerable overlap between some of these steps. For this reason, we will treat steps 2 and 4 together as well as large parts of steps 1 and 3.[5] All operations take an (atomic) rensub from $\hat{\Gamma}$ to $\hat{\Delta}$ and an SFMTT expression in scoping context $\hat{\Delta}$ to produce an SFMTT expression in scoping context $\hat{\Gamma}$.

3.2.1 Atomic rensubs acting on non-variable expressions

We first discuss the application of atomic rensubs on SFMTT expressions other than variables. In general, if we have an atomic rensub $\vdash_{\mathsf{sf}} \sigma\ \mathsf{aren/asub}(\hat{\Gamma} \to \hat{\Delta})\,@\,m$ and an SFMTT expression $\hat{\Delta} \vdash_{\mathsf{sf}} t\ \mathsf{expr}\,@\,m$ (other than a variable), we describe how to construct an expression $\hat{\Gamma} \vdash_{\mathsf{sf}} t\ [\,\sigma\,]_{\mathsf{aren/asub}}\ \mathsf{expr}\,@\,m$. Note that in order for this construction to be well-defined on intrinsically-scoped syntax, one must verify that it does indeed preserve well-scopedness.

$$
\begin{aligned}
\langle \mu \mid A \rangle\ [\,\sigma\,]_{\mathsf{aren/asub}} &= \langle \mu \mid A\ [\,\sigma\,.\,🔒_{\mu}\,]_{\mathsf{aren/asub}} \rangle \\
\mathsf{mod}_{\mu}\,(t)\ [\,\sigma\,]_{\mathsf{aren/asub}} &= \mathsf{mod}_{\mu}\left(t\ [\,\sigma\,.\,🔒_{\mu}\,]_{\mathsf{aren/asub}}\right) \\
((\mu \mid A) \to B)\ [\,\sigma\,]_{\mathsf{aren/asub}} &= \left(\mu \mid A\ [\,\sigma\,.\,🔒_{\mu}\,]_{\mathsf{aren/asub}}\right) \to B\ \left[\,\sigma^{+}\,\right]_{\mathsf{aren/asub}} \\
(\lambda^{\mu}\,(t))\ [\,\sigma\,]_{\mathsf{aren/asub}} &= \lambda^{\mu}\left(t\ \left[\,\sigma^{+}\,\right]_{\mathsf{aren/asub}}\right) \\
\mathsf{app}_{\mu}\,(f;t)\ [\,\sigma\,]_{\mathsf{aren/asub}} &= \mathsf{app}_{\mu}\left(f\ [\,\sigma\,]_{\mathsf{aren/asub}}\,;t\ [\,\sigma\,.\,🔒_{\mu}\,]_{\mathsf{aren/asub}}\right)
\end{aligned}
$$

3.2.2 Atomic renamings acting on variables

We now turn to the case for variables. This is where we distinguish between atomic renamings and atomic substitutions. We first discuss the action of an atomic renaming on a variable, producing another variable. The intuitive "type signature" of this operation is too weak to make recursion work. In particular, it does not allow us to go under locks in renamings. Therefore, we have a result that generalises over a lock telescope Λ, but we can recover the desired result by taking the empty lock telescope for Λ. Note that for the remainder of Section 3 we will state the signatures of the different parts of the substitution algorithm in lemmas and theorems. The actual description of the algorithm can be found in the corresponding proofs (which we will call constructions to make it clear that they contain computationally interesting content).

▶ **Lemma 3.** *If we have an SFMTT atomic renaming* $\vdash_{\mathsf{sf}} \sigma\ \mathsf{aren}(\hat{\Gamma} \to \hat{\Delta})\,@\,n$*, a lock telescope* $\Lambda : \mathsf{LockTele}(n \to m)$ *and an SFMTT variable* $\hat{\Delta}\,.\,\Lambda \vdash_{\mathsf{sf}} v\ \mathsf{var}\,@\,m$*, then we can construct a variable* $\hat{\Gamma}\,.\,\Lambda \vdash_{\mathsf{sf}} v\ [\,\sigma\,]^{\Lambda}_{\mathsf{aren,var}}\ \mathsf{var}\,@\,m$

Lemma 3 is a core lemma for this paper. Our substitution algorithm crucially relies on identifying a notion of renamings that can be recursively applied to MTT terms. It is this lemma that establishes that our choices achieve this and we include the construction below because it clarifies well why atomic renamings should be defined as they are.

In the construction for Lemma 3 we will make use of the following result.

▶ **Lemma 4.** *Let* $\Theta, \Psi : \mathsf{LockTele}(n \to m)$ *be two lock telescopes and* $\alpha \in \mathsf{locks}\,(\Theta) \Rightarrow \mathsf{locks}\,(\Psi)$ *a 2-cell. Then we can transform a variable* $\hat{\Gamma}\,.\,\Theta \vdash_{\mathsf{sf}} v\ \mathsf{var}\,@\,m$ *to a variable* $\hat{\Gamma}\,.\,\Psi \vdash_{\mathsf{sf}} v\ [\,\alpha\,]^{\Theta \Rightarrow \Psi}_{\text{2-cell}}\ \mathsf{var}\,@\,m$*.*

[5] In fact, the action of regular renamings is not really used anywhere. Only atomic renamings will be important. However, as already mentioned the treatment of regular renamings and regular substitutions is entirely the same.

Construction. We proceed by structural recursion on the variable v (i.e. the annotated De Bruijn index).

- CASE $\hat{\Gamma} \,.\, \Theta \vdash_{\mathsf{sf}} \mathbf{v}_0^{\beta}\ \mathsf{var} \mathbin{@} m$ with $\hat{\Gamma} = \hat{\Delta} \,.\, \mu \,.\, \Lambda$ (SF-VAR-ZERO, Λ is a lock telescope so it only contains locks)
  We know that $\hat{\Delta} \,.\, \mu \,.\, \Lambda \,.\, \Theta \vdash_{\mathsf{sf}} \mathbf{v}_0^{\beta}\ \mathsf{var} \mathbin{@} m$, so $\beta \in \mu \Rightarrow \mathsf{locks}\,(\Lambda \,.\, \Theta) = \mathsf{locks}\,(\Lambda) \circ \mathsf{locks}\,(\Theta)$. Using the horizontal composition $\star$, we can construct a 2-cell $1_{\mathsf{locks}(\Lambda)} \star \alpha \in \mathsf{locks}\,(\Lambda) \circ \mathsf{locks}\,(\Theta) \Rightarrow \mathsf{locks}\,(\Lambda) \circ \mathsf{locks}\,(\Psi)$. Hence we use the rule SF-VAR-ZERO again to obtain $\mathbf{v}_0^{\beta}\ [\,\alpha\,]_{\text{2-cell}}^{\Theta \Rightarrow \Psi} = \mathbf{v}_0^{(1_{\mathsf{locks}(\Lambda)} \star \alpha) \circ \beta}$.[6]
- CASE $\hat{\Gamma} \,.\, \Theta \vdash_{\mathsf{sf}} \mathsf{suc}\,(v)\ \mathsf{var} \mathbin{@} m$ with $\hat{\Gamma} = \hat{\Delta} \,.\, \mu \,.\, \Lambda$ (SF-VAR-SUC, Λ is a lock telescope)
  In this case we have that $\hat{\Delta} \,.\, \Lambda \,.\, \Theta \vdash_{\mathsf{sf}} v\ \mathsf{var} \mathbin{@} m$. By recursion we then obtain a variable $\hat{\Delta} \,.\, \Lambda \,.\, \Psi \vdash_{\mathsf{sf}} v\ [\,\alpha\,]_{\text{2-cell}}^{\Theta \Rightarrow \Psi}\ \mathsf{var} \mathbin{@} m$. Applying the rule SF-VAR-SUC again to this result gives us the desired variable, so $\mathsf{suc}\,(v)\ [\,\alpha\,]_{\text{2-cell}}^{\Theta \Rightarrow \Psi} = \mathsf{suc}\left(v\ [\,\alpha\,]_{\text{2-cell}}^{\Theta \Rightarrow \Psi}\right)$. ◀

Construction for Lemma 3. We proceed by structural recursion on σ.

- CASE $\vdash_{\mathsf{sf}} !\ \mathsf{aren}(\hat{\Gamma} \to \cdot) \mathbin{@} n$
  In this case, $\hat{\Delta}$ is the empty scoping context. We can see from Figure 7 that there can be no variables in the empty scoping context (the scoping contexts in conclusions of both inference rules both contain at least a variable annotation). Hence we do not have to deal with this case further.[7]
- CASE $\vdash_{\mathsf{sf}} \mathsf{id}^{\mathsf{a}}\ \mathsf{aren}(\hat{\Gamma} \to \hat{\Gamma}) \mathbin{@} n$
  Now $\hat{\Gamma} \,.\, \Lambda \vdash_{\mathsf{sf}} v\ \mathsf{var} \mathbin{@} m$, so we can just say $v\ [\,\mathsf{id}^{\mathsf{a}}\,]_{\mathsf{aren,var}}^{\Lambda} = v$.
- CASE $\vdash_{\mathsf{sf}} \mathsf{weaken}(\sigma)\ \mathsf{aren}(\hat{\Gamma} \,.\, \mu \to \hat{\Delta}) \mathbin{@} n$
  We know that $\hat{\Delta} \,.\, \Lambda \vdash_{\mathsf{sf}} v\ \mathsf{var} \mathbin{@} m$, so we can use recursion for σ and obtain a variable $\hat{\Gamma} \,.\, \Lambda \vdash_{\mathsf{sf}} v\ [\,\sigma\,]_{\mathsf{aren,var}}^{\Lambda}\ \mathsf{var} \mathbin{@} m$. Since Λ is a lock telescope not containing variable annotations, we can then apply the rule SF-VAR-SUC from Figure 7 with $\Theta = \Lambda$ to obtain a variable in $\hat{\Gamma} \,.\, \mu \,.\, \Lambda$ as required. In other words, $v\ [\,\mathsf{weaken}(\sigma)\,]_{\mathsf{aren,var}}^{\Lambda} = \mathsf{suc}\left(v\ [\,\sigma\,]_{\mathsf{aren,var}}^{\Lambda}\right)$.
- CASE $\vdash_{\mathsf{sf}} \sigma \,.\, 🔒_{\mu}\ \mathsf{aren}(\hat{\Gamma} \,.\, 🔒_{\mu} \to \hat{\Delta} \,.\, 🔒_{\mu}) \mathbin{@} n$
  Adding the $🔒_{\mu}$ to the left of the lock telescope Λ, we get $v\ [\,\sigma \,.\, 🔒_{\mu}\,]_{\mathsf{aren,var}}^{\Lambda} = v\ [\,\sigma\,]_{\mathsf{aren,var}}^{🔒_{\mu} \,.\, \Lambda}$.
- CASE $\vdash_{\mathsf{sf}} 🗝_{\hat{\Gamma}}^{\beta \in \Theta \Rightarrow \Psi}\ \mathsf{aren}(\hat{\Gamma} \,.\, \Psi \to \hat{\Gamma} \,.\, \Theta) \mathbin{@} n$
  We have that $\hat{\Gamma} \,.\, \Theta \,.\, \Lambda \vdash_{\mathsf{sf}} v\ \mathsf{var} \mathbin{@} m$ and that $\beta \in \mathsf{locks}\,(\Theta) \Rightarrow \mathsf{locks}\,(\Psi)$. This means that $\beta \star 1_{\mathsf{locks}(\Lambda)} \in \mathsf{locks}\,(\Theta \,.\, \Lambda) \Rightarrow \mathsf{locks}\,(\Psi \,.\, \Lambda)$. Using Lemma 4, we can use this 2-cell to obtain a variable in $\hat{\Gamma} \,.\, \Psi \,.\, \Lambda$, so $v\ \left[\,🗝_{\hat{\Gamma}}^{\beta \in \Theta \Rightarrow \Psi}\,\right]_{\mathsf{aren,var}}^{\Lambda} = v\ \left[\,\beta \star 1_{\mathsf{locks}(\Lambda)}\,\right]_{\text{2-cell}}^{\Theta \,.\, \Lambda \Rightarrow \Psi \,.\, \Lambda}$.
- CASE $\vdash_{\mathsf{sf}} \sigma.w\ \mathsf{aren}(\hat{\Gamma} \to \hat{\Delta} \,.\, \mu) \mathbin{@} n$
  We know that $\hat{\Delta} \,.\, \mu \,.\, \Lambda \vdash_{\mathsf{sf}} v\ \mathsf{var} \mathbin{@} m$ (where Λ contains only locks) and perform a case split on v.
  - CASE $\hat{\Delta} \,.\, \mu \,.\, \Lambda \vdash_{\mathsf{sf}} \mathbf{v}_0^{\alpha}\ \mathsf{var} \mathbin{@} m$
    In this case we have a 2-cell $\alpha \in \mu \Rightarrow \mathsf{locks}\,(\Lambda)$. Moreover, as one of the premises of SF-AREN-EXTEND we know that $\hat{\Gamma} \,.\, 🔒_{\mu} \vdash_{\mathsf{sf}} w\ \mathsf{var} \mathbin{@} m$. We can then use Lemma 4 with lock telescopes $\Theta = 🔒_{\mu}$ and $\Psi = \Lambda$ to transform w to a variable in $\hat{\Gamma} \,.\, \Lambda$. In other words, $\mathbf{v}_0^{\alpha}\ [\,\sigma.w\,]_{\mathsf{aren,var}}^{\Lambda} = w\ [\,\alpha\,]_{\text{2-cell}}^{🔒_{\mu} \Rightarrow \Lambda}$.

[6] This definition seems to imply a dependency of $\mathbf{v}_0^{\beta}\ [\,\alpha\,]_{\text{2-cell}}^{\Theta \Rightarrow \Psi}$ on Λ, but note that Λ is completely determined by the scoping context and the variable.

[7] This case illustrates why it is advantageous to use intrinsically scoped syntax. It makes sure that the codomain of the renaming and the scoping context of the expression match, so we do not have to cover insensible cases.

- CASE $\hat{\Delta} \,.\, \mu \,.\, \Lambda \vdash_{\mathsf{sf}} \mathsf{suc}\,(v)\ \ \mathsf{var} \mathbin{@} m$
  Now we know that $\hat{\Delta} \,.\, \Lambda \vdash_{\mathsf{sf}} v\ \mathsf{var} \mathbin{@} m$ and that $\vdash_{\mathsf{sf}} \sigma\ \mathsf{aren}(\hat{\Gamma} \to \hat{\Delta}) \mathbin{@} n$. Consequently, we can recursively obtain a variable in $\hat{\Gamma} \,.\, \Lambda$, so $\mathsf{suc}\,(v)\ [\,\sigma.w\,]^{\Lambda}_{\mathsf{aren,var}} = v\ [\,\sigma\,]^{\Lambda}_{\mathsf{aren,var}}$. ◀

Note that the algorithm presented in the construction for Lemma 3 is indeed structurally recursive: in every recursive call the renaming gets structurally smaller (and moreover the algorithm in the construction for Lemma 4 does not depend on that of Lemma 3).

Together with the equations from Section 3.2.1, we get the following result.

▶ **Lemma 5** (Atomic renaming for SFMTT expressions). *If* $\vdash_{\mathsf{sf}} \sigma\ \mathsf{aren}(\hat{\Gamma} \to \hat{\Delta}) \mathbin{@} m$ *and* $\hat{\Delta} \vdash_{\mathsf{sf}} t\ \mathsf{expr} \mathbin{@} m$*, then we can construct* $\hat{\Gamma} \vdash_{\mathsf{sf}} t\ [\,\sigma\,]_{\mathsf{aren}}\ \mathsf{expr} \mathbin{@} m$.

3.2.3 Atomic substitutions acting on variables

We now describe the action of atomic substitutions on variables. This will produce an SFMTT expression that is not necessarily a variable anymore (as was the case for atomic renamings). We have a result very similar to Lemma 3.

▶ **Lemma 6.** *If we have an SFMTT atomic substitution* $\vdash_{\mathsf{sf}} \sigma\ \mathsf{asub}(\hat{\Gamma} \to \hat{\Delta}) \mathbin{@} n$*, a lock telescope* $\Lambda : \mathsf{LockTele}(n \to m)$ *and an SFMTT variable* $\hat{\Delta} \,.\, \Lambda \vdash_{\mathsf{sf}} v\ \mathsf{var} \mathbin{@} m$*, then we can construct an expression* $\hat{\Gamma} \,.\, \Lambda \vdash_{\mathsf{sf}} v\ [\,\sigma\,]^{\Lambda}_{\mathsf{asub,var}}\ \mathsf{expr} \mathbin{@} m$.

Construction. Again we proceed by case distinction and recursion over σ. The cases for $!$, id^{a}, $\sigma \,.\, \mathbin{🔒}_{\mu}$ and $\mathbin{🗝}^{\beta \in \Theta \Rightarrow \Psi}_{\hat{\Gamma}}$ are similar to the construction for Lemma 3 so we omit them.

- CASE $\vdash_{\mathsf{sf}} \mathsf{weaken}(\sigma)\ \mathsf{asub}(\hat{\Gamma} \,.\, \mu \to \hat{\Delta}) \mathbin{@} n$
  We have that $\hat{\Delta} \,.\, \Lambda \vdash_{\mathsf{sf}} v\ \mathsf{var} \mathbin{@} m$ and $\vdash_{\mathsf{sf}} \sigma\ \mathsf{asub}(\hat{\Gamma} \to \hat{\Delta}) \mathbin{@} n$, so we can use recursion to obtain an expression in $\hat{\Gamma} \,.\, \Lambda$. Then we can apply Lemma 5 with the atomic renaming $\pi \,.\, \Lambda$ (i.e. applying all the locks from Λ to π) to obtain an expression in $\hat{\Gamma} \,.\, \mu \,.\, \Lambda$ as required. Consequently, we have $v\ [\,\mathsf{weaken}(\sigma)\,]^{\Lambda}_{\mathsf{asub,var}} = \Big(v\ [\,\sigma\,]^{\Lambda}_{\mathsf{asub,var}}\Big)\ [\,\pi \,.\, \Lambda\,]_{\mathsf{aren}}$.
- CASE $\vdash_{\mathsf{sf}} \sigma.t\ \mathsf{asub}(\hat{\Gamma} \to \hat{\Delta} \,.\, \mu) \mathbin{@} n$
  We know that $\hat{\Delta} \,.\, \mu \,.\, \Lambda \vdash_{\mathsf{sf}} v\ \mathsf{var} \mathbin{@} m$ and perform a case split on v.
  - CASE $\hat{\Delta} \,.\, \mu \,.\, \Lambda \vdash_{\mathsf{sf}} \mathbf{v}^{\alpha}_{0}\ \mathsf{var} \mathbin{@} m$
    In this case $\alpha \in \mu \Rightarrow \mathsf{locks}\,(\Lambda)$ and $\hat{\Gamma} \,.\, \mathbin{🔒}_{\mu} \vdash_{\mathsf{sf}} t\ \mathsf{expr} \mathbin{@} m$. Therefore, we can apply Lemma 5 with the renaming $\mathbin{🗝}^{\alpha \in \mathbin{🔒}_{\mu} \Rightarrow \Lambda}_{\hat{\Gamma}}$ and the expression t to obtain an expression in $\hat{\Gamma} \,.\, \Lambda$. In other words $\mathbf{v}^{\alpha}_{0}\ [\,\sigma.t\,]^{\Lambda}_{\mathsf{asub,var}} = t\ \Big[\,\mathbin{🗝}^{\alpha \in \mathbin{🔒}_{\mu} \Rightarrow \Lambda}_{\hat{\Gamma}}\,\Big]_{\mathsf{aren}}$.
  - CASE $\hat{\Delta} \,.\, \mu \,.\, \Lambda \vdash_{\mathsf{sf}} \mathsf{suc}\,(v)\ \ \mathsf{var} \mathbin{@} m$
    Now $\hat{\Delta} \,.\, \Lambda \vdash_{\mathsf{sf}} v\ \mathsf{var} \mathbin{@} m$, so we can apply recursion (with both the variable and the substitution getting structurally smaller) to get $\mathsf{suc}\,(v)\ [\,\sigma.t\,]^{\Lambda}_{\mathsf{asub,var}} = v\ [\,\sigma\,]^{\Lambda}_{\mathsf{asub,var}}$. ◀

Note that all of the cases in the previous construction are similar to the corresponding cases in the construction for Lemma 3. The most important difference is that the result of applying a substitution is an expression and not a variable. To transform the results from recursive calls, we therefore make use of the fact that atomic renamings act on expressions as shown in Lemma 5 (unlike the direct manipulation of variables as in the construction for Lemma 3). This is reminiscent of how renaming gets used in the definition of substitution in [23, 4].

Combining the previous result with the equations in Section 3.2.1, we get the following.

▶ **Lemma 7** (Atomic substitution for SFMTT expressions). *If* $\vdash_{\mathsf{sf}} \sigma\ \mathsf{asub}(\hat{\Gamma} \to \hat{\Delta}) \mathbin{@} m$ *and* $\hat{\Delta} \vdash_{\mathsf{sf}} t\ \mathsf{expr} \mathbin{@} m$*, then we can construct* $\hat{\Gamma} \vdash_{\mathsf{sf}} t\ [\,\sigma\,]_{\mathsf{asub}}\ \mathsf{expr} \mathbin{@} m$.

▶ **Example 8.** In order to illustrate the substitution algorithm described in this section, we reconsider the MTT function f from Example 1. In the MTT context $\Gamma \,.\, (\mathbb{1} \mid y : (\rho \mid B) \to A) \,.\, (\rho \mid z : B) \,.\, \text{🔒}_{\mathbb{1}}$ we can construct a term $t = \mathsf{app}_\rho \left(y^{1_1} ; z^{1_\rho}\right)$ of type A to which f can be applied. Although neither SFMTT nor WSMTT have built-in β-equivalence, we can still construct the term to which the this application of f should reduce. First of all, the SFMTT version of the function f is $\lambda^{\mathbb{1}} \left(\mathsf{mod}_\rho \left(\mathsf{mod}_\mu \left(\mathbf{v}_0^\eta\right)\right)\right)$ and t becomes $\mathsf{app}_\rho \left(\mathsf{suc}\left(\mathbf{v}_0^{1_1}\right) ; \mathbf{v}_0^{1_\rho}\right)$. If we write π^2 for $\mathsf{weaken}(\pi)$, then we can compute the desired term as follows

$$
\begin{aligned}
&\left(\mathsf{mod}_\rho \left(\mathsf{mod}_\mu \left(\mathbf{v}_0^\eta\right)\right)\right) \left[\, \pi^2.\ \mathsf{app}_\rho \left(\mathsf{suc}\left(\mathbf{v}_0^{1_1}\right) ; \mathbf{v}_0^{1_\rho}\right) \right]_{\mathsf{asub}} \\
&= \mathsf{mod}_\rho \left(\mathsf{mod}_\mu \left(\mathbf{v}_0^\eta \left[\left(\pi^2.\ \mathsf{app}_\rho \left(\mathsf{suc}\left(\mathbf{v}_0^{1_1}\right) ; \mathbf{v}_0^{1_\rho}\right)\right) \,.\, \text{🔒}_\rho \,.\, \text{🔒}_\mu \right]_{\mathsf{asub,var}}\right)\right) \\
&= \mathsf{mod}_\rho \left(\mathsf{mod}_\mu \left(\mathbf{v}_0^\eta \left[\, \pi^2.\ \mathsf{app}_\rho \left(\mathsf{suc}\left(\mathbf{v}_0^{1_1}\right) ; \mathbf{v}_0^{1_\rho}\right) \right]_{\mathsf{asub,var}}^{\text{🔒}_\rho \,.\, \text{🔒}_\mu}\right)\right) \\
&= \mathsf{mod}_\rho \left(\mathsf{mod}_\mu \left(\left(\mathsf{app}_\rho \left(\mathsf{suc}\left(\mathbf{v}_0^{1_1}\right) ; \mathbf{v}_0^{1_\rho}\right)\right) \left[\, \text{🔑}^{\eta \in \text{🔒}_{\mathbb{1}} \Rightarrow \text{🔒}_\rho \,.\, \text{🔒}_\mu}_{\hat\Gamma \,.\, \mathbb{1} \,.\, \rho} \right]_{\mathsf{aren}}\right)\right) \\
&= \mathsf{mod}_\rho \left(\mathsf{mod}_\mu \left(\mathsf{app}_\rho \left(\mathsf{suc}\left(\mathbf{v}_0^{1_1} \left[\, \text{🔑}^{\eta \in \text{🔒}_{\mathbb{1}} \Rightarrow \text{🔒}_\rho \,.\, \text{🔒}_\mu}_{\hat\Gamma \,.\, \mathbb{1} \,.\, \rho} \right]_{\mathsf{aren,var}}\right) ; \mathbf{v}_0^{1_\rho} \left[\, \text{🔑}^{\eta \in \text{🔒}_{\mathbb{1}} \Rightarrow \text{🔒}_\rho \,.\, \text{🔒}_\mu}_{\hat\Gamma \,.\, \mathbb{1} \,.\, \rho} \right]_{\mathsf{aren,var}}^{\text{🔒}_\rho}\right)\right)\right) \\
&= \mathsf{mod}_\rho \left(\mathsf{mod}_\mu \left(\mathsf{app}_\rho \left(\mathsf{suc}\left(\mathbf{v}_0^\eta\right) ; \mathbf{v}_0^{\eta \star 1_\rho}\right)\right)\right) .
\end{aligned}
$$

3.2.4 Regular renamings/substitutions

We now turn to regular renamings and substitutions. There is no need to distinguish between these two as the procedure for renamings and substitutions will be exactly the same. Since a regular rensub is a sequence of atomic rensubs, we can just sequentially apply the results from the previous sections. We therefore get the following.

$$
t \left[\, \mathsf{id} \,\right]_{\mathsf{ren/sub}} = t \qquad\qquad t \left[\, \sigma \mathbin{⓪} \tau \,\right]_{\mathsf{ren/sub}} = \left(t \left[\, \sigma \,\right]_{\mathsf{ren/sub}}\right) \left[\, \tau \,\right]_{\mathsf{aren/asub}}
$$

As a conclusion, we have finished the algorithm for renaming and substitution in SFMTT.

▶ **Theorem 9** (Renaming and substitution for SFMTT expressions)**.** *Given a renaming or substitution* $\vdash_{\mathsf{sf}} \sigma\ \mathsf{ren/sub}(\hat\Gamma \to \hat\Delta) \mathbin{@} m$ *and an SFMTT expression* $\hat\Delta \vdash_{\mathsf{sf}} t\ \mathsf{expr} \mathbin{@} m$*, we can construct an expression* $\hat\Gamma \vdash_{\mathsf{sf}} t \left[\, \sigma \,\right]_{\mathsf{ren/sub}}\ \mathsf{expr} \mathbin{@} m$*.*

Note that we do not actually need the action of full renamings on SFMTT expressions in order to define the action of atomic substitutions, atomic renamings suffice for that purpose.

Although we are not really concerned with performance in this paper, we note that optimisations are certainly possible. For example, as it is currently described, the algorithm will, when applying a regular substitution consisting of n atomic ones to an expression t, perform n traversals of t, one for every atomic substitution. This could be reduced by traversing the expression just once and applying lifting ($^+$) or locks to all atomic substitutions simultaneously when required.

3.3 Interpretation of WSMTT Expressions in SFMTT

We now turn to the relation between WSMTT and SFMTT. Using the substitution algorithm just defined, we will show that WSMTT expressions can be translated to SFMTT expressions, essentially proving that explicit substitutions can be computed away. The reverse direction is easier: apart from variables, every SFMTT expression constructor also appears in WSMTT

so we can almost trivially embed the former system into the latter. We define the two translations here and consider their meta-theoretical properties (particularly soundness and completeness) in the next sections.

3.3.1 Translation from WSMTT to SFMTT

The translation from WSMTT to SFMTT is defined mutually recursively for both expressions and substitutions. In other words, for any WSMTT expression $\hat{\Gamma} \vdash_{\mathsf{ws}} t\ \mathsf{expr} \mathbin{@} m$ we get an SFMTT expression $\hat{\Gamma} \vdash_{\mathsf{sf}} [\![t]\!]\ \mathsf{expr} \mathbin{@} m$ and for any WSMTT substitution $\vdash_{\mathsf{ws}} \sigma\ \mathsf{sub}(\hat{\Gamma} \to \hat{\Delta}) \mathbin{@} m$ we get an SFMTT (regular) substitution $\vdash_{\mathsf{sf}} [\![\sigma]\!]\ \mathsf{sub}(\hat{\Gamma} \to \hat{\Delta}) \mathbin{@} m$. We only show some of the cases for the different expression constructors. Again, in order for $[\![\_]\!]$ to be well-defined, we should check that the definition below preserves well-scopedness.

$$
\begin{aligned}
[\![\mathbf{v}_0]\!] &= \mathbf{v}_0^{1_\mu} & [\![\pi]\!] &= \mathsf{id} \mathbin{ⓐ} \mathsf{weaken}(\mathsf{id}^{\mathsf{a}}) \\
[\![(\mu \mathbin{\triangleright} A) \to B]\!] &= (\mu \mathbin{\triangleright} [\![A]\!]) \to [\![B]\!] & [\![\sigma \circ \tau]\!] &= [\![\sigma]\!] +\!\!+ [\![\tau]\!] \\
[\![t\ [\,\sigma\,]_{\mathsf{ws}}]\!] &= [\![t]\!]\ [\,[\![\sigma]\!]\,]_{\mathsf{sub}} & [\![\sigma\,.\,🔒_\mu]\!] &= [\![\sigma]\!]\,.\,🔒_\mu \\
[\![!]\!] &= \mathsf{id} \mathbin{ⓐ} ! & \left[\!\!\left[🗝_{\hat{\Gamma}}^{\alpha \in \Theta \Rightarrow \Psi} \right]\!\!\right] &= \mathsf{id} \mathbin{ⓐ} 🗝_{\hat{\Gamma}}^{\alpha \in \Theta \Rightarrow \Psi} \\
[\![\mathsf{id}]\!] &= \mathsf{id} & [\![\sigma.t]\!] &= [\![\sigma]\!]^{+} \mathbin{ⓐ} (\mathsf{id}^{\mathsf{a}}.\,[\![t]\!])
\end{aligned}
$$

When translating an (explicitly) substituted WSMTT expression $t\ [\,\sigma\,]_{\mathsf{ws}}$, we translate both the expression t and the substitution σ and then apply Theorem 9 (i.e. the algorithm from the previous section). Translation of a composite substitution involves the concatenation of the two translated substitutions, which are regular SFMTT substitutions so sequences of atomic SFMTT substitutions. Recall that the operations $\_\,.\,🔒_\mu$ and $^{+}$ for regular SFMTT substitutions are defined at the end of Section 3.1. Finally, one could wonder why in the translation of $\sigma.t$ we first add $[\![t]\!]$ to the identity atomic substitution and then apply the lifted version of $[\![\sigma]\!]$ where it would seem easier to first apply (the non-lifted) $[\![\sigma]\!]$ and then extend id^{a} with $[\![t]\!]$. The answer is that in that case $[\![t]\!]$ would live in the wrong scoping context: if $[\![\sigma]\!]$ goes from $\hat{\Gamma}$ to $\hat{\Delta}$, then $[\![t]\!]$ lives in $\hat{\Gamma}\,.\,🔒_\mu$ but if we want the translation of $\sigma.t$ to be of the form $(\mathsf{id}^{\mathsf{a}}.?) \mathbin{ⓐ} [\![\sigma]\!]$, then we need some term in scoping context $\hat{\Delta}\,.\,🔒_\mu$ at the place of the question mark.

3.3.2 Embedding of SFMTT into WSMTT

We only provide an embedding of SFMTT expressions to WSMTT expressions (so not for substitutions). Apart from the constructor for variable expressions, all SFMTT expression constructors also occur in WSMTT. We therefore only specify how to embed variables.

$$
\mathsf{embed}(\mathbf{v}_0^{\alpha}) = \mathbf{v}_0\ \left[🗝_{\hat{\Gamma}}^{\alpha \in 🔒_\mu \Rightarrow \Theta} \right]_{\mathsf{ws}} \qquad \mathsf{embed}(\mathsf{suc}\,(v)) = \mathsf{embed}(v)\ [\,\pi\,.\,\Theta\,]_{\mathsf{ws}}
$$

The lock telescopes Θ in both cases are inferred from the scoping context (recall that we consider SFMTT expressions to be intrinsically scoped).

As a result, for every SFMTT expression $\hat{\Gamma} \vdash_{\mathsf{sf}} t\ \mathsf{expr} \mathbin{@} m$ we get a corresponding WSMTT expression $\hat{\Gamma} \vdash_{\mathsf{ws}} \mathsf{embed}(t)\ \mathsf{expr} \mathbin{@} m$.

4 Soundness & Completeness

In the previous section, we introduced a translation from WSMTT to SFMTT that uses our substitution algorithm to translate away WSMTT's explicit substitution. In this section, we establish the translation's key properties: soundness and completeness with respect to σ-equivalence in WSMTT.

4.1 Soundness

In our setting, soundness is the property that starting from a WSMTT expression, applying the translation where all explicit substitutions are computed away, and then embedding the result back into WSMTT, we get a result that is σ-equivalent to the original expression. In order to prove this, we will make use of an embedding of SFMTT substitutions into WSMTT, which was not provided in Section 3.3.2. We therefore define the following for both atomic and regular SFMTT substitutions.

$$\begin{aligned}
\mathsf{embed}(!) &= ! & \mathsf{embed}\left(\mathsf{key}_{\hat{\Gamma}}^{\alpha\in\Lambda\Rightarrow\Theta}\right) &= \mathsf{key}_{\hat{\Gamma}}^{\alpha\in\Lambda\Rightarrow\Theta}\\
\mathsf{embed}(\mathsf{id}^{\mathsf{a}}) &= \mathsf{id} & \mathsf{embed}(\sigma.t) &= \mathsf{embed}(\sigma)\,.\mathsf{embed}(t)\\
\mathsf{embed}(\mathsf{weaken}(\sigma)) &= \mathsf{embed}(\sigma)\circ\pi & \mathsf{embed}(\mathsf{id}) &= \mathsf{id}\\
\mathsf{embed}(\sigma\,.\,\mathsf{lock}_{\mu}) &= \mathsf{embed}(\sigma)\;.\mathsf{lock}_{\mu} & \mathsf{embed}(\sigma\mathbin{ⓐ}\tau) &= \mathsf{embed}(\sigma)\circ\mathsf{embed}(\tau)
\end{aligned}$$

The crucial case in the proof of the soundness theorem is when the WSMTT expression is of the form $t\,[\,\sigma\,]_{\mathsf{ws}}$. In that case we use the following lemma.

▶ **Lemma 10.** *Given an SFMTT expression* $\hat{\Delta} \vdash_{\mathsf{sf}} t\ \mathsf{expr}\,@\,m$ *and substitution* $\vdash_{\mathsf{sf}} \sigma\ \mathsf{sub}(\hat{\Gamma} \to \hat{\Delta})\,@\,m$*, we have that* $\hat{\Gamma} \vdash_{\mathsf{ws}} \mathsf{embed}(t\,[\,\sigma\,]_{\mathsf{sub}}) \equiv^{\sigma} \mathsf{embed}(t)\,[\,\mathsf{embed}(\sigma)\,]_{\mathsf{ws}}\ \mathsf{expr}\,@\,m$.

Lemma 10 tells us that computing away a substitution in SFMTT and embedding the result in WSMTT gives an expression that is σ-equivalent to the result of explicitly applying the embedded substitution in WSMTT. The proof of this lemma is technically quite involved (it proceeds by induction on t and σ, the most difficult cases being weakening and key substitutions) and can therefore be found in the technical report [13].

▶ **Theorem 11** (Soundness). *For every WSMTT expression* $\hat{\Gamma} \vdash_{\mathsf{ws}} t\ \mathsf{expr}\,@\,m$ *we have* $\hat{\Gamma} \vdash_{\mathsf{ws}} \mathsf{embed}([\![t]\!]) \equiv^{\sigma} t\ \mathsf{expr}\,@\,m$ *and for every WSMTT substitution* $\vdash_{\mathsf{ws}} \sigma\ \mathsf{sub}(\hat{\Gamma} \to \hat{\Delta})\,@\,m$ *we have* $\vdash_{\mathsf{ws}} \mathsf{embed}([\![\sigma]\!]) \equiv^{\sigma} \sigma\ \mathsf{sub}(\hat{\Gamma} \to \hat{\Delta})\,@\,m$.

Idea of proof. This proof proceeds by induction on the expression t and the substitution σ. We only show one case for t, the other cases can be found in the technical report [13].

- CASE $\hat{\Gamma} \vdash_{\mathsf{ws}} t\,[\,\sigma\,]_{\mathsf{ws}}\ \mathsf{expr}\,@\,m$
  We have $\mathsf{embed}([\![t\,[\,\sigma\,]_{\mathsf{ws}}]\!]) = \mathsf{embed}([\![t]\!]\,[\,[\![\sigma]\!]\,]_{\mathsf{sub}}) \equiv^{\sigma} \mathsf{embed}([\![t]\!])\,[\,\mathsf{embed}([\![\sigma]\!])\,]_{\mathsf{ws}}$ where the last σ-equivalence holds because of Lemma 10. The induction hypothesis for t and σ gives us that $\mathsf{embed}([\![t]\!]) \equiv^{\sigma} t$ and $\mathsf{embed}([\![\sigma]\!]) \equiv^{\sigma} \sigma$, which proves the desired result. ◀

4.2 Completeness

Completeness of our algorithm with respect to σ-equivalence means that whenever two WSMTT expressions are σ-equivalent, the results when computing away all substitutions via $[\![\_]\!]$ are the same. Recall that σ-equivalence for WSMTT expressions is defined mutually recursively with σ-equivalence for WSMTT substitutions (see Figure 6). Therefore, to prove completeness we will simultaneously need to prove a similar result about σ-equivalent WSMTT substitutions. However, in SFMTT, syntactic equality of substitutions is not a good notion of equivalence. Instead, we will use the following.

▶ **Definition 12** (Observational equivalence). *We say that two SFMTT substitutions* $\vdash_{\mathsf{sf}} \sigma, \tau\ \mathsf{sub}(\hat{\Gamma} \to \hat{\Delta})\,@\,m$ *are observationally equivalent when* $t\,[\,\sigma\,]_{\mathsf{sub}} = t\,[\,\tau\,]_{\mathsf{sub}}$ *for every expression* $\hat{\Delta} \vdash_{\mathsf{sf}} t\ \mathsf{expr}\,@\,m$*. We will write this as* $\sigma \approx^{\mathsf{obs}} \tau$.

This notion of observational equivalence is actually quite strong because it quantifies over all possible SFMTT expressions. That means that both substitutions might get pushed under a lot of expression constructors, with locks or lifts added along the way. The technical report [13] shows the following lemma, which makes it easier to prove observational equivalence.

▶ **Lemma 13.** *Let* $\vdash_{\mathsf{sf}} \sigma, \tau\ \mathsf{sub}(\hat{\Gamma} \to \hat{\Delta})\ @\, n$ *be two SFMTT substitutions and suppose that* $v\ [\,\sigma\,.\,\Lambda\,]_{\mathsf{sub}} = v\ [\,\tau\,.\,\Lambda\,]_{\mathsf{sub}}$ *for every lock telescope* $\Lambda : \mathsf{LockTele}(n \to m)$ *and every variable* $\hat{\Delta}\,.\,\Lambda \vdash_{\mathsf{sf}} v\ \mathsf{var}\ @\, m$*. Then* $\sigma \approx^{\mathsf{obs}} \tau$*.*

▶ Remark 14. Lemma 13 essentially says that a substitution is uniquely determined, up to observational equivalence, by its action on De Bruijn indices. In plain dependent type theory, substitutions are often *defined* as mappings from variables to terms, or at least it is clear that they can be uniquely represented in this way. The technical report [13] provides an example that this is impossible for SFMTT: not every such mapping arises from an SFMTT substitution. In other words, the structure of substitutions in modal type theory is fundamentally more complex than in plain dependent type theory.

▶ **Theorem 15** (Completeness)**.** *If we have two* σ*-equivalent WSMTT expressions* $\hat{\Gamma} \vdash_{\mathsf{ws}} t \equiv^{\sigma} s\ \mathsf{expr}\ @\, m$*, then* $[\![t]\!] = [\![s]\!]$*. Furthermore, given two* σ*-equivalent WSMTT substitutions* $\vdash_{\mathsf{ws}} \sigma \equiv^{\sigma} \tau\ \mathsf{sub}(\hat{\Gamma} \to \hat{\Delta})\ @\, m$*, we have that* $[\![\sigma]\!] \approx^{\mathsf{obs}} [\![\tau]\!]$*.*

Idea of proof. We proceed by induction on a derivation of the σ-equivalence judgement, going over all inference rules from Figure 6. Only one case is presented here, the others can be found in the technical report [13].

- CASE $\hat{\Gamma} \vdash_{\mathsf{ws}} t\ [\,\tau\,]_{\mathsf{ws}} \equiv^{\sigma} s\ [\,\sigma\,]_{\mathsf{ws}}\ \mathsf{expr}\ @\, m$
  The premises of this inference rule are $\hat{\Gamma} \vdash_{\mathsf{ws}} t \equiv^{\sigma} s\ \mathsf{expr}\ @\, m$ and $\vdash_{\mathsf{ws}} \tau \equiv^{\sigma} \sigma\ \mathsf{sub}(\hat{\Delta} \to \hat{\Gamma})\ @\, m$, so by the induction hypothesis we have $[\![t]\!] = [\![s]\!]$ and $[\![\tau]\!] \approx^{\mathsf{obs}} [\![\sigma]\!]$. Using the definition of $\approx^{\mathsf{obs}}$ we then get that $[\![t\ [\,\tau\,]_{\mathsf{ws}}]\!] = [\![t]\!]\ [\,[\![\tau]\!]\,]_{\mathsf{sub}} = [\![s]\!]\ [\,[\![\sigma]\!]\,]_{\mathsf{sub}} = [\![s\ [\,\sigma\,]_{\mathsf{ws}}]\!]$. ◀

A consequence of soundness and completeness is the following result.

▶ **Theorem 16.** *Given two WSMTT expressions* $\hat{\Gamma} \vdash_{\mathsf{ws}} t, s\ \mathsf{expr}\ @\, m$*, then* $\hat{\Gamma} \vdash_{\mathsf{ws}} t \equiv^{\sigma} s\ \mathsf{expr}\ @\, m$ *if and only if* $[\![t]\!] = [\![s]\!]$*. From this it follows that SFMTT expressions are the* σ*-normal forms of WSMTT expressions, and* $[\![-]\!]$ *is the normalisation function.*

Proof. The direction from left to right is exactly Theorem 15. Conversely, suppose that $[\![t]\!] = [\![s]\!]$. Then we know that $t \equiv^{\sigma} \mathsf{embed}([\![t]\!]) = \mathsf{embed}([\![s]\!]) \equiv^{\sigma} s$. To show that SFMTT expressions are the σ-normal forms of WSMTT expressions, we only need to prove that every SFMTT expression is in the image of the $[\![-]\!]$ function. This is indeed the case since $[\![\mathsf{embed}(t)]\!] = t$ for all $\hat{\Gamma} \vdash_{\mathsf{sf}} t\ \mathsf{expr}\ @\, m$ (which is provable via a trivial induction on t). ◀

5 Related and Future Work

5.1 Normalisation by Evaluation for MTT

Normalisation of MTT with respect to σβη-equality had already been proven by Gratzer [17] [18, ch. 8]. He uses a normalisation by evaluation (NbE) argument [5, 3], structured using the more recent technique of Synthetic Tait Computability (STC) [31][18, ch. 4]. We compare Gratzer's work with ours both in terms of approach and of implications.

Implications. An NbE algorithm will take as input a term $\Gamma \vdash t : T$ (considered up to σβη-equality) and a *value environment* $\rho : \mathsf{env}(\Delta \to \Gamma)$ and return a σβη-normal form $\Delta \vdash \mathsf{nbe}(t, \rho) : T[\rho]$. When we instantiate ρ with the identity environment, which substitutes every variable with itself or its η-expansion, then we are really just normalising t. When instead we are only interested in syntax up to σβη-equality, and thus not in σβη-normalisation which is inobservable up to σβη-equality, then the algorithm really just applies the substitution ρ to the term t. So in this sense an NbE algorithm already allows for substitution and indeed this is sufficient for a proof-of-concept implementation of MTT [30].

However, for conceptual, didactical and practical reasons, we see a role for a substitution and σ-normalisation algorithm unreliant on βη-equality as presented in the current paper. Conceptually, there is the fact that substitution originates as a find-replace operation that replaces every occurrence of a given variable with a term of the same type. While the definition of such an operation becomes more difficult with the introduction of variable binding, dependent types, ..., it is still a reasonable expectation and indeed a sanity check to ask that this operation be definable, without referring to computation or βη-equality. It ensures that, even before considering computation, variables can be thought of as placeholders, and that programs are not permanently tied to the context in which they are defined, but merely use the context as an interface. Didactically, since computation relies on substitution, it is desirable to be able to explain substitution *first*, and especially without having to introduce NbE. Practically, when working in a dependently typed proof assistant, we want to get type goals that are *not* in σβη-normal form. For example, an η-normal form of an advanced algebraic structure will typically be a big nested record type listing all carriers and implementing all available operations, which may not be quite as readable as the more intensional way in which the algebra was constructed. A proof assistant that relies on NbE for substitution, will not be able to type a function application $f\,a$ of a dependently typed function f without normalising the codomain of f. Our algorithm, on the other hand, will cleanly push substitutions through all non-substitution-related syntax constructors and merely find and replace variables.

Approach. A first stark difference between NbE and the current work is that NbE considers a type system's syntax up to σβη-equality, i.e. it considers the type system's initial model in which important type formers can be characterised by their universal properties. In order to speak about σ-equality, we need to distinguish βη-equal terms and lose some of the categorical tooling. In particular, the category of models of a type system is of little use and most type formers do not satisfy their universal properties up to σ- or syntactic equality.

Similarly, because typing relies on βη-equality and we want to get the complications of substitution out of the way *before* considering βη-equality (e.g. because of the conceptual and didactical reasons above), we work with intrinsically scoped untyped syntax, whereas NbE generally works with intrinsically typed syntax.

NbE arguments generally feature at least five "collections of program representations": variables, neutrals, normal forms, values, and σβη-equivalence classes[8] of terms. An NbE proof involves several operations on and between these collections, and each of them is stable under renaming, which is necessary to deal with λ-abstraction and application. In the current work, we do not ever need to construct or eliminate functions, so while we do need to apply lock telescopes to renamings and substitutions, it turns out there is no need to prove that

[8] When formalising type theory in type theory, one would not use set-theory-style quotients based on equivalence classes, but instead use quotient-inductive-inductive types [6].

every operation featured in the construction is stable under renaming. Furthermore, while MTT and SFMTT can be regarded as the collections of terms and normal forms respectively, and we also have a definition of SFMTT variables, we do not need to distinguish between values and normal forms (which in NbE has mostly to do with η-equality) and we do not need a separate collection of neutrals (as σ-reduction, unlike β-reduction, is never stuck on a variable).

5.2 Second-order Algebraic Theories

Allais, Atkey, Chapman, McBride and McKinna [4] implement renaming and substitution (among many other things) at once for a large class of languages, which Fiore and Szamozvancev [16] identify to be what is often called second-order multisorted algebraic theories (SOMATs). Here, multisorted means simply-typed, and second-order means that they accommodate variable-binding, but no other context features, i.e. it is assumed that contexts, renamings and substitutions are lists of types, variables and terms respectively. More recently and in a more categorical perspective, Uemura has defined the corresponding class of dependently typed languages, which in the larger naming scheme would be called second-order generalised algebraic theories (SOGATs). A similar general substitution result should be possible for SOGATs, and in any case it is very well understood (but considered tedious) how to define substitution for specific SOGATs, which is why there is nowadays little attention for this problem in the metatheory of specific *non-modal* languages. The necessity of the current work arises from the fact that, due to the presence of modal locks, MTT is not a SOGAT (it is a generalised algebraic theory or GAT [11], as are WSMTT and SFMTT). A generalisation of second-order algebraic theories that would subsume MTT or at least Multimode Simple Type Theory (MSTT) [12] is work in progress [24] and will be informed by our current findings.

5.3 Other Approaches to Modal Contexts and/or Substitution

Lock calculi. Bahr, Grathwohl and Møgelberg [7] introduce Clocked Type Theory (CloTT), a system for guarded type theory which features a *later* modality $\triangleright$ for every clock listed in the clock context. If we keep the clock context fixed, then to a large extent CloTT can be regarded as an instance of MTT,[9] but the "lock" operation for each later modality is *named*. To clarify, we put the introduction rules for the later types for a clock κ in MTT and CloTT side by side:

$$\frac{\Gamma\,.\,🔒_{\triangleright^\kappa} \vdash t : T}{\Gamma \vdash \mathsf{mod}_{\triangleright^\kappa}\,(t) : \langle \triangleright^\kappa \mid T \rangle} \qquad \frac{\Gamma, \alpha : \kappa \vdash t : T}{\Gamma \vdash \lambda(\alpha : \kappa).t : \triangleright(\alpha : \kappa).T}$$

The variable α is called a tick of the clock κ, but we can more generally call it a lock variable. The specific mode theory for CloTT is enforced by requiring that α be used substructurally. This slightly complicates the type system but on the bright side, substitutions in CloTT are simply variable and tick replacement operations and do not have the complex categorical structure they have in MTT, facilitating implementation in Agda [33]. Dependent quantification over an affine or cartesian interval variable in cubical homotopy or parametric type theory [9, 15, 8] can also be regarded as an instance of this approach, with the interval

[9] Alternatively, we could regard the clock context as the mode, in which case we have an instance of MTT where clock substitution and quantification are also modalities. However, our discussion about lock calculi does not apply if we take that perspective.

variable being analogous to the tick. We could similarly try to assign a lock variable to every lock in MTT and extend MTT with a substructural lock calculus [25]. This is challenging however, as we need to deal with arbitrarily complex mode theories and the lock calculus admits in general neither weakening, exchange nor contraction.

2-posetal MTT. If MTT is instantiated on a mode theory that is a 2-poset, meaning that the 2-cell of a given domain and codomain is unique if it exists, and if moreover this existence is decidable, then rather than listing 2-cell information on variables and in substitutions, the unique existence of the necessary 2-cells can be checked. Then all the remaining *information* in a substitution is a list of terms, and the substitution operation is again merely a find-replace operation. In the implementation of the proof assistant Mitten [30], this fact is used to optimise the NbE algorithm (Section 5.1) for implementation.

Left division. MTT is based on a line of work on type systems using a *left division* operation [2, 28, 27, 26], which in turn can be regarded as a generalisation of a dual-context approach [29]. Rather than having a context *constructor* $🔒_\mu$ which is semantically left adjoint to the modality, it is assumed that there exists a left division operation $\mu\backslash\_$ left adjoint to $\mu\circ\_$ on modalities, and this operation extends to contexts by applying it to the modal annotation of every variable. In systems based on left division, contexts are lists of modality-annotated types, and substitutions are lists of terms. The difficult question there is not whether substitution is definable, but whether left division of contexts is functorial. This question has to our knowledge never been properly studied for general mode theories. Moreover, left division of contexts is itself a defined operation on syntax and, unlike substitution, typically does not have clean denotational semantics.

Fitch-style calculi. Logics and type systems that feature typically a single modality $\Box$ and a left adjoint context constructor 🔒, but no modal annotations on variables, are referred to as Fitch-style calculi [14]. Given the presence of only a single modality, the proof of Theorem 2 only stands if there is a non-trivial and non-horizontally-decomposable 2-cell between powers of $\Box$, e.g. the duplication $\delta \in \Box \Rightarrow \Box\Box$ of a comonad. Gratzer, Sterling and Birkedal [21] implement type theory with an S4-style $\Box$-modality (i.e. an applicative comonad) and indeed our counterexample applies. They do not define a substitution operation and instead use NbE. Valliappan, Ruch and Cortiñas [32] prove NbE for four modal systems, where $\Box$ is an applicative functor with optionally a co-unit $\varepsilon \in \Box \Rightarrow \mathbb{1}$ and/or a duplication δ. Each time, they define a *modal accessibility relation* $\Delta \lhd \Gamma$ on contexts which entails the existence of a substitution $\Gamma \to \Delta\,.🔒$ involving only weakening and 2-cells. As such, unlike MTT, their system has a composition-free substitution $\Gamma\,.🔒\,.\,A\,.🔒 \to \Gamma\,.🔒$ that forgets the variable of type A and fuses the locks all at once. Still, they do not claim definability of composition of substitution (only identity), nor do they define substitution, instead using NbE. For pointed modalities and monads, on the other hand, we refer back to the lock calculi discussed above, with the later modality and interval quantification as examples.

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