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Verified Extraction from Coq to OCaml

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One of the central claims of fame of the Coq proof assistant is extraction, i.e., the ability to obtain efficient programs in industrial programming languages such as OCAML, Haskell, or Scheme from programs written in Coq’s expressive dependent type theory. Extraction is of great practical usefulness, used crucially e.g., in the CompCert project. However, for such executables obtained by extraction, the extraction process is part of the trusted code base (TCB), as are Coq’s kernel and the compiler used to compile the extracted code. The extraction process contains intricate semantic transformation of programs that rely on subtle operational features of both the source and target language. Its code has also evolved since the last theoretical exposition in the seminal PhD thesis of Pierre Letouzey. Furthermore, while the exact correctness statements for the execution of extracted code are described clearly in academic literature, the interoperability with unverified code has never been investigated formally, and yet is used in virtually every project relying on extraction.

In this paper, we describe the development of a novel extraction pipeline from Coq to OCaml, implemented and verified in Coq itself, with a clear correctness theorem and guarantees for safe interoperability. We build our work on the MetaCoq project, which aims at decreasing the TCB of Coq’s kernel by re-implementing it in Coq itself and proving it correct w.r.t. a formal specification of Coq’s type theory in Coq. Since OCAML does not have a formal specification, we make use of the Malfunction project specifying the semantics of the intermediate language of the OCaml compiler.

Our work fills some gaps in the literature and highlights important differences between the operational semantics of Coq programs and their extracted variants. In particular, we focus on the guarantees that can be provided for interoperability with unverified code, identify guarantees that are infeasible to provide, and raise interesting open question regarding semantic guarantees that could be provided. As central result, we prove that extracted programs of first-order data type are correct and can safely interoperate, whereas for higher-order programs already simple interoperations can lead to incorrect behaviour and even outright segfaults.

CCS Concepts:
- Software and its engineering → Compilers; Functional languages: Formal software verification; • Theory of computation → Type theory.

Additional Key Words and Phrases: Coq, verified compilation, extraction, interactive theorem proving, functional programming

1 INTRODUCTION

Extraction of programs written with a proof assistant based on type theory can be seen as a compilation process from a high-level language to a low-level one (e.g., OCAML, HASKELL, or C). This is the standard way to get a certified executable code from a Coq formalisation [Letouzey 2004], that is used for instance by the CompCert compiler [Leroy 2006], the CertiCoq project [Anand et al. 2017], the verified Javascript reference interpreter JSCert [Bodin et al. 2014], or the Velús verified compiler for Lustre [Bourke et al. 2017]. From this point of view, extraction is part of the trusted code base (TCB) of the proof assistant and thus should come with strong guarantees.

Since the behavior of the extraction process is crucial for the trust in formally verified software, it seems natural to have clear and formally verifiable guarantees about this process. Precisely, one would expect two guarantees: First, preservation of the operational semantics, that is if a program evaluated to a value in the proof assistant, its extracted version evaluates to a corresponding value in the target language. Second, preservation of typing, that is any extracted program is well-typed in the target language.

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Unfortunately, there are severe limitations to both properties. For the preservation of operational semantics, one needs to first capture the operational semantics of the target language, and notions such as “corresponding value”. For the case of OCAML, there is no agreed upon formal semantics, and defining correspondence relations is intricate. Of course, on values of first-order data type such as natural numbers or booleans, the definition is straightforward, but users of extraction are usually interested in extracting programs that take arguments as inputs and produce values. This means that we need to define what it means for a function written in the low-level target language to be equivalent to a program written in a proof assistant to give any interesting operational specification of extraction.

The situation on the typing side is even less satisfactory. For extraction, the type system of the source language usually features general polymorphism or even dependent types, and is thus much more expressive that the one of the target language. In practice, the extracted code thus needs to use unsafe typing features to produce a piece of code that may be accepted by the typechecker of the target language. For instance, the extraction from Coq to OCAML quickly makes use of the unsafe type cast operation \texttt{Obj.magic}. If one wants to formally specify the behaviour of such programs, one quickly encounters Xavier Leroy’s famous motto:

\textit{”Repeat after me: \texttt{Obj.magic} is not part of the OCAML language.”} 

Indeed, as soon as one starts using such unsafe features, one has absolutely no guarantee from the type checker anymore, and efforts to make the rest of the extracted code welltyped seem more or less useless.

Letouzey’s seminal PhD thesis [Letouzey 2004] presents the current extraction mechanism of the Coq proof assistant and discusses correctness guarantees. The mathematical development is mainly centered around an intermediate language called $\lambda_\square$, which has a formal semantics that is similar to Coq’s operational semantics. The translation from $\lambda_\square$ to languages such as OCAML is then left unspecified, due to a lack of formal semantics for OCAML. However, the discrepancy between provided guarantees and uses of extraction in practice can already be explained in terms of $\lambda_\square$. Letouzey proves two central theorems: First, that the operational behaviour of erased $\lambda_\square$ terms and Coq terms is in agreement through a (non-deterministic) erasure relation [Letouzey 2004, Thm. 6, pg. 60]. Secondly, that higher order functions, e.g., of type $(\mathbb{N} \to \mathbb{N}) \to \mathbb{N}$, behave correctly when they are called on $\lambda_\square$ functions that extensionally agree on a Coq function of the same type [Letouzey 2004, Thm. 9, pg. 74]. The second result is proved using a logical relation, and, provided a formal semantics of OCAML and a proof of the first result regarding OCAML, could be extended to OCAML as well. However, this means that the only safe interoperability of extracted Coq functions is, in practice, with other extracted Coq functions.

We address three shortcomings of the state of the art in the present paper:

1. Due to a lack of formal semantics for OCAML, the extraction process is not and cannot be formally specified and thus not proved correct.
2. Interoperation of higher-order functions with (potentially) nonterminating or effectful OCAML programs is not captured by the correctness guarantees, because they do not extensionally agree with a Coq program.
3. Even though a type interface is provided by extraction, the use of \texttt{Obj.magic} means that there are no guarantees by OCAML’s type checker.

We propose to address those issues in the particular setting of extraction from programs written in the Coq proof assistant to the OCAML programming language. For other proof assistants such as Lean or Agda, and other target languages such as Scheme or Haskell, similar but subtly different

1Message on the OCAML mailing list: https://sympa.inria.fr/sympa/arc/caml-list/2009-10/msg00181.html
issues arise. We however hope that by the exposition of this special case, our techniques can be transported and reused for other source and target languages.

To solve the issue of trust regarding operational correctness (1), we contribute a formal semantics of the Malfunction language by Dolan [2016]. Malfunction has three central design goals:

- it is "a thin wrapper around OCaml 's [...] intermediate representation", and thus trivial to compile to it,
- its "syntax is simplified, to allow easy code generation",
- and its semantics is stricter in most cases than that of the OCaml intermediate representation, to be robust to future changes to OCaml.

We then give a machine-checked proof of preservation of evaluation behaviour, connecting the formal semantics of Coq to the formal semantics of Malfunction by a proof in Coq. The proof is split into a long pipeline of intermediate passes to make the proof engineering overhead manageable. The central theorem talks about terms of first-order data type, i.e., of inductive type were all constructors arguments are of first-order data type.

To solve the issue of interoperability (2), we prove that for first-order functions, i.e., functions from first-order data types to first-order data types, any interoperation with OCaml code is safe, even if the Coq code internally uses higher-order features and proofs. In the next section, we provide a counter-examples that show that outside this setting, it is possible to get extracted code that produces a segmentation fault when called with a well-typed OCaml argument. This is because most of the target languages of extraction can perform effects such as writing to reference cells, and the strong guarantees provided by the proof assistant only apply to pure functions.

To solve the typing issue (3), we advocate for a drastic change of perspective on extracted code: Instead of hoping that the extracted code is well-typed in the target language and correcting problems heuristically using unsafe casts, we advocate for just exposing safe first-order function interfaces as discussed in the previous paragraph, and using untyped but verified code for the internal, higher-order parts of the code. Running the typechecker of the target language is superfluous anyways: the generated code is already type checked by the proof assistant, providing strong guarantees. Thus what we contribute in this paper is a definition of a semantic typing judgment for the target language [Dreyer 2018] à la realizability, and a formal proof that the extracted code from a Coq program with a simple enough type realizes the corresponding erased type in OCaml. The type system of OCaml is one way to statically check that a program realises a type, but Coq’s type system plus the extraction mechanism should be seen as another way to guarantee realizability, eliminating the need to use the OCaml type checker for our purposes. Targeting Malfunction is in line with these considerations, since it is untyped but supports exposing a typed interface.

Overall, our compilation chain is depicted in Fig. 1 and can be summarised as follows. A program is type-checked by the Coq kernel (red area). It is then quoted using a quotation mechanism that is essentially the identity function into MetaCoq’s term representation of Coq itself [Sozeau et al. 2019a], with the assumption that the quotation yields a program that is well-typed according to MetaCoq’s typing judgment. The theory of the kernel of Coq formalised in MetaCoq is called PCUIC. We perform verified type and proof erasure [Sozeau et al. 2019b], targeting the untyped \(\lambda\)-calculus \(\lambda_D\). We then perform several transformation steps on \(\lambda_D\), namely to change the representation of fixpoints, to remove parameters, to remove case analysis on proofs, to implement native projections, to treat constructors as blocks, to implement erasure residues as functions, and to annotate names. All this is in the grey area. The final transformation is a translation to representation of Malfunction in Coq. To get an executable (blue area), we finally print

\[2\] The OCaml compiler’s intermediate language is called Lambda. To avoid confusion with \(\lambda_D\), we do not use the name.
The s-expression representation of the resulting MALFUNCTION program to a file and use the MALFUNCTION compiler to compile to OCAML compilation units (.cmx).

Before diving into the technical details of our formal setting, let us look into examples that illustrate our claims and the current limitations of Coq’s official extraction mechanism to OCAML.

1.1 Scope and Limitations of Extraction to OCAML

We here discuss general limitations of any extraction to OCAML, to which any extraction process – and thus Coq’s current extraction process as well as our verified replacement – are subject to.

First, a situation where OCAML’s type system is too weak arrives as soon as one uses higher-order dependent types and exposes this function to be called from unverified OCAML code. We are going to develop a function assumes_purity : (unit → B) → B where applying it to an (effectful) OCAML function impure leads to a segmentation fault. We here consider the example of a function function_or_N that expects a boolean value b and returns a a function from B to B if b is true and a natural number otherwise, inspired by Letouzey’s discussion [2004, §3.1.3, 3.2.1.].

\[
\text{Definition function_or_N : } \forall (b : B), \text{if } b \text{ then } B \rightarrow B \text{ else } N := \\
\text{fun } b \Rightarrow \\
\text{match } b \text{ with } \\
\text{| true } \Rightarrow \text{fun } x \Rightarrow x \\
\text{| false } \Rightarrow S 0 \\
\text{end.}
\]

From VerifiedExtraction
Require Import Loader.

\[
\text{Definition function_or_N \_true := fun b } \Rightarrow \\
\text{match b with } \\
\text{| true } \Rightarrow \text{fun } x \Rightarrow x \\
\text{| false } \Rightarrow S 0 \\
\text{end.}
\]

MetaCoq Verified Extraction
function.
MetaCoq Run Print mli function.

(* Prints:
  type B = True | False
  val function : B → B *)

Output in file out.mlf:

(module
  ($def_function_or_nat
    (lambda ($b)
      (let ($discr $b)
        (switch $discr
          ((0 0) (lambda ($x) $x))
          ((1 1) (block (tag 0) 0)))))
    ($def_function
      (apply $def_arity_function 0))
    ($function $def_function)
    (export $function))

Fig. 1. Left: Overview of the extraction process. Red background indicates parts of the Coq proof assistant implementation in OCAML, grey parts implemented and verified in Coq, blue parts of the MALFUNCTION compiler implementation in OCAML. Green font means the implementations are part of the TCB. Blue font means that we are using work by Sozeau et al. [2019b].

Right: Example invocation of the verified extraction plugin and its output.
Since OCAML’s type system does not support type-on-term dependency, there is no way to give a type to the extracted version of function_or_N and thus the extraction implemented in Coq as of today reads:

```coq
(** val function_or_N : B → Obj.t **)  
let function_or_N = function|True → Obj.magic (fun x → x)|False → Obj.magic (S O)
```

The type Obj.t is actually a synonym to the universal type, which can be used to type any term using Obj.magic, meaning that function_or_N cannot be typed in OCAML without unsafe casts. The use of Obj.magic, besides annihilating the interest of the type system, also pollutes the rest of the code, because any use of function_or_N must then be enclosed in an Obj.magic invocation to cast the return type to B → B or N. In practice, the extraction tries to avoid the greedy use of Obj.magic which has the even less satisfactory consequence of producing ill-typed terms in some complex situations [Sozeau et al. 2019b, §3.6].

This taken aside, let us continue our example and define a function that takes a boolean value b and, as input, again either function from B to B or a natural number (depending on b) and applies the function to an argument in the first case while just returning a default value in the second:

```coq
Definition apply_function_or_N : ∀ b : B, (if b then B → B else N) → B :=  
  fun b ⇒ match b with true ⇒ fun f ⇒ f true | false ⇒ fun _ ⇒ false end.
```

Again, the OCAML extraction has to use unsafe casts:

```coq
(** val apply_function_or_N : B → _ → B **)  
let apply_function_or_N b f = match b with |True → Obj.magic f True |False → False
```

We now use apply_function_or_N with function_or_N as argument, while letting the boolean be determined by a function from unit to B applied to the only element tt of unit:

```coq
Definition assumes_purity : (unit → B) → B :=  
  fun f ⇒ apply_function_or_N (f tt) (function_or_N (f tt)).
```

This function can be extracted to an OCAML function whose type is a perfectly valid OCAML type:

```ocaml
(** val assumes_purity : (unit → B) → B **)  
let assumes_purity f = apply_function_or_N (f ()) (function_or_N (f ()))
```

Now on the Coq side the function assumes_purity is well-typed under the invariant that f tt always returns the same value. Thus, nothing will go wrong in OCAML as long as assumes_purity is always called with an OCAML function of type unit → B that always returns the same value.

If this invariant however is broken, the internal unsafe casts Obj.magic become invalid, and all guarantees are lost. And indeed, it is easy to break this invariant in OCAML by using a reference:

```ocaml
let impure : unit → B = let x : B ref = ref False in  
  fun _ → match !x with False → (x := True; False) | True → True
```

The function impure returns False the first time it is called and True afterwards. When applied to assume_purity, the execution is essentially equivalent to apply_function_or_N True (function_or_N False), meaning apply_function_or_N expects a function as argument, but gets a natural number. Thus, the program tries to evaluate the application of Obj.magic False True which induces a segmentation fault:

```ocaml
assume_purity impure  
(** Segmentation fault: 11 **)
```

This examples illustrates the fact that even if an extracted program has a valid OCAML interface, this does not mean that its interaction with well-typed OCAML pieces of code will not go wrong.
1.2 What Guarantees Can We Expect From Extracted Code?

The situation looks pretty bad. On one side, the target type system is fundamentally too weak to support extraction of dependently typed programs. On the other side, even on the common part of the type system, the semantics associated to the type is very different between the two systems. In particular, because CIC is a pure language, it satisfies strong invariants, such as the fact that a function always returns the same output on the same input. But by using dependent types, those invariants at the computational level can be lifted at the type level. This is the case for instance for the pure_apply function. Thus, one can wonder whether we can expect any guarantee at all for the interaction between an extracted program and OCaml pieces of code?

This paper provides the first positive answer in two steps. First, we do not expect extraction to produce a well-typed OCaml program, but rather we prove that it produces an untyped low-level functional code that operationally behaves the same as Coq’s initial program. Then, by defining a realisability semantics for low-level pieces of functional code over the OCaml type system, we can show that for first order types (i.e., functions whose domain and codomain are first-order data types) the extracted code actually meets its specification and can thus interact safely with any pieces of OCaml code.

Note that this result is significantly less restrictive than it might seem, e.g., the benchmarks used for evaluation of compilation times in CertiCoq readily satisfy the constraints.

Major programs relying on extraction as of today might not all be in this shape, but for reasons related to convenience and thus they could be brought to this shape. For instance for CompCert, the main compilation function would satisfy this condition if not for a representation of integers as unbounded numbers with an explicit proof of a bound (which could easily be re-organised into a syntax type without this bounding constraint and a first translation phase that establishes it). For our own extraction procedure, the only hinderance is representing non-empty lists (for universe instances) via \(X \cdot 1\text{list } X\) rather than a pair of a list and a non-emptiness proofs.

1.3 A General Plan to Support Certified Extraction Towards Several Languages

In the process of proving operational correctness and realisability properties of extraction, there is a sizable part that is independent of the target language and can be defined commonly. To make this explicit, \(\lambda_\square\) has been introduced by Letouzey [2004] as a common intermediate untyped language in which an original Coq term can be erased. Sozeau et al. [2019b] have mechanised a weak call-by-value variant of \(\lambda_\square\) in Coq based on the MetaCoq project. They give a machine-checked proof of type and proof erasure, removing type information and proof terms that are in Prop (or SProp), and replace everything with a canonical \(\square\) term.

In this paper, we show how to define a compilation pipeline that gradually transform a \(\lambda_\square\) term to a term that computes the same values, but is operationally closer to the semantics of the target language. These different phases correspond to compilation phases usually provided by compilers and are not specific to extraction to OCaml. They consist for instance in removing the parameters of constructors of inductive types that are required in Coq for type inference but have no computational content and thus can be discarded in a simply typed or untyped setting. There are also other phases such as \(\eta\)-expansion of constructors of inductive types that are not fully syntactic and require typing to be defined. Those phases need thus to be performed before erasure to \(\lambda_\square\).

As of today, this pipeline based on \(\lambda_\square\) is already use in the CertiCoq project [Anand et al. 2017]. It could easily be used to target other call-by-value languages as well, e.g., blockchain-based languages as covered in the ConCert project [Annenkov et al. 2020], or even languages like Rust.

---

3https://compCert.org/doc/html/compCert.driver.Compiler.html#transf_c_program
It could also be used as a target for other proof assistants. Indeed, it seems feasible to get extraction from the Agda or Lean proof assistants to OCAML via MALFUNCTION by implementing type and proof erasure from Agda or Lean to \( \lambda_\square \).

1.4 Malfunction vs. Other Target Languages

In order to give a machine-checked implementation of extraction, we require a specification of the target language in Coq. This specification will remain part of the TCB: it has to be correct for the verification to be meaningful. Thus, it is desirable to have a clear, easy-to-review specification.

One path would be to specify the operational semantics of OCAML in Coq. Such a semantics could be obtained by translating the semantics of OCAML given in prose, or by reverse-engineering a specification from a compiler, interpreter, or an abstract machine for OCAML. However, the semantics of OCAML is complex, and it would require a major amount of trust to believe that the specification indeed is correct. Furthermore, several parts of OCAML are intentionally unspecified, e.g., the evaluation order of function call arguments.

Another path would be to directly specify the operational semantics of Lambda, the intermediate language of the OCAML compiler. However, the semantics of the OCAML intermediate representation is intentionally unspecified (even the -dlambda option of the compiler to generate the intermediate representation from OCAML code is undocumented), and changes between releases.

Lastly, it is also desirable that the chosen semantics be economical, in the sense that it can be used in a verification project without generating an overhead which lets even easy tasks take months.

Thus, to have a clear and economical specification, it seems natural to choose MALFUNCTION as target language for extraction: MALFUNCTION has a clear semantics provided by an interpreter, it has been around the (scientific part of the) OCAML community for several years, and it can serve as a stable interface to deal with changes of the semantics of Lambda. Furthermore, MALFUNCTION is fully specified: e.g., evaluation order of operators is clearly specified to be left-to-right.

1.5 Plan of the Paper

In Section 2, we present the statement and main idea of the proof of the main correctness theorem. Then we proceed in Section 3 to a phase-by-phase description of each necessary transformation outlined in Fig. 1. We then discuss in Section 4 our contribution as a practical tool to replace current Coq’s extraction to OCAML. Section 5 explains how we bootstrap our extraction mechanism to obtain a self-hosted compiler. We compare the performance of our extraction to Coq’s extraction and CertiCoq in Section 6. Finally, we discuss related and future work and conclude.

Links to the available online formalisation are provided using the syntax "myNotion [myFile.v]". The links are voluntarily obfuscated for double blind but they are explicit enough so that they can be mapped to the anonymous supplementary material provided with this paper.

2 THE CORRECTNESS THEOREMS

In this section, we technically explain the statement of our two central theorems, providing key elements of their proofs. From a bird’s-eye view, the first central theorem is a simple simulation theorem for a compiler, saying that if a Coq program \( t \) of first-order data type is convertible to an irreducible term \( v \), then its translation to MALFUNCTION evaluates to the value translation of \( v \). A first-order data type (\code{firstorder_ind [PCUIFirstOrder.v]}) is a mutual inductive type whose constructors only have arguments of first-order data type. The value translation is a a simple function translating a constructor application to either an integer if all arguments are parameters of the constructor, or to an applied tagged block if they are not. The second central theorem deals with first-order functions, that is functions whose arguments and return value are of first-order data types. It states that the MALFUNCTION program obtained by extracting a Coq first-order
function can be applied safely to any pieces of OCAML (compiled to MALFUNCTION) that has the right corresponding type. In particular, we prove that the kind of counter-examples such as assumes_purity of Section 1.1 cannot be produced for first-order functions. So interoperability with unverified OCAML programs is safe for this fragment.

2.1 MALFUNCTION and COQ

The internal language of the kernel of COQ (Fig. 2, top) is formalised in MetaCoq [Sozeau et al. 2019a] as the inductive type term [Ast.v]. On the computational level, it features basic constructs of functional language such as (DeBruijn) variables (tRel), lambda abstraction (tlambda), (n-ary) application (tApp) and a letIn construct. It also features inductive and co-inductive features, tConstruct for constructors of (co-)inductive types, tCase for pattern-matching, fixpoints (tFix) and co-fixpoints (tCoFix), and a notion of projections (tProj) which corresponds to a negative presentation of record types. COQ also features constructions that are very specific to dependent type theory. In particular, types appear in the syntax of terms and can be manipulated as any other terms. Thus, it features terms tSort for universe, tInd for inductive types (it takes as arguments on inductive definition and a universe Instance.t) and tProd for dependent function types and a tCast function to explicitly cast a term to a given type. Finally, COQ features a primitive notion of integers (tInt) and floats (tFloat). The syntax comes with a notion one-step reduction red [PCUICTyping.v], noted Σ; Γ ⊢ t ⇝ t’, of a term t into t’ in the global env_ext [PCUICAst.v] Σ and in the local context Γ. The reflexive, transitive closure of one-step reduction is noted Σ; Γ ⊢ t ⇝∗ t’. It also comes with a specification of typing [PCUICTyping.v], Σ; Γ ⊢ t : T. All of these definitions are quite complex in detail, but a deep understanding is not required to understand the rest of this paper and we refer the interested reader to Sozeau et al. [2019b] for further explanations.

MALFUNCTION (Fig. 2, bottom) specifies the following syntactic constructs relevant for extraction: named variables, n-ary abstraction and application, mutual recursion via Mlet rec, tagged n-ary Mblock, an operation to project out the i-th field of a block, and a Mswitch statement branching over the tag of a block. Besides MALFUNCTION features lazyness, primitive integers and mutable vectors that are not relevant to extraction from COQ.

Operationally, MALFUNCTION and COQ are relatively simple. However, since COQ is a dependent type theory, it has first-class types and proofs that can play roles in computations and have no
counterpart in MALFUNCTION, i.e., they have to be erased. The further semantic differences are subtle. We take care of them one-by-one, to avoid combinatorial explosion in proofs.

Still, combinatorial explosion lurks behind every corner. After all, we are dealing with the real semantics of Coq rather than an idealised type theory. We thus put focus on finding economical proofs, often proving a slightly weaker property than what could be proven which is however still strong enough to establish the wanted theorem. Standard techniques like using observational equivalence of programs are for instance not economical: An induction over the derivation of observational equivalence would have to deal with far more than 50 cases. Instead, our results are all stated w.r.t. a big-step evaluation relation of programs.

The reasons we restrict to values of first-order data types then become apparent: First, those are the only values where one can meaningfully talk about their normal form w.r.t. evaluation, because they are just constructor applications. Second, it becomes possible to prove that a weak call-by-value evaluation relation computes the same values—rather than just observationally equivalent ones—as Coq’s unrestricted conversion becomes possible. Third, type and proof erasure is only complete in this fragment, because detecting whether a certain term is erasable sometimes requires evaluating it fully, and full evaluation being to inefficient is a central reason extraction processes are needed.

2.2 Operational Semantics of MALFUNCTION in Coq

MALFUNCTION [Dolan 2016] is a “thin wrapper” around the untyped intermediate language of the OCAML compiler. It comes with an interpreter written in OCAML, and a compiler hooking into the OCAML compiler’s pipeline to either produce bytecode or native cmx files. Thus, it can make use of OCAML’s optimisations. Both interpreter and compiler expect its input in s-expression format. As such, MALFUNCTION is supposed to be easy to generate rather than easy to read, and thus fits our purpose perfectly. Explicitly, whenever the interpreter computes a value, the compiled code is expected to produce the same value. Thus, we can derive MALFUNCTION’s semantics in Coq purely from the interpreter, and as long as the derived semantics indeed matches, we have a guarantee that the compiled code behaves correctly by adding the MALFUNCTION compiler to the intermediate representation (which is essentially the identity function) and the OCAML compiler to our TCB.

The interpreter is defined in less than 300 lines of (impure) OCAML code and serves as the specification. It uses an environment for variables and a higher-order abstract syntax (HOAS) representation [Pfenning and Elliott 1988] of values for function thunks, i.e., reuses OCAML functions to represent MALFUNCTION function thunks. Most other features of MALFUNCTION are specified using the corresponding feature in OCAML and mutable references: The operational semantics of the Mlazy constructor is defined using the corresponding lazy primitive in OCAML, mutable vectors are defined using mutable references and for let rec constructs, the mutual recursive knot is tied via references.

To define a specification for MALFUNCTION in Coq, we need to define a semantics matching the interpreter in Coq, and for this, we cannot rely on impure features of the language. This means that we need to make explicit the notion of heap [SemanticsSpec.v] in the operational semantics. To make sure that our notion of semantics is closely related to the initial version in OCAML, we proceed in two steps.

First, to disentangle the (non-terminating) interpreter from our formal proof, we provide an inductive, weak call-by-value evaluation relation eval [SemanticsSpec.v] in Coq, closely following the OCAML interpreter, but using the heap explicitly instead of relying on imperative feature of the language. This relation requires a local environment locals to be defined on open terms. We simply specify it using a function in Coq:

\[
\text{Inductive eval (locals : Ident.t → value) : heap → t → heap → value → Prop := ...}
\]
We also provide a functional interpretation of `let rec` instead of relying on the imperative one. It depends on an explicit strictly-positive representation of values.

Second, as a sanity check, we define a Coq function acting exactly as the interpreter for MALFUNCTION implemented in OCaml, with the difference that we use an explicit heap and provide a machine-checked proof that whenever a program evaluates to a value for this predicate, then the interpreter computes this value. This is only possible by switching off termination checking in Coq locally because the evaluated term may be non terminating so there is no guarantee that the interpreter will terminate in Coq.

Then, to trust that the resulting semantics matches the intended semantics as specified in Malfunction (i) the reference interpreter of MALFUNCTION written in OCAML has to be correct w.r.t. the compiler, (ii) our pure Coq implementation of the interpreter has to be correct, which can be validated by extracting it to OCAML and unit testing against the reference interpreter.

The unsafe proof that our relational semantics relates to the MALFUNCTION interpreter is just a sanity check that our formal semantics relates to the proposal of [Dolan 2016] and is not required in our correctness theorems. Therefore, the fact that it switches off the termination checker is not crucial. However, it should be noticed that by making this proof, we actually found a bug in the bound check for vectors of MALFUNCTION reference interpreter. The interpreter was performing an out of bounds vector access and subsequently crashing rather than reporting the access. We also discovered a miscompilation of pattern matchings in the MALFUNCTION compiler due to a change in OCaml 4.14+flambda (compiled programs were computing the wrong value or even segfaulting).

2.3 Extraction Theorem For First-Order Data Types

We now explain the exact statement of the first correctness theorem about terms of first-order data type detailing the exact pre-conditions.

We use Coq syntax to ease the task of ensuring that the theorem is exactly as claimed also for readers with less experience reading Coq code of the theorem verified_malfunction_pipeline_theorem [Pipeline.v].

We assume that we are working in a well-formed global environment containing declarations of definitions and inductive types, where all definitions are $\eta$-expanded. We explain the need for $\eta$-expanded terms in the next section.

Variable $\Sigma$: global_env_ext.
Variable $\Sigma H$: wf_ext $\Sigma$.
Variable $\Sigma exp$: expanded_global_env $\Sigma$.

We then fix a Coq-term $t$, which is also $\eta$-expanded and whose type in this environment is a first-order data type $i$ at some universe level $u$ with parameters and arguments $args$:

Variable $t$: term.
Variable $expt$: expanded $\Sigma [[]] t$.
Variables ($i$: inductive) ($u$: Instance.t) ($args$: list PCUICAst.term).
Variable $fo$: firstorder_ind $\Sigma$ (firstorder_env $\Sigma$ $i$).
Variable $typing$: $\Sigma; [[]] t \mapsto \map {mkApps (tInd i u)} args$.

To simplify the proof slightly, we also assume that all inductives in the environment have no parameters. This assumption could be removed at the cost of a slightly more tedious proof, we plan to do so for the final version of this paper.4

4Note that the restriction however does not really inhibit the expressivity of the theorem, since instead of parameters all inductives could simply declare their parameters as indices.
Verified Extraction from Coq to OCaml

Variable noParam : ∀ i mdecl, lookup_env Σ i = Some (InductiveDecl mdecl) → ind_npars mdecl = 0.

We then assume that t reduces using Coq’s reduction to a term v that is irreducible. Note that Coq’s reduction relations is maximally general and thus agnostic towards the specific reduction order used.

Variable v : term.
Variable v_red : Σ ; [] ⊢ t ⇝ ∗ v.
Variable v_irred : ∀ t’, (Σ ; [] ⊢ v ⇝ t’) → False.

We then define the environment Σ’ as the result of applying the middle-end of the extraction pipeline to the environment Σ and assume that there is a MALFUNCTION environment containing exactly the values of every definition of Σ’ compiled to MALFUNCTION.

Lastly, we assume that after erasure, only extractable inductive types remain in the global environment. Concretely, this enforces some numerical maximums on number of constructor and number of arguments of constructors and that the environment contains no axioms. This numerical checks are here because for instance Coq’s inductive types can have as many constructors as needed, whereas in OCAML and MALFUNCTION there are explicit bounds on their numbers. For technical reasons, we prefer to deal with it as an axiom that is invoked exactly once in the proof of the erasure pipeline. This approach allows us to still get an (unsafe) extraction procedure for Coq’s terms that do not meet those restriction. See Section 3 for more details.

We can then prove that in this environment, the compilation of t evaluates to the value translation of v in MALFUNCTION, leaving the heap h it is run in unchanged:

Theorem verified_malfunction_pipeline_theorem : ∀ (h : heap),
  eval Σ’ empty_locals h (compile_malfunction_pipeline expt typing) h (compile_value_mf Σ v).

In the above, compile_malfunction_pipeline is the function compiling a Coq term to a MALFUNCTION term and compile_value_mf is the function compiling a Coq first-order value (i.e., a value in a first-order data type) to a MALFUNCTION value. The function empty_locals is used to encode the empty local environment and returns an error on every identifier.

For instance, the irreducible Coq term @cons B true (@cons B false (@nil B)) (i.e., the list [true, false]) is translated to block (tag 0) 0 (block (tag 0) 1) 0, because cons is the first constructor of list with arguments (thus tag 0), true is the first constructor of B not taking arguments (thus 0), false is the second constructor of B not taking arguments (thus 1), and nil is the first constructor of list not taking arguments (thus 0). This semantics follows OCAML’s internal representation of values in order to enable interoperability.

2.4 Extraction Theorem For First-Order Functions

Outside the first-order data type fragment, there is no hope to state and prove a meaningful theorem in terms of evaluation to particular values because there is no control on the translation of the body of functions, which are open terms. But we can however characterise the compilation of first-order functions in terms of interoperability—or to phrase it in a more foundational manner, in terms of realisability semantics. To this end, we define a notion of values realising in MALFUNCTION a first-order data type coming from Coq. Concretely, we define a notion of OCAML type, camlType [RealizabilitySemantics.v], that only contains function types (Arrow) and algebraic data types (Adt).

Inductive camlType : Set :=
  Arrow : camlType → camlType → camlType
  | Rel : N → camlType
  | Adt : kername → N → list camlType → camlType.
The type $\text{Rel}_n$ refers to the $n$-th mutually defined data type in an $\text{Adt}$. We can construct a function $\text{CoqType}\_\text{to}_\text{camlType}$ [Firstorder.v] that builds an $\text{Adt}$ from any first-order data type of Coq. Finally, to state the correctness theorem for firstorder function, we need to define what it means for a value $v$ to be a realiser of $\text{adt}$ at number $\text{ind}$, noted $v \vdash (\text{adt}, \text{ind})$. The number specifies which type of the potentially mutually defined $\text{Adt}$ is realised.

Then, with similar hypothesis as in Section 2.3, we can prove the following interoperability theorem (interoperability_firstorder_function [Firstorder.v]$^5$) for a first-order function $f$. To reduce technical details, we assume a function that maps one type of a mutual first-order inductive type $\text{mind}$ to another—the generalisation to arbitrary first-order functions is mathematically straightforward, but contains a lot of tedious technical manipulations.

**Theorem** interoperability_firstorder_function:

$\forall \text{typing} : \Sigma; [] \vdash f : \text{tProd} \text{na} (\text{tInd} (\text{mkInd kn ind}) []) (\text{tInd} (\text{mkInd kn ind'}) [])$,

let $\text{adt} := \text{CoqType}\_\text{to}_\text{camlType} \text{mind fo in}$

let $\text{compile}_f := \text{compile}_\text{malfunction}\_\text{pipeline} \text{expt typing in}$

$\forall \text{arg : t}$,

$(\forall (h \text{ h'} : \text{heap}) (v : \text{value}), \text{eval} [] \text{ empty_locals h arg h' v} \rightarrow v \vdash (\text{adt}, \text{ind})) \rightarrow$

$(\forall (h \text{ h'} : \text{heap}) (v : \text{value}), \text{eval} [] \text{ empty_locals h (Mapply (compile}_f, [\text{arg}]) h' v} \rightarrow v \vdash (\text{adt}, \text{ind})).$

The crux of the proof lies in three main ingredients. First, se show that compilation to MALFUNCTION is modular in the sense that a non-erasable application (e.g., of firstorder type) in Coq is compiled to the application of the compiled function to its compiled argument in MALFUNCTION. Second, it uses the fact that any value realising an $\text{Adt}$ coming from a first-order data type can be obtained by the compilation of a Coq term (camlValue\_to\_CoqValue [Firstorder.v]), i.e., we prove a decompilation theorem from MALFUNCTION values to COQ values. Lastly, it crucially uses the fact that the evaluation of compiled terms does not change the heap; i.e., compilation to MALFUNCTION produces pure terms.

Note that the second aspect is not valid outside the first-order fragment, because the function $\text{impure}$ defined in Section 1.1 does not correspond to the compilation of any Coq function.

3 THE MAN IN THE MIDDLE: $\lambda_\square$, AN INTERMEDIATE PLATFORM FOR EXTRACTION

In this section, we describe the middle-end of the extraction process. The language $\lambda_\square$ was introduced by Letouzey [2004] as an operational model of Coq after computationally irrelevant parts—i.e., types and proofs—are all erased to the same particular value $\square$. It was first mechanised by Sozeau et al. [2019b] in their correctness proof of type and proof erasure, with a focus on weak call-by-value semantics. We integrate this erasure procedure into a pipeline with multiple translation steps to finally extract to OCAML.

Those multiple steps are necessary because, like Coq, $\lambda_\square$ has higher-order constructors, structural fixpoints with principal arguments that have to reduce to a constructor for the fixpoint to unfold, and no dedicated evaluation strategy. On the other hand, constructors in OCAML are blocks (e.g., cons by itself is not well-typed, only cons$(x, 1)$ is), let $\text{rec}$ does not indicate a special principal argument, and evaluation is a variant of weak call-by-value reduction. These subtle differences pose challenges for machine-checked reasoning, since they are traditionally ignored in proofs on paper. We parametrise the evaluation relation of $\lambda_\square$ in various flags which can be used to alter it to avoid code duplication, and give separate correctness proofs while gradually translating the

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$^5$At the time of writing, the proof of this theorem is done over an abstract notion of compilation that satisfies the properties mentioned in the text. The formal connection with our concrete pipeline properties—in particular dealing with the concrete pre- and post-conditions of the pipeline—requires still few days of work.
which is a well-typed function in Coq.

The erasure pipeline as a whole transforms a program from TemplateCoq (an environment and
program) into an erased program, with term asts representing the value types and evaluation relations from TemplateCoq (weak call-by-value evaluation of Gallina terms) being simulated by evaluation of erased programs, where evaluation has no rule for pattern-matching on □ and uses an unguarded fixpoint expansion rule (i.e., one argument is enough to trigger fixpoint
unfolding) and a representation of constructors as blocks.

In this section, we concisely outline the different phases, focusing on the pre-conditions for their
correctness, the post-conditions they establish, as well as the evaluation relations and observational
equivalence on values they use when it is not simply syntactic equality. A more detailed overview
of the passes is given in Appendix A.

**Eta-expand.** This phase η-expands all fixpoints and constructors. For instance, the term map cons,
which is a well-typed function in Coq but not in OCaml, is η-expanded to the convertible term

\[
\text{map cons} : \text{List} T \rightarrow \text{List} T \rightarrow \text{List} T
\]
map (fun x => cons x) which is also well-typed in OCaml. Because METACoq does not include \( \eta \)-expansions in its theory yet, for reasons discussed by Lennon-Bertrand [Lennon-Bertrand 2022], the correctness proof of this phase is just assumed together with the correctness of the quotation phase. The pre-condition is well-typedness of \( t \) in the global environment \( \Sigma \), written \( \exists T, \Sigma ; [] \vdash t : T \) in the Coq formalisation. The post-condition is well-typedness of the return term \( t' \) and \( \eta \)-expandedness of all constant definition in \( \Sigma \) and \( t' \). Both evaluation relations are weak call-by-value evaluation of the formalisation of Coq in Coq.

**Translation to PCUIC.** PCUIC is the idealised calculus underlying Coq used in METACoq. Technically, this translation removes casts and makes application unary to ease meta-theoretical proofs. The translation is always valid there is no pre-condition, and the post-condition is that the translated term and environment do not contain casts. The main property of this phase is that it preserves well-typedness. The evaluation relation of the target is weak call-by-value evaluation of PCUIC.

**Lets in constructor types.** Constructors in Coq can be defined as \( C (x_1 : X_1) (x_2 := t_2) (x_3 : X_3) \) where \( X_3 \) can use both \( x_1 \) and \( x_2 \), and dually, pattern-matching can bind these defined arguments, while these let-bindings are not actually stored in constructor applications. We translate away such bindings via substitution to ease several verifications later on. As far as we know, Coq is the only language supporting let-bindings in constructor types, which is a useful feature when specifying inductive relations. This translation brings the language closer to usual presentations of algebraic datatypes. The phase has no pre-condition and ensures that in the translated term, constructor types are functional and pattern-matching reduction only involves a simple substitution. It preserves well-typedness and \( \eta \)-expandedness of fixpoints and constructors and the evaluation relation is simplified. This phase is the least economical in terms of proof-engineering as we must show a type preservation theorem for the whole theory of PCUIC: the proofs amount to 10kLoC.

**Type and proof erasure.** This phase goes from PCUIC to \( \lambda_\Box \). We use the verified type and proof erasure procedure due to Sozeau et al. [2019b]. The pre-condition of this phase requires well-typedness of the term. The post-condition cannot be well-typedness anymore because \( \lambda_\Box \) is untyped and erasure breaks typing. However, to still control the shape of the output term, the post-condition gives a well-scopedness condition. This phase preserves \( \eta \)-expandedness of constructors and fixpoints and the target evaluation relation is the weak call-by-value relation of \( \lambda_\Box \), with structural fixpoints, match on \( \Box \), and higher-order constructors. The observational equivalence on values for this phase is more complex and makes use of an erasure relation, which only agrees with the syntactic equality on first-order values. This weaker notion of equivalence is however enough to get our final theorem because it will ultimately be restricted to first-order values.

**Unary fix translation.** The evaluation of fixpoints in Coq and up-to this point of the pipeline is performed by evaluating its structural argument to a constructor application and then unfolding the fixpoint. The structural argument is the one guaranteeing termination and thus other unfolding strategies are not safe. However, in OCAML, evaluation of fixpoints is performed in a similar way as \( \beta \)-reduction, by always evaluating its first argument to a value and then unfolding the fixpoint. This rule is called the “unary fixpoint rule”. So the purpose of this phase, which is the identity on programs, is to justify that enabling the unary fixpoint rule in the target preserves evaluation of programs. It crucially relies on fixpoints being eta-expanded so that when they get unfolded in an evaluation path, we have a guarantee that their structural argument already evaluates to a constructor.

**No parameters.** This phase removes parameters from inductive types in the global context and from constructor applications. It requires \( \eta \)-expandedness of constructors to be performed. As an output, it guarantees that programs are well-formed, when the use of parameters is disallowed.
Remove match on □. This phase removes case analysis on □, the residue of erased computational case analysis on proofs, by replacing occurrences of the term `match □ with C a₁ ... aₙ ⇒ t end` immediately by t applied to n-many □. This is necessary, because we are going to implement □ as a recursive function in MALFUNCTION, meaning a naive translation of the case analysis would produce segmentation faults. This phase has no pre- and post-conditions as it is purely syntactic. Its unique interest is to justify disabling the rule for `match □` in the target.

Inline projections. Primitive projections correspond to a negative treatment of pattern-matching when the inductive type under consideration is a record type. This produces more efficient code and enables η-conversion for record types that have at least one constructor. This transformation phase inlines primitive projections as `match`, it requires no pre-condition and guarantees syntactically that no projections are left in the translated program.

Constructors as blocks. Because constructors of inductive types are fully applied in OCAML and MALFUNCTION, this phase translates any application of a constructor C n [] (where n is the name and [] is the a priori empty list of fields of the constructor) to a full list of arguments a₁,...,aₙ to C[a₁,...,aₙ]. This transformation has no specific pre- and post-conditions, and its puporse is to enable the rules treating constructors as blocks in the evaluation of a program.

Enforce extractability. For extraction in MALFUNCTION to be correct, we need to check that

1. inductives have at most as many constructors as fit into OCAML’s integer type,
2. inductives have at most 200 constructors non-constant constructors,
3. constructors have at most as many arguments as fit into OCAML’s array type,
4. no axioms occur in the global environment,
5. no □, named or existential variables, projections, or co-fixpoints remain in the term or context.

Note that we explicitly assume these conditions are fulfilled for the proof an Axiom and do not abort extraction if they are not fulfilled. This is in order to ensure that also programs that do not fall in the scope of the correctness theorem can be extracted, especially ones which have axioms.

Implement □. This phase implements □ as a fixpoint that consumes its argument, i.e., as `fix f x := f`. It requires well-formedness as pre- and post-conditions and ensures that □ does not appear anymore in the translated program.

Linearise case. Let-binds the discriminee of cases, i.e., replaces `match d with ... end` by `let x := d in match x with ... end`. This makes the translation to `switch` and `field` later in MALFUNCTION preserve complexity of programs. The reason we perform this translation at this stage is that it is easier to verify with variables represented as de Bruijn indices, but harder once variables are names as it will be the case in next phase.

Named variables and environment semantics. This phase translates terms with de Bruijn indices to non-capturing, named terms. For named terms, an environment semantics with a dedicated value type (containing amongst others closures and recursive closures) is used. We use two unfolding relations, unfolding respectively a named term or a value in an environment to a term with de Bruijn variables. This phase has no pre-condition and ensures as post-condition that there exists a well-formed term s such that t (with names) unfolds to s. After this phase, evaluation is switched to a named environment semantics.

Global environments. Several of the passes need to do lookups on the global environment, e.g., to compute the number of parameters of an inductive type. Global environments are represented as an association list of unique identifiers to declarations of constants and inductive types in MetaCoq. While this allows a straightforward formalisation of the well-formedness predicate on global contexts naturally representing dependencies between declarations, this is a very suboptimal datastructure to use when transforming programs, as they generally need to lookup information in the global environment, which can contain thousands of declarations. This problem is well-known
in the literature about compiler programming in Coq, with specialists resorting to highly optimised
tree datastructures [Appel and Leroy 2023] to avoid performance issues inside Coq and after
extraction. Hence we intersperse transformations that turn a well-formed environment represented
as a list into a lookup table based on AVL trees that can be used for fast lookups. Some of our
transformations, e.g., erasure itself, are nested, so they need to follow the order of declarations
given by the association list and likewise produce association lists as outputs, while relying on the
efficient environment representation for lookups. A subtlety that appears during formalisation is
that we generally need to show global environment weakening lemmas on our transformations so
that we don’t need to extend our efficient global environment structures after handling each entry
in the environment but can leave it untouched for a whole pass. This solely rests on the fact that
identifiers are globally unique in a well-formed environment, with this well-formedness condition
being carried around throughout the pre- and post-conditions of all our transformations.

Compilation from $\lambda\Box$ to Malfunction. The last pass in our extraction pipeline replaces the
case analysis $\text{match } x \text{ with } C_1 a_1 ... a_n \Rightarrow t_1 | ... \text{ end}$ by $\text{switch } x \text{ with } C_1 \Rightarrow (\text{fun } a_1 ... a_n \Rightarrow t_1) (\text{field } 1 x) ... (\text{field } n x) | ... \text{ end}$, translates constructors without arguments to integers, constructors with
arguments to $\text{block (tag n) ...}$, and mutual fixpoints to mutual $\text{let rec}$ blocks. Its precondition
is that the term is extractable, i.e., the five conditions explained above for the enforce extractability
phase. The post-condition ensures that the resulting Malfunction program is well-formed, mean-
ing there are no free variables, all constants are declared, blocks are tagged with an integer less
than 200, and every occurring $\text{switch}$ does not have an empty list of branches.

4 VERIFIED EXTRACTION AS A DROP-IN REPLACEMENT
In this section, we discuss our contribution from the point of view of a practical tool, neglecting
its formal guarantees, and thereby comparing it to Coq’s current extraction to OCaml [Letouzey
2004] which is not formally verified.

Coq’s current extraction has several features that we have not discussed until now:

1. It allows the user to enable optimisations of the generated code via $\text{Set Extraction Optimize}$. Optimisations are e.g., commutation of function application and $\text{match}$, simplifying $\text{let}$s
where the bound term only occurs once in the body, etc.

2. It generates a .mli interface by re-inferring types of the generated code using the type
inference algorithm $\mathcal{M}$ [Lee and Yi 1998]. Because the code might be ill-typed in OCaml’s
type system, $\text{Obj.magic}$ is heuristically inserted, resulting in the types of extracted code to
contain $\text{Obj.t}$.

3. It supports separate extraction to .ml files matching the module structure of the corresponding
Coq code.

4. It allows fine-tuning of the extracted code by the user providing $\text{Extract Constant}$ and $\text{Extract
Inductive}$ directives. This is for instance used to map Coq’s $\text{B}$ type to the one of OCAML
(whcih has an exactly swapped memory representation).

5. It allows fine-tuning of the extracted code by the user providing a $\text{Extract Inline}$ directive,
meaning a constant is always unfolded.

6. It extracts terms of type $\{ x : A \mid P x \}$ where $P$ is a propositional predicate to terms of type
corresponding to $A$ in OCAML.

Regarding (1), the benchmarks in Section 6 indicate that the optimisations do not have a relevant
impact on performance. Instead, they seem mainly to have readability and following standard
certain OCAML programming paradigms of the generated code in mind. This is not relevant to our
work because we provide low level code with formal guarantees instead.
Regarding (2), since we bypass OCaml’s type checker, we only have to generate .mli files for the parts of the extracted code that can and should be exposed, i.e., for first-order functions. We provide an .mli printer for such functions, which has a simple implementation since it has to solve a significantly simpler problem than the type reinference algorithm. Nevertheless, we support extracting higher-order code, but require the user to annotate the types in the .mli file manually.

Regarding (3), separate extraction is mainly a concern for readability of code, which we have not considered. However, we could easily implement it if users demand for it.

Regarding (4), the reason we do not provide such directives is that it is almost impossible to guarantee their correctness. However, it would not be hard to do so if users demand for it—with the cost that it is easy to break correctness. There are three frequent use cases:

First, to direct extraction to extract Coq’s \(B\) to OCaml’s bool, which is a subtly different type: Coq’s \(\text{Inductive } B := \text{true} | \text{false}\) has true as first constructor, which will thus be represented as integer 0 in memory, whereas OCaml’s type bool = false | true has false as first constructor, thus true being represented as integer 1. Here, we advocate for using such type conversion explicitly when calling and receiving arguments of an extracted Coq function explicitly, i.e., by converting between the two types.

Secondly, to direct extraction to extract Coq’s unbounded \(\mathbb{N}\) to OCaml’s int. However, this extraction is plain wrong, because int is not unbounded. It is however still correct on small enough numbers. Here, we thus advocate for proving this property for small enough numbers explicitly on the Coq side. This is possible because Coq features a primitive integer type, see below.

Thirdly, to direct extraction to extract Coq’s primitive integer and float types to the corresponding types in OCaml. This use case is already supported since Coq’s primitive types are declared as axioms, and our extraction just maps all axioms to a call to a module called Axioms that has to be provided by the user. We however lack a correctness proof, see Section 8.

Regarding (5), inlining definitions during extraction is mainly concerned with readability of code and thus not relevant for us. Where inlining is performance-critical, it will likely be performed by OCaml’s compiler.

Regarding (6), unboxing such types would potentially even be beneficial for performance, see Section 8 on future work.

Thus, we estimate that our verified re-implementation of Coq’s extraction is almost ready to replace Coq’s current extraction mechanism on safe use-cases.

5 BOOTSTRAPPING A SELF-HOSTING COMPILER

A compiler is called self-hosting if it is implemented in the same language it is a compiler for. This is the case for us: Our extraction process is implemented in Coq, and translates Coq to MALFUNCTION. The process to obtain a first executable (e.g., by using a different) compiler is called bootstrapping.

Since Coq is a dependent type theory, already its type checker comes with the ability to execute programs. Thus, in principle, two ways of bootstrapping are conceivable:

First, using the existing, unverified extraction from Coq to OCaml (implemented in OCaml). This means that in the bootstrapping process, this unverified extraction algorithm becomes part of the TCB.

Secondly, by executing the extraction pipeline live in Coq using Coq’s execution mechanisms once on itself. Unfortunately, execution in Coq is not very performant (which, of course, is the main reason why extraction is needed). In this case, we could not manage to make the process terminate, because Coq is exhausting its stack. Even setting ulimit -s unlimited does not help on our working machines—but it would be an interesting experiment to let it run longer on a more performant server.
Our bootstrapping method via the existing extraction to OCAML works. However, we have to patch the generated OCAML files to circumvent some bugs of the current extraction mechanism. Patching is fine because we have no guarantee on this phase anyway, but it illustrates the limitations of current extraction mechanism. By statically adding the resulting .mlf file to the repository, and using it to re-extract new future versions of the extraction pipeline, the use of the existing extraction can be limited to the initial bootstrapping once and for all, meaning it is not crucial that it is kept a part of Coq in the future.

Note that our correctness theorem does not yet apply to the bootstrapped extraction pipeline. Concretely, we would have to (i) slightly change the input format to be a first-order data type by modelling annotated universe instances with potentially empty lists instead of provably non-empty lists, and then do a validation pass on the new input format ensuring the lists are not empty. (ii) cover primitive operations for integers and floats in the theorem, because they are needed for printing integers and floats to strings in the output.

Especially the second part requires a global change to MetaCoq, most crucially to its operational semantics and typing judgment, so we leave it for future work.

6 BENCHMARKS

We compare the performance of extracted code comparing Coq’s current extraction to OCAML, CertiCoq’s extraction to C, and our verified extraction to Malfunction. All benchmarks are run on a 11th Gen Intel(R) Core(TM) i7-1165G7 @ 2.80GHz and Coq version 8.17.1. We use the same benchmark set as used in the evaluation of CertiCoq by Paraskevopoulos [2020], namely:

- **demo1**, appending two lists of booleans of length 500 and 300.
- **demo2**, mapping negation on a list of 100 booleans (using the higher-order function map).
- **list_sum**, computing the sum of a list containing 100 times the number 1.
- **vs_easy**, compiling the VeriStar [Stewart et al. 2012] prover for a fragment of separation logic and deciding the validity of an easy entailment.
- **vs_hard**, same as **vs_easy**, but with a harder entailment.
- **binom**, constructing two binomial queues, merging them, and finding the maximum element, using a verified implementation of binomial queues [Appel 2023; Vuillemin 1978].
- **color**, coloring a graph using a formally verified implementation of the Kempe/Chaitin algorithm [Appel 2023; Chaitin et al. 1981]. Note that this benchmark is not executed with OCAML extraction, because the generated code contains type errors.
- **sha**, computing the SHA-256 hash of a string consisting of 484 characters.

For OCAML we use version 4.14.0 with f1ambda enabled and both the bytecode and native-code compilers. We set and unset the (heuristic, unproved) optimisations Coq’s current extraction performs on the code. For CertiCoq, we use commit version a5323b8 from November 2023. We compile the resulting code with gcc with both no optimisations and gcc -O1. For verified extraction to Malfunction, we compare performance by disabling optimisations when calling the OCAML compiler pipeline, or calling it with the default of two rounds of optimisations.

In total, we compile code by eight different means (the results are depicted in Table 1): By Coq’s current extraction to OCAML, with Set Extraction Optimize and using the ocamlc bytecode compiler (1st column) or the ocamlopt native-code compiler (2nd column). By Coq’s current extraction to OCAML, with Unset Extraction Optimize and using the ocamlc bytecode compiler (3rd column) or the ocamlopt native-code compiler (4th column). By CertiCoq, using gcc for C compilation (5th column) or gcc -O1 for C compilation (6th column). By verified extraction to Malfunction, using malfunction cmx -O0 compilation (7th column) or malfunction cmx -O2 compilation (8th column).
We observe that compiling our code with the default optimisations has performance very similar to using the OCaml native-code compiler ocamlopt. On some benchmarks our extraction produces slightly faster code vs_easy, whereas on others it produces slightly less performant code. The performance difference can be explained for instance by differences in pattern matching compilation, where the OCaml compiler tries to optimise heavily and MALFUNCTION performs some mild optimisations. In all cases, we outperform CertiCoq with gcc.

Unrelated to the contributions of this paper, we observe that Set Extraction Optimize has a somewhat unpredictable effect on the performance: Sometimes it leads to a slight performance gain (e.g., for the vs_easy benchmark), sometimes it leads to a slight slowdown (e.g., for the binom benchmark). However, this means that the current optimisations are mainly of cosmetical nature, i.e., are concerned with obtaining more efficient code. The notable exception could be unboxing dependent pair types \{x : A \mid P x\} with a propositional predicate P (which can be seen as refinement or subset types) such that elements of this type are treated as elements of type A, rather than as pairs of an element of type A and a □. In future work, we would like to analyse whether performing such an optimisation at type and proof erasure time is beneficial.

7 RELATED WORK

There are several ongoing projects on obtaining correct programs in industrial programming languages like OCaml, Haskell, or C from programs in richly typed dependent programming languages like Coq, Lean, Idris, and Agda, or the simple type theories underlying Isabelle/HOL, HOL light, or HOL4. Our project is closely related to all of them, but has a separable motivation. We want to replace the current extraction process of Coq to OCaml [Letouzey 2004] with a verified process, without causing maintenance issues in the projects using extraction.

The ConCert project [Annenkov et al. 2021, 2020] is a platform to extract Coq code to ML-like and blockchain languages. Since most target languages they consider are not specified and their implementation is under constant evolution, the final phase of their extraction process is trusted pretty-printing.

The CertiCoq project [Anand et al. 2017; Appel et al. 2022] aims at extracting Coq code to the C light interface of CompCert. The objectives of the project are different in that it is not supposed to replace Coq’s extraction, but rather supplement it. CertiCoq relies on the \(\lambda_0\) pipeline presented in and contributed by this paper. Most but not all following phases of CertiCoq are verified, meaning it still lacks an end-to-end theorem.

The Candle project [Abrahamsson et al. 2022] provides a verified implementation of HOL light in CakeML, and automatic extraction from HOL4 to CakeML is available [Myreen and Owens 2014]. Similarly, functions defined in Isabelle can be extracted [Hupel and Nipkow 2018], and a proof
checker of Isabelle has been verified in Isabelle based on this [Nipkow and Roßkopf 2021]. Euf [Mullen et al. 2018] formalises a subset of Coq and provides a verified compiler from this language to Assembly code. Pit-Claudel et al. [Pit-Claudel et al. 2022] report on a proof-producing translation of functional models into low-level code via relational compilation.

8 FUTURE WORK

Our current extraction pipeline makes the axiomatic assumption that \( \eta \)-expanding fixpoints and constructors does not change the values of first-order data types w.r.t. weak call-by-value evaluation. The easiest way to prove this is to extend MetaCoq’s reduction relation with a suitable notion of \( \eta \)-conversion. The difficulties of this are discussed by Lennon-Bertrand [2022].

Regarding features of Coq we support, we are missing two central syntactic constructs: Primitive operations on integers, floats, and arrays and co-fixpoints. For the former, one would have to extend the reduction semantics of MetaCoq with primitive operations, and thread the corresponding correctness proofs through the pipeline. In the target, one then has to prove that these functions can be correctly implemented using certain \textsc{MALFUNCTION} programs. Most likely, a program logic for \textsc{MALFUNCTION} would be helpful here, or alternatively a program logic for an envisioned variant of \textsc{OCaml} with formal semantics that can be compiled to \textsc{MALFUNCTION}. For the latter, there are different options: One is to implement co-fixpoints without sharing as thunked fixpoints. A second would be to use \textsc{MALFUNCTION}’s lazy construct, at the cost of letting extraction produce impure programs altering the heap.

Regarding an extension of our correctness theorem, we would like to work in the direction of proving a theorem of interoperability with an arbitrary higher-order fragment as long as the only effect used by the unverified \textsc{OCaml} program is nontermination, i.e., requiring that the heap remains unchanged. However, such properties cannot be enforced by \textsc{OCaml}’s type-checker automatically, meaning they would have to be manually verified by the user.

Regarding optimisations implemented in Coq’s current extraction mechanism, our benchmarks seem to indicate that they have no impact on performance. Thus, the only optimisation we plan on implementing is the one unboxing elements of subset types, i.e., extracting terms of type \( \{ x : A \mid P x \} \) to the type corresponding to \( A \).

Lastly, the middle-end of our extraction pipeline based on \( \lambda \square \) could be used as a more general platform for verified extraction. It is conceivable to implement type and proof erasure from other type theory-based proof assistants such as Lean or Agda to \( \lambda \square \), and it is conceivable to implement back ends to other programming languages than \textsc{OCaml}/\textsc{MALFUNCTION}. The CertiCoq project in its current stage can already be seen as such a back end to C.

9 CONCLUSION

We contribute a verified extraction process from Coq to the \textsc{OCaml} ecosystem via \textsc{Malfunction}, implemented and verified in Coq itself. Our proofs consider the actual semantics of Coq and the actual semantics of \textsc{Malfunction}, with no idealisations. Including the reusable intermediate pipeline based on \( \lambda \square \), our contributed code has about 40k lines of code.

Our central theorem covers first-order function, i.e., functions that take elements of ground type as input and output. We observe that this is the strongest possible theorem for interaction with unverified programs type-checked by the \textsc{OCaml} type checker \( \dagger \) since even slightly more higher-order functions cannot be safely called from \textsc{OCaml} programs under all circumstances.

Besides the specific results for extraction of programs from Coq to \textsc{OCaml}, we believe that the exposition has several valuable contributions: (i) it discusses proof techniques that should scale to \( \dagger \)With the exception of also covering Coq’s primitive integers, floats and arrays, which we leave to future work.
get similar results for other proof assistants and other target languages, (ii) it gives an exposition how to extract from type theory to (call-by-value) programming languages in general, and makes the invariants explicit and (iii) it collects known techniques for compilation, which are however nowhere presented in a unified, accessible way.

REFERENCES


A DETAILS ON $\lambda\Box$ PASSES

We here give more details for selected passes of the middle-end of our extraction process.

A.1 Eta-Expansion

The correctness proof of the translation of higher-order constructors to constructors as blocks in Appendix A.6 is straightforward if constructor applications are eta-expanded, in the sense that constructors are never only partially applied. Similarly, the translation from structural fixpoints to unary fixpoints benefits from fixpoints being syntactically fully applied.

It is straightforward to implement a translation which on the fly eta-expands constructors and fixpoints. However, lacking $\eta$-expansion in MetaCoq, proving correctness is not for free. Three strategies suggest themselves:

1. Eta-expand on the fly e.g., during type and proof erasure, and prove that the result computes correctly, which will require defining observational equivalence in the (untyped) target language $\lambda\Box$.
2. Eta-expand Coq terms first, and prove that the result is observationally equivalent, which will require defining observation equivalence in the source, i.e., either TemplateCoq or PCUIC.
3. Use a translation validation approach by expanding the Coq term and using $\eta$-conversion of the Coq kernel (not the verified MetaCoq conversion check).

Inspired by the ConCert project [Annenkov et al. 2020], which uses a similar approach for similar reasons, we choose to work with the last option. Once MetaCoq supports $\eta$-expansion, the translation validation can be replaced by a correctness proof of the translation following option (2).

The crucial theorem proves that the result of the translation is expanded, with the following definition (where we only show the interesting cases):

The expanded predicate is parameterised by a context $\Gamma$ that records for each de Bruijn variable how much it should be eta-expanded: this is used to force the eta-expansion of fixpoint variables. For constructors, we ensure that they are applied to at least the sum of the number of parameters of their inductive type and the number of assumptions of their argument context (definitions in the context of arguments do not appear at applications). Together with the typing precondition of eta_expand_expanded, we can strengthen this claim and guarantee that each constructor takes exactly the right number of arguments. However, expanded is stable by substitution while the more stringent requirement is not, unless we only work with well-typed terms. The precondition on the contexts $\Gamma'$ and $\Gamma$ ensures that each variable that is expanded $n$ times indeed has a universally quantified type which allows at least $n$ applications. Finally, the condition on $\Sigma g$ provides the connection between the association list of declarations $\Sigma$ and the efficient lookup table $\Sigma g$: they are observationally equivalent with respect to lookups.

The $\eta$-expansion functions themselves are relatively straightforward: eta_single builds an $n$-ary $\eta$-expansion of a term $\text{mkApps} t\ARGS$ starting with its type $ty$. Indeed we need to decorate the newly introduced $\lambda$-abstractions with their appropriate type for the expansion to be type preserving. For constructors, we lookup their type and expected number of arguments from the global environment in eta_constructor. For fixpoints, in eta_fixpoint, we only need to $\eta$-expand them up to their recursive argument, which is stored as $d.(rarg)$ in the fixpoint block definition. Finally, the eta_expand function maps through a term and applies $\eta$-expansion in the variable, constructor and fixpoint cases.

A.2 Type and Proof Erasure

The next pass is type and proof erasure, described by Letouzey [Letouzey 2004] and proved correct in Coq for the case of weak call-by-value evaluation by Sozeau et al. [Sozeau et al. 2019b, 2023]. We
briefly recall the structure of the proofs and the relevant theorems, but use mathematical syntax rather than Coq code to indicate that the results do not form a part of the contribution of the present paper.

Following Letouzey, we define an erasure function $\mathcal{E}$ yielding a $\lambda\Box$ term provided a well-typed term of Coq’s type theory. However, this erasure function is not closed under (weak call-by-value) evaluation, i.e., if $t$ evaluates to $v$, then not necessarily $\mathcal{E}t$ evaluates to $\mathcal{E}v$. Due to polymorphism such a property could only be reached by letting $\mathcal{E}$ perform (partial) evaluation on the source, which is contrary to the goals of extraction. Thus, Letouzey sets up a non-deterministic erasure relation which we write as “$t$ erases to $t’$” and proves the following theorem, which Sozeau et al. verify in MetaCoq.

**Theorem A.1.** Well-typed terms $t$ erase to $\mathcal{E}t$, and if a well-typed term $t$ evaluates to $v$ and erases to $t’$, then $v$ erases to $v’$ to which $t’$ evaluates.

The erasure function and relation only agree on terms if there is nothing to erase: this is the case for first-order values, i.e., the values of Coq types which neither contain proofs nor functions. We say that a term is a first-order value if it is the application of a constructor to first-order values. We say that a type is first-order if it is inductive, and all its parameters, indices, and field types are first-order.

**Lemma A.2.** (1) If $t$ is of first-order type and evaluates to $v$, then $v$ is a first-order value. (2) If $v$ is well-typed, a first-order value, and erases to $v’$, then $\mathcal{E}v = v’$.

In general, reduction in Coq is not specified to follow any particular strategy or path. However, evaluation specified by Malfunction is weak (i.e., no evaluation under function binders) and call-by-value (i.e., arguments are always evaluated before a function call). We prove the following:

**Theorem A.3.** If $t$ is of first-order type and reduces to the irreducible term $v$, then $t$ weak call-by-value evaluates to $v$. And in particular, then $\mathcal{E}t$ evaluates to $\mathcal{E}v$.

### A.3 Unary Fix Translation

The next pass is the identity as transformation, but changes a flag in the evaluation relation to use a unary rule for fixpoints, rather than a structural rule. Having a structural fixpoint rule with one argument being identified as the primary argument is one of the most special peculiarities of Coq, and, consequently, $\lambda\Box$.

Letouzey explains how this rule does not pose problems when extracting to OCAML and Haskell informally. He relies on two arguments [Letouzey 2004, §2.6.4]:

- that in the user syntax of Coq, the body of a fixpoint with the $n$-th argument being the principal argument has to start with $n$ abstractions syntactically. While this is indeed true for the user syntax, it is not true for the type theory implemented in Coq, and thus not true for PCUIC. Here, the lambdas only have to occur after reduction.
- that one can implement a translation of general structural reduction to recursors by using the accessibility predicate $\text{Acc}$, as suggested by Paulin-Mohring [Paulin-Mohring 1996, p. 103] in 1996. However, with the current implementation of Coq’s guardedness checker updated by Gimenez [Giménez 1996] in 1998, no such translation is currently known.

Instead of solving this generally hard problem in type theory, we work around it by observing that for eta-expanded fixpoints the two semantics indeed agree. Eta-expandedness of fixpoints was already established in the first pass, we make use of this as a pre-condition here. We omit details of the proof, which is straightforward.
Since the translation is the identity, we do not have to define any function and can immediately state the correctness theorem:

**Lemma** eval opt to target $\Sigma t v : isEtaExp_env \Sigma \rightarrow wf_glb \Sigma \rightarrow eval \Sigma t v \rightarrow isEtaExp \Sigma [] t \rightarrow eval \Sigma t v$.

The crux of the proof is that if all fixpoint applications are $\eta$-expanded, then during weak call-by-value evaluation, if we encounter a fixpoint application it will always have the structural argument reduce to a value. As the fixpoint body start with at least as many $\lambda$-abstractions as the structural argument, the unary fixpoint expansion rule plus as many $\beta$-reduction steps simulates the guarded fixpoint rule.

### A.4 Removal of Parameters

This pass removes parameters from inductives in the global context and from constructor applications. This is mainly an optimisation.

As the constructors are $\eta$-expanded and the parameters never participate to the reduction, they can be removed without affecting the evaluation. They just will not appear in values of inductive types anymore.

We do not go into details.

### A.5 Remove Match on $\square$

To ensure that the application $\square \square$ reduces to $\square$ we will implement $\square$ as a recursive function in the target that consumes and ignores its argument. We then need to ensure that subexpressions of the form `match $\square$ with $Ca_1 \ldots a_n \Rightarrow t$ end` do not occur, since case analysis on a function will result in a segfault. Thus, we statically replace such case analyses immediately by $t$ applied to $n$ times $\square$. We do however keep empty pattern-matchings on $\square$ as they correspond to case analysis on empty types. These are stuck terms that are guaranteed never to occur on the evaluation path to a value, i.e. dead code.

This translation checks if a singleton case analysis or projection is performed on a propositional inductive type (in Prop or SProp) and expands it according to the number of arguments of its single constructor. Similarly to let-binding expansion, this statically performs a reduction that is otherwise performed by evaluation using a specific case-on-prop rule, so it is straightforward to show preservation of evaluation.

### A.6 Constructors as Blocks

The syntax of $\lambda\square$ allows two forms of applying a constructor with name $n$ to an argument $a$. First, via explicit application `tApp (tConstruct c []) a`. Secondly, via the fields of the constructor `tConstruct c [a]`. Depending on which switch is set, the evaluation semantics will treat them differently. In this pass, we translate from the first to the second representation.

We first show the adapted rules of the evaluation relation which treats constructors as blocks:

```plaintext
Definition atom [wfl : WcbvFlags] $\Sigma t ::=$
  match t with
  | tBox | tCoFix _ | tLambda _ | tFix _ | tPrim _ => true
  | tConstruct ind c [] => negb (with_constructor_as_block wfl) \& isSome (lookup_constructor $\Sigma ind c)
  | _ => false
end.
```
Inductive eval [wfl: WcbvFlags]: term → term → Set :=
  (** Case *)
  | eval_iota_block ind pars cdecl discr c args brs br res :
  @with_constructor_as_block wfl = true →
  eval discr (tConstruct ind c args) →
  constructor_isprop_pars_decl Σ ind c = Some (false, pars, cdecl) →
  nth_error brs c = Some br →
  #|args| = pars + cdecl.(cstr_nargs) →
  #|skipn pars args| = #|br| →
  eval (iota_red pars args br) res →
  eval (tCase (ind, pars) discr brs) res

  (** Constructor congruence *)
  | eval_construct_block ind c mdecl idecl cdecl args args' :
  @with_constructor_as_block wfl = true →
  lookup_constructor Σ ind c = Some (mdecl, idecl, cdecl) →
  #|args| = cstr_arity mdecl cdecl →
  All2_Set eval args args' →
  eval (tConstruct ind c args) (tConstruct ind c args')

Note that the application constructor in $\lambda_\square$ is unary, i.e., it applies a function to exactly one argument. However, for the present translation, we need to accumulate all arguments to a function. This pattern can easily be implemented using an accumulator argument. We here show how to solve it once and for all in Coq, by using a view and the equations plugin [Sozeau and Mangin 2019]:

Section transform_blocks.
Variable (Σ: GlobalContextMap.t).

Section Def.
Import TermSpineView.

Equations? transform_blocks (t: term): term
by wf t (fun x y : EAst.term ⇒ size x < size y):=
  | e with TermSpineView.view e := |
  | tApp u v napp nnil with construct_viewc u := |
  | view_construct ind i block_args with GlobalContextMap.lookup_constructor_pars_args Σ ind i := |
  | Some (npars, nargs) ⇒
  | let args := map_InP v (fun x H ⇒ transform_blocks x) in
  | let' (args, rest) := MCList.chop nargs args in
  | EAst.mkApps (EAst.tConstruct ind i args) rest |
  | None ⇒
  | let args := map_InP v (fun x H ⇒ transform_blocks x) in
  | EAst.tConstruct ind i args |
  | view_other _ _ ⇒ mkApps (transform_blocks u) (map_InP v (fun x H ⇒ transform_blocks x)) |
  | |
  | tConstruct ind i block_args ⇒ EAst.tConstruct ind i [] |
  | (* ... *).

Definition switch_constructor_as_block fl: WcbvFlags :=
EWcbvEval.Build_WcbvFlags fl.(@with_prop_case fl.@with_guarded_fix) true.

End Def.

The definition is done by well-founded induction on the size of the term, and we immediately apply a view of the term which decomposes it into a (non-applicative) head and a spine of arguments. We can then check if the head of the term is a constructor and move the application’s arguments to the argument field of the tConstruct constructor. We rely on $\eta$-expandedness of constructors to ensure correctness. The application of the resulting constructor to the rest arguments might seem uncanny, as it would mean that constructors can be over-applied. This is only a trick used
Section Wcbv.
Context Σ.(global_declarations).

Inductive eval (E : environment): term → value → Set :=
| eval_var na v : lookup E na = Some v →
  eval E (tVar na) v
| eval_fix mfix idx nms : ∀ (Hlen : (idx < #| mfix |)),
  List.Vb (isLambda ◦ dbody) mfix →
  NoDup nms →
  Forall2 (fun d n ⇒ nNamed n = d) mfix nms →
  eval E (tFix mfix idx) (vRecClos (map2 (fun n d ⇒ (n, d.(dbody))) nms mfix) idx E)
| eval_fix_unfold f mfix idx a na na' av fn v E :
  eval E f (vRecClos mfix idx E') →
  Vb (fun x ⇒ isLambda (snd x)) mfix →
  NoDup (map fst mfix) →
  nth_error mfix idx = Some (na', tLambda (nNamed na) fn) →
  ∼ In na (map fst mfix) →
  eval E a av →
  eval (add na av (add_multiple (List.rev (map fst mfix)) (fix_env mfix E')(E'))) fn v →
  eval E (tApp f a) v

Fig. 4. Evaluation semantics for named terms

to facilitate the commutation lemmas of this transformation with substitution, which otherwise
would require a typing argument.

A.7 Named Variables and Environment Semantics

We describe a variant of λ□ with named variables, which is based on environments rather than
explicit substitution, and consequently uses a dedicated value type. We use a notion of unfolding a
dedicated value in a given environment to a term.

We first describe the type of values, which comes with four constructors:

Inductive value : Set :=
| vBox
| vConstruct (ind : inductive)(c : N)(args : list value)
| vClos (na : ident)(b : term)(env : list (ident × value))
| vRecClos (b : list (ident × term))(idx : N)(env : list (ident × value)).

The vBox constructor represents the value of the □ construct of λ□. The constructor constructor
represents the construct of an inductive ind with index c with a list of its arguments, which are
fully evaluated as well. The vClos constructor represents a closure, i.e., the value of an abstraction.
It carries the bound name na of the closure, the body b which is a (non-evaluated) term, and an
environment env with bindings for the names of b. Similarly, the vRecClos constructor contains a
list of (mutual) names and bodies as well as an index idx, indicating which body is represented,
and an environment env once again binding names in the mutual bodies.

Next, we describe the evaluation relation on named terms in a global environment Σ and named
environment E in Fig. 4.

The eval_var rule states that a variable evaluates to a value v according to the environment E. The
eval_fix rule states that a fixpoint tfix mfix idx evaluates to a recursive closure in environment E
which carries the names nms and bodies of the fixpoint mfix as well as the number idx and
the environment E, where nms is the list of names bound in the fixpoint (ruling out anonymous
Reserved Notation "\( \Gamma ; E \vdash s \sim t \)" (at level 50, \( E, s, t \) at next level).

Inductive represents : list ident \rightarrow \text{environment} \rightarrow \text{term} \rightarrow \text{term} \rightarrow \text{Set} :=
\begin{align*}
&| \text{represents_bound}_\text{tRel} \, \Gamma \, n \, a \, E : \text{nth_error} \, \Gamma \, n \, = \, \text{Some} \, \, n \, a \, \rightarrow \, \Gamma ; E \vdash \text{tVar} \, n \sim \text{tRel} \, n \\
&\text{|\text{represents_unbound}_\text{tRel} \, E \, v \, \Gamma \, s : \text{lookup} \, E \, n \, = \, \text{Some} \, v \rightarrow \text{represents}_\text{value} \, v \, s \rightarrow \Gamma ; E \vdash \text{tVar} \, n \sim s \\
&\text{|represents}_\text{tLambda} \, \Gamma \, n \, a \, E \, n \, a' \, b' : \text{na} \rightarrow \Gamma ; E \vdash \text{tLambda} \, \text{nNamed} \, \text{na} \, b \sim \text{tLambda} \, \text{na} \, b' \\
&\text{|represents}_\text{tFix} \, \Gamma \, E \, \text{func} \, \text{idx} \, n \, E \rightarrow \text{represents}_\text{value} \, \text{func} \, \text{idx} \, n \, E \\
\end{align*}

\text{NoUp} \, n \, E \rightarrow
\begin{align*}
&\text{All2_Set} \, \text{fun} \, d \, n \, = \, \text{d(name)} = \text{Named} \, n \rightarrow \text{mfix} \, n \, E \rightarrow \\
&\text{All2_Set} \, \text{fun} \, d \prime \rightarrow \text{(List} \, \text{rev} \, \text{mfix} \, \text{++} \, \Gamma ; E \, \text{d(dbody}) \sim d'} \text{(dbody)} \text{mfix} \, \text{mfix'} \rightarrow \\
&\Gamma ; E \vdash \text{mfix} \, \text{func} \, \text{idx} \sim \text{mfix} \, \text{func} \, \text{idx} \\
\end{align*}

\text{with} \, \text{represents}_\text{value} \, : \text{value} \rightarrow \text{term} \rightarrow \text{Set} :=
\begin{align*}
&\text{represents}_\text{value}_\text{tBox} \, : \text{represents}_\text{value} \, \text{vBox} \, \text{tBox} \\
&\text{represents}_\text{value}_\text{tClos} \, \text{na} \, E \, s \, \text{t} \, \text{na} : \text{na} \rightarrow \text{represents}_\text{value} \, \text{vClos} \, \text{na} \, s \, E \, \text{tClos} \, \text{na} \, t \\
&\text{represents}_\text{value}_\text{tConstruct} \, \text{vs} \, \text{ind} \, c \rightarrow \text{All2_Set} \, \text{represents}_\text{value} \, \text{vs} \, \text{ts} \rightarrow \text{represents}_\text{value} \, \text{vClos} \, \text{ind} \, c \, \text{vs} \, \text{tClos} \, \text{ind} \, c \, \text{ts} \\
&\text{represents}_\text{value}_\text{tFix} \, \text{vfix} \, \text{func} \, \text{idx} \, \text{e} \\
&\text{All2_Set} \, \text{fun} \, d \rightarrow \text{isLambda} \, \text{snd} \, \text{vfix} \rightarrow \text{List} \, \text{rev} \, \text{(map} \, \text{fst} \, \text{vfix}) ; E \vdash \text{snd} \, \text{vfix} \rightarrow \text{d(dbody)} \, \text{vfix} \, \text{mfix} \rightarrow \text{represents}_\text{value} \, \text{vRecClos} \, \text{vfix} \, \text{func} \, \text{idx} \, \text{e} \, \text{tFix} \, \text{func} \, \text{idx} \\
&\text{where} \, \text{\"} \, \Gamma ; E \vdash s \sim t \, \text{\"} := \text{represents} \, \Gamma \, E \, s \, t.
\end{align*}

\text{Fig. 5. Unfolding relation between named terms / values and de Bruijn terms}

binders via wildcards). Furthermore, there is a precondition ensuring that that every mutual body is syntactically an abstraction. Lastly, the eval\_fix\_unfold rule states that an application tApp f a evaluates to value v if f evaluates to a recursive closure vRecClos mfix idx E' where all bodies in mfix are syntactically abstractions, where the names in mfix are duplicate-free, the mutual body at position idx in mfix is an abstraction binding na with body fn, and na is not occurring in the recursive names of the fixpoint. Furthermore, a has to evaluate to a value av, and evaluating fn yields v in the environment E' extended with all recursive bindings of mfix and na bound to av.

Next, we describe a representation relation between de Bruijn terms s and named terms t in a context \( \Gamma \) and environment \( E \). Intuitively \( \Gamma; E \vdash s \sim t \) means that given a term \( t \) with free variables in \( \Gamma \), unfolding the term \( s \) in the environment \( E \) yields \( t \). The relation is mutually inductive with a relation \( \vdash_{\text{v}} s \sim_{\text{v}} t \) between values \( v \) and de Bruijn terms \( t \). We describe the rules for tRel and tFix, as well as all rules for the value relation in Fig. 5.

The represents\_bound\_tRel rule unfolds a (bound) named variable tVar na to a de Bruijn variable tRel n by looking up the n-th name in \( \Gamma \). The represents\_unbound\_tRel rule unfolds an (unbound) named variable coqetVar na to a de Bruijn term s by looking up the value v at name na in the environment E, and by then unfolding \( v \) to \( s \). The represents\_tFix rule ensures unfolds tFix mfix idx to t Fix mfix' idx by ensuring that all bodies in mfix are syntactically tLambdas, ensuring that all bound names in mfix are indeed explicit names (identified by the list nms) rather than wildcards, and that these names are duplicate-free. Lastly, the bodies have to unfold pointwise, in the context List\_rev nms ++ \( \Gamma \). Note that the List\_rev comes in since the last mutual fixpoint bound in mfix will have de Bruijn index 0.

We first prove that if a value unfolds to a de Bruijn term \( s \) and \( s \) evaluates to \( t \), then \( v \) also unfolds to \( t \).

\text{Lemma eval\_represents\_value} \, \Sigma \, s \, t:
\begin{align*}
&\text{EWcbEval}\_\text{eval}\_\text{val} \, \Sigma \, s \, t \rightarrow \forall v, \vdash_{\text{v}} v \sim s \rightarrow v \sim_{\text{v}} t.
\end{align*}

Next, we prove a theorem relating unfolding and substitution:
Lemma represents_subst E s s' t v na:
~ In na (map fst E) →
≡ v ~ t →
[na]: E ⊩ s ~ s' →
[]: add na v E ⊩ s ~ csubst t 0 s'.

By induction, we can then lift the theorem about parallel substitution with a list:

Lemma represents_substl_rev E s s' ts nms vs Γ:
∀ na, In na nms → ~ In na (map fst E) →
NoDup nms → #| nms | = #| vs | →
All2 represents_value vs ts →
(nms ++ Γ): E ⊩ s ~ s' →
Γ; add_multiple nms vs E ⊩ s ~ substl ts s'.

Next, we introduce a well-formedness predicate wf v on values:
The predicate relies on a definition of sunny terms, see Fig. 6, which are terms that are not shadowing. For instance, an abstraction tLambda (nNamed na) M is not shadowing a list of names Γ if na does not occur in Γ and M does not shadow the extended context na :: Γ. We first prove that evaluating a sunny term yields a well-formed value:

Lemma eval_wf Σ E s v:
∀ d, match d.2 with ConstantDecl (Build_constant_body (Some d)) ⇒ sunny [] d | _ ⇒ true end Σ →
All (fun x ⇒ wf (snd x)) E →
map fst E ⊩ s →
E ⊩ s ~ s' →
wf v.

Lastly, we introduce an annotation function turning any term into a sunny term:

Fixpoint annotate (s: list ident) (u: term) {struct u}:
match u with
| tRel n → match nth_error s n with
| Some na ⇒ tVar na
| None ⇒ tRel n end
| tLambda na M →
  let na' :=
  match na with
  | nNamed na ⇒ if in_dec (ReflectEq_EqDec _) na s then gen_fresh na s else na
  | nAnon ⇒ gen_fresh "wildcard" s
  end
  in
  tLambda (nNamed na') (annotate (na' :: s) M)
(* ... *) end.

Lemma nclosed_represents Σ Γ E s:
wellformed Σ Γ || s → Γ; E ⊩ annotate Γ s ~ s.

Lemma sunny_annotate Γ s:
sunny Γ (annotate Γ s).

We can then prove the central theorem:

Lemma eval_to_eval_named_full Σ (Σ : global_context) s t:
wf_glob Σ →
∀ u, match u with
| tRel n → match nth_error s n with
| Some na ⇒ tVar na
| None ⇒ tRel n end
| tLambda na M →
  let na' :=
  match na with
  | nNamed na ⇒ if in_dec (ReflectEq_EqDec _) na s then gen_fresh na s else na
  | nAnon ⇒ gen_fresh "wildcard" s
  end
  in
  tLambda (nNamed na') (annotate (na' :: s) M)
(* ... *) end.

The actual proof of the theorem is by a generalised induction for any term u with Γ; E ⊩ u ~ s and sunny (map fst E) u.
Fixpoint sunny \( \Gamma (t:\text{term}) : \mathbb{B} := \)
match \( t \) with
| tRel i \Rightarrow \text{true}  
| tLambda (nNamed na) M \Rightarrow \text{fresh na} \land \text{sunny} (\text{na} :: \Gamma) M 
| tApp u v \Rightarrow \text{sunny} \Gamma u \land \text{sunny} \Gamma v 
(* ... *)
end.

Inductive \( \text{wf} : \text{value} \rightarrow \text{Type} := \)
| \( \text{wf}_v\Box \): \( \text{wf} \ v\Box \)
| \( \text{wf}_v\Clos \text{na} \text{b} \ E \): \( \sim \text{In} \text{na} (\text{map} \text{fst} \ E) \rightarrow \text{sunny} (\text{na} :: \text{map} \text{fst} \ E) \text{b} \rightarrow \text{All} (\text{fun} \ v \Rightarrow \text{wf} (\text{snd} \ v)) E \rightarrow \text{wf} (\text{vClos} \text{na} \text{b} \ E) 
| \( \text{wf}_v\Construct \text{ind} \text{c} \text{args} : \text{All} \text{wf} \text{args} \rightarrow \text{wf} (\text{vConstruct} \text{ind} \text{c} \text{args}) 
| \( \text{wf}_v\RecClos \text{vfix idx} \text{E} : \text{NoDup} (\text{map} \text{fst} \text{vfix}) \rightarrow 
\forall \text{nm}, \text{In} \text{nm} (\text{map} \text{fst} \text{vfix}) \rightarrow \sim \text{In} \text{nm} (\text{map} \text{fst} \ E) \rightarrow 
\text{All} (\text{fun} \ t \Rightarrow \text{sunny} (\text{map} \text{fst} \text{vfix} ++ \text{map} \text{fst} \ E) (\text{snd} \ t)) \text{vfix} \rightarrow 
\text{All} (\text{fun} \ v \Rightarrow \text{wf} (\text{snd} \ v)) E \rightarrow 
\text{wf} (\text{vRecClos} \text{vfix idx} \text{E}).

Fig. 6. Non-shadowing terms

A.8 Translation to Malfunction

We now describe the final translation of the version of \( \lambda_{\square} \) with unary fixpoints, constructors as blocks, no case analysis on \( \square \), using named variables with an environment semantics and an explicit value type to Malfunction in more details.

Three aspects of the translation functions are interesting:

First, constructors without arguments are solely represented as integers in OCAML, rather than as empty blocks with only a tag.\(^7\) To be able to interface with OCAML programs in the next section we use the same representation, even though not technically necessary for the first-order correctness theorem to hold. Since constructors are fully eta expanded, we can check whether they take arguments or not by case analysis on their field. See the first highlighted block in Fig. 7.

Secondly, \( \lambda_{\square} \) has an explicit case analysis construct, whereas Malfunction only has native \texttt{switch} and \texttt{proj} constructs. The operational idea is to use \texttt{switch} to decide on the branch, and then to replace the variables bound in the branches by the respective projections.

match \( d \) with
| A \Rightarrow x  
| C a b \Rightarrow f 
end

switch \( d \) with
| 0 \Rightarrow x |
| (\text{tag} 0) \Rightarrow (\text{fun} a b \Rightarrow f) (\text{proj} 0 d) (\text{proj} 1 d) |
end

Note that due to the weak call-by-value semantics we cannot substitute the variables directly, because such a translation would only be correct up to observational congruence. The introduced beta-redices might be unnecessary, but we leave it to the OCAML compiler to simplify them. As a result, our correctness statement can be stated again in terms of evaluation semantics only.

\(^7\)https://v2.ocaml.org/manual/intfc.html#ss:c-concrete-datatypes
Section Compile.
Context Σ: (global_declarations).

Definition Mapply_u t a := match t with Mapply(fn, args) ⇒ Mapply(fn, list.app.args[a] | _ ⇒ Mapply(t, [a]) end.

Equations compile (t: term): Malfunction.t
by wf t (fun x y: EAst.term ⇒ size x < size y) :=
  | tRel n ⇒ Mstring "tRel"
  | tBox ⇒ Mstring "Box"
  | tletIn nn fn bo ⇒ Mlet (t: (BasicAst.string_of_name nn, compile fn), compile bo)
  | tApp fn arg ⇒ Mapply_u (compile fn)(compile arg)
  | tCase i mch bars ⇒
    match lookup_constructor_args Σ i with
    | [] ⇒ Mnnum (numconst_Int (nonblocks until m num_args))
    | _ ⇒ Mblock (int_of Int num_args, map_InP args (fun x H ⇒ compile x))
  | None ⇒ Mstring "inductive not found"
end
| tfix mfix idx ⇒
  let bodies := map_InP mfix (fun d H ⇒ (BasicAst.string_of_name d.(dname)), compile d.(dbody)) in
  Mlet ([Recursive bodies], Mvar (fun n ⇒ compile (n.1)))
| tProj (Kernames.mkProjection ind _ nargs) bod with lookup_record_projs Σ ind :=
  | [] ⇒
    | let len := Lst.length args in
    | Mfield (int_of Int (len - 1 - nargs), compile bod)
  | None ⇒ Mstring "Proj"
| tCoFix mfix idx ⇒ Mstring "TCofix"
| tVar _ _ ⇒ Mstring "Evar"
| tPrim p ⇒ to primitive p.
Proof.
all: try (cbn; lia).
- unfold id in H. change size with (fun x ⇒ size x) at 2. cbn [size]. exact H.
- eapply (in_size snd size) in H. cbn in ↔ lia.
- eapply (in_size dbody size) in H. cbn in ↔ lia.
Qed.

End Compile.

Fig. 7. Final compilation phase to Malfunction

Definition blocks_until i (num_args: list N) :=
  | filter (fun x ⇒ match x with 0 ⇒ false | _ ⇒ true end)(firstn i num_args).

Definition nonblocks_until i num_args :=
  | filter (fun x ⇒ match x with 0 ⇒ true | _ ⇒ false end)(firstn i num_args).

Definition Mcase : list N • t • list (list Ident • t) • t :=
  fun (num_args, discr, brs) ⇒
  Mswitch (discr, mapi (fun i ⇒ [nms, b] ⇒
  match nth_error num_args i with
  | Some 0 ⇒ [Malfunction.Inrange (int_of Int (nonblocks until i num_args), int_of Int (nonblocks until i num_args))]
  | _hasargs ⇒ [Malfunction.Tag (int_of Int (blocks until i num_args))]
end,
  Mapply_u (Mlambda][(nms, b), mapi (fun i _ ⇒ Mfield (int_of Int i, discr))(nms))] brs).
we use recursive closures as values, rather than trying to build a function closure

\begin{verbatim}
Fixpoint compile_value 'H:Heap) Σ (\Sigma:EAst.global_declarations) (s:EMcbvEvalNamed.value) : SemanticsSpec.value :=
  match s with
  | vBox ⇒
    RClos (fun _ ⇒ fail "empty", ["reccall"], [RFunc ("_", MalfunctionMvar "reccall")], 0)
  | vClos na b env ⇒ Func (fun x ⇒ match lookup (map (fun 'x,v ⇒ (x, compile_value Σ v)) env) x with Some v ⇒ v | None ⇒ fail "notfound" end), na, compile Σ b)
  | vConstruct i m [] ⇒
    match lookup_constructor_args Σ i with
    | Some num_args ⇒ let num_args_until_m := first n m num_args in
      let index := #| filter (fun x ⇒ match x with 0 ⇒ true | _ ⇒ false end) num_args_until_m in
      SemanticsSpec.value_Int (Malfunction.Int, BinInt.Z.of_N index)
    | None ⇒ fail "inductive not found"
  end
  | vRecClos mfix idx env ⇒
    RClos ((fun x ⇒ match lookup (map (fun 'x,v ⇒ (x, compile_value Σ v)) env) x with Some v ⇒ v | None ⇒ fail "notfound" end), (map fst mfix),
      map (fun \_\_ ⇒ b) ⇒
      match b with
      | EAst.tLambda na bd ⇒ RFunc ((BasicAst.string_of_name na), compile Σ bd)
      | _ ⇒ Bad_recursive_value
  end
  end.
\end{verbatim}

Fig. 8. Compilation function for values

Thirdly, to translate Coq’s `fix`, we use a recursive `let` in Malfunction, as highlighted in Fig. 7. We show the compilation function of values in Fig. 8. The translation is straightforward and should not require more explanation.

To get an elegant verification of the correctness of the translation of fixpoints it is crucial that we use recursive closures as values, rather than trying to build a function closure `Func` with a circularity in the body, e.g., through a fixed-point combinator.

The correctness statement reads:

\begin{verbatim}
Lemma compile_correct 'H:Heap) Σ Σ' s t Σ Γ h :
  \(∀\Sigma'b, EGlobalEnv.lookup_inductive Σ i = Some (mb, ob) → (\#\Sigma\Sigma'EAst.ind_constructors| \Sigma'\to\Sigma\Sigma'Malfunction.Int63.wB ∧ ∃\Sigma'b, nth_error ob (EAST.ind_constructors) n = Some b → b(EAST.cstr_nargs) < int_to_N Array.max_length) → (∃\Sigma\Sigma'b, Malfunction.Ident.Map.find na Γ = match lookup Γ na with Some v ⇒ compile_value Σ v | _ ⇒ fail "notfound" end) → (∃\Sigma\Sigma'b, decl_body na EGlobalEnv.declared_constant Σ c dec1 = \Σ\Σ'EAst.cst_body decl = Some body → EMcbvEvalNamed.eval Σ [] body v ← In ((Kernames.string_of_kername c, compile_value Σ v) Σ) →
  EMcbvEvalNamed.eval Σ Σ' s t → SemanticsSpec.eval Σ Γ h (compile Σ s) h (compile_value Σ t).\)
\end{verbatim}

The first two lines state preconditions about the global environment: All declared inductives can have at most as many constructors as there are machine integers (in order for tags to still fit into a block), and the arity of constructors cannot be higher than the maximal length of an array (in order for the arguments to fit into a block).

The third line relates the local `\(\lambda_Ω\)` environment `Γ` with the Malfunction environment `Γ'`, whereas the fourth line relates the global `\(\lambda_Ω\)` environment `Σ` with the Malfunction environment `Σ'`.

The final line then states the correctness: Whenever a `\(\lambda_Ω\)` term evaluates, the compiled term evaluates to the value produced by `compile_value`. 