Certified Symbolic Transducer with Applications in String Solving

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Abstract

Finite Automata (FAs) are fundamental components in the domains of programming languages. For instance, regular expressions, which are pivotal in languages such as JavaScript and Python, are frequently implemented using FAs. Finite Transducers (FTs) extend the capabilities of FAs by enabling the transformation of input strings into output strings, thereby providing a more expressive framework for operations that encompass both recognition and transformation. Despite the various formalizations of FAs in proof assistants such as Coq and Isabelle/HOL, these formalizations often fall short in terms of applicability to real-world scenarios. A significant limitation of classical FAs and FTs is that transition labels are typically defined as a single character from a finite alphabet. However, in practical applications, the alphabet of an FA or FT can be enormously large or even *infinite*. The classical approach to formalizing transitions can result in transition explosion, leading to critical performance bottlenecks of FA and FT operations.

A more pragmatic approach involves the formalization of symbolic FAs [12] and FTs [34], where transition labels are symbolic and potentially infinite. While the formalization of symbolic FAs has been explored in the work of CertiStr [17], the formalization of symbolic FTs in interactive proof assistants remains largely unexplored due to the increased complexity challenges. In this paper, we aim to formalize symbolic FTs within the Isabelle/HOL framework. This formalization is refinement-based and is designed to be extensible with various symbolic representations of transition labels. To assess its performance, we applied the formalized symbolic FTs to an SMT string solver for modeling replacement operations. The experimental results indicate that the formalized symbolic transducer can efficiently and effectively solve string constraints with replacement operations.

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1 Introduction

Finite Automata (FA) and Finite Transducers (FT) are fundamental constructs in the theory of formal languages, with extensive applications in programming languages and software engineering. For example, recent advancements in string solvers, as demonstrated by [8], have illustrated the relationship between regular expressions in modern programming languages and various forms of FAs and FTs. Additionally, FAs and FTs find significant industrial applications, such as in the verification of AWS access control policies [3].

Even though there are various formalizations of FAs and FTs in interactive proof assistants such as Isabelle [2] and Coq [1], these are predominantly based on classical definitions. However, these traditional approaches present certain limitations when applied to practical scenarios. One significant drawback is that transition labels are typically non-symbolic and finite. A conventional transition is represented as $q \xrightarrow{a} q'$, where a is a character from a finite alphabet. This simplistic representation can lead to a phenomenon known as transition explosion. For example, if the alphabet Σ encompasses the entire Unicode range, which is common in modern programming languages, it consists of `0x110000` distinct characters. Defining a transition from state q to q' that accepts any character in Σ would require splitting into `0x110000` individual transitions, rendering the FA and FT operations highly inefficient. Furthermore, in practical applications, it is often necessary to consider infinite alphabets, such as the set of all integers.

Symbolic Finite Automata (SFA) and Symbolic Finite Transducers (SFT) [12, 34] represent advanced extensions of classic FAs and FTs, enhancing their applicability in practical scenarios. These symbolic models utilize transition labels defined by first-order predicates over boolean algebras, allowing for more expressive representations. For example, a transition label might be specified as an interval ($'\mathtt{a}' -' \mathtt{z}'$), encompassing all characters from $'\mathtt{a}'$ to $'\mathtt{z}'$, or as an arithmetic condition ($x \mod 2 = 0$), denoting all even numbers. This symbolic approach not only provides a more succinct representation but also supports infinite alphabets, thereby extending the expressive capabilities of FAs and FTs.

However, the formalization of transition labels in SFAs and SFTs presents significant challenges within interactive proof assistants. Two fundamental considerations arise: first, the representation of transition labels must be sufficiently expressive to accommodate diverse predicate representations of boolean algebras; second, the formalization framework must be designed with extensibility in mind to facilitate the incorporation of new boolean algebras while minimizing redundant proof efforts.

Prior work of CertiStr [17] has successfully formalized SFAs within Isabelle/HOL, demonstrating both the efficiency and effectiveness of SFAs in practice. However, the formalization of SFTs remains an open challenge, primarily due to their inherent complexity in two aspects: the formalization of transition labels and the specification of transition output functions. SFTs constitute a significantly more expressive and powerful theoretical framework compared to SFAs, as evidenced by their capability to model complex string transformations such as replacement operations. Furthermore, numerous studies have demonstrated the broad applicability of SFTs across diverse domains. The work of [34] showcases SFTs in security-critical applications, particularly for cross-site scripting (XSS) prevention. [15] extends this security focus by applying SFTs to web application sanitizer analysis. In system verification, [36] employs SFTs for runtime behavior monitoring, while [16] demonstrates their utility in automated program transformation through systematic inversion techniques.

In this work, we present a comprehensive formalization of SFTs. To address the extensibility challenges inherent in supporting diverse transition label theories, we adopt a refinement-based approach. At the abstraction level, transition labels are formalized through the fundamental mathematical concept of *sets*. This abstraction facilitates subsequent refinement to various representations of Boolean algebras, such as intervals and arithmetic predicates, while maintaining theoretical consistency.

The key operation of our formalization is the product operation between an SFT and an input regular language. Specifically, given an SFA $\mathcal{A}$ representing a regular language and an SFT $\mathcal{T}$, we define the product operation $\mathcal{T} \times \mathcal{A}$ that characterizes the output language generated by $\mathcal{T}$ when processing inputs from the language recognized by $\mathcal{A}$.

In the refinement level, we implemented transition labels using an interval-based representation to examplify the refinement process. The formalization of interval algebra provides efficient set-theoretic operations—including membership checking, intersection, and difference computations—facilitating the refinement of transition labels from abstract sets to concrete intervals. Furthermore, leveraging the data refinement framework [20] in Isabelle/HOL, we store states and transitions using sophisticated data structures such as hashmaps and red-black trees, ensuring efficient automata manipulation.

To evaluate the effectiveness and efficiency of our formalization, we developed a string solver compliant with SMT-LIB language [4], focusing particularly on replacement operations. We evaluated our implementation using a set of benchmarks from the SMT-LIB repository [26]. The experimental results demonstrate that our formalization achieves computational efficiency in constraint-solving scenarios.

In summary, our formalization makes the following contributions:

1. We present the first formalization of symbolic finite transducers in Isabelle/HOL proof assistant.
2. We leverage the refinement framework to create an extensible SFT formalization that is capable of accommodates various boolean algebras, ensuring adaptability to future transition label developments.
3. We develop an interval algebra with efficient set-theoretic operations, enabling refinement of transition labels from abstract sets to concrete intervals.
4. We demonstrate the practical utility of our formalization through its application to string constraint solving, specifically in modeling replacement operations with verified correctness guarantees.

The remainder of this paper is organized as follows: Section 2 introduces the formalization of symbolic finite transducers. Section 3 presents the product operation at the abstract level. Section 4 details the algorithmic refinement of the product operation. Section 5 demonstrates the application to string constraint solving. Section 6 discusses related work. Section 7 concludes with future directions.

2 Formalization of SFTs

We begin by presenting a mathematical definition of SFTs [34], abstracting from the specific implementation details of Isabelle/HOL.

2.1 The Mathematical Definition of SFTs

Let $\mathcal{U}$ be a multi-sorted carrier set or background universe, which is equipped with functions and relations over the elements. We use τ as a sort and $\mathcal{U}^\tau$ denotes the sub-universe of elements of type τ. We have a special type $\mathbb{B}$ with $\mathcal{U}^\mathbb{B} = \{\top, \bot\}$, which corresponds to the boolean type.

A lambda term is defined as $\lambda x.\ t$ of type $\tau_1 \to \tau_2$. When τ_2 is $\mathbb{B}$, this lambda term is a predicate. Let ϕ be a predicate. We write $a \in [\![\phi]\!]$ if $\phi\ a = \top$. For non-predicate lambda terms, we view them as functions that generate output elements of type τ_2 given input terms of type τ_1. With these notations and the above definitions, we can define SFTs as follows.

▶ **Definition 1** (Symbolic Finite Transducer). *A Symbolic Finite Transducer over $\tau_1 \to \tau_2$ is a quadruple $\mathcal{T} = (\mathcal{Q}, \Delta, \mathcal{I}, \mathcal{F})$, where*

- *$\mathcal{Q}$ is a finite set of states,*
- *$\mathcal{I} \subseteq \mathcal{Q}$ is the set of initial states,*
- *$\mathcal{F} \subseteq \mathcal{Q}$ is the set of accepting states,*
- *Δ is the set of transition relations. Each element in Δ is of the form (q, ϕ, f, q') or written as $q \xrightarrow{\phi, f} q'$, where q and q' are states in $\mathcal{Q}$. ϕ is a predicate of type $\tau_1 \to \mathbb{B}$. f is a lambda term of type $\tau_1 \to \tau_2$. f is called an* output function.

For each transition $q \xrightarrow{\phi, f} q'$, if there exists an element $a \in [\![\phi]\!]$, where a is called an input, then the application $(f\ a)$ is the output.

SFTs accept an input word and generate an output word. This can be defined by *runs* of SFTs. An SFT run σ is a sequence $(q_0, \phi_0, f_0, q_1), (q_1, \phi_1, f_1, q_2), \ldots, (q_{n-1}, \phi_{n-1}, f_{n-1}, q_n)$ such that $q_0 \in \mathcal{I}$ and $(q_i, \phi_i, f_i, q_{i+1}), 0 \leq i \leq n-1$ is a transition in Δ. σ is an accepting run when q_n is an accepting state.

For a word $w = a_0, \ldots, a_{n-1}$, it is accepted by σ if and only if $a_i \in [\![\phi_i]\!]$ for $0 \leq i \leq n-1$. When w is accepted, run σ generates an output sequence $w' = f_0\ a_0, \ldots, f_{n-1}\ a_{n-1}$. We define:

- $(a_0, (f_0\ a_0)), \ldots, (a_{n-1}, (f_{n-1}\ a_{n-1}))$ a *trace*,
- $a_0, \ldots, a_{n-1}$ the *input* of the trace and $(f_0\ a_0), \ldots, (f_{n-1}\ a_{n-1})$ the *output* of the trace.

If $a_0, \ldots, a_{n-1}$ is accepted by an accepting run in $\mathcal{T}$, we say that the trace is an accepting trace of $\mathcal{T}$. For a trace π, we denote its input as $in(\pi)$ and its output as $out(\pi)$. Given an SFT $\mathcal{T}$ and a word w, we define the *product* operation of $\mathcal{T}$ and w (denoted as $\mathcal{T} \times \{w\}$) as the set of outputs generated by $\mathcal{T}$ with input w. More precisely,

$$\mathcal{T} \times \{w\} = \{w' \mid \exists \pi.\ \pi \text{ is an accepting trace of } \mathcal{T} \wedge in(\pi) = w \wedge out(\pi) = w'\}.$$

To make the operation *product* more general, we extend the operation to an SFT and a set of input words represented by a regular language, which can be denoted by an SFA $\mathcal{A}$. More precisely,

$$\mathcal{T} \times \mathcal{A} = \{w' \mid \exists w.\ w \in \mathcal{L}(\mathcal{A}) \wedge w' \in \mathcal{T} \times \{w\}\},\ \text{where } \mathcal{L}(\mathcal{A}) \text{ denotes the language of } \mathcal{A}.$$

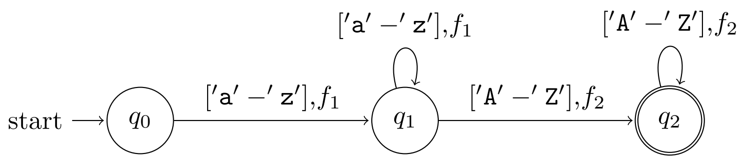

Figure 1 An example of SFT

Figure 1 illustrates an SFT that accepts words matching the regular expression $/['\texttt{a}' -' \texttt{z}'] + ['\texttt{A}' -' \texttt{Z}'] + /$. The transition labels utilize intervals of the form $[i\text{-}j]$, which are interpreted as predicates $\lambda x.\ i \leq x \leq j$. The output functions f_1 and f_2 perform case transformations: $f_1 = \lambda x.\ \texttt{toUpper}(x)$ converts lowercase letters to uppercase, while $f_2 = \lambda x.\ \texttt{toLower}(x)$ performs the inverse operation. For example, given the input string `"bigSMALL"`, this SFT produces the output `"BIGsmall"`.

2.2 The Isabelle/HOL Formalization of SFTs

As we have discussed the diversity of transition labels in Section 1, we now present an extensible formalization of SFTs that accommodates this variety. Our approach leverages the refinement framework (Refine_Monadic [19]) in Isabelle/HOL to achieve the flexibility and extensibility of transition labels modeling.

Figure 2 presents our formalization of SFTs in Isabelle/HOL. While the elements $\mathcal{Q}_t$, $\mathcal{I}_t$, and $\mathcal{F}_t$ directly correspond to their counterparts ($\mathcal{Q}$, $\mathcal{I}$, and $\mathcal{F}$) in Definition 1, the transition relations are not exactly the same. The transition relations are formalized through `LTTS` (Labeled Transducer Transition System), where each transition is represented as a triple $'q \times ('a\ \texttt{set option}\ \times' i) \times' q$. This representation reflects several key design decisions aimed at enhancing the abstraction and flexibility of our SFT formalization.

```
record ('q, 'a, 'i, 'b) NFT =
         𝒬_t :: "'q set"
         Δ_t :: "('q, 'a, 'i) LTTS"
         ℐ_t :: "'q set"
         ℱ_t :: "'q set"
         ℳ_t :: "'i ⇒ ('a, 'b) Tlabel"
type_synonym ('q, 'a, 'i) LTTS = "('q × ('a set option ×' i) ×' q) set"
type_synonym ('a, 'b) Tlabel = "'a option ⇒ 'b set option"
```

Figure 2 The formalization of $SFTs$ in Isabelle/HOL

Firstly, $'a$ set option is the input type of the transition, it accepts a set of elements of type $'a$ or `None` corresponding to empty string ε. Accepting a set of $'a$ elements aims to express the same but more abstract semantics of the input labels in Definition 1, in which an input label is a predicate. A predicate's semantics as introduced before represents a set of elements that make the predicate true. But predicates have various different forms. For instance, the interval $[1-9]$ represents the set $\{e \mid 1 \leq e \leq 9\}$. The predicate $\lambda b.\ b[7] = 1$, where b is a bit vector of length 8, denotes the set of bit vectors that have a 1 in the 7th position. All these different forms of labels are abstracted as sets in our formalization. The value `None` represents the empty string ε in our formalization, indicating a transition that consumes no input but may still produce output elements. This design choice facilitates the modeling of real-world applications in SFTs, as we will demonstrate in our application to string solvers.

The second element of type $'i$ serves as an index into the output function space. We use indices instead of functions themselves to enable the reuse of the same output functions for different transitions. The mapping $\mathcal{M}_t$ associates each index with a specific output function. These output functions, formalized by `Tlabel`, map a single input element to a set of possible output elements rather than to a single element. This design enables non-deterministic output behavior, where the transducer may select any element from the output set randomly or according to specified criteria. Additionally, output functions can produce the empty string ε by returning `None`, providing further flexibility in transition behavior.

3 The Product Operation of SFTs

In this section, we formalize the product operation between an SFT $\mathcal{T}$ and an SFA $\mathcal{A}$, denoted as $\mathcal{T} \times \mathcal{A}$ in Section 2. An additional consideration in this operation is the presence of ε-transitions in our SFT formalization, which implies that the resulting automata may also contain ε-transitions. Since CertiStr [17] does not include a formalization of SFAs with ε-transitions, we extend the framework in CertiStr with a formalization of symbolic SFAs with ε-transitions (denoted as εSFA) and provide a verified conversion to standard SFAs. In this paper, we present only the definitions of εSFAs and SFAs, while the complete formalization, including correctness proofs, is available in our Isabelle development.

Figure 3 presents the formalization of both SFAs and εSFAs using Isabelle/HOL record types `NFA` and `eNFA`, respectively. The εSFA formalization extends the standard SFA structure by introducing Δ'_e, which captures ε-transitions as pairs of states, while maintaining the same labeled transition relation Δ as in standard SFAs.

Having established these foundational definitions, we can now formalize the product operation.

```
record ('q, 'a) NFA =
        𝒬 :: "'q set"
        Δ :: "('q, 'a) LTS"
        ℐ :: "'q set"
        ℱ :: "'q set"

record ('q, 'a) eNFA =
        𝒬_e :: "'q set"
        Δ_e :: "('q, 'a) LTS"
        Δ'_e :: "('q *' q) set"
        ℐ_e :: "'q set"
        ℱ_e :: "'q set"

type_synonym ('q,' a) LTS = "'q ×' a set ×' q"
```

Figure 3 The formalization of εSFAs and SFAs

```
definition productT :: "('q,' a,' i,' b)" NFT ⇒ ('q,' a) NFA ⇒
            (('a,' b) Tlabel ⇒' a set ⇒' b set option) ⇒
            ('q ×' q, 'b) eNFA where
  "productT 𝒯 𝒜 F = ⦇
    𝒬e = 𝒬_t 𝒯 × 𝒬 𝒜,
    Δ_e = {((p,p'), the (((ℳ_t 𝒯) f) None), (q,p')) | p,p',q,f. p' ∈ 𝒬 𝒜 ∧
            (p,(None,f),q) ∈ Δ_t 𝒯 ∧ ∃S. (ℳ_t 𝒯) f None = Some S} ∪
          {((p,p'), the (F ((ℳ_t 𝒯) f) (σ1 ∩ σ2)), (q,q')) | p,p',q,σ1,σ2,q',f.
            (p,(Some σ1,f),q) ∈ Δ_t 𝒯 ∧ (p',σ2,q') ∈ Δ 𝒜 ∧ σ1 ∩ σ2 ≠ ∅ ∧
              ∃S. F ((ℳ_t 𝒯) f) (σ1 ∩ σ2) = Some S},
    Δ'_e = {((p,p'), (q,p')) | p,p',q,f. p' ∈ 𝒬 𝒜∧
            (p,(None,f),q) ∈ Δ_t 𝒯 ∧ (ℳ_t 𝒯) f None = None} ∪
          {((p,p'), (q,q')) | p,p',q,σ1,σ2,q',f.
            (p,(Some σ1,f),q) ∈ Δ_t 𝒯 ∧ (p',σ2,q') ∈ Δ 𝒜 ∧ σ1 ∩ σ2 ≠ ∅ ∧
              ∃x ∈ (σ1 ∩ σ2). ((ℳ_t 𝒯) f) (Some x) = None},
    ℐ_e = ℐ_t 𝒯 × ℐ 𝒜
    ℱ_e = ℱ_t 𝒯 × ℱ 𝒜 ⦈"
```

Figure 4 The formalization of product operation

Figure 4 depicts the abstract level formalization for the product of an SFT and an SFA. The parameters $\mathcal{T}$ and $\mathcal{A}$ are an SFT and an SFA, respectively. The result of the product operation is an εSFA. But we need to explain the role of parameter `F`. The output function f for each transition in Δ_t is of type "$'a$ option $\Rightarrow' b$ set option", which applies to a *single* element of type $'a$ or ε. `F` extends f to apply f to a set of elements. More precisely, let f be an output function, the semantics of `F` is defined as follows:

$$\texttt{F}\ f\ A = \texttt{Some}\ \left(\bigcup_{a\in A}(\text{if } f\ a = \text{Some } S \texttt{ then } S \texttt{ else } \emptyset)\right)$$

.

The transition relations Δ_e and Δ'_e are determined by considering two distinct cases based on the nature of transitions in the SFT: ε-transitions and non-ε-transitions. In both cases, the transition labels in the resulting εSFA are derived from the composition of the SFT's output function and the SFA's input labels. Let us consider Δ_e first.

1. When $(p, (\text{None}, f), q)$ is a transition in Δ_t, i.e. the input character is ε, and f None $\neq$ None. Consequently, the SFA $\mathcal{A}$ remains in its current state, and the product transition produces the output "$((\mathcal{M}_t\ \mathcal{T})\ f)$ None". Remember that f is just an index, $(\mathcal{M}_t\ \mathcal{T})\ f$ is the output function.
2. When $(p, (\text{Some}\ \sigma_1, f), q)$ is a transition in Δ_t, synchronization is possible only with SFA transitions that share characters with σ_1, i.e., $\sigma_1 \cap \sigma_2 \neq \emptyset$, where σ_2 represents the input label of the corresponding SFA transition. The resulting output is `F` $((\mathcal{M}_t\ \mathcal{T})\ f)\ (\sigma_1 \cap \sigma_2)$.

The transitions in Δ'_e follow a similar pattern with analogous cases for ε and non-ε transitions.

To establish the correctness specification of the product operation, we begin by formalizing the concept of SFT *traces* as introduced in Definition 1. In our formalization, traces are represented by the type $('a\ \text{option} \times' b\ \text{option})$ `list`, as shown in Figure 5. Given a trace π, we define two key projection functions: (1) `inputE`, which corresponds to $in(\pi)$ and extracts the input sequence (2) `outputE`, which corresponds to $out(\pi)$ and extracts the output sequence.

The definition `outputL` generalizes `outputE` to characterize the set of all possible outputs that an SFT $\mathcal{T}$ can generate when processing inputs from the language accepted by the SFA $\mathcal{A}$. The reachability of a trace π between states q and q' in an SFT $\mathcal{T}$ is verified by the predicate `LTTS_reachable` $\mathcal{T}\ q\ \pi\ q'$.

```
fun inputE :: ('a option × 'b option) list ⇒ 'a list where
  "inputE [] = []" |
  "inputE ((Some a, _) # l) = a # (inputE l)" |
  "inputE ((None, _) # l) = (inputE l)"

fun outputE :: "('a option ×' b option) list ⇒' b list" where
  "outputE [] = []" |
  "outputE ((_, Some a) # l) = a # (outputE l)" |
  "outputE ((_, None) # l) = (outputE l)"

definition outputL :: "('q,' a,' i,' b) NFT ⇒ ('q,' a) NFA ⇒' b list set"
 where
  "outputL 𝒯 𝒜 = {outputE π | π q q'. q ∈ ℐt 𝒯 ∧ q' ∈ ℱt 𝒯∧
                  LTTS_reachable 𝒯 q π q' ∧ inputE π ∈ ℒ 𝒜}"
```

Figure 5 The formalization of traces in SFTs

Figure 6 presents Lemma `productT_correct`, which establishes the correctness of the product operation. The lemma's assumptions, `F_ok1` and `F_ok2`, specify the essential properties of function `F`. The assumptions `NFT_wf` $\mathcal{T}$ and `NFA` $\mathcal{A}$ ensure that the SFT $\mathcal{T}$ and the SFA $\mathcal{A}$ are well-formed. The conclusion, marked by `shows`, demonstrates that the language of the constructed εSFA ($\mathcal{L}_e$ denotes the language of εSFA) from $\mathcal{T} \times \mathcal{A}$ coincides with the mathematical semantics defined by `outputL`, thereby establishing semantic preservation of the product construction.

```
lemma productT_correct:
  fixes 𝒯 𝒜 F
  assumes F_ok1: "∀ f s. (∀e ∈ s. f (Some e) = None) ⟷ F f s = None"
      and F_ok2: "∀ f s. F f s ≠ None ⟶ F f s =
         Some (∪ {S | e S. e ∈ s ∧ f (Some e) = Some S})"
      and wfTA: "NFT_wf 𝒯 ∧ NFA 𝒜"
    shows "ℒe (productT 𝒯 𝒜 F) = outputL 𝒯 𝒜"
```

Figure 6 The correctness lemma of the product operation

4 Algorithm Level Refinement

Having established the abstract definition of the SFT product operation in Section 3, we now present its algorithmic refinement. This section introduces an efficient implementation of the product construction and refines the abstract representation of transition labels to a concrete interval algebra, enabling practical computation.

4.1 Intervals

An interval is defined as a pair (i, j) (represented as $[i-j]$ as well in the paper) representing the set $\{e \mid i \leq e \leq j\}$. To achieve greater expressiveness, our formalization extends this notion to interval lists of the form $[(i_1, j_1), \ldots, (i_n, j_n)]$, which denote the set $\bigcup_{1 \leq k \leq n} \{e \mid i_k \leq e \leq j_k\}$. This generalization offers two key advantages: it enables more compact representation of transitions in SFAs and SFTs through merging, and it allows for efficient handling of interval operations without unnecessary splitting. For example, the set difference between intervals $(1, 5)$ and $(3, 4)$ can be directly represented as the interval list $[(1, 2), (5, 5)]$, which is also an interval.

Throughout the following discussion, we use the term "interval" to refer to interval lists. Our formalization provides a collection of interval operations through the following interface:

1. `semIs` i: Defines the semantic interpretation of an interval as a set. For an interval (i, j), `semIs` $(i, j) = \{e \mid i \leq e \leq j\}$.
2. `emptyIs` i: Tests whether an interval represents an empty set, i.e., whether `semIs` $i = \emptyset$.
3. `nemptyIs` i: Tests whether an interval represents a non-empty set, i.e., whether `semIs` $i \neq \emptyset$.
4. `intersectIs` i_1 i_2: Computes the intersection of two intervals, yielding an interval i such that `semIs` $i =$ `semIs` $i_1 \cap$ `semIs` i_2.
5. `diffIs` i_1 i_2: Computes the set difference of two intervals, yielding an interval i such that `semIs` $i =$ `semIs` $i_1 \setminus$ `semIs` i_2.

To facilitate formal reasoning and optimize performance, we introduce a canonical form for interval. An interval $[(i_1, j_1), \ldots, (i_n, j_n)]$ is in canonical form if it satisfies two key properties:

1. Each (i_k, j_k) is well-formed: $i_k \leq j_k$ for all $k \in \{1, \ldots, n\}$
2. Intervals are ordered and non-overlapping: $j_k < i_{k+1}$ for all $k \in \{1, \ldots, n-1\}$

We prove that all interval operations preserve canonical form when applied to canonically-formed inputs. This invariant serves two purposes: it simplifies formal proofs by eliminating the need to reason about malformed or overlapping intervals, and it enables more efficient implementations of interval operations by reducing the number of cases to consider.

4.2 Algorithmic Implementation of the Product Operation

In this subsection, we present the algorithmic implementation of the product operation between an SFT and an SFA[1]. Figure 7 illustrates the core algorithm `productT_impl`, which is implemented using the *Refine_Monadic* framework. Note that in the implementation, there are some refined operations: `nfa_states`, `nfa_trans`, `nfa_initial`, `nfa_accepting`, and `nft_tranfun`. These are corresponding to the states, transitions, initial states, accepting states, and output function mapping of the SFT.

The operation `prods_imp`, shown in Figure 8, computes the Cartesian product of two state sets. This function employs the `FOREACH` construct, a higher-order iteration operator analogous to OCaml's `Set.fold`. Specifically, given a set S, a function f of type $'a \Rightarrow' b \Rightarrow' b$, and an initial accumulator I of type $'b$, the expression `FOREACH` S f I systematically applies f to each element in S, accumulating results in a principled manner.

```
definition productT_impl where
  "productT_impl 𝒯 𝒜 F fe = do {
    Q ← prods_imp (nft_states 𝒯) (nfa_states 𝒜);
    (D1, D2) ← trans_comp_imp (nft_tranfun 𝒯) F fe
        (nft_trans 𝒯) (nfa_trans 𝒜) (nfa_states 𝒜);
    I ← prods_imp (nft_initial 𝒯) (nfa_initial 𝒜);
    F ← prods_imp (nft_accepting 𝒯) (nfa_accepting 𝒜);
    RETURN (Q, D1, D2, I, F)
  }"
```

Figure 7 The computation of SFT product

```
definition prods_imp where
  "prods_imp Q1 Q2 =
   FOREACH {q. q ∈ Q1} (λ q Q. do {
    S ← FOREACH {q. q ∈ Q2}
         (λ q′ Q′. RETURN ({(q,q′)} ∪ Q′)) ∅;
    RETURN (Q ∪ S)
   }) ∅"
```

Figure 8 The computation of Cartesian product of two state sets

A central algorithmic challenge in our implementation lies in the computation of transition sets `D1` (corresponding to Δ_e) and `D2` (corresponding to Δ'_e) in Figure 7. As shown in Figure 9, we implement this computation through the function `trans_comp_imp`, which computes the synchronization of transitions between the SFT and SFA. This function decomposes the synchronization process into two distinct cases, each handled by a specialized function:

1. `subtrans_comp_`ε: Processes ε-transitions in the SFT, where transitions consume no input but may produce output

[1] For clarity of presentation, we show a simplified version of the Isabelle/HOL implementation while preserving the essential algorithmic structure.

```
definition trans_comp_imp where
  "trans_comp_imp M F fe T1 T2 Q =
    FOREACH {t. t ∈ T1}
      (λ (q, (α, f), q′) (D1, D2).
        (if (α = None) then
          (subtrans_comp_ε M q f q′ F fe T2 D1 D2)
        else
          (subtrans_comp M q (the α) f q′ F fe T2 D1 D2)
      )) (∅, ∅)"
```

Figure 9 The computation of `trans_comp_imp`

2. `subtrans_comp`: Processes standard transitions in the SFT, where both input consumption and output generation may occur

```
definition subtrans_comp where
  "subtrans_comp M q α f q′ F fe T D1 D2 =
    FOREACH
      {t. t ∈ T} (λ (q1, α′, q1′) (D1, D2).
        (if (nemptyIs (intersectIs α α′)) then do {
          D1 ← (if (F (M f) (intersectIs α α′)) ≠ None)
            then
            let αi = the (F (M f) (intersectIs α α′)) in
            RETURN {((q,q1), αi, (q′,q1′))} ∪ D1
            else RETURN D1);
          D2 ← (if fe (M f) (intersectIs α α′) then
            RETURN {((q,q1), (q′,q1′))} ∪ D2 else RETURN D2);
          RETURN (D1, D2)
        }
        else (RETURN (D1, D2)))) (D1, D2)"
```

Figure 10 The computation of `subtrans_comp`

We now present the implementation of `subtrans_comp` in detail, as shown in Figure 10 (the implementation of `subtrans_comp_ε` follows analogous principles). For a transtion $(q, (\text{Some } \alpha, f), q')$ in the SFT, this function traverses all transitions in the SFA, represented by the set `T`. For each transition $(q_1, \alpha', q_1') \in$ `T`, the function performs two key operations when the intersection of input labels is non-empty ($\alpha \cap \alpha' \neq \emptyset$, verified using `nemptyIs`):

1. Computes non-ε-transitions (`D1`): When the output function applied to the intersection $\alpha \cap \alpha'$ yields a non-empty set, a new transition is added to `D1` with the computed output label.
2. Generates ε-transitions (`D2`): When there exists at least one input in the intersection $\alpha \cap \alpha'$ that produces an empty string (verified by checking if `M` f maps any element to `None`. The checking is implemented by `fe`), a corresponding ε-transition is added to `D2`.

The correctness of the product computation is established through a refinement proof, demonstrating that `productT_imp` (Figure 7) correctly implements the abstract specification

```
lemma productT_imp_correct:
assumes finite_TT: "finite (Δ_t 𝒯)"
    and finite_TA: "finite (Δ 𝒜)"
    and finite_Q: "finite (𝒬 𝒜)"
    and finite_TQ: "finite (𝒬_t 𝒯)"
    and finite_I: "finite (ℐ 𝒜)"
    and finite_TI: "finite (ℐ_t 𝒯)"
    and finite_F: "finite (ℱ 𝒜)"
    and finite_TF: "finite (ℱ_t 𝒯)"
shows "productT_imp 𝒯 𝒜 F fe ≤ SPEC (λA. A = productT 𝒯 𝒜 F)"
```

Figure 11 The refinement relation between `productT_imp` and `productT`

`productT` (Figure 4). This refinement relationship is formally specified in Figure 11, where we leverage the *Refine_Monadic* framework's data refinement.

The refinement is expressed through the relation $\mathbf{C} \leq \texttt{SPEC}\ \mathbf{A}$, which asserts that the concrete implementation $\mathbf{C}$ is an element of the abstract specification $\mathbf{A}$. More precisely, the concrete implementation must produce an εSFA that is structurally equivalent or isomorphic to the one produced by the abstract algorithm `productT`.

To establish this equivalence, we must prove that the εSFAs produced by `productT_imp` and `productT` are isomorphic in all essential components: the set of states, transition relations, ε-transition relations, initial and accepting state sets.

The implementation of `productT_imp` follows *Refine_Monadic* framework's interfaces for sets to store states and transition relations. The *Refine_Monadic* framework provides a way to automatically refine these interfaces to more efficient data structure, such as red-black trees or hashmaps. In our formalization, we refine the sets of storing states and transitions to red-black trees.

5 An Application to String Solving

In this section, we demonstrate the practical application of our formalized SFTs to string constraint solving, specifically focusing on replacement operations. While CertiStr [17] provides a verified framework for string constraint solving using SFAs, its capabilities are inherently limited by the expressiveness of SFAs. In particular, SFAs cannot directly model string transformation operations such as replacement.

Our string solver is based on CertiStr [17] by extending it with the modeling of replacement operations. CertiStr exploits forward-propagation to solve the string constraints. Our SFT modeling for replacement operations can seamlessly be integrated into CertiStr's forward-propagation framework.

5.1 Modeling the Replacement Operation

The string replacement operation, denoted as `replace(str, pattern, replacement)`, is a fundamental string transformation that takes three parameters:

- `str`: The input string to be transformed.
- `pattern`: A regular expression defining the matching criteria.
- `replacement`: The string to be substituted for the matched substring.

The semantics of the replacement operation can be formally characterized by two distinct cases:

1. When there exists at least one substring s' in `str` such that s' matches `pattern`, then s' is replaced with `replacement`.
2. When no substring of `str` matches `pattern`, the operation returns `str` unchanged.

The first case can be modeled by SFTs. We illustrate this case by an example. Given a replacement operation `replace`(s,`/[0-9]+/`,`"NUM"`), which means replacing a occurrence of the substring that matches the regular expression `/[0-9]+/` with the string `"NUM"`. We model this replacement operation by an SFT with the following 3 steps:

1. First, construct an SFA that recognizes the regular expression pattern `/[0-9]+/`. Transform this SFA into an SFT by augmenting each transition with an output function $f = \lambda x.$ `None` that produces the empty string.
2. Second, construct an SFA that accepts the replacement string `"NUM"`. Since a constant string can be viewed as a specialized regular expression, we can construct its SFA representation. Convert this SFA into an SFT by adding ε-transitions and appropriate output functions that emit the characters of `"NUM"` in sequence.
3. Finally, compose the two SFTs through concatenation and augment the resulting transducer with self-loop transitions at the initial and final states. These additional transitions, labeled with Σ (the set of all characters in the alphabet) and the identity function `id` $= \lambda x.\ x$, enable the SFT to process arbitrary prefixes and suffixes of the input string while preserving the replacement behavior on matched substrings.

Step 1. Figure 12 illustrates the construction of the pattern-matching component. The left side shows the SFA that recognizes the regular expression `/[0-9]+/`, while the right side presents its transformation into an SFT. This transformation is achieved by augmenting each transition with the output function `f` $= \lambda x.$ `None`, which consistently produces the empty string, effectively "consuming" the matched digits without generating output.

Figure 12 Corresponding SFA and SFT for `/[0-9]+/`

Step 2. Figure 13 depicts the automata for the replacement string `"NUM"`. The left side shows the SFA that accepts this constant string, while the right side presents its SFT transformation. The transformation employs an indexed output function `g` that emits characters of the replacement string sequentially:

$$\texttt{g} = \lambda\ i\ x.\ \texttt{match}\ i\ \texttt{with} \begin{cases} 1 \mapsto [(78,78)] & \text{(ASCII for 'N')} \\ 2 \mapsto [(85,85)] & \text{(ASCII for 'U')} \\ 3 \mapsto [(77,77)] & \text{(ASCII for 'M')} \\ \_ \mapsto \texttt{None} \end{cases}$$

This function maps transition indices to their corresponding character outputs, using ASCII codes to represent the string `"NUM"` character by character.

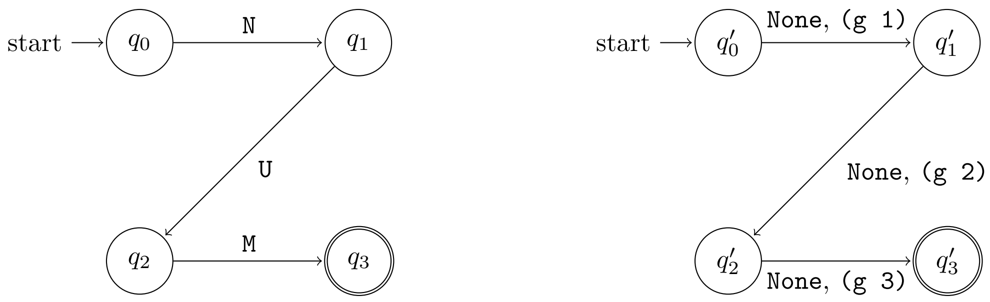

Figure 13 Corresponding SFA and SFT for `"NUM"`

Step 3. Figure 14 presents the complete SFT construction, obtained by composing the pattern-matching SFT (Fig. 12) with the replacement-generating SFT (Fig. 13). The composition process involves two key modifications:

1. Connect the two SFTs by adding ε-transitions (labeled with "`None, f`") from each accepting state of the pattern-matching SFT to the initial state of the replacement-generating SFT
2. Augment the resulting transducer with self-loop transitions at both ends, labeled with "Σ, `id`", where Σ represents the full alphabet. For the string solver, Σ is the set of all unicode characters. These transitions enable the SFT to process arbitrary input prefixes and suffixes while preserving the matched substring for replacement

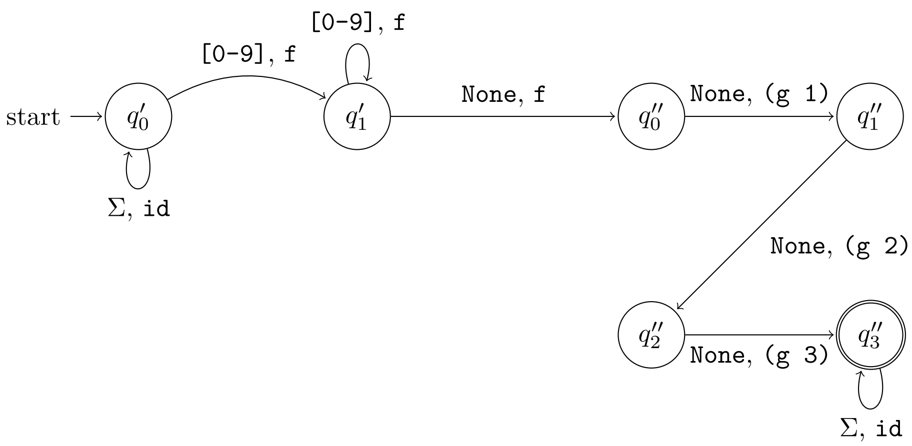

Figure 14 The SFT for the replacement operation `replace`(s,`/[0-9]+/`,NUM)

Having constructed the SFT, we can now compute the forward image of the replacement operation. Consider the string constraint $s' =$ `replace`(s, `/[0-9]+/`, `"NUM"`), where we aim to characterize the possible values of s'. Let $\mathcal{T}$ denote the constructed SFT modeling the replacement operation, and let $\mathcal{A}$ be the SFA representing the domain of possible values for the input string s. The forward image of this replacement operation is given by the product $\mathcal{T} \times \mathcal{A}$, which precisely captures the set of all possible output strings that can be produced by applying the replacement operation to any input string accepted by $\mathcal{A}$. Our string solver uses this forward image to do forward propagation for further string solving.

Comparison with SMT-LIB Semantics. It is important to note that our formalization differs from the standard SMT-LIB semantics for the replacement operation. In SMT-LIB, the `str.replace` operation is defined to replace only the *first* occurrence of a substring matching the given pattern. In contrast, our semantics allows for a more general interpretation where any matching substring may be replaced. But it still replaces only one occurrence of them.

5.2 Experiments

We have implemented CertiStrR, an extension of CertiStr [17], to support string replacement operations While the core solving algorithm maintains the certification guarantees of CertiStrR, the frontend components are implemented using established non-certified OCaml libraries: dolmen [24] for SMT-LIB parsing and ocaml-re-nfa [35] for regular expression to NFA conversion.

CertiStrR implements two kinds of SMT-LIB's replacement operations: `str.replace s p r`: a string-based replacement where pattern `p` is a constant string. `str.replace_re s p r`: a regular expression-based replacement where pattern `p` is a regular expression

Listing 1 demonstrates the regular expression variant through an example that replaces numeric sequences with the string `"NUM"`. The constraints are satisfiable because the input string `a` = `"2024,2025"` contains a substring `"2025"` that matches the regular expression `re.+ (re.range "0" "9")` (equivalent to `/[0-9]+/`), and replacing this match with `"NUM"` yields the expected output string `b` = `"2024,NUM"`.

As discussed in the previous subsection, our replacement semantics differs from the SMT-LIB standard semantics. Run the SMT solver CVC5 [30] with the code in Listing 1, the result is UNSAT because CVC5 only matches the first occurrence of the pattern.

```
(set-logic QF_S)
(declare-fun a () String)
(declare-fun b () String)
(assert (= a "2024,2025"))
(assert (= b "2024,NUM"))
(assert (= b (str.replace_re a (re.+ (re.range "0" "9")) "
   NUM")))
(check-sat)
```

Listing 1 Example SMT-LIB Code

We evaluate CertiStrR using benchmarks from SMT-LIB 2024 [26], focusing on the QF_S and QF_SLIA logic fragments. The benchmarks are divided into two categories based on the replacement operations: (1) string-based replacement (`str.replace`) and (2) regular expression-based replacement (`str.replace_re`). Due to CertiStrR's current front-end limitations in supporting the full SMT-LIB language, we preprocess certain operations. For instance, conjunctive assertions of the form `(assert (and c1 c2))` are decomposed into separate assertions `(assert c1)` and `(assert c2)` when `c1` and `c2` are string constraints supported by CertiStrR.

	SAT	UNSAT	Inconclusive	Time	Number of Tests
`replace_str`	142	173	8	0.27	323
`replace_re`	84	4	10	0.36	98

Table 1 Experimental results

The experimental evaluation was conducted on a laptop with an Apple M4 processor and 24 GB of memory, with a time limit of one minute per test. The results show average execution times of 0.27 seconds for `str.replace_str` and 0.36 seconds for `str.replace_re` operations. Test outcomes were classified into three categories: SAT (satisfiable), UNSAT (unsatisfiable), and Inconclusive. An "Inconclusive" result indicates that the solver cannot determine satisfiability, not due to timeout (all tests are finished in one minute) but rather due to inherent limitations of the forward-propagation algorithm inherited from CertiStr [17]. Specifically, when the string constraints do not satisfy the tree property defined in [17], the forward-propagation algorithm may be unable to reach a definitive conclusion, even when the variable domains remain non-empty after propagation.

Our performance analysis revealed that while the SFT-based replacement operation modeling is efficient, the primary computational bottleneck stems from automata accumulation during forward-propagation. Consider the following string constraints:

$$x = x_1\texttt{++}x_2;\; x = \texttt{replace}(x_3, p, r);\; x = x_4;\; x = \texttt{replace\_re}(x_5, p_1, r_1);$$

where `++` denotes string concatenation. The variable x appears multiple times on the left-hand side of the equations, causing the forward-propagation algorithm to accumulate automata representations for all constraints: $x_1\texttt{++}x_2$, $\texttt{replace}(x_3, p, r)$, x_4, and $\texttt{replace\_re}(x_5, p_1, r_1)$. Each accumulation step requires computing the product of the current automaton with the previous result. Given that the product operation has a worst-case complexity of $O(n^2)$, where n represents the automaton size, this repeated accumulation can lead to state explosion.

5.3 Effort of Certified Development

We discuss the effort of certified SFT development in this subsection. Table 2 provides an overview. The abstract-level development means all formalizations in Section 2 and 3, including SFTs and εSFAs . The implementation-level development means all formalizations in Section 4 including the refinement of the product operation. The last row corresponds to the effort of the interval formalization. The most difficult part is the correctness proof of the product operation at the abstract level (Figure 6). Interval formalization complexity dramatic increase in CertiStrR compared to the interval formalization in CertiStr [17] due to the extension of intervals to a list.

	Definitions	**Lemmas**	**Proofs** (lines of code)
Abstract-level	17	21	3274
Implementation-level	51	43	2700
Interval	15	29	1500

Table 2 Overview of the effort of certified development

6 Related Work

Symbolic Automata and Transducers. Symbolic Automata and Transducers [12, 34, 11, 10, 27] represent a significant advancement in automata theory, offering improved efficiency in operations and enhanced expressiveness through algebraic theories that support infinite alphabets. This symbolic framework has been progressively extended to accommodate more complex structures: symbolic tree transducers [32] handle hierarchical data structures, while symbolic pushdown automata [9] manage nested word structures. Recent developments in 2024 have further expanded the scope of symbolic techniques to include Büchi automata and omega-regular languages [31], enabling verification of infinite-state systems and analysis of non-terminating computations.

Applications of Symbolic Transducers. The efficiency, scalability, and expressive power of symbolic automata and transducers have led to their widespread adoption in numerous real-world applications. These applications span diverse domains, including: constraint solving for program analysis [33], security-critical sanitizer analysis for web applications [15], runtime verification of system behaviors [36], and automated program inversion for software transformation [16]. Each application leverages the symbolic approach's ability to handle complex patterns and infinite alphabets efficiently.

Formalization of Symbolic Automata and Transducers. While classical automata theories have been extensively formalized in interactive theorem provers [29, 18, 7, 13], with some work on transducer formalization [21], the symbolic variants of automata and transducers remain largely unexplored in formal verification. To our knowledge, CertiStr [17] represents the only existing work on symbolic automata formalization in a proof assistant. Our work advances this frontier by extending the formal treatment to both SFTs and εSFAs.

String Solving. A significant application of our certified transducer framework is in string constraint solving, a field that has seen intensive research development over the past decade. While our work provides formal verification guarantees, there exists a rich ecosystem of non-certified string solvers, each with distinct capabilities: Kaluza [23] specializes in JavaScript analysis, CVC5 [30], Z3-str3 [5] builds on the Z3 framework, S3P [28], Ostrich [8], and SLOTH [14]. As more and more bugs have beein uncovered in existing string solvers [6] and SMT solvers [22] We believe that our work will benefit the community by providing a formal foundation for string solvers development.

Certified SMT Solvers. Beyond string theories, certification efforts in SMT solving have extended to other domains. For example, the work by Shi et al. [25], who developed a certified SMT solver for quantifier-free bit-vector theory, demonstrating the broader applicability of interactive theorem proving in certified SMT solver development.

7 Conclusion

In this paper, we have presented the first formalization of symbolic finite transducers in the proof assistant Isabelle/HOL. Our formalization provides flexible interfaces that facilitate diverse applications through two key features: support for ε-transitions in both inputs and outputs, and extensibility to various boolean algebras via the refinement framework.

To demonstrate the practical utility of our formalization, we developed CertiStrR, an extension of CertiStr [17]. This implementation adds support for string replacement operations and has been evaluated on benchmarks from SMT-LIB 2024 [26]. The experimental results confirm both the efficiency and effectiveness of our approach. While we focused on string solving applications, our extensible framework for transition labels is broadly applicable to other domains, including program verification.

Future work includes extending our symbolic formalization in two key directions: (1) Enriching the boolean algebra framework to support more complex theories, such as arithmetic constraints. (2) Incorporating prioritized transitions into SFTs, which would enable precise modeling of SMT-LIB's standard semantics for replacement operations, particularly the first-match behavior. These extensions will further enhance the expressiveness and practical applicability of our formalization while maintaining its formal verification guarantees.

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