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HAL Id: hal-00189137
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Submitted on 20 Nov 2007

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A System for the Static Analysis of XPath

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XPath is the standard language for navigating XML documents and returning a set of matching nodes. We present a sound and complete decision procedure for containment of XPath queries as well as other related XPath decision problems such as satisfiability, equivalence, overlap and coverage. The considered XPath fragment covers most of the language features used in practice. Specifically, we propose a unifying logic for XML, namely the alternation-free modal µ-calculus with converse. We show how to translate major XML concepts such as XPath and regular XML types (including DTDs) into this logic. Based on these embeddings, we show how XPath decision problems, in the presence or the absence of XML types, can be solved using a decision procedure for µ-calculus satisfiability. We provide a complexity analysis together with practical experiments of our system that illustrate the efficiency of the approach for realistic scenarios.

Categories and Subject Descriptors: H.3.3 [Information Storage and Retrieval]: Information Search and Retrieval; H.2.3 [Database Management]: Systems—Query Processing; D.3.1 [Programming Languages]: Formal Definitions and Theory—Semantics

General Terms: Algorithms, Languages, Standardization, Theory

Additional Key Words and Phrases: Containment, Equivalence, Logic, Query, XML, XPath

1. INTRODUCTION

XPath [Clark and DeRose 1999] is the standard declarative language for querying an XML tree and returning a set of nodes. It is increasingly popular due to its expressive power and its compact syntax. These advantages have given XPath a central role both in other key XML specifications and XML applications. It is used in XQuery as a core query language; in XSLT as node selector in transformations; in XML Schema to define keys; in XLink and XPointer to reference portions of XML data. XPath is also used in many applications such as update languages [Sur et al. 2004] and XML access control [Fan et al. 2004].

Several XPath decision problems arise naturally in these use cases. The most basic decision problem for a query language is satisfiability [Benedikt et al. 2005]: whether or not an expression yields a non-empty result. XPath satisfiability is important for optimization of host languages implementations: for instance, if one can decide at compile time that a query is not satisfiable then subsequent bound computations can be avoided. Another basic decision problem is the XPath equiv-
ence problem: whether or not two queries always return the same result. It is important for reformulation and optimization of the query itself [Genevès and Vion-Dury 2004a], which aim at enforcing operational properties while preserving semantic equivalence [Abiteboul and Vianu 1999; Levin and Pierce 2005]. These two decision problems are reducible to XPath containment: whether or not, for any tree, the result of a particular query is included in the result of another one. Query containment is itself critical for static analysis of XML specifications and especially for type-checking transformations [Martens and Neven 2004; Tozawa 2001]. Such applications introduce XPath decision problems in the presence of XML types such as DTDs [Bray et al. 2004] or XML Schemas [Fallside and Walmsley 2004]. Other decision problems needed in applications include for example XPath overlap (whether two expressions select common nodes) and coverage (whether nodes selected by an expression are always contained in the union of the results selected by several other expressions).

In the literature, much of the attention has been paid to classifying the containment problem for simple XPath subfragments in complexity classes. This allowed to identify subsets of XPath for which the containment can be efficiently decided.

In this paper, our goal is to describe sound, complete and efficient decision procedures usable in practice for a large XPath fragment in the presence or absence of XML types. We first briefly introduce the XPath language, and present the approach and outline of the paper.

1.1 Introduction to XPath

XPath [Clark and DeRose 1999] has been introduced by the W3C as the standard query language for retrieving information in XML documents. It allows to navigate in XML trees and return a set of matching nodes. In their simplest form XPath expressions look like “directory navigation paths”. For example, the XPath

```
/book/chapter/section
```

navigates from the root of a document (designated by the leading slash “/”) through the top-level “book” element to its “chapter” child elements and on to its “section” child elements. The result of the evaluation of the entire expression is the set of all the “section” elements that can be reached in this manner, returned in the order they occurred in the document. At each step in the navigation the selected nodes for that step can be filtered using qualifiers. A qualifier is a boolean expression between brackets that can test path existence. So if we ask for

```
/book/chapter/section[citation]
```

then the result is all “section” elements that have a least one child element named “citation”. The situation becomes more interesting when combined with XPath's capability of searching along “axes” other than the shown “children of” axis. Indeed the above XPath is a shorthand for

```
/child::book/child::chapter/child::section[child::citation]
```

where it is made explicit that each path step is meant to search the “child” axis containing all children of the previous context node. If we instead asked for

```
/child::book/descendant::*[child::citation]
```

then the last step selects nodes of any kind that are among the descendants of the top element "book" and have a "citation" sub-element.

Previous examples are all absolute XPath expressions. The meaning of a relative expression (without the leading "/") is defined with respect to a context node in the tree. A key to XPath success is its compactness due to the powerful navigation made possible by the various axes. Starting from a particular context node in a tree, every other nodes can be reached. Axes define a partitioning of a tree from any context node. Figure 1 illustrates this on a sample tree. More informal details on the complete XPath standard can be found in the W3C specification [Clark and DeRose 1999].

A variety of factors contribute to the complexity of XPath decision problems such as the operators allowed in XPath queries and the combination of them. We present here the common distinctions between XPath fragments found in the literature, taken from [Benedikt et al. 2005]:

—positive vs. non-positive: depending whether the negation operator is considered or not inside qualifiers.
—downward vs. upward: depending whether queries specify downward or upward traversal of the tree, or both.
—recursive vs. non-recursive: depending whether XPath transitive closure axes (for instance "descendant" or "ancestor") are considered or not.
—qualified vs. non-qualified: depending whether queries allow filtering qualifiers or not.
—with vs. without data values: depending whether comparisons of data values expressing joins are allowed or not.
From the results of [Benedikt et al. 2005; Schwentick 2004], we know that the combination of some previous factors with data values may lead to undecidability of decision problems such as the containment. In the remaining part of the paper, we focus on a large XPath fragment covering all previous factors except data values. This fragment, detailed in Section 3, is the largest considered so far in the literature, and covers most features of XPath 1.0.

1.2 Approach and Outline

In this paper, we propose the alternation free modal µ-calculus with converse as the appropriate logic for effectively solving XPath decision problems in the presence or absence of XML types. We show how XPath can be linearly translated into the µ-calculus. We also show how to embed regular tree types (including DTDs) in the µ-calculus. We express XPath decision problems (containment, satisfiability, equivalence, overlap, coverage) as formulas in this logic. We use an EXPTIME decision procedure for µ-calculus satisfiability to solve the generated formula and construct relevant example and/or counter-example XML trees. We provide experimental results which shed light, for the first time, on the cost of solving XML decision problems in practice. The system has been fully implemented [Genevès and Layaida 2006] and can be used for the static analysis of XML specifications.

The remaining part of the paper is organized as follows: in Section 2 we introduce the logic we propose for reasoning on XML trees; in Section 3 we describe the translation of XPath queries into this logic; Section 4 embeds regular XML types into the logic. Based on these translations, Section 5 explains how to formulate and solve the considered decision problems. We present an implementation of the system along with practical experiments in Section 6, before discussing related work in Section 7 and concluding in Section 8.

2. A LOGIC FOR XML

In this section we introduce a specific variant of the modal µ-calculus as a formalism for reasoning on XML trees.

2.1 XML Documents and Finite Binary Trees

We consider an XML document as a finite ordered and labeled tree of unbounded depth and arity. Since there is no a priori bound on the number of children of a node; such a tree is therefore unranked [Neven 2002b]. Tree nodes are labeled with symbols taken from a countably infinite alphabet Σ. There is a straightforward isomorphism between sequences of unranked trees and binary trees [Hosoya et al. 2005; Neven 2002a]. In order to describe it, we first define the set $T^n_Σ$ of unranked trees:

$$T^n_Σ \ni t ::= \sigma(h)$$

where $\sigma \in \Sigma$ and $h$ is a hedge, i.e. a sequence of unranked trees, defined as follows:

$$H_Σ \ni h ::= \sigma(h), h' \mid ()$$

---

1. The fragment also includes two extensions from the forthcoming XPath 2.0 [Berglund et al. 2006] language: qualified paths (e.g. $(p)[q]$) instead of XPath 1.0 qualified steps (e.g. $a::n[q]$) and path intersection $(p_1 \cap p_2)$. 

A binary tree $t$ is either a $\sigma$-labeled root of two subtrees ($\sigma \in \Sigma$) or the empty tree:

$$T_\Sigma^2 \ni t ::= \sigma(t, t') | \epsilon$$

Unranked trees can be translated into binary trees with the following function:

$$\beta(\cdot) : \mathcal{H}_\Sigma \rightarrow T_\Sigma^2$$
$$\beta(\sigma(h), h') = \sigma(\beta(h), \beta(h'))$$
$$\beta(\epsilon) = \epsilon$$

The inverse translation function converts a binary tree into a sequence of unranked trees:

$$\beta^{-1}(\cdot) : T_\Sigma^2 \rightarrow \mathcal{H}_\Sigma$$
$$\beta^{-1}(\sigma(t, t')) = \sigma(\beta^{-1}(t), \beta^{-1}(t'))$$
$$\beta^{-1}(\epsilon) = ()$$

For example, Figure 2 illustrates how a sample unranked tree is mapped to its binary representation and vice-versa.

![Fig. 2. Unranked and Binary Tree Representations.](image)

Note that the translation of a single unranked tree results in a binary tree of the form $\sigma(t, \epsilon)$. Reciprocally, the inverse translation of such a binary tree always yields a single unranked tree. When modeling XML, we therefore restrict our attention to binary trees of the form $\sigma(t, \epsilon)$, without loss of generality.

We now introduce the logic we propose for reasoning over these structures.

### 2.2 The $\mu$-Calculus

The *propositional $\mu$-calculus* is a propositional modal logic extended with least and greatest fixpoint operators [Kozen 1983]. A *signature* $\Xi$ for the $\mu$-calculus consists of a set $\text{Prop}$ of atomic propositions, a set $\text{Var}$ of propositional variables, and a set $\text{FProg}$ of atomic programs. In the XML context, atomic propositions represent the symbols of the alphabet $\Sigma$ used to label XML trees. Atomic programs allow navigation in trees.

The $\mu$-calculus with converse\(^2\) [Vardi 1998] augments the propositional $\mu$-calculus by associating with each atomic program $a$ its converse $\overline{a}$. A *program* $\alpha$ is either an atomic program or its converse. We note $\text{Prog}$ the set $\text{FProg} \cup \{\overline{a} | a \in \text{FProg}\}$. This is the only difference between the propositional $\mu$-calculus that lacks converse programs. It is important to note that the addition of converse programs preserves the EXPTIME upper bound for the satisfiability problem [Vardi 1998].

\(^2\)The $\mu$-calculus with converse is also known as the *full* $\mu$-calculus, or alternatively as the *two-way* $\mu$-calculus in the literature.
The set \( \mathcal{L}_\mu \) of formulas of the \( \mu \)-calculus with converse over the signature \( \Xi \) is defined as follows:

\[
\mathcal{L}_\mu \ni \phi ::= T \mid \bot \mid p \mid p \land \phi_1 \lor \phi_2 \mid \phi_1 \land \phi_2 \mid \langle \alpha \rangle \phi \mid \langle X \rangle \phi \mid \mu X.\phi \mid \nu X.\phi
\]

where \( p \in \text{Prop} \), \( X \in \text{Var} \) and \( \alpha \) is a program. Note that \( X \) should not occur negatively in \( \mu X.\phi \) and in \( \nu X.\phi \).

The semantics of the full \( \mu \)-calculus is given with respect to a Kripke structure \( K = \langle W, R, L \rangle \) where \( W \) is a set of nodes, \( R : \text{Prog} \rightarrow 2^W \times W \) assigns to each atomic program a transition relation over \( W \), and \( L \) is an interpretation function that assigns to each atomic proposition a set of nodes.

The formal semantics function \( \llbracket \cdot \rrbracket^K \) shown on Figure 3 defines the semantics of a \( \mu \)-calculus formula in terms of a Kripke structure \( K \) and a valuation \( V \). A valuation \( V : \text{Var} \rightarrow 2^W \) maps each variable to a subset of \( W \). For a valuation \( V \), a variable \( X \), and a set of nodes \( W' \subseteq W \), \( V[X/W'] \) denotes the valuation that is obtained from \( V \) by assigning \( W' \) to \( X \).

\[
\begin{align*}
\llbracket \top \rrbracket^K &= W \\
\llbracket \bot \rrbracket^K &= \emptyset \\
\llbracket p \rrbracket^K &= L(p) \\
\llbracket \neg \phi \rrbracket^K &= W \setminus \llbracket \phi \rrbracket^K \\
\llbracket \phi_1 \lor \phi_2 \rrbracket^K &= \llbracket \phi_1 \rrbracket^K \cup \llbracket \phi_2 \rrbracket^K \\
\llbracket \phi_1 \land \phi_2 \rrbracket^K &= \llbracket \phi_1 \rrbracket^K \cap \llbracket \phi_2 \rrbracket^K \\
\llbracket \langle \alpha \rangle \phi \rrbracket^K &= \{ w : \exists w' \in R(\alpha) \land w' \in \llbracket \phi \rrbracket^K \} \\
\llbracket \langle X \rangle \phi \rrbracket^K &= \{ w : \forall w' \in W : \llbracket \phi \rrbracket^{W 	imes W}[X/w] \subseteq w' \} \\
\llbracket \mu X.\phi \rrbracket^K &= \bigcap \{ W' \subseteq W : \llbracket \phi \rrbracket^K[X/W'] \subseteq W' \} \\
\llbracket \nu X.\phi \rrbracket^K &= \bigcup \{ W' \subseteq W : \llbracket \phi \rrbracket^K[X/W'] \supseteq W' \} \\
\llbracket X \rrbracket^K &= V(X)
\end{align*}
\]

Fig. 3. Semantics of the \( \mu \)-Calculus.

Note that if \( \phi \) is a sentence (i.e. all propositional variables occurring in \( \phi \) are bound), then no valuation is required. For a node \( w \in W \) and a sentence \( \phi \), we say that \( \phi \) holds at \( w \) in \( K \), denoted \( K, w \models \phi \) iff \( w \in \llbracket \phi \rrbracket^K \).

The two modalities \( \langle \alpha \rangle \phi \) (possibility) and \( [\alpha] \phi \) (necessity) are operators for navigating the structure.

The syntax of \( \mathcal{L}_\mu \) formulas as given previously is in fact redundant. Actually, we only have to deal with a subset of \( \mathcal{L}_\mu \) composed of formulas in negation normal form. We say that a formula is in negation normal form if and only if all negations in the formula appear only before atomic propositions. Every formula is equivalent to a formula in negation normal form [Kozen 1983], which can be obtained by expanding negations using De Morgan’s rules together with standard dualities for modalities and fixpoints (c.f. Figure 4). For readability purposes, translations of XPath expressions given in Section 3 are not given in negation normal form.

For reasoning on XML trees, we are in fact interested in a specific subset of \( \mathcal{L}_\mu \), namely the alternation-free modal \( \mu \)-calculus with converse over finite binary trees.
\[
\begin{align*}
\neg \langle \alpha \rangle \varphi &= (\alpha) \neg \varphi \\
\neg [\alpha] \varphi &= [\alpha] \neg \varphi \\
\mu X . \varphi &= \nu X . \neg \varphi[X/\neg X] \\
\nu X . \varphi &= \mu X . \neg \varphi[X/\neg X] \\
\neg (\varphi_1 \land \varphi_2) &= \neg \varphi_1 \lor \neg \varphi_2 \\
\neg (\varphi_1 \lor \varphi_2) &= \neg \varphi_1 \land \neg \varphi_2 \\
\neg \neg \varphi &= \varphi \\
\end{align*}
\]

Fig. 4. Dualities for Negation Normal Form.

We recall that a \( L_{\mu} \) formula \( \varphi \) in negation normal form is \textit{alternation-free} whenever the following condition holds\(^3\): if \( \mu X . \varphi_1 \) (respectively \( \nu X . \varphi_1 \)) is a subformula of \( \varphi \) and \( \nu Y . \varphi_2 \) (respectively \( \mu Y . \varphi_2 \)) is a subformula of \( \varphi_1 \) then \( X \) does not occur freely in \( \varphi_2 \).

The following section now introduces the additional restrictions of \( L_{\mu} \) related to finite binary trees.

### 2.3 XML Constraints on Kripke Structures

In this section, we restrict the satisfiability problem of \( L_{\mu} \) over Kripke structures to the satisfiability problem over finite binary trees.

The propositional \( \mu \)-calculus has the \textit{finite tree model property}: a formula that is satisfiable, is also satisfiable on a finite tree [Kozen 1988]. Unfortunately, the introduction of converse programs causes the loss of the finite model property [Vardi 1998]. Therefore, we need to reinforce the finite model property and introduce some others to ensure we work on finite binary trees encoding XML structures.

First, each XML node has at most one \( \Sigma \)-label, i.e. \( p \land p' \) never holds for distinct atomic propositions \( p \) and \( p' \). This can be easily incorporated in a \( \mu \)-calculus satisfiability solver.

Second, for navigating binary trees, we only use two atomic programs 1 and 2, and their associated relations \( R(1) = \prec_{fc} \) and \( R(2) = \prec_{ns} \) whose meaning is to respectively connect a node to its left child and to its right child. For any \((x,y) \in W \times W\), \( x \prec_{fc} y \) holds iff \( y \) is the left child of \( x \) (i.e. the first child in the unranked tree representation) and \( x \prec_{ns} y \) holds iff \( y \) is the right child of \( x \) in the binary tree representation (i.e. the next sibling in the unranked tree representation).

For each atomic program \( a \in \{1,2\} \) we define \( R(\overline{a}) \) to be the relational inverse of \( R(a) \), i.e., \( R(\overline{a}) = \{(v,u) : (u,v) \in R(a)\} \). We thus consider programs \( \alpha \in \{1,2,T,F\} \) inside modalities for navigating downward and upward in trees.

We now define restrictions for a Kripke structure to form a finite binary tree. A Kripke structure \( t = \langle W, R, L \rangle \) is a finite binary tree if it satisfies the following conditions:

1. \( W \) is finite
2. the set of nodes \( W \) together with the accessibility relation \( \prec_{fc} \cup \prec_{ns} \) define a tree
3. \( \prec_{fc} \) and \( \prec_{ns} \) are partial functions, i.e. for all \( m \in W \) and \( j \in \{1,2\} \) there is at most one \( m_j \in W \) such that \((m,m_j) \in R(j)\).

\(^3\)For instance, \( \nu X . (\langle \mu Y . (1) Y \land p \rangle \lor (2) X \) is alternation-free but \( \nu X . (\langle \mu Y . (1) Y \land X \rangle \lor p \) is not since \( X \) bound by \( \nu \) appears freely in the scope of \( \mu Y \).
We say that a finite binary tree $t = \langle W, R, L \rangle$ satisfies $\varphi$ if $t, r \models \varphi$ where $r \in W$ is the root of the tree $t$.

For accessing the root, we use the $L_\mu$ formula

$$\varphi_{\text{root}} = [\top] \perp \land [\top] \perp$$

which selects a node provided it has no parent.

For ensuring finiteness, we rely on König's lemma which states that a finitely branching infinite tree has some infinite path or, in other words, a finitely branching tree in which every branch is finite is finite. The expression $\nu X. (1) X \lor (2) X$ is only satisfied by structures containing infinite or cyclic paths. To prevent the existence of such paths, we negate the previous formula and, by propagating negation using the rules presented on Figure 4, we obtain:

$$\varphi_{\text{ft}} = \mu X. [1] X \land [2] X$$

$\varphi_{\text{ft}}$ states that all descending branches are finite from the current context node ($\varphi_{\text{ft}}$ is vacuously satisfied at the leaves). In our case we need $\varphi_{\text{ft}}$ to hold at the root (i.e. $\varphi_{\text{root}} \land \varphi_{\text{ft}}$ must hold), in order to ensure we work with a finite structure. This is for condition (1) to be satisfied.

We still need to enforce (2) and (3). We do this by rewriting existential modalities in such a way that if a successor is supposed to exist, then there exists at least one, and if there are many all verify the same property. This is a way to overcome the difficulty that in $\mu$-calculus, one cannot naturally express a property like “a node has exactly $n$ successors”. Technically, we denote by $\varphi_{\text{FBT}}$ the formula $\varphi$ where all occurrences of $\langle \alpha \rangle \psi$ are replaced by $\langle \alpha \rangle \top \land [\alpha] \psi_{\text{FBT}}$. This replacement is enough to enforce conditions (2) and (3).

**Proposition 2.1.** A $L_\mu$ formula $\varphi$ is satisfied by a finite binary tree model if and only if the formula $\varphi_{\text{root}} \land \varphi_{\text{ft}} \land \varphi_{\text{FBT}}$ is satisfied by a Kripke structure.

The proof of the “if” part iteratively constructs a tree model and proceeds by induction on the structure on $\varphi$. The “only if” part is almost immediate [Tanabe et al. 2005].

Proposition 2.1 gives the adequate framework for formulating decision problems on XML structures in terms of a $\mu$-calculus formula.

3. LOGICAL INTERPRETATION OF XPATH QUERIES

We consider a large and realistic XPath fragment which includes negation, both downward and upward navigation, recursion, union, intersection and qualifiers. The abstract syntax of our XPath fragment is shown below:

- **Leaf** $e ::= /p \mid p \mid e_1 \cdot e_2 \mid e_1 \cap e_2$
- **Path** $p ::= p_1 / p_2 \mid p[q] \mid a.n$
- **Qualifier** $q ::= q \land q \mid q \lor q \mid \neg q \mid p$
- **Axis** $a ::= \,$ child $\mid$ descendant $\mid$ self $\mid$ parent $\mid$ ancestor $\mid$ following $\mid$ preceding $\mid$ descendant-or-self $\mid$ ancestor-or-self $\mid$ preceding-sibling $\mid$ following-sibling
- **NodeTest** $n ::= \sigma \mid *$
XPath expressions are directly used for querying unranked XML trees. We first recall XPath denotational semantics over unranked trees [Wadler 2000]. The evaluation of an XPath query returns a set of nodes reachable from a context node \( x \) in a tree \( t \). The formal semantics functions \( S_c \) and \( S_p \) define the set of nodes respectively returned by expressions and paths:

\[
S_c[\cdot] \quad : \quad \mathcal{L}_{\text{XPath}} \times \text{Node} \times \mathcal{T}_\Sigma^t \rightarrow \text{Set(Node)}
\]

\[
S_p[\cdot]_x \quad = \quad S_p[p]_{\text{root}}(t)
\]

\[
S_c[\cdot]_x \quad = \quad S_c[p]_{\text{root}}(t)
\]

\[
S_c[e_1 \cdot e_2]_x \quad = \quad S_c[e_1]_{e_2}[x]
\]

\[
S_c[e_1 \cap e_2]_x \quad = \quad S_c[e_1]_{e_2}[x]
\]

\[
S_p[p_1/p_2]_x \quad = \quad \{ x \mid x_1 \in S_p[p_1]_x \land x_2 \in S_p[p_2]_x \}
\]

\[
S_p[p\cdot q]_x \quad = \quad \{ x \mid x_1 \in S_p[p]_x \land S_q[q]_x \}
\]

\[
S_p[a::\sigma]_x \quad = \quad \{ x \mid x_1 \in S_a[a]_x \land \text{name}(x_1) = \sigma \}
\]

\[
S_p[p\cdot 1]_x \quad = \quad \{ x \mid x_1 \in S_p[p]_x \}
\]

The function \( S_q \) defines the semantics of qualifiers that basically state the existence (or absence) of one or more paths from a context node \( x \):

\[
S_q[\cdot] \quad : \quad \text{Qualifier} \times \text{Node} \times \mathcal{T}_\Sigma^t \rightarrow \text{Boolean}
\]

\[
S_q[q_1 \text{ and } q_2]_x \quad = \quad S_q[q_1]_x \land S_q[q_2]_x
\]

\[
S_q[q_1 \text{ or } q_2]_x \quad = \quad S_q[q_1]_x \lor S_q[q_2]_x
\]

\[
S_q[\text{not } q]_x \quad = \quad \neg S_q[q]_x
\]

\[
S_p[p\cdot 1]_x \quad = \quad S_p[p]_x \neq \emptyset
\]

Eventually the function \( S_a \) gives the denotational semantics of axes:

\[
S_a[\cdot] \quad : \quad \text{Axis} \times \text{Node} \times \mathcal{T}_\Sigma^t \rightarrow \text{Set(Node)}
\]

\[
S_a[\text{child}]_x \quad = \quad \text{children}(x)
\]

\[
S_a[\text{parent}]_x \quad = \quad \text{parent}(x)
\]

\[
S_a[\text{descendant}]_x \quad = \quad \text{children}^+(x)
\]

\[
S_a[\text{ancestor}]_x \quad = \quad \text{parent}^+(x)
\]

\[
S_a[\text{self}]_x \quad = \quad \{ x \}
\]

\[
S_a[\text{descendant-or-self}]_x \quad = \quad S_a[\text{descendant}]_x \cup S_a[\text{self}]_x
\]

\[
S_a[\text{ancestor-or-self}]_x \quad = \quad S_a[\text{ancestor}]_x \cup S_a[\text{self}]_x
\]

\[
S_a[\text{preceding}]_x \quad = \quad \{ y \mid y \ll x \} \setminus S_a[\text{ancestor}]_x
\]

\[
S_a[\text{following}]_x \quad = \quad \{ y \mid x \ll y \} \setminus S_a[\text{descendant}]_x
\]

\[
S_a[\text{preceding-sibling}]_x \quad = \quad \{ y \mid y \in \text{children}^+(\text{parent}(x)) \land x \ll y \}
\]

\[
S_a[\text{following-sibling}]_x \quad = \quad \{ y \mid y \in \text{children}^+(\text{parent}(x)) \land y \ll x \}
\]

in which \( \text{root}() \), \( \text{children}(x) \) and \( \text{parent}(x) \) are primitives for navigating unranked trees, \( \ll \) is the ordering relation (\( x \ll y \) holds if and only if the node \( x \) is before the node \( y \) in the depth-first traversal order of the tree), and \( \text{name}() \) is the mean for accessing the labeling of the tree.

3.1 A Translation into the \( \mu \)-Calculus

We now explain how an XPath expression can be translated into an equivalent formula in \( \mathcal{L}_\mu \) over binary trees. The translation adheres to XPath formal semantics.
in the sense that the translated formula holds for nodes which are selected by the XPath query. Navigation as performed by XPath in unranked trees is thus translated in terms of navigation in the binary tree representation.

For example, Figure 5 gives the intuition of the translation of the XPath expression “child::a[child::b]”. In an unranked tree, this expression selects all “a” child nodes of a given context which have at least one “b” child. The translated $L_\mu$ formula holds for “a” nodes which are selected by the expression. By navigating upward in the binary tree from these nodes (specifically, any number of steps upward from a right child, and then once upward from a left child), we must reach the initial context. Then, starting back from the candidate “a” nodes we must navigate downward in the tree in order to verify the existence of a “b” child.

Translated Query: child::a[child::b]

$\phi \land (1)X. (\langle 1 \rangle \chi \lor (2)X) \land (1)\mu Y.b \lor (2)Y)

Fig. 5. XPath Translation Example.

Note that without converse programs, we would have been unable to differentiate selected nodes from nodes whose existence is tested. This is because we must state properties on both the ancestors and the descendants of the selected node. Therefore, equipping the $L_\mu$ logic with converse programs is crucial for supporting XPath\textsuperscript{4}. Logics without converse programs may only be used for solving XPath satisfiability but not other decision problems such as containment.

3.1.1 Logical Interpretation of Axes. We first translate navigational primitives, namely XPath axes. The translation is formally specified on Figure 6 as a translation function noted “$A^{-\llbracket [\cdot] \rrbracket (\cdot)$” which takes an XPath axis as input, and returns its translation in $\mu$-calculus, in terms of the $\mu$-calculus formula given as a parameter to allow further composition. $A^{-\llbracket [\cdot] \rrbracket (\chi)}$ holds for all nodes that can be accessed through the axis $a$ from some node verifying $\chi$. The formal parameter $\chi$ allows to express composition of formulas needed for translating path composition.

For readers more familiar with PDL and CPDL (PDL with converse programs) both defined in [Fischer and Ladner 1979], we give a correspondence of notations on Figure 7.

\textsuperscript{4}One may ask whether it is possible to eliminate upward navigation at the XPath level. It is well known that such XPath rewritings may cause exponential blow-ups of expression sizes.

3.1.2 Logical Interpretation of Expressions. The translation of XPath expressions into \( \mu \)-calculus is given on Figure 8. It is formally expressed as a translation function noted “\( E^- \cdot [] \cdot () \)" which takes an XPath expression as input, a \( \mu \)-calculus formula as a parameter which indicates the context from which the expression is applied. Absolute XPath expressions are interpreted from the root (selected by the \( \mu \)-calculus expression \( \varphi_{\text{root}} \)), whereas relative expressions are interpreted relatively to any context node. We use a fresh atomic proposition named \( \varphi_{\text{context}} \) for distinguishing context nodes.

The translation of expressions relies on the translations of paths shown on Figure 9. XPath most essential construct \( p_1/p_2 \) translates into formula composition in \( L_\mu \), such that the resulting formula holds for all nodes accessed through \( p_2 \) from those nodes accessed from \( \chi \) by \( p_1 \).

The translation of the branching construct \( p[q] \) significantly differs. The resulting formula must hold for all nodes that can be accessed through \( p \) and from which \( q \) holds (c.f. XPath denotational semantics given previously in Section 3). To
 preserves semantics, the translation of $p[q]$ stops the “selecting navigation” to those nodes reached by $p$, then filters them depending whether $q$ holds or not. We express this by introducing a dual formal translation function for XPath qualifiers, noted $Q^-$ [·] (·) (and shown on Figure 10), which performs “filtering” instead of navigation. Specifically, $P^- [·] (·)$ can be seen as the “navigational” translating function: the translated formula holds for target nodes of the given path. On the opposite, $Q^- [·] (·)$ can be seen as the “filtering” translating function: it states the existence of a path without moving to its result. The translated formula $Q^- [q] (χ)$ (respectively $P^- [p] (χ)$) holds for nodes from which there exists a qualifier $q$ (respectively a path $p$) leading to a node verifying $χ$.

XPath translation into $μ$-calculus is based on these two translating “modes”, the first one being used for paths and the second one for qualifiers. Note that whenever the “filtering” mode is entered, it will never be left. This differs from the denotational semantics given previously in Section 3 in which the formal semantics functions for paths and qualifiers are mutually recursive (and cause naïve implementations to be unnecessarily complex, as pointed out by [Gottlob et al. 2005]). Translations of paths inside qualifiers are also given on Figure 10. They use the specific translations for axes inside qualifiers, based on XPath symmetry, shown on Figure 11.

The cost of the translation is linear in the length of the XPath expression since there is no duplication of subformulas of arbitrary length in the formal translations. Formulas in which the formal parameter $χ$ appears twice (see Figure 8 and Figure 10) do not cause such duplication since the value of $χ$ is either $ϕ_\text{context}$ or $ϕ_\text{root}$ constants.

Note that the translation of an XPath expression is a sentence. Indeed, for absolute XPath expressions, the translation starts from the root (the initial formal parameter is $ϕ_\text{root}$). For relative expressions, the translated formula is closed by the initial formal parameter $ϕ_\text{context}$ modeling context nodes.
where \( y \) is the counterpart of \( \sigma \) and \( \mu \) is a countably infinite set of type variables. Abbreviated type expressions can be defined as follows:

\[
\begin{align*}
T^? & = () \mid T \\
T^* & = \text{let } X \rightarrow T \text{ in } T, X \mid () \\
T^+ & = T, T^*
\end{align*}
\]

Fig. 11. Symmetry of Axes inside Qualifiers.

We can prove that the translated \( L_\mu \) formula over binary trees is semantically equivalent to the original XPath expression over corresponding unranked trees. For instance, if we relate our translations in \( L_\mu \) to the XPath denotational semantics given previously in Section 3:

**Proposition 3.1.** Let \( T' \) be an XML tree, and \( e \) an XPath expression, then for all \( y' \in T' \), the followings are equivalent:

- There exists \( x' \in T' \) such that \( y' \in S_e[e]^T_x \)
- \( T, y \models \varphi \land \varphi \land (E^{-}[e](\varphi_{context}))^{FBT} \)

where \( y \) is the counterpart of \( y' \) in the binary tree representation \( T \) of \( T' \).

The proof is done by a straightforward structural induction that “peels off” the compositional layers of each set of rules. This result links XPath decision problems in the absence of XML types to satisfiability in \( L_\mu \). We now show how XML types can also be translated in the \( \mu \)-calculus.

4. XML TYPES

XML types describe structural constraints for XML documents. Several formalisms exist for describing classes of XML documents (see [Murata et al. 2005] for an overview). In this paper, we translate the class of regular tree languages, that gathers all widely used formalisms for describing classes of XML documents (including the well-known DTDs and XML Schemas) into \( L_\mu \) over binary trees.

We begin with the syntactic definition of tree type expressions. We define a type \( T \) as follows:

\[
L_{CFT} \ni T ::= \emptyset \mid (X \mid l[T]) \mid T_1, T_2 \mid T_1 \cup T_2 \\
\text{let } (X_i \rightarrow T_i)_{1 \leq i \leq m} \text{ in } T
\]

where \( l \in \Sigma \) and \( X \in TVar \) assuming that \( TVar \) is a countably infinite set of type variables.
Given an environment $\theta$ of type variable bindings, the semantics of tree types is given by the denotation function $\llbracket \cdot \rrbracket_\theta$:

<table>
<thead>
<tr>
<th>Syntax</th>
<th>Semantics</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\llbracket \cdot \rrbracket_\theta$</td>
<td>$\mathcal{L}_{CFT} \times (TVar \to 2 \mathbb{T}^\Sigma) \to 2 \mathbb{T}^\Sigma$</td>
</tr>
<tr>
<td>$\llbracket \emptyset \rrbracket_\theta$</td>
<td>$\emptyset$</td>
</tr>
<tr>
<td>$\llbracket (\cdot) \rrbracket_\theta$</td>
<td>${()}$</td>
</tr>
<tr>
<td>$\llbracket X \rrbracket_\theta$</td>
<td>$\theta(X)$</td>
</tr>
<tr>
<td>$\llbracket [t][T] \rrbracket_\theta$</td>
<td>${t'(l) \mid t' &lt; l \land t \in \llbracket T \rrbracket_\theta}$</td>
</tr>
<tr>
<td>$\llbracket T_1, T_2 \rrbracket_\theta$</td>
<td>${t_1, t_2 \mid t_1 \in \llbracket T_1 \rrbracket_\theta \land t_2 \in \llbracket T_2 \rrbracket_\theta}$</td>
</tr>
<tr>
<td>$\llbracket \text{let } (X_i \rightarrow T_i)<em>{1 \leq i \leq m} \text{ in } T \rrbracket</em>\theta$</td>
<td>$\llbracket T \rrbracket\text{lfp}(S)$</td>
</tr>
</tbody>
</table>

where $\prec$ is a global subtagging relation: a reflexive and transitive relation on labels\(^5\), and $S(\theta') = \theta[X_i \rightarrow [T_i]_\theta]_\theta$. Note that each function $S$ is monotone according to the ordering $\subseteq$ on $TVar \to 2 \mathbb{T}^\Sigma$, and thus has a least fixpoint $\text{lfp}(S)$.

Types as defined above actually correspond to arbitrary context-free tree types, for which the decision problem for inclusion is known to be undecidable [Hopcroft et al. 2000]. We impose the additional restriction used in [Hosoya et al. 2005] to reduce the expressive power of considered types so that they correspond to regular tree languages. The restriction consists in a simple syntactic condition that allows unguarded (i.e. not enclosed by a label) recursive uses of variables, but restricts them to tail positions\(^6\). This condition ensures regularity, and we name $\mathcal{L}_{RT}$ the resulting class of regular tree languages. From an XML point of view, regular tree types form a superset of standards such as XML Schemas and DTDs. We further detail the connection with the widely used DTD standard.

### 4.1 Document Type Definitions

As they are defined in the W3C recommendation, DTDs [Bray et al. 2004] are local tree grammars\(^7\), which are strictly less expressive than regular tree types. In the XML terminology, a type expression is often called the content model. DTD content models are described by the following syntax:

$$T ::= l \mid T_1 : T_2 \mid T_1 ; T_2 \mid T? \mid T^* \mid T^+ \mid ()$$

where $l \in \Sigma$. From the W3C specification, we see a DTD as a function that associates a content model to each label taken from a subset $\Sigma'$ of $\Sigma$, such that $\Sigma'$ gathers all labels used in content models. We thus represent the set $\mathcal{L}_{DTD}$ of tree types described by DTDs as follows:

$$\mathcal{L}_{DTD} \ni T ::= l \mid T_1 : T_2 \mid T_1 ; T_2 \mid T? \mid T^* \mid T^+ \mid () \mid \text{let } (l_i \rightarrow T_i)_{1 \leq i \leq m} \text{ in } T$$

---

\(^5\)Subtagging goes beyond the expressive power of DTDs but a similar notion called “substitution groups” exists in XML Schemas (see [Hosoya et al. 2005] for more details on subtagging).

\(^6\)For instance the type “let $(X \rightarrow [a][Y \rightarrow b], X : ())$ in $X^*$” is allowed.

\(^7\)A local tree grammar is a regular tree grammar without competing non-terminals. Two non-terminals $A$ and $B$ of a tree grammar are said to compete with each other if one production rule has $A$ in its left-hand side, one production rule has $B$ in its left-hand side, and these two rules share the same terminal symbol in the right-hand side.
4.2 Binarization of Types

In section 2.1, we used a straightforward isomorphism between binary trees and sequences of unranked trees. There is also an isomorphism between unranked and binary tree types, which follows exactly the same intuition as for trees.

Binary tree types are described by the following syntax:

\[ \mathcal{L}_{BT} \ni T ::= \emptyset \mid \epsilon \mid T_1 : T_2 \mid l(X_1, X_2) \mid \text{let } (X_i \rightarrow T_i)_{1 \leq i \leq m} \text{ in } T \]

For any type, there is an equivalent binary type, and vice-versa. We use the translation function shown in Figure 12 (adapted from the one found in [Hosoya et al. 2005]) to convert a type into its corresponding binary representation. The function considers the environment \( \theta : TVar \rightarrow \mathcal{L}_{RT} \) for accessing the type bound to a variable \( X_i \) by constructs of the form “let \( (X_i \rightarrow T_i)_{1 \leq i \leq m} \) in \( T \)".  

4.3 Translation into \( \mu \)-Calculus

We now introduce the translation of regular tree types into \( \mu \)-calculus, which is based on the binary representation of types. In order to simplify translations, we introduce a notion for a \( n \)-ary least fixpoint binder:

\[ \text{let}_\mu (X_i, \varphi_i)_{1 \leq i \leq m} \text{ in } \psi \]

This notation is actually a syntactic sugar for \( \psi \) where all free occurrences of \( X_i \) have been replaced by \( \mu X_i. \varphi_i \) until \( \psi \) becomes closed (that is all \( X_i \) in \( \psi \) are in scope of their corresponding unary \( \mu \)-binder). This provides a shorthand for denoting a \( \mathcal{L}_\mu \) formula which would be of exponential size if expressed using only the unary least fixpoint construct. Such a naive expansion contains unnecessary duplicate formulas whereas the satisfiability solver operates only on a single copy of them (see Section 6.1). Therefore, the \( n \)-ary binder is a useful compact notation for representing \( \mathcal{L}_\mu \) translations of recursive types, without introducing useless blow-ups between representation of formulas and their satisfiability test.

Note that \( \mathcal{L}_{DTD} \subseteq \mathcal{L}_{RT} \) is obvious, by associating a unique type variable to each label. In the following, we therefore do not distinguish DTDs from general regular tree types anymore.

![Figure 12. Binarization of Tree Types.](image-url)
The translation from binary regular tree types into \( \mathcal{L}_\mu \) formulas is given by the following rules:

\[
\begin{align*}
\{\}\, & : \mathcal{L}_{BT} \to \mathcal{L}_\mu \\
\{\emptyset\}\, & = \bot \\
\{\cdot\}\, & = \bot \\
\{T_1 \mid T_2\}\, & = \{T_1\} \lor \{T_2\} \\
\{l(X_1, X_2)\}\, & = l \land \text{succ}_1(X_1) \land \text{succ}_2(X_2) \\
\{\text{let } (X_i \to T_i)_{1 \leq i \leq m} \text{ in } T\}\, & = \text{let} \mu (X_i, \{T_i\}_{1 \leq i \leq m} \text{ in } \{T\})
\end{align*}
\]

where there is an implicit bijective correspondence between \( \mathcal{L}_{BT} \) variables from \( \mathcal{TVar} \) and \( \mathcal{L}_\mu \) variables from \( \mathcal{Var} \). Note that the translations of the empty tree type and the empty tree are the same since we choose not to mention explicitly empty trees in satisfiability results. The function \( \text{succ}(\cdot) \) sets the tree frontier accordingly:

\[
\text{succ}(\cdot) : \mathcal{Prog} \times \mathcal{TVar} \to \mathcal{L}_\mu
\]

\[
\text{succ}_o(X) = \begin{cases} 
\{\alpha\}X & \text{if nullable}(X) \\
\langle\alpha\rangle X & \text{if not nullable}(X)
\end{cases}
\]

The predicate \( \text{nullable}(\cdot) \) indicates if a type contains the empty tree:

\[
\begin{align*}
\text{nullable}(\cdot) : & \mathcal{TVar} \cup \mathcal{L}_{BT} \to \{\text{true, false}\} \\
\text{nullable}(X) & = \text{nullable}(\emptyset(X)) \\
\text{nullable}(\emptyset) & = \text{false} \\
\text{nullable}(\epsilon) & = \text{true} \\
\text{nullable}(l) & = \text{false} \\
\text{nullable}(T_1 \mid T_2) & = \text{nullable}(T_1) \lor \text{nullable}(T_2) \\
\text{nullable}(l(X_1, X_2)) & = \text{false} \\
\text{nullable}(\text{let } (X_i \to T_i)_{1 \leq i \leq m} \text{ in } T) & = \text{nullable}(T)
\end{align*}
\]

5. XML DECISION PROBLEMS

We have translated both XPath over unranked trees, and regular unranked tree types in the unifying \( \mathcal{L}_\mu \) logic over binary trees. Owing to these embeddings, we now reduce XML decision problems (such as XPath containment, equivalence, satisfiability, overlap and coverage) to satisfiability in \( \mathcal{L}_\mu \).

We first introduce some simplified notations. For an XPath expression \( e \in \mathcal{L}_{XPath} \), we note \( \varphi_e \) the translated formula \( E^{-}[e][\varphi_{\text{context}}] \in \mathcal{L}_\mu \). Furthermore, we note \( T \) the set of trees: by default, \( T = T_{\Sigma}^{\emptyset} \), and whenever an optional DTD \( d \in \mathcal{L}_{DTD} \) is specified \( T = \llbracket d \rrbracket^d \). Finally, we note \( \varphi_T \) the \( \mathcal{L}_\mu \) embedding of the tree language \( T \). In the absence of DTDs \( \varphi_T = \top \), and \( \varphi_T = \llbracket \emptyset \rrbracket^d \) in the presence of \( d \in \mathcal{L}_{DTD} \).

Several decision problems needed in applications can be expressed in terms of \( \mathcal{L}_\mu \) formulas:

---XPath Containment

---Input: \( e_1, e_2 \in \mathcal{L}_{XPath} \) and optional \( d \in \mathcal{L}_{DTD} \)

---Problem: Does \( e_2 \) always select all nodes selected by \( e_1 \)?

---Definition: \( \forall t \in T, \forall x \in t, S_t[e_1] = S_t[e_2] \)

Tested $L_\mu$ formula: $\varphi_{e_1} \land \neg \varphi_{e_2}$

XPath Equivalence

- Input: $e_1, e_2 \in L_{XPath}$ and optional $d \in L_{DTD}$
- Problem: Does $e_2$ always select exactly the same nodes than $e_1$?
- Definition: $\forall t \in T, \forall x \in t, S_e[e_1]_t^x = S_e[e_2]_t^x$
- Equivalence can be tested by two successive and separate containment checks

XPath Satisfiability:

- Input: $e \in L_{XPath}$ and optional $d \in L_{DTD}$
- Problem: Will $e$ ever return a non-empty set of nodes?
- Definition: $\forall t \in T, \forall x \in t, S_e[e]_t^x = \emptyset$
- Tested $L_\mu$ formula: $\varphi_e$

XPath Overlap:

- Input: $e_1, e_2 \in L_{XPath}$ and optional $d \in L_{DTD}$
- Problem: May $e_1$ and $e_2$ select common nodes?
- Definition: $\forall t \in T, \forall x \in t, S_e[e_1]_t^x \cap S_e[e_2]_t^x = \emptyset$
- Tested $L_\mu$ formula: $\varphi_{e_1} \land \varphi_{e_2}$

XPath Coverage:

- Input: $e_1, e_2, \ldots, e_n \in L_{XPath}$ and optional $d \in L_{DTD}$
- Problem: Are nodes selected by $e_1$ always selected by one of the $e_2, \ldots, e_n$?
- Definition: $\forall t \in T, \forall x \in t, S_e[e_1]_t^x \subseteq \bigcup_{2 \leq i \leq n} S_e[e_i]_t^x$
- Tested $L_\mu$ formula: $\varphi_{e_1} \land \bigwedge_{2 \leq i \leq n} \neg \varphi_{e_i}$

Note that for the containment problem, we actually test the unsatisfiability of $\varphi_{e_1} \land \neg \varphi_{e_2}$. Indeed, checking that an XPath expression $e_1$ is contained into another expression $e_2$ consists in checking that the implication $\varphi_{e_1} \Rightarrow \varphi_{e_2}$ holds for all trees.

In other terms, there exists no tree for which the results of $e_1$ are not included in those of $e_2$, i.e. the negated implication $\varphi_{e_1} \land \neg \varphi_{e_2}$ is unsatisfiable.

Since we need to enforce the finite binary tree model property (as seen in Section 2.1), we formulate decision problems from the root, and the actually checked formula becomes:

$$
\varphi_{\text{root}} \land \varphi_{\text{ft}} \land (\varphi_T \land \mu X. \varphi_{\text{tested}} \lor (1) X \lor (2) X)^{\text{FBT}}
$$

where $\varphi_{\text{tested}}$ corresponds to a particular XPath decision problem from those given above. Intuitively, the fixpoint is introduced for “plunging” XPath navigation performed by $\varphi_{\text{tested}}$ at any location in the tree. It is for example necessary for relative XPath expressions that involve upward navigation in the tree.

It is important to note that formula (1) is always alternation-free since both embeddings of XPath and tree types produce alternation-free formulas, and the negation of an alternation free sentence remains alternation-free. In practice, negated sentences introduced by XPath embeddings are turned into negation normal form, by applying the rules given on Figure 4.

6. SYSTEM EVALUATION

The proposed approach has been fully implemented and the working system is available [Genevès and Layaida 2006]. A compiler takes XPath expressions as input, and translates them into $L_\mu$ formulas. Another compiler takes regular tree types
as input (DTDs) and outputs their $L_\mu$ translation. The formula of a particular decision problem is then composed, normalized and solved.

### 6.1 Complexity Analysis and Implementation Principles

Our $\mu$-calculus satisfiability solver is specialized for the alternation-free $\mu$-calculus with converse. A detailed description of the solver is beyond the scope of the paper. We rather focus on its aspects which allow to establish precise complexity results for XML decision problems considered in this paper. The $L_\mu$ satisfiability solver is closely inspired from the tableau methods described in [Tanabe et al. 2005] and [Pan et al. 2002]. The algorithm relies on a top-down tableau method which attempts to construct satisfying Kripke structures by a fixpoint computation. Nodes of the tableau are specific subsets of a set called the Lean [Pan et al. 2002]. Given a formula $\psi \in L_\mu$, the Lean is the subset of the Fischer-Ladner closure [Fischer and Ladner 1979] of $\psi$ composed of atomic and modal subformulas of $\psi$ [Pan et al. 2002]. The algorithm starts from the set of all possible nodes, and repeatedly removes inconsistent nodes until a fixpoint is reached. At the end of the computation, if $\psi$ is present in a node of the fixpoint, then $\psi$ is satisfiable. In this case, the fixpoint contains a satisfying model that can be easily extracted and used as a satisfying example XML tree.

We can now state the complexity of XML decision problems addressed in this paper:

**Proposition 6.1.** XPath containment, equivalence, satisfiability, overlap and coverage decision problems, in the presence or absence of regular tree constraints, can be solved in time complexity $2^{O(n \cdot \log n)}$, where $n$ is the Lean size of the corresponding $L_\mu$ formula.

This upper-bound is derived from:

1. the linear translations of XPath and regular tree types into the $\mu$-calculus;
2. the $2^{O(n \cdot \log n)}$ time complexity of our solver, which corresponds to the best known complexity for deciding alternation-free $\mu$-calculus with converse over Kripke structures [Tanabe et al. 2005]. Note that it is more efficient than the complexity for the whole $\mu$-calculus with converse [Vardi 1998] which is known to be $2^{O(n^4 \cdot \log n)}$ [Grädel et al. 2002].

The key observation for the linear translation of regular tree types is that only distinct atomic and modal subformulas of the translated formula are present in the Lean, even for a $n$-ary binder $\varphi = \text{let}_\mu (X_i.\varphi_i)_{1 \leq i \leq m}$ in $X_k$. More precisely, the Lean corresponding to the translation of $\varphi$ contains at most:

— the two eventualities $\langle a \rangle \top$ for $a = 1, 2$
— $2 \cdot m$ universalities $[a] \varphi$ where $m$ is the number of binary tree type variables in the binder and the constant factor corresponds to the downward programs $a = 1, 2$
— the atomic propositions representing the alphabet symbols used in $\varphi$

Deriving complexity from properties of the closure of a formula was first used by Fischer and Ladner for establishing decidability of PDL in single exponential time [Fischer and Ladner 1979]. Analog observations have also been made for the modal
logic K [Pan et al. 2002], and the $\mu$-calculus over general Kripke structures [Tanabe et al. 2005]. Our results can be seen as an application of this technique to the case where regular tree types are combined with XPath bidirectional queries over finite trees.

Keys of the efficiency of the method for large practical instances are as follows:

1. Nodes of the tableau contain only modal formulas and exactly one atomic proposition (for XML), which greatly reduces the number of enumerated nodes for large alphabets.

2. Negation in the $\mu$-calculus is rather straightforward compared to automata techniques. Indeed, handling $\mathcal{L}_\mu$ formulas in negation normal form simply reduces to checking membership of atomic propositions in tableau nodes. This contrasts with tree automata techniques which require for every negation the full construction and complementation of automata with an exponential blow-up. As pointed out in [Baader and Tobies 2001] and [Pan et al. 2002], tableau methods for logics with the tree model property can be viewed as implementations of the automata-theoretic approach which avoids an explicit automata construction.

3. Our implementation relies on representing sets of nodes and operating on them symbolically using Binary Decision Diagrams (BDDs) [Bryant 1986]. BDDs provide a canonical representation of boolean functions and their effectiveness is well known in formal verification of systems [Edmund M. Clarke et al. 1999]. In our approach, BDD variables encode truth status of Lean formulas. The cost of BDD operations is very sensitive to variable ordering. Finding the optimal variable ordering is known to be NP-complete [Hojati et al. 1996], however several heuristics are known to perform well in practice [Edmund M. Clarke et al. 1999]. Choosing a good initial variable order does significantly improve performance. We found out that preserving locality of the initial problem is essential. We observed that the variable order determined by the breadth-first traversal of the initial formula (thus keeping sister subformulas in close proximity while ordering Lean formulas) yields better results in practice.

6.2 Experimental Results

The objective of the section aims at testing the practical performance of our method. We carried out several testing scenarios. First, we used an XPath benchmark [Franceschet 2005] whose goal is to cover XPath features by gathering a significant variety of XPath expressions met in real-world applications. In this first test series, we do not consider types yet, and only focus on the XPath containment problem, since its logical formulation (presented in Section 5) is the most complex, as it requires the logic to be closed under negation. The first test series consists in finding the relation holding for each pair of queries from the benchmark. This means checking the containment of each query of the benchmark against all the others. We note $q_i \subseteq q_j$ whenever the query $q_i$ is contained in the query $q_j$. Comparisons of two queries $q_i$ and $q_j$ may yield to three different results:

\[q_i \subseteq q_j\]
(1) \( q_i \subseteq q_j \) and \( q_j \subseteq q_i \), the queries are semantically equivalent, we note \( q_i \equiv q_j \)
(2) \( q_i \subseteq q_j \) but \( q_j \nsubseteq q_i \), we denote this by \( q_i \subset q_j \) or alternatively by \( q_j \supset q_i \)
(3) \( q_i \nsubseteq q_j \) and \( q_j \nsubseteq q_i \), queries are not related, we note \( q_i \nsim q_j \)

Queries are presented on Figure 13. Corresponding results together with running times of the decision procedure are summarized on Table I. Times reported in milliseconds correspond to the actual running time of the \( \mu \)-calculus satisfiability solver without the extra time spent for parsing XPath nor the (linear) cost of the translation into \( \mu \)-calculus. Obtained results show that all tests are solved in several milliseconds. This suggests that XPath expressions used in real-world scenarios can be efficiently handled in practice.

\[
q_1 /site/regions/*/item \\
q_2 /site/closedauctions/closedauktion/description/parlist/listitem/text/keyword \\
q_3 //keyword \\
q_4 /descendant-or-self::listitem/descendant-or-self::keyword \\
q_5 /site/regions/*/item[parent::namerica or parent::samerica] \\
q_6 //keyword/ancestor::listitem \\
q_7 /keyword/ancestor-or-self::mail \\
q_8 /site/regions/namerica/item /site/regions/samerica/item \\
q_9 /site/people/person/address and (phone or homepage)]
\]

Fig. 13. XPath Queries Taken from the XPathmark Benchmark.

<table>
<thead>
<tr>
<th>Relation</th>
<th>Time (ms)</th>
<th>Relation</th>
<th>Time (ms)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( q_1 \napprox q_2 )</td>
<td>16</td>
<td>( q_3 \napprox q_4 )</td>
<td>12</td>
</tr>
<tr>
<td>( q_1 \napprox q_3 )</td>
<td>14</td>
<td>( q_3 \napprox q_5 )</td>
<td>14</td>
</tr>
<tr>
<td>( q_1 \napprox q_4 )</td>
<td>9</td>
<td>( q_3 \napprox q_9 )</td>
<td>13</td>
</tr>
<tr>
<td>( q_1 \subset q_5 )</td>
<td>16</td>
<td>( q_4 \napprox q_5 )</td>
<td>24</td>
</tr>
<tr>
<td>( q_1 \napprox q_6 )</td>
<td>22</td>
<td>( q_4 \napprox q_9 )</td>
<td>9</td>
</tr>
<tr>
<td>( q_1 \napprox q_7 )</td>
<td>15</td>
<td>( q_4 \napprox q_7 )</td>
<td>22</td>
</tr>
<tr>
<td>( q_1 \supset q_8 )</td>
<td>9</td>
<td>( q_4 \napprox q_8 )</td>
<td>14</td>
</tr>
<tr>
<td>( q_1 \napprox q_9 )</td>
<td>16</td>
<td>( q_4 \napprox q_9 )</td>
<td>13</td>
</tr>
<tr>
<td>( q_2 \subset q_3 )</td>
<td>32</td>
<td>( q_5 \napprox q_6 )</td>
<td>14</td>
</tr>
<tr>
<td>( q_2 \subset q_4 )</td>
<td>38</td>
<td>( q_5 \napprox q_7 )</td>
<td>11</td>
</tr>
<tr>
<td>( q_2 \napprox q_5 )</td>
<td>24</td>
<td>( q_5 \napprox q_7 )</td>
<td>11</td>
</tr>
<tr>
<td>( q_2 \napprox q_6 )</td>
<td>22</td>
<td>( q_5 \napprox q_9 )</td>
<td>8</td>
</tr>
<tr>
<td>( q_2 \napprox q_7 )</td>
<td>31</td>
<td>( q_5 \napprox q_9 )</td>
<td>18</td>
</tr>
<tr>
<td>( q_2 \napprox q_8 )</td>
<td>26</td>
<td>( q_6 \napprox q_7 )</td>
<td>21</td>
</tr>
<tr>
<td>( q_2 \napprox q_9 )</td>
<td>34</td>
<td>( q_6 \napprox q_8 )</td>
<td>15</td>
</tr>
<tr>
<td>( q_3 \supset q_4 )</td>
<td>17</td>
<td>( q_6 \napprox q_9 )</td>
<td>14</td>
</tr>
<tr>
<td>( q_3 \napprox q_5 )</td>
<td>5</td>
<td>( q_7 \napprox q_8 )</td>
<td>26</td>
</tr>
<tr>
<td>( q_3 \napprox q_6 )</td>
<td>4</td>
<td>( q_8 \napprox q_9 )</td>
<td>11</td>
</tr>
</tbody>
</table>

Table I. Results and Total Computation Times.

As a second test series, we compare expressions found in research papers on the containment of XPath expressions. Figure 14 presents the expressions we collected. For this set of expressions, the tree pattern homomorphism technique [Miklau and Suciu 2004] returns false negatives, whereas our approach is complete. Figure 14
also shows the results obtained with our system. They suggest that our system is able to reasonably handle containment instances which are difficult to solve using other techniques.

\[
e_1 \quad /a[.]/b[c]/d]/b[c]/d]/b[c]/d]\n\[
e_2 \quad /a[.]/b[c]/d]/b[c]/d]\n\[
e_3 \quad a[b]/d*/g\n\[
e_4 \quad a[b]/(b[c]/d)(e[f])/g\n\[
e_5 \quad a[b]/d/e/g/a/b/d/f/g\n\[
e_6 \quad a/b/s/c/b/s/c]/d\n\[
e_7 \quad a/b*/c/*/d\n\[
e_8 \quad a[b][c][b][f][c]\n\[
e_9 \quad a[b][e][b][f]\n\[
e_{10} \quad \text{/descendant::editor[parent::journal]}\n\[
e_{11} \quad \text{/descendant-or-self::journal/child::editor}\n\]

Fig. 14. Results on XPath Containment Instances Found in Research Papers.

Figure 15 presents the results of a third test series including examples with intersection, and axes such as “following” and “preceding”, which are not illustrated in the previous series.

\[
e_{12} \quad a/b//c/following-sibling::d/e\n\[
e_{13} \quad a/d[preceding-sibling::c]/e\n\[
e_{14} \quad /a/b//c/following-sibling::d/e\n\[
e_{15} \quad /b/ancestor::a[/][preceding-sibling::c]/e\n\[
e_{16} \quad /b[preceding::a]/following::c\n\[
e_{17} \quad /a/b//c/following::e\n\[
e_{18} \quad a/b[/c]/following::d/e\n\[
e_{19} \quad a/d[preceding::c]/e\n\[
e_{20} \quad a/b/[d][preceding-sibling::c]/e\n\[
e_{21} \quad a/c/following::d/e\n\[
e_{22} \quad a/d[preceding::c]/e\n\[
e_{23} \quad a/b/[c]/following::d/e\cap a/d[preceding::c]/e\n\[
e_{24} \quad a/c/following::d/e\cap a/d[preceding::c]/e\n\]

Fig. 15. Results on Examples Including “following” and “preceding” Axes.

The fourth test series aims at evaluating the effectiveness of the system for XPath decision problems in the presence of DTDs. We used a small recursive DTD (given on Figure 16), and real-world DTDs of the SMIL [Hoschka 1998] and XHTML [Pemberton 2000] standards. Table II gives the size of each DTD by presenting the number of symbols used (alphabet size) and the number of grammar production rules (type variables) in the unranked and binary representations.

For each DTD, we built several XPath decision problems using the expressions shown on Figure 17. Some decision problems and their results are presented on Table III. The system performs well for the respectively small, medium and large recursive DTDs.
Table II. DTDs Used in Practical Experiments.

<table>
<thead>
<tr>
<th>DTD Examples</th>
<th>Symbols</th>
<th>Type Variables</th>
<th>Binary Type Variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>People.dtd (Figure 16)</td>
<td>8</td>
<td>15</td>
<td>11</td>
</tr>
<tr>
<td>SML 1.0 [Hoschka 1998]</td>
<td>19</td>
<td>29</td>
<td>11</td>
</tr>
<tr>
<td>XHTML 1.0 Strict [Pemberton 2000]</td>
<td>77</td>
<td>104</td>
<td>325</td>
</tr>
</tbody>
</table>

Fig. 16. (People.dtd) A Simple Recursive DTD.

\[
\begin{align*}
p_1 & \quad \text{people/} \\
p_2 & \quad //\text{person} \\
p_3 & \quad /\text{descendant-or-self}/\text{people}/\text{person} \\
p_4 & \quad //\text{children}/\text{person} \\
p_5 & \quad \text{switch}/\text{layout} \\
p_6 & \quad \text{smil}/\text{head}/ //\text{layout} \\
p_7 & \quad \text{smil}/\text{head}/ //\text{layout} [\text{ancestor::switch}] \\
p_8 & \quad /*//\text{switch} [\text{ancestor::head}]/\text{descendant::seq}/\text{descendant::audio} [\text{preceding-sibling::video}] \\
p_9 & \quad \text{descendant::a}[\text{ancestor::a}] \\
p_{10} & \quad /\text{descendant::} * \\
p_{11} & \quad \text{html}/(\text{head} /\text{body}) \\
p_{12} & \quad \text{html}/\text{head}/\text{descendant::} * \\
p_{13} & \quad \text{html}/\text{body}/\text{descendant::} * \\
p_{14} & \quad //\text{img} \\
p_{15} & \quad //\text{img}[\text{not *}] \\
\end{align*}
\]

Fig. 17. XPath Expressions used in the presence of DTDs.

The satisfiability test for \( p_9 \) illustrates an additional benefit of our technique which automatically outputs a satisfying XML document (shown on Figure 18), enriched with XPath context and target information. Interestingly, this example also shows that the official XHTML DTD does not syntactically prohibit the nesting of anchors.

For the large XHTML case, we observe that the time needed is significantly more important, but deciding XPath problems remains practically feasible, especially for static analysis purposes where such operations are performed at compile-time.

These preliminary measurements shed light, for the first time, on the cost of solving XPath decision problems in practice.

7. RELATED WORK

Relatively close in spirit to our work is the constructive connection between XPath and formal logics, which is actively studied [Marx 2004b; Benedikt et al. 2005; Bar-
Table III. Some Decision Problems in the Presence of DTDs and Results.

<table>
<thead>
<tr>
<th>XPath Decision Problem</th>
<th>Instance</th>
<th>DTD</th>
<th>Answer</th>
<th>Time (ms)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Containment</td>
<td>( p_1 \subseteq p_2 )</td>
<td>People.dtd</td>
<td>true</td>
<td>32</td>
</tr>
<tr>
<td>Containment</td>
<td>( p_2 \subseteq p_3 \cup p_4 )</td>
<td>People.dtd</td>
<td>true</td>
<td>41</td>
</tr>
<tr>
<td>Coverage</td>
<td>( p_5 \subseteq p_3 \cup p_4 )</td>
<td>SMIL 1.0</td>
<td>true</td>
<td>32</td>
</tr>
<tr>
<td>Satisfiability</td>
<td>( p_5 \subseteq p_7 )</td>
<td>SMIL 1.0</td>
<td>true</td>
<td>41</td>
</tr>
<tr>
<td>Overlap</td>
<td>( p_6 \cap p_7 \neq \emptyset )</td>
<td>SMIL 1.0</td>
<td>false</td>
<td>174</td>
</tr>
<tr>
<td>Satisfiability</td>
<td>( p_8 \subseteq p_7 )</td>
<td>SMIL 1.0</td>
<td>true</td>
<td>120</td>
</tr>
<tr>
<td>Containment</td>
<td>( p_9 \subseteq p_11 \cup p_12 \cup p_13 )</td>
<td>XHTML 1.0</td>
<td>true</td>
<td>2630</td>
</tr>
<tr>
<td>Containment</td>
<td>( p_9 \subseteq p_12 \cup p_13 )</td>
<td>XHTML 1.0</td>
<td>true</td>
<td>2872</td>
</tr>
<tr>
<td>Containment</td>
<td>( p_9 \subseteq p_15 )</td>
<td>XHTML 1.0</td>
<td>true</td>
<td>2931</td>
</tr>
</tbody>
</table>

Fig. 18. Generated XML Tree for Satisfiability of \( p_9 \) in Presence of the XHTML DTD.

celó and Libkin 2005]. From [Marx 2004a; Genevès and Vion-Dury 2004b], we know that XPath expressive power is close to first-order logic (FO). However, FO does not fully capture regular tree types [Benedikt and Segoufin 2005]. Thus, attempts to characterize XPath subfragments in terms of FO variants like Computational Tree Logic (CTL) [Marx 2004b; Miklau and Suciu 2004], which is equivalent to FO over tree structures [Marx 2004a; Barceló and Libkin 2005], are not intended to support regular XML types. The work found in [Afanasiev et al. 2005] proposes a variant of Propositional Dynamic Logic (PDL) [Fischer and Ladner 1979] with a similar EXPTIME complexity for reasoning about ordered trees, but whose exact expressive power is still under study.

One of the most expressive (yet decidable) known logic is Monadic Second Order Logic (MSO) over tree structures, which extends FO by quantification over sets of nodes. Specifically, the appropriate MSO variant which exactly captures regular tree types is the weak monadic second-order logic of two successors (WS2S) [Thatcher and Wright 1968; Doner 1970]. From [Arnold and Niwiński 1992; Kupferman and Vardi 1999], we know that WS2S is exactly as expressive as the alternation-free fragment (AFMC) of the propositional modal \( \mu \)-calculus introduced in [Kozen...
However, the satisfiability problem for WS2S is non-elementary\(^9\) while in EXPTIME\(^{10}\) for AFMC. Moreover, the AFMC subsumes all early logics such as CTL [Clarke and Emerson 1981] and PDL [Fischer and Ladner 1979]. Furthermore, the work in [Vardi 1998] adds converse programs to the propositional modal \(\mu\)-calculus and shows that the resulting logic still admits an EXPTIME decision procedure for satisfiability. It follows that the alternation-free modal \(\mu\)-calculus with converse sounds as an appropriate logic for XML: it is expressive enough to capture a significant class of XPath decision problems, while potentially providing efficient and practically effective decision procedures.

From the point of view of computational complexity, some EXPTIME upper bounds are already known for satisfiability and containment of specific subsets of our XPath fragment. The complexity of XPath satisfiability in the presence of DTDs is studied in [Benedikt et al. 2005]. XPath containment has specifically attracted a lot of research attention [Amer-Yahia et al. 2001; Deutsch and Tannen 2001; Miklau and Suciu 2004; Neven and Schwentick 2003; Schwentick 2004; Wood 2000; 2003]. Prior work concentrated on various combinations of the previous factors for obtaining complexity results (see [Schwentick 2004] for an overview). Specifically, the focus was given to restricted positive XPath subfragments without upward axes. In particular, [Neven and Schwentick 2003] proves an EXPTIME upper-bound for containment (in the presence of DTDs) of queries containing the “child” and “descendant” axes, and union of paths. [Deutsch and Tannen 2001] considers XPath containment in the presence of DTDs and simple XPath integrity constraints (SXICS). They obtain that this problem is undecidable in general and in the presence of bounded SXICS and DTDs. Containment for the fragment \(\text{XP}^{\{\cdot,//,\}^*}\) is shown to be coNP-complete in [Miklau and Suciu 2004], where the containment mapping technique relies on a polynomial time tree homomorphism algorithm, which gives a sufficient but not necessary condition for containment of \(\text{XP}^{\{\cdot,//,\}^*}\) in general. Additionally, the containment problem is shown to be in EXPTIME for the fragments \(\text{XP}^{\{\cdot,//,\}}\), \(\text{XP}^{\{\cdot,\}^*}\), \(\text{XP}^{\{\cdot,\}^*}\), \(\text{XP}^{\{\cdot,\}^*}\) in the presence of DTDs in [Wood 2003].

Compared to all these previous works, the XPath fragment we consider is far more complete and much more realistic. We also present a single unifying logical framework in which all major XPath features but also regular tree types fit together. Moreover, our framework yields effective decision procedures usable in practice for real world scenarios (whereas no usable working system has been reported in prior work).

Finally, from a theoretical perspective, we see the connection between XML and

---

\(^9\)We recall that the term \textit{elementary} introduced by Grzegorczyk [Grzegorczyk 1953] refers to functions obtained from some basic functions by operations of limited summation and limited multiplication. Consider the function \(\text{tower}(n)\) defined by:

\[
\begin{align*}
\text{tower}(n, 0) &= n \\
\text{tower}(n, k + 1) &= 2^{\text{tower}(n, k)}
\end{align*}
\]

Grzegorczyk has shown that every elementary function in one argument is bounded by \(\lambda n.\text{tower}(n, c)\) for some constant \(c\). Hence, the term \textit{non-elementary} refers to a function that grows faster than any such function.

\(^{10}\)The complexity class EXPTIME is the set of all decision problems solvable by a deterministic Turing machine in \(O(2^{p(n)})\) time, where \(p(n)\) is a polynomial function of the input size \(n\).
the $\mu$-calculus as a simple way of deriving the precise upper-bound time complexity $2^{O(n \cdot \log n)}$ of XML decision problems, where $n$ is the combined size of considered XPath queries and tree types.

8. CONCLUSION

We propose a new logical approach for XPath decision problems. XPath queries and regular tree types are translated into the $\mu$-calculus. XML decision problems are expressed as formulas in this logic, then decided using an efficient decision procedure for $\mu$-calculus satisfiability. This paper makes several contributions. First, we propose a specific variant of the $\mu$-calculus, namely the alternation-free modal $\mu$-calculus with converse, as the appropriate logic for reasoning on XML trees, XPath queries and XML types. As a valuable outcome, we show how both XPath and regular tree types can be linearly translated in the $\mu$-calculus. Second, we take advantage of these translations to reduce several XML decision problems to satisfiability in $L_\mu$. We obtain effective EXPTIME decision procedures, usable in practice. The considered XPath fragment includes union, intersection, path composition together with all downward and upward axes, branching, boolean connectives, wildcards, and negation, in the presence or absence of DTDs. This fragment is far more complete than other fragments addressed in previous studies. We provide practical experiments and detailed results that corroborate our claim that this approach is efficient in practice for real-world XPath expressions and DTDs. Our system has been fully implemented [Genevès and Layaida 2006] and can be used for the static analysis of XML specifications. This strengthens the hope for an effective analysis of standard XML transformations in the near future.

Eventually, an additional advantage of the technique is to allow generation of XML tree examples when the containment does not hold. We believe this makes our method of special interest for many applications including debuggers, or applications that can benefit from a precise reporting during static analysis stages.

One direction of future work consists in specifically tuning the $\mu$-calculus satisfiability solver for XML. Incorporating XML peculiarities directly in the core of the $\mu$-calculus solver (instead of general Kripke structures) may yield even more efficient decision procedures.

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A System for the Static Analysis of XPath

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