A space– and time–efficient Implementation of the Merkle Tree Traversal Algorithm

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Abstract. We present an algorithm for the Merkle tree traversal problem which combines the efficient space-time trade-off from the fractal Merkle tree [3] and the space efficiency from the improved log space-time Merkle trees traversal [8]. We give an exhaustive analysis of the space and time efficiency of our algorithm in function of the parameters $H$ (the height of the Merkle tree) and $h$ ($h = \frac{H}{2}$ where $L$ is the number of levels in the Merkle tree). We also analyze the space impact when a continuous deterministic pseudo–random number generator (PRNG) is used to generate the leaves. We further program a low storage–space and a low time–overhead version of the algorithm in Java and measure its performance with respect to the two different implementations cited above. Our implementation uses the least space when a continuous PRNG is used for the leaf calculation.

Keywords: Merkle tree traversal, Authentication path computation, Merkle signatures

1 Introduction

Merkle’s binary hash trees are currently very popular, because their security is independent from any number theoretic conjectures [6]. Indeed their security is based solely on two well defined properties of hash functions: (i) Pre-image resistance: that is, given a hash value $v$, it is difficult to find a message $m$ such that $v = \text{hash}(m)$. The generic pre-image attack requires $2^n$ calls to the hash function, where $n$ is the size of the output in bits. (ii) Collision resistance: that is, finding two messages $m_1 \neq m_2$ such that $\text{hash}(m_1) = \text{hash}(m_2)$ is difficult. The generic complexity of such an attack is given by the birthday bound which is $2^{n/2}$ calls to the hash function. It is interesting to note that the best quantum algorithm to date for searching $N$ random records in a data base (an analogous problem to hash pre-image resistance) achieves only a speedup of $O(\sqrt{N})$ to the classical one $O(N)$ [15]. More to the point in [14] the speedup of a quantum algorithm that finds collisions in arbitrary r-to-one functions is $O(\sqrt[3]{N/r})$ to the classical one.

A Merkle tree is a complete binary tree with a $n$-bit hash value associated with each node. Each internal node value is the result of a hash of the node values of its children. Merkle trees are designed so that a leaf value can be verified with respect to a publicly known root value given the authentication path of the respective leaf. The authentication path for a leaf consists of one node value at each level $l$, where $l = 0, \ldots, H - 1$, and $H$ is the height of the Merkle tree ($H \leq 20$ in most practical cases). The chosen nodes are siblings of the nodes on the path connecting the leaf to the root.

The Merkle tree traversal problem answers the question of how to calculate efficiently\(^1\) the authentication path for all leaves one after another starting with the first Leaf\(_0\) up to the last Leaf\(_{2^H-1}\), if there is only a limited amount of storage available (e.g. in Smartcards).

\(^1\) The authors of [7] proved that the bounds of space ($O(\log(H/\log(l)))$) and time ($O(H/\log(l)))$) for the output of the authentication path of the current leaf are optimal ($l$ is a freely choosable parameter).
The generation of the root of the Merkle tree (the public key in a Merkle signature system) requires the computation of all nodes in the tree. This means a grand total of $2^H$ leaves’ evaluations and of $2^H - 1$ hash computations. The root value (the actual public key) is then stored into a trusted database accessible to the verifier.

The leaves of a Merkle tree are used either as a one–time token to access resources or as building block for a digital signature scheme. Each leaf has an associated private key that is used to generate either the token or a signature building block (see 4.2). The tokens can be as simple as a hash of the private key. In the signature case, more complex schemes are used in the literature (see for example [2] for a review).

Related work

Two solutions to the Merkle tree traversal problem exist. The first is built on the classical tree traversal algorithm but with many small improvements [8] (called log algorithm from now on). The second one is the fractal traversal algorithm [3] (called fractal algorithm from now on). The fractal algorithm trades efficiently space against time by adapting the parameter $h$ (the height of both Desired and Exist subtrees, see Fig. 1), however the minimal space it uses for any given $H$ (if $h$ is chosen for space optimality) is more than what the log algorithm needs. The log algorithm cannot as effectively trade space for performance. However, for small $H$ it can still achieve a better time and space trade-off than the fractal algorithm.

A study [7] analyses theoretically the impact on space and time–bounds of some enhancements to both the log and fractal algorithm, which are important to our implementation.

Our contributions

We developed an algorithm for the Merkle tree traversal problem which combines the efficient space-time trade-off from [3] with the space efficiency from [8]. This was done by applying all the improvements discussed in [8] to the fractal algorithm [3]. We have also analyzed the space impact of a continuous deterministic pseudo–random number generator (PRNG)\footnote{A deterministic pseudo–random number generator which can not access any random number in its range without first computing all the preceding ones.} on the algorithms. All these improvements lead to an algorithm with a worst case storage of $[L \times 2^h + 2H - 2h]$ hash values (Sec. 4.4). The worst case time bound for the leaves’ computation per authentication path, amounts to $\frac{2^h - 1}{2^h} \times (L - 1) + 1$ (Sec. 4.4). This means a reduction in space of about a factor 2 compared with the fractal algorithm [3] (see Fig. 5 and Fig. 4).

Although on first sight our enhancements are predated by [7] three main differences distinguish our contribution vis-à-vis [7]: (i) Our use of a different TreeHash and metrics; (ii) Our special computation of the Desired tree (see Section 4.2) and (iii) Our use of a continuous PRNG in leaf computation.

We further implemented the algorithm in Java with focus on a low space and time overhead [1] and we measured its performance (Sec. 6).

2 Preliminaries

The idea of the fractal algorithm [3] is to store only a limited set of subtrees within the whole Merkle tree (see Fig. 1). They form a stacked series of $L$ subtrees $\{Subtree_i\}_{i=0}^{L-1}$. Each subtree
consists of an \textit{Exist} tree \{\textit{Exist}_i\} and a \textit{Desired} tree \{\textit{Desired}_i\}, except for \textit{Subtree}_{L-1}, which has no \textit{Desired} tree. The \textit{Exist} trees contain the authentication path for the current leaf. When the authentication path for the next leaf is no longer contained in some \textit{Exist} trees, these are replaced by the \textit{Desired} tree of the same subtree. The \textit{Desired} trees are built incrementally after each output of the authentication path algorithm, thus minimizing the operations needed to evaluate the subtree.

![Fractal Merkle tree structure and notation](image)

**Fig. 1:** Fractal Merkle tree structure and notation (Figure courtesy of [3]). A hash tree of height \(H\) is divided into \(L\) levels, each of height \(h\). The leaves of the hash tree are indexed \(\{0, 1, \ldots, 2^H - 1\}\) from left to right. The height of a node is defined as the height of the maximal subtree for which it is the root and ranges from \(0\) (for the leaves) to \(H\) (for the root). An \(h\)-subtree is "at level \(i\)" when the height of its root is \((i + 1)h\) for some \(i \in \{0, 1, \cdots, L - 1\}\).

The nodes in a Merkle tree are calculated with an algorithm called \textit{TreeHash}. The algorithm takes as input a stack of nodes, a leaf calculation function and a hash function and it outputs an updated stack, whose top node is the newly calculated node. Each node on the stack has a height \(i\) that defines on what level of the Merkle tree this node lies: \(i = 0\) for the leaves and \(i = H\) for the root. The \textit{TreeHash} algorithm works in small steps. On each step the algorithm looks at its stack and if the top two elements have the same height it pops them and puts the hash value of their concatenation back onto the top of stack which now represents the parent node of the two popped ones. Its height is one level higher than the height of its children. If the top two nodes do not have the same height, the algorithm calculates the next leaf and puts it onto the stack, this node has a height of zero.

We quickly summarize the three main areas where our improvements were critical for a better space–time performance of the original fractal algorithm:

1. Left nodes have the nice property, that when they first appear in an authentication path, their children were already on an earlier authentication path (see Fig. 2). For right nodes this property does not hold. We can use this fact to calculate left nodes just before they are needed for the authentication path without the need to store them in the subtrees. So we can save half of the space needed for the subtrees, but compared to the fractal algorithm one additional leaf
calculation has to be carried out every two rounds (one round corresponds to the calculation of one authentication path).

2. In most practical applications, the calculation of a leaf is more expensive than the calculation of an inner node. This can be used to design a variant of the \textit{TreeHash} algorithm, which has a worst case time performance that is nearer to its average case for most practical applications. The improved \textit{TreeHash} (see Algorithm 1) given one leaf, calculates as many inner nodes as possible per update (see Section 4.1) before needing a new leaf, instead of processing just one leaf or one inner node as in the normal case.

3. In the fractal Merkle tree one \textit{TreeHash} instance per subtree exists for calculating the nodes of the Desired trees and each of them gets two updates per round. Therefore all of them have nodes on their stacks which need space of the order of $O(H^2 h)$. We can distribute the updates in another way, so that the associated stacks are mostly empty [5]. This reduces the space needed by the stacks of the \textit{TreeHash} instances to $O(H - h)$.

It is easy enough to adapt point one and two for the fractal algorithm, but point three needs some changes in the way the nodes in a subtree are calculated (see Sec. 4.2).

\begin{algorithm}
\caption{Listing: Generic version of \textit{TreeHash} that accepts different types of Process$_i$ (See Appendix A for a thorough definition of Process$_i$). A node has a height and an index, where the index indicates where a node is positioned in relation to all nodes with the same height in the Merkle tree.}
\begin{algorithmic}
\State \textbf{INPUT} : StackOfNodes, Leaf, Process$_i$, SubtreeIndex
\State \textbf{OUTPUT} : updated StackOfNodes
\State Node $\leftarrow$ Leaf
\If{Node.index \text{ (mod 2)} == 1}
\State continue $\leftarrow$ Process$_i$(Node, SubtreeIndex)
\Else
\State continue $\leftarrow$ 1
\EndIf
\While{continue $\neq$ 0 \text{ AND} (Node.height $\neq$ StackOfNodes.top.height)}
\State Node $\leftarrow$ hash(StackOfNodes.pop||Node)
\State continue $\leftarrow$ Process$_i$(Node, SubtreeIndex)
\EndWhile
\If{continue $\neq$ 0}
\State StackOfNodes.push(Node)
\EndIf
\end{algorithmic}
\end{algorithm}

3 Algorithm’s overview

In this Section we will give an overview of the complete algorithm and explain how all its components work together. The algorithm is divided into two phases. The first phase is the initialisation phase in which the public key is calculated (see Alg. 2). We run in this phase the improved \textit{TreeHash} (see 3 A inner node is a node with height greater than zero.)
Fig. 2: The colored lines mark the different authentication paths. The index $I$ at the start of each line indicates how many times a node on level $L$ of the authentication path has changed. An authentication path whose node has changed $I$ times on level $L$ has changed $I \times (2^L)$ times on level 0 (which changes each round). The dotted circles are left nodes or the root of a subtree which are not stored in a subtree.

Alg. 1) from [8], step by step until the root node is computed. The improved $TreeHash$ algorithm needs $Leaf_i$ where $i \in \{0, 1, \ldots, 2^H - 1\}$ as an input.

The value of $Leaf_i$ is dependent on the usage of the Merkle tree. It could be as simple as a token, where the leaf is a hash of the tokens private key, or a one time signature scheme like Winternitz [6] where the leaf is the public key of the one–time signature. The private keys needed to compute the leaves are provided by a PRNG, whose key corresponds to the private key of the complete Merkle tree.

In the initialisation phase each node is computed exactly once. This fact is used to store all right nodes in the first $Exist$ tree of each subtree and all the nodes in the authentication path for the $Leaf_0$. The second phase iteratively generates the authentication paths for all the remaining $Leaf_i$ (from left to right) where $i \in \{1, 2, \ldots, 2^H - 1\}$ (see Alg. 8 and Alg. 7). Each authentication path can be computed by changing the previous one [6]. The authentication path for $Leaf_i$ changes on a level $k$ if $2^k | i$. If the node changes to a right node, it can be found in one of the $Exist$ trees. If it changes to a left node, it can be computed from its two children. The right child can be found in the $Exist$ trees and the left child is on the previous authentication path (see Fig. 2).

When a node in the $Exist$ tree is no longer needed for the computation of any upcoming authentication path, it is removed. To prevent the $Exist$ tree running out of nodes, all the nodes in the $Desired$ tree have to be computed before the $Exist$ tree has no nodes left. This is done with the help of two $TreeHash$ instances per subtree. One, called the lower $TreeHash$, calculates all nodes on the bottom level\(^4\) of a $Desired$ tree (called bottom level nodes) from the leaves of the Merkle tree. The other, called the higher $TreeHash$, calculates all the remaining $Desired$ nodes\(^5\) (called non-bottom level nodes) from the bottom level ones. All the lower $TreeHash$ instances use the same scheduling algorithm as in [8] with $L - 1$ updates per round. The higher $TreeHash$ uses a custom

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\(^4\) The bottom level is the lowest level in a $Desired$ tree.

\(^5\) $Desired$ nodes are all the nodes stored in a $Desired$ tree.
scheduling algorithm which executes an update every $2^{\text{bottomLevel}}$ rounds. The higher TreeHash produces a node on a level $k$ in the Desired tree every $2^k$ rounds, which corresponds to the rate at which the authentication path changes on that level. When the last node from the Exist tree is removed, all the nodes in the Desired tree are computed and the Exist tree can be replaced with the Desired tree. In section 4.3 we will prove that the lower TreeHashes produce the nodes on the bottom level before the higher TreeHashes need them, if $L - 1$ updates are done per round. A lower TreeHash, which has terminated, is initialized again as soon as the generated node is used as input for the higher TreeHash. Because only the right nodes are stored in the subtrees, the TreeHashes do only have to compute right nodes and those left nodes which are used to calculate a right node contained in the Desired tree. The only left nodes never used to compute a right node in a Desired tree are the first left node at each level in each Desired tree. To ensure that no unneeded nodes are computed, the lower TreeHash does not compute nodes for its first $2^{\text{bottomLevel}}$ updates per Desired tree and so does the higher TreeHash for its first update per Desired tree. These skipped updates are nevertheless counted without the scheduling algorithm assigning them to another TreeHash. Therefore from the point of view of the scheduling algorithm the TreeHash behaves as if the nodes would have been computed.

4 Analysis

4.1 TreeHash Metrics

Below we give some definitions that will firstly permit a better understanding of our analysis and secondly, unify all the similar concepts scattered in the literature. We define as classical TreeHash the algorithm used in [3]. In that paper a step$_C$ is defined as the calculation of either one leaf or the node’s hash. We define as improved TreeHash the algorithm used in [8]. Therein a step$_I$ is defined as the calculation of the sum of one leaf and X hashes (where X is the number of nodes’ computations before a new leaf is needed). We define update $= 2 \times \text{step}_C$ in the case of the classical TreeHash and update $= 1 \times \text{step}_I$ in the case of the improved TreeHash.

Since in our work we assume that the hash computation time is very small compared to a leaf’s computation (an assumption certainly valid for MSS (Merkle Signature Scheme)), we use as the basic time unit (metrics) for this work the time we need to compute a leaf.

So we can claim that in the worst case condition a classical TreeHash update takes 2 leaves’ computations whereas an improved TreeHash update takes only one. For the calculation of all nodes in a tree of height $H$, the classical TreeHash needs $2^H - 2^{-1}$ updates ($2^{-1}$ because the last update needs only to do one step$_C$). On the contrary the improved TreeHash needs $2^H$ updates to reach the same goal.

4.2 Computation of the Desired tree

In this section we will explain how the nodes in a Desired tree are computed and stored which marks the main difference of our algorithm to the algorithm in [7]. Recall that in [7] the TreeHash algorithm of a Desired tree gets $2^h \times (2^{\text{bottomLevel}})$ updates for calculating its nodes. The $2^h$ bottom level nodes of a Desired tree are calculated during the first $2^h \times (2^{\text{bottomLevel}} - 2^{-1})$ updates. After calculating the bottom level nodes there are $2^{h-1}$ updates left (from: $(2^h \times (2^{\text{bottomLevel}})) -$

$^6$ Remember that a classical TreeHash needs $2^{\text{bottomLevel}} - 2^{-1}$ updates to compute a bottom level node. Furthermore in all our derivation $h|H$ and $h \leq H$ hold.
\((2^h \times (2^{\text{bottomLevel}} - 2^{-1})) = 2^{h-1}\). These are used to calculate the non-bottom level nodes of the Desired tree \([7]\). There is no additional space needed to calculate the non-bottom level nodes from the bottom level nodes. This because after calculating a new node, the left child is dropped and the new value can be stored instead \([7]\). This approach can not be used with the improved TreeHash from \([8]\) without increasing the amount of updates the TreeHash of a Desired tree gets before the Desired tree has to be finished. This is due to the fact, that the improved TreeHash needs \(2^h \times (2^{\text{bottomLevel}})\) updates to compute all bottom level nodes of the Desired tree, which would leave 0 updates for the calculation of the non-bottom level nodes.

As described in Section 3 our algorithm uses a lower TreeHash and a higher TreeHash per subtree. All the lower TreeHash instances use the same scheduling algorithm as in \([8]\) with \(L - 1\) updates per round. The higher TreeHashes use a custom scheduling algorithm which executes an update every \(2^{\text{bottomLevel}}\) rounds. The main difference vis-à-vis \([7]\) is that we compute the nodes in the Desired tree continuously during the calculations of the Desired tree, and not only at the end. This approach distributes the leaf computations during the computation of a Desired tree more equally than the one from \([7]\).

**Space analysis for Desired tree computation** We will show that our algorithm needs \(L \times (2^h - 1)\) hash values for the Exist and Desired tree, when the authentication path is taken into account, instead of \(L \times (2^h)\) hash values needed by the algorithm in \([7]\).

The authentication path is a data structure which can store one node per level. Because the authentication path is contained in all the Exist trees (which store only right nodes), right nodes on the authentication path are contained in both structures and thus have to be held only once in memory. The authentication path changes on a level \(k\) every \(2^k\) rounds and the higher TreeHash produces a node on a level \(k'\) every \(2^{k'}\) rounds. Whenever a left node enters the authentication path, its right sibling leaves the authentication path and can be discarded (with one exception discussed below). From this we can conclude (ignoring the exception for now), that every \(2^{k+1}\) rounds the Exist tree discards a right node on level \(k\) and the higher TreeHash produces a left node on the same level. This means the higher TreeHash can store one left node on each level using the space of the discarded nodes in the Exist tree. The right nodes the higher TreeHash produces can be stored using the space of the left node from which they have been computed.

We will now look at the exception mentioned above: a right node on level \(k\) which has a left node as parent, cannot be discarded when it leaves the authentication path, because it is needed for the computation of its parent as explained in \([8]\). It will be discarded \(2^k\) rounds after it left the authentication path. During these \(2^k\) rounds there can be a left node with height \(k\) on the higher TreeHash, for which fresh storage space must be provided. Fortunately this situation can only occur if there is a right node on the authentication path (the sibling of the parent of the node which could not be discarded). This right node is stored in both the Exist tree and the authentication path and must be held in memory only once.

The special scheduling of the lower TreeHash (see Sec. 4.3) may compute a node on the bottom level that is not immediately consumed by the higher TreeHash and therefore should be stored until needed. We can store this node in the space reserved for the higher TreeHash, because the left node with the highest level on a higher TreeHash is never stored, for the simple reason that it is not needed for the calculation of any right node in the Desired tree (see Fig. 3).

From this we conclude that the authentication path and all the subtrees together use no more than \(L \times (2^h - 1) + H\) space, where \(h\) is the height of a subtree, \((2^h - 1)\) is the amount of nodes a tree of
Sharing the same Data structure in both Exist and Desired Trees  We now show that we can store the nodes of the Exist tree and the Desired tree in one single tree data structure. This is the case, because we can store two related\(^7\) nodes in the same slot. We can do this because when a node in the Desired tree is stored, its related node in the Exist tree was already discarded. This is trivial for left nodes, because they are never stored in the Exist or Desired tree. In the previous section we showed that with one exception, the Exist tree discards a right node on a level in the same round the higher TreeHash computes a left node on that level. The sibling of the left node a higher TreeHash computes every \(2^{l+1}\) rounds on a level \(l\), is the node related to the right node the Exist tree discards during this round. The right node which is computed \(2^l\) rounds later on the level \(l\) is the node related to the discarded one and so it can be stored in the same slot of the data structure. We now look at the special case: right nodes with a left node as parent (see Sec. 4.2). Such a right node on level \(k\) will be discarded \(2^k\) rounds later than the other right nodes. It will be discarded in the same round as the higher TreeHash produces its related node. We ensure that the slot in the data structure is free by calculating left nodes in the authentication path before we update the higher TreeHash (see Algorithm 8).

In Fig. 3 we show how the different nodes of the Desired and Exist trees are managed.

Space used for the key generation of the leaves  In this section we will analyse the space used by the deterministic PRNG, which calculates the private keys used in the leaf calculations. Supposing the PRNG algorithm can generate any random number within its range without first calculating all the preceding ones (indexed PRNG), then only one instance of the PRNG would be needed to calculate the private keys for all the leaves. No PRNG’s currently recommended by NIST [9] have this property. For both, the log and the fractal algorithms, solutions exist that use a PRNG which calculates the leaves’ private keys in sequential order (continuous PRNG). This requires storing multiple internal states of the continuous PRNG during the generation of the authentication paths. The fractal algorithm stores as many continuous PRNG internal states as it has subtrees, whereas the log algorithm stores two continuous PRNG internal states per TreeHash [8] plus one for calculating the leaves that are left nodes. Our algorithm uses the same PRNG-approach as the fractal one. When our algorithm skips a leaf calculation (because it would not contribute to the calculation of a right node stored in a subtree, see Sec. 3), it still calculates the leaf’s private key and thus advances the state of the PRNG. Therefore, our algorithm and the fractal one, store \(L\) additional continuous PRNG states, whereas the log algorithm needs to store \(2 \times (H - K) + 1\) continuous PRNG states [8]. For the space analysis we choose the state size of the PRNG equal to the output size of the hash function used.

4.3 The TreeHash Algorithm

In this section we will explain the reason why we use the same TreeHash scheduling as in [8] together with the improved TreeHash from [8] and what impact this has on the performance of the algorithm. A TreeHash instance which calculates a node on height \(i\) and all its children, is called

\(^7\) Two nodes of either a Desired or an Exist tree are said to be related if they have the same position relative to their root.
The basic idea is to start a freshly initialized $TreeHash_k$ only if there is no $TreeHash$ with nodes of height smaller than $k$ on their stack. This is achieved by assigning each update to the $TreeHash$ instance with the smallest tail height (see Algorithm 3). The tail height is the smallest height for which there is a node on the stack of the $TreeHash$. A terminated $TreeHash_k$ is considered to have an infinite tail height and an empty one is considered to have a tail height of $k$. Furthermore, the improved $TreeHash$ from [8] we use, changes the definition of a step as compared to the classical one. A $step_C$ was originally considered in [6] as either calculating a leaf node or an inner node. This is fine as long as a hash computation can be considered to be as expensive as a leaf calculation. More often though, a leaf computation is significantly more expensive than the computation of an inner node. This leads to a larger difference between the average and worst case time needed for a $step_C$. In [8], a $step_I$ consists of one leaf’s calculation and of as many inner node computations as
possible before needing a new leaf, instead of processing just one leaf or one inner node as in the classic case (see Algorithm 1).

**Nodes’ supply for the higher TreeHash** We wish to prove, that when we spend \( L - 1 \) updates on the lower TreeHash (see Alg. 1), it produces nodes before the higher TreeHash needs them for computing nodes in the Desired tree. To prove this we use the same approach as in [8]. We focus on a subtree \( ST_k \) with a lower TreeHash\(_h\) (bottom level of \( ST_k \) is \( h \)). We consider a time interval starting at the initialization of TreeHash\(_h\) and ending at the time when the next node at height \( h \) is required by the higher TreeHash of \( ST_k \). We call this node Need\(_h\). The higher TreeHash is updated every \( 2^h \) rounds and requires a bottom level node in each update. This means that in the time considered we execute \((L - 1) \times 2^h\) updates. A higher TreeHash of a subtree on a lower level needs new nodes more frequently, because their authentication nodes change more often. For any given TreeHash\(_i\) with \( i < h \), \( \frac{2^h}{2^i} \) nodes are needed during the time interval defined above: \( 2^i \) updates are used up to complete a node on height \( i \). Therefore TreeHash\(_i\) requires \( \frac{2^h}{2^i} \times 2^i = 2^h \) updates to produce all needed nodes. If there are \( N \) TreeHash\(_i\) with \( i < h \), then all of them together need at most \( N \times 2^h \) updates to compute all their nodes. They may need less, because they may already have nodes on their stack. There may be a partial contribution to any TreeHash\(_j\) with \( j > h \). But they can only receive updates as long as they have nodes at height \( < h \) (tail height \( < h \)). A TreeHash\(_j\) needs at most \( 2^h \) updates to raise its tail height to \( h \). There are \( L - N - 2 \) TreeHash\(_j\) with \( j > h \) (the top subtree has no TreeHash). Together they need at most \((L - N - 2) \times 2^h\) updates. All TreeHash\(_h\) with \( k \neq h \) need at most \((L - N - 2) \times 2^h + N \times 2^h = (L - 2) \times 2^h\) updates. This leaves \( 2^h \) updates for TreeHash\(_h\), which are enough to compute Need\(_h\).

**Space and time analysis for the lower TreeHashes** In [8], it was shown that when the improved scheduling algorithm is used with \( n \times \frac{1}{2} \) updates per round, a TreeHash\(_l\) terminates at most \( 2^{l+1} \) rounds after its initialization (\( n \) corresponds to the actual number of TreeHash instances). This is clearly enough for the log algorithm, because the authentication path needs a new right node on level \( l \) every \( 2^{l+1} \) rounds. For our algorithm the higher TreeHash needs a new node every \( 2^l \) rounds which is twice as often. We thus need to distribute twice as many updates per lower TreeHash instances with the improved scheduling algorithm from [8]. That means \( L - 1 \) updates per round in total.

In addition, when the improved scheduling algorithm is used to calculate nodes with a set of TreeHash\(_i\) (where all \( i \)'s are different), these nodes can share a stack [8]. The amount of space needed by this shared stack is the same as that of the TreeHash\(_i\) with the highest \( i \) [8]. Since the highest subtree (bottom level: \( H - h \)) does not have a lower TreeHash instance, the highest level on which any node has to be computed by a lower TreeHash is the bottom level of the second highest subtree (with bottom level: \( H - h - h \)). So, the shared stack of our algorithm stores at most \( H - 2h \) hash values.

### 4.4 The space and time gains of our approach

In this section we will give the total space and time bounds of our algorithm, and compare them with the log and fractal ones under the condition that a continuous PRNG with an internal state equal in size of the hash value is used. We obtain the total space of our algorithm by summing up the contributions of its different parts: \( L \times (2^h - 1) + H \) from the subtrees and authentication path
(see Sec. 4.2), $H - 2h$ from the lower TreeHashes (see Sec. 4.3) and $L$ from the PRNG internal states (see Sec. 4.2). This sums up to $L \times 2^h + 2H - 2h$ times the hash value size.

For the time analysis we look at the number of leaves’ calculations per round. The improved TreeHash makes one leaf calculation per update and we make at most $(L - 1)$ lower TreeHash updates per round. The higher TreeHash never calculates leaves. So in the worst case all TreeHashes together need $(L - 1)$ leaves’ calculations per round. We need an additional leaf calculation every two rounds to compute the left nodes as shown in [8]. Thus we need $L$ leaves’ calculations per round in the worst case. In the average case however, we need less, as the first node of the $2^h$ bottom level nodes of a Desired tree is not computed, since it is not needed to compute any right node in the Desired tree.

This reduces the average–case time by a factor $\frac{2^h - 1}{2^h - 2}$ and leads to a total of $\frac{2^h - 1}{2^h - 2} \times (L - 1) + \frac{1}{2}$ leaves’ computations per round. The term $\frac{1}{2}$ enters the expression because the left node computation needs a leaf every two rounds. The average case time bound holds true for only the first $2^H - 2^{H-h}$ rounds. Thereafter less leaf computations would be needed on average, because some subtrees no longer need a Desired tree. Table 1 summarizes the above results and Table 2 does the same for the log space– and fractal–algorithm when a continuous PRNG with an internal state equal to the size of a hash value used.

Table 1: Space–time trade–off of our Merkle tree traversal algorithm as a function of $H$ (height of the tree) with $h$ (height of a subtree) as parameter.

| Bounds | $h = 1, L = H$ | $h = 2, L = \frac{H}{2}$ | $h = \log(H), L = \frac{H}{\log(H)}$ |
|--------|----------------|------------------------|-----------------------------------|
| Worst case: space | $4H - 2$ | $4H - 4$ | $\frac{H^2}{\log(H)} + 2H - 2\log(H)$ |
| Average case: time | $\frac{H}{2}$ | $\frac{H}{2} - \frac{1}{2}$ | $\frac{H}{\log(H)} + \frac{1}{2}$ |
| Worst case: time | $H$ | $\frac{H}{2}$ | $\frac{H}{\log(H)} - 1$ |

Table 2: Space–time trade–off of log algorithm [8] and fractal algorithm [3] optimized for storage space. The values in the Table include the space needed by the continuous PRNG.

| Bounds | Log [8] $K = 2$ | Fractal [3] $h = \log(H)$ |
|--------|----------------|-------------------|
| Worst case: space | $5.5H - 7$ | $\frac{5H^2 + 2H}{2\log(H)}$ |
| Average case: time | $\frac{H}{2} - \frac{1}{2}$ | $\frac{H}{\log(H)} - 1$ |
| Worst case: time | $\frac{H}{2}$ | $\frac{H}{\log(H)} - 2$ |

When $h = 2$ our algorithm has better space and time bounds (or at least as good as in the case of worst–case time) than the log algorithm [8]. When we choose the same space–time trade-off parameter as in the fractal algorithm [3] (column $h = \log(H)$ in Table 1), our algorithm needs less storage space.
5 Implementation

There are several aspects which are by purpose unspecified by the Merkle tree traversal algorithms. These are the hash function, the deterministic pseudo-random number generator and the algorithm used for the leaf calculation. The latter is defined by the usage of the tree. Although the hash function and PRNG are independent of the trees’ usage, both have an impact on the cryptographic strength and the performance. The hash function used for the traversal algorithm must be collision-resistant as shown in [13]. Thus the main selection criteria for the hash function are good performance and strong security. A suitable candidate is BLAKE [4].

As a PRNG we chose an algorithm based on a hash function. This choice has the advantage that we do not need another cryptographic primitive. In [9], NIST has recommended two continuous hash based PRNG’s named HASH_DBRG and HMAC_DBRG. Both of them have an internal state composed of two values with the same length as the output length of the used hash function. HASH_DBRG has the advantage that one of its two internal values solely depends on the seed and does not change until a reseeding occurs. For Merkle trees, there is no reseeding necessary as long as less than $2^{48}$ leaves exist [9]. Hence, in our application one of its two internal values is the same for all used HASH_DBRG instances within the same Merkle tree. We prefer HASH_DBRG over HMAC_DBRG because it uses less space and is more performant.

6 Results

We compared the performance of our algorithm with both, the log algorithm from [8] and the fractal algorithm from [3]. We chose as performance parameters the number of leaf computations and the number of stored hash values. This choice is reasonable because the former is the most expensive operation if the Merkle tree is used for signing, and the latter is a good indicator of the storage space needed. Operations like computing a non-leaf node or generating a pseudo-random value have nearly no impact on the performance in the range of $H$ values of practical interest. A leaf computation is exactly the same in each of the three algorithms and therefore only dependent on the underlying hardware for its performance.

To be able to present cogently the results, each data point represents an aggregation over $2^{10}$ rounds. Recall that one round corresponds to the calculation of one authentication path. In the case of storage measurements one point represents the maximal amount of stored hash values at any time during these $2^{10}$ rounds. In the case of the leaf computation one point represents the average number of leaves’ computations done in one round during the $2^{10}$ rounds.

We will present the results for two sets of measurements with $2^{16}$ leaves. For the first set we choose the parameter such that each algorithm uses its minimal space. For our and the fractal algorithm the minimal space for $H = 16$ is achieved with $h = 2$. In the case of the log algorithm we have set $K$ (defined in [8]) to 2 in order to achieve minimal space usage. The second set uses $h = \log(H)$ as it was proposed in [3]. For the fractal and our algorithm this means $h = 4$ for $H = 16$ and $K = 2$ for the log algorithm. The NIST recommendation HASH_DBRG is used as PRNG for both sets of measurements. The results of these measurements are shown in Fig. 5 for a similar space–time trade-off as the fractal tree and in Fig. 4 for minimal storage space.

We see that in a setting where a good space–time trade-off is needed, our algorithm uses less space and slightly more leaf calculations than the fractal algorithm (at most $\frac{1}{2}$ more on average per round). If a minimal space solution is needed, our algorithm with $h = 2$ uses less space and less leaf calculations than both the log and the fractal algorithm.
In addition, the plots show a weak point of our algorithm compared with the log algorithm: the number of leaves’ calculations is not constant. The fractal algorithm for similar parameter shows even greater fluctuations, but they are not visible in Fig. 5, because they cancel each other out over the $2^{10}$ rounds. If we measure the first $2^7$ rounds with no aggregation we see that the deviations of our algorithm decrease markedly (see Fig. 6) compared to the fractal one.

The full package with source code and measurements results is available at [1].

## 7 Conclusion

We developed an algorithm for the Merkle tree traversal problem which combines the efficient space-time trade-off from the fractal algorithm and the space efficiency from the log algorithm. An exhaustive analysis of the space and time efficiency of our algorithm in function of the parameters $H$ and $h$ has shown that if a continuous PRNG is used, our algorithm has a space advantage over the log and fractal algorithms and a time advantage over the log algorithm.
Fig. 6: Number of calculated leaves as function of rounds for similar space–time trade-off (first 128 rounds in detail). Parameters: \( H = 16 \) and \( h = 4 \). HASH_DRBG is used as pseudo–random number generator. One round corresponds to the calculation of one authentication path.

We further programmed a low storage–space and a low time–overhead version of the algorithm in Java and measured its performance with respect to the two different implementations. Our implementation needs about a factor 2 less space than the fractal algorithm, when minimum space is required.

Ours as well as the log and fractal algorithms suffer from a long initialisation time for large values of \( H \). This problem was solved by the CMSS [10] and GMSS [11] algorithms. These two algorithms use a stacked series of Merkle trees where the higher trees sign the roots of their child trees and the lowest tree is used for the real cryptographic purpose. Both of them thus rely on a solution of the Merkle traversal problem for each layer, for which our algorithm could be used instead of the current ones. It is possible to use different parameters for different layers in the CMSS or GMSS. In addition, the higher trees used in these schemes favor Winternitz as leaf calculation function which is significantly more expensive than an inner node computation, and thus can profit from the improved TreeHash used in our algorithm. The XMSS [12] is an extension to the Merkle signature scheme (MSS) which allows to use a hash function which is only second-pre–image resistant instead of collision resistant. It is based on the log algorithm and the usage of a forward secure continuous PRNG. Under these circumstances, our algorithm would be a good replacement for the log algorithm: it would use less space and provide greater flexibility.

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A Appendix

A.1 Algorithms

The algorithm descriptions use an oracle for the leaves’ computations. The oracle gets the leaf’s index as input. We should modify the algorithms (as explained in Sec. 4.2) in the case that the leaf’s computation is based on a continuous PRNG and it needs a private key as input.

Our algorithm uses the following data structures:
1. \( \text{Auth}_h, h = 0, \ldots, H - 1 \). An array of nodes that stores the current authentication path.
2. \( \text{Subtree}_h, h = 0, \ldots, L - 1 \). An array of subtree structures with the following properties:
   (a) \( \text{bottomLevel} \): the minimal height for which the subtree stores nodes.
   (b) \( \text{rootLevel} \): the height of the root of the subtree.
   (c) \( \text{tree} \): the data structure for the \textit{Exist} and \textit{Desired} tree with the following functions:
      i. \( \text{get}(j, k) \): get \( k \)th node (from left to right) with height \( j \) in the subtree
      ii. \( \text{add}(\text{node}) \): store node in the subtree
      iii. \( \text{remove}(j, k) \): remove \( k \)th node (from left to right) with height \( j \) in the subtree
   (d) \( \text{stackHigh} \): the stack for the higher \textit{TreeHash}.
   (e) \( \text{nextIndex} \): the index of the next leaf needed by the lower \textit{TreeHash}.
   (f) \( \text{bottomLevelNode} \): the node of lower \textit{TreeHash} which is stored outside the shared stack \[8\].
   (g) \( \text{stackLow} \): the stack for the lower \textit{TreeHash} (the part of the shared stack currently containing
      nodes for this \textit{Subtree} \[8\]).
3. \( \text{LeafCalc}(i), i = 0, \ldots, 2^H - 1 \). Oracle for calculating the leaf \( i \).

Our algorithm has the following phases:

1. \textbf{Init}: \textit{TreeHash} computes the root node. During this process it stores right nodes of the left–most
   \textit{Exist} trees and the nodes of the first authentication path (Algorithm \[2\])
2. \textbf{Generation of the authentication paths}: repeat \( 2^H \) times:
   (a) Output current authentication path \( \text{Auth}_h, h = 0, \ldots, H - 1 \)
   (b) Update lower \textit{TreeHashes} (Algorithm \[7\])
   (c) Compute next authentication path (Algorithm \[8\])
**Algorithm 2** Key generation (PK) and Merkle tree setup.

**INPUT**: 
**OUTPUT**: PK

{Initialize L-1 subtrees}

for all Subtree, with \( i \in \{0, \ldots, L-1\} \) do

Subtree.tree ← empty

if \( i < (L-1) \) then

Subtree.stackHigh ← empty

Subtree.stackLow ← empty

end if

Subtree.bottomLevel ← \( i \times h \)

Subtree.rootLevel ← Subtree.bottomLevel + \( h \)

Subtree.nextIndex ← \( 2^{Subtree.rootLevel} - 1 \)

end for

{Initialize Stack, set Leaf level \( k = 0 \)}

\( k \leftarrow 0 \)

Stack ← empty

Stack.push(LeafCalc(k))

\( k \leftarrow k + 1 \)

while Stack.peek.height < \( H \) do

TreeHash(Stack, LeafCalc(k), Process0, null)

\( k \leftarrow k + 1 \)

end while

PK ← Stack.pop

return PK

---

**Algorithm 3** TailHeight: Calculation of the height of the lowest node on a stackLow

**INPUT**: subtree index \( i \)

**OUTPUT**: height

if Subtree has a stackHigh \& \( \sim\) (Subtree, bottomLevelNode) then

if Subtree.stackLow == empty then

height ← Subtree.bottomLevel

else

height ← Subtree.stackLow.tosNode.height

end if

else

height ← \( \infty \)

end if

return height
Algorithm 4 Process$_0$

\begin{verbatim}
INPUT : Node, index j
OUTPUT : continue
if Node.index \leq 2^{SubTreeForLevel(Node.height).rootLevel−Node.height} \& Node.index (mod 2) == 1 then
    SubTreeForLevel(Node.height).tree.add(Node)
end if
if Node.index == 1 then
    AuthNode.height ← Node
end if
return continue ← 1
\end{verbatim}

Algorithm 5 Process$_1$:

\begin{verbatim}
INPUT : Node; subtree index j
OUTPUT : continue
if Node.height == Subtree$_j$.bottomLevel then
    Subtree$_j$.bottomLevelNode ← Node
    continue ← 0
else
    continue ← 1
end if
return continue
\end{verbatim}

Algorithm 6 Process$_2$:

\begin{verbatim}
INPUT : Node; subtree index i
OUTPUT : continue
if Node \neq dummy then
    continue ← 1
if Node.index (mod 2) == 1 then
    Subtree$_i$.tree.add(Node)
    if Node.index/2 (mod 2^{Subtree$_i$.rootLevel−Node.height−1}) == 0 then
        continue ← 0
    end if
end if
if Node.height == Subtree$_i$.rootLevel − 1 then {Current Desired tree becomes new Exist tree}
    if Subtree$_i$.nextIndex + 1 >= 2^i then {It was the last Desired}
        Subtree$_i$.stackHigh ← remove
    end if
end if
else
    continue ← 0
end if
return continue
\end{verbatim}
**Algorithm 7** Distribution of updates to the active lower TreeHash instances:

```plaintext
INPUT: leaf index \( i \in \{1, \cdots, 2^H - 1\} \)

\( \text{updates} \leftarrow \text{number of desiredTree in SubTrees} \)

repeat
  \( \text{Find TreeHash instance with lowest tail height, on a tie use the one with lowest index} \)
  \( s \leftarrow \min \{ l : \forall \text{TailHeight}(l) = \min_{j=0, \ldots, L-2} \{\text{TailHeight}(j)\} \} \)
  \( \text{Subtree}.\text{nextIndex} \leftarrow \text{Subtree}.\text{nextIndex} + 1 \)
  if \( \text{Subtree}.\text{nextIndex} \mod 2^{\text{Subtree}.\text{rootLevel}} \geq 2^{\text{Subtree}.\text{bottomLevel}} \) then
    \( \text{TreeHash}((\text{Subtree}.\text{stackLow}, \text{LeafCalc}(\text{Subtree}.\text{nextIndex}), \text{Process1}, s)) \)
  else
    if \( \text{Subtree}.\text{nextIndex} + 1 \mod 2^{\text{Subtree}.\text{rootLevel}} = 2^{\text{Subtree}.\text{bottomLevel}} \) then
      \( \text{Subtree}.\text{bottomLevelNode} \leftarrow \text{dummy} \)
    end if
  end if
  \( \text{updates} \leftarrow \text{updates} - 1 \)
until \( \text{updates} == 0 \)
```

**Algorithm 8** Generation of the next authentication path. (SubTreeForLevel(l) is the Subtree containing level l.)

```plaintext
INPUT: leaf index \( i \in \{1, \cdots, 2^H - 1\} \)

\( k \) is 0 if leaf \( i \) is a right node and \( k \neq 0 \) means the height of the first parent of leaf \( i \) that is a right node

\( k \leftarrow \max_{m=0, \cdots, H} \{m : i \mod 2^m == 0\} \)

if \( k == 0 \) then
  \( \text{Auth}_0 \leftarrow \text{LeafCalc}(i - 1) \)
else
  leftNode \( \leftarrow \text{Auth}_{k-1} \)
  rightNode \( \leftarrow \text{SubTreeForLevel}(k-1).\text{tree}.\text{get}(\text{leftNode}.\text{index} \oplus 1, k-1) \)
  \( \text{Auth}_k \leftarrow \text{hash(leftNode[|rightNode|]} \)
  \( \text{SubTreeForLevel}(k-1).\text{tree}.\text{remove}(j, k-1) \)
end if

if \( \text{Auth}_k.\text{index}/2 \mod 2 == 1 \) then
  \( \text{SubTreeForLevel}(k).\text{remove}(\text{Auth}_k.\text{index} \oplus 1, k) \)
end if

for all \( r \in \{0 \cdots L - 2\} \) where \( \text{Subtree}.\text{bottomLevel} \leq k \) do
  if \( \text{SubTree}[r] \) has a desiredTree then
    \( \text{TreeHash}((\text{Subtree}.\text{stackHigh}, \text{Subtree}.\text{bottomLevelNode}, \text{Process2}, r)) \)
    \( \text{Subtree}.\text{bottomLevelNode} \leftarrow \text{remove} \)
  end if
end for

for all \( t \in \{0 \cdots k - 1\} \) do
  \( \text{Auth}_t \leftarrow \text{SubTreeForLevel}(t).\text{tree}.\text{get}(n, (i/2^t) \oplus 1) \)
end for

return \( \text{Auth}_j \forall j \in \{0, \cdots, H - 1\} \)
```
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