

# End-to-End Formal Verification of Ethereum 2.0 Deposit Smart Contract

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**Abstract.** We report our experience in the formal verification of the deposit smart contract, whose correctness is critical for the security of Ethereum 2.0, a new Proof-of-Stake protocol for the Ethereum blockchain. The deposit contract implements an incremental Merkle tree algorithm whose correctness is highly nontrivial, and had not been proved before. We have verified the correctness of the compiled bytecode of the deposit contract to avoid the need to trust the underlying compiler. We found several critical issues of the deposit contract during the verification process, some of which were due to subtle hidden bugs of the compiler.

## 1 Introduction

The deposit smart contract [23] is a gateway to join Ethereum 2.0 [24] that is a new sharded Proof-of-Stake (PoS) protocol which at its early stage, lives in parallel with the existing Proof-of-Work (PoW) chain, called Ethereum 1.x chain. Validators drive the entire PoS chain, called Beacon chain, of Ethereum 2.0. To be a validator, one needs to deposit a certain amount of Ether, as a “stake”, by sending a transaction (over the Ethereum 1.x network) to the deposit contract. The deposit contract records the history of deposits, and locks all the deposits in the Ethereum 1.x chain, which can be later claimed at the Beacon chain of Ethereum 2.0.<sup>3</sup> Note that the deposit contract is a one-way function; one can move her funds from Ethereum 1.x to Ethereum 2.0, but not vice versa.

The deposit contract, written in Vyper [28], employs the Merkle tree [40] data structure to efficiently store the deposit history, where the tree is *dynamically* updated (i.e., leaf nodes are incrementally added in order from left to right) whenever a new deposit is received. The Merkle tree employed in this contract is very large: it has height 32, so it can store up to  $2^{32}$  deposits. Since the size of the Merkle tree is huge, it is not practical to reconstruct the whole tree every time a new deposit is received.

To reduce both time and space complexity, thus saving the gas<sup>4</sup> cost significantly, the contract implements an *incremental Merkle tree algorithm* [56]. The incremental algorithm enjoys  $O(h)$  time and space complexity to reconstruct

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<sup>3</sup> This deposit process will change at a later stage.

<sup>4</sup> In Ethereum, gas refers to the fee to execute a transaction or a smart contract on the blockchain. The amount of gas fee depends on the size of the payloads.

(more precisely, compute the root of) a Merkle tree of height  $h$ , while a naive algorithm would require  $O(2^h)$  time or space complexity. The efficient incremental algorithm, however, leads to the deposit contract implementation being unintuitive, and makes it non-trivial to ensure its correctness. The correctness of the deposit contract, however, is critical for the security of Ethereum 2.0, since it is a gateway for becoming a validator. Considering the utmost importance of the deposit contract for the Ethereum blockchain, formal verification is demanded to ultimately guarantee its correctness.

In this paper, we present our formal verification of the deposit contract.<sup>5</sup> The scope of verification is to ensure the correctness of the contract bytecode within a single transaction, without considering transaction-level or off-chain behaviors. We take the compiled bytecode as the verification target to avoid the need to trust the compiler.<sup>6</sup>

We adopt a refinement-based verification approach. Specifically, our verification effort consists of the following two tasks:

- Verify that the incremental Merkle tree algorithm implemented in the deposit contract is *correct* w.r.t. the original full-construction algorithm.
- Verify that the compiled bytecode is *correctly generated* from the source code of the deposit contract.

Intuitively, the first task amounts to ensuring the correctness of the contract source code, while the second task amounts to ensuring the compiled bytecode being a sound refinement of the source code (i.e., translation validation of the compiler). This refinement-based approach allows us to avoid reasoning about the complex algorithmic details, especially specifying and verifying loop invariants, directly at the bytecode level. This separation of concerns helped us to save a significant amount of verification effort.

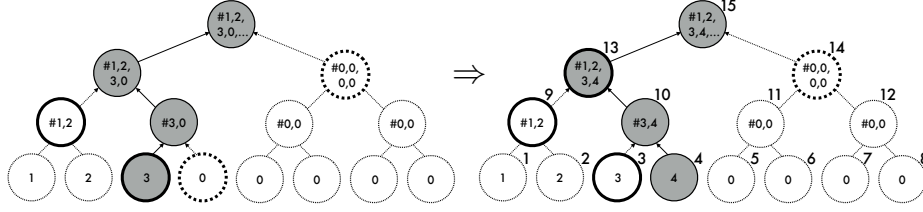
*Challenges* Formally verifying the deposit contract was challenging. First, the algorithm employed in the contract is sophisticated and its correctness is not straightforward to prove. Indeed, we found a critical bug in the algorithm implementation which had been not detected by existing tests. (Section 4.1)

Second, we had to take the compiled bytecode as the verification target, which is much larger (consisting of  $\sim 3,000$  instructions) and more complex than the source code. The source-code-level verification was not accepted by the customer for the end-to-end correctness guarantee, especially considering the fact that the compiler is not mature enough [10]. Indeed, we found several critical bugs in the compiler during the formal verification process. (Section 4.2)

Third, we had to consider not only the functional correctness, but also security properties of the contract. That is, we had to identify the behaviors of the contract in exceptional cases, and check if they are exploitable. We found a bug of the contract in case that it receives invalid inputs. (Section 4.3)

<sup>5</sup> This was done as part of a contract funded by the Ethereum Foundation [25].

<sup>6</sup> Indeed, we found several critical bugs [18,19,20,21] of the Vyper compiler in the process of formal verification. See Section 4 for more details.



**Fig. 1.** Illustration of the incremental Merkle tree algorithm. The left tree is updated to the right tree by inserting a new data hash in the fourth leaf (node 4). Only the path from the new leaf to the root (i.e., the gray nodes) are computed by the algorithm (hence linear-time). The bold-lined (and bold-dotted-lined) nodes denote the **branch** (and **zero\_hashes**) array, respectively, which are only nodes that the algorithm maintains (hence linear-space). The # symbol denotes the hash value, e.g., “#1,2” (in node 9) denotes “hash(1,2)”, and “#1,2,3,4” (in node 13) denotes “hash(hash(1,2),hash(3,4))”. Node numbers are labeled in the upper-right corner of each node.

Finally, we had to take into account potential future changes of the Ethereum blockchain system (called hard-forks). That is, we had to verify that the compiled bytecode will work not only in the current system, but also in any future version of the system that employs a different gas fee schedule. Considering such potential changes of the system required us to generalize the semantics of bytecode execution. We also found a bug regarding that. (Section 4.4)

## 2 Correctness of the Incremental Merkle Tree Algorithm

In this section, we briefly describe the incremental Merkle tree algorithm of the deposit contract, and formulate its correctness. Both the formalization of the algorithm and the formal proof of the correctness are presented in Appendix A.

A Merkle tree [40] is a perfect binary tree where leaf nodes store the hash of data, and non-leaf nodes store the hash of their children. A *partial Merkle tree up-to  $m$*  is a Merkle tree whose first (leftmost)  $m$  leaves are filled with data hashes and the other leaves are empty and filled with zeros. The incremental Merkle tree algorithm takes as input a partial Merkle tree up-to  $m$  and a new data hash, and inserts the new data hash into the  $(m + 1)^{\text{th}}$  leaf, resulting in a partial Merkle tree up-to  $m + 1$ .

Figure 1 illustrates the algorithm, showing how the given partial Merkle tree up-to 3 (shown in the left) is updated to the resulting partial Merkle tree up-to 4 (in the right) when a new data hash is inserted into the 4<sup>th</sup> leaf node. Here are a few key observations to the algorithm.

1. The only difference between the two Merkle trees is the path from the new leaf node (i.e., node 4) to the root. All the other nodes are identical between the two trees.
2. The path can be computed by using only the left (i.e., node 3 and node 9) or right (i.e., node 14) sibling of each node in the path. All the other nodes are *not* needed for the path computation.

3. All the left siblings (i.e., node 3 and node 9) of the path are “finalized” in that they will never be updated in any subsequent execution of the algorithm. All the leaves that are a descendant of the finalized node are non-empty.
4. All the right siblings (i.e., node 14) are zero-hashes, that is, 0 for leaf nodes (at level 0), “hash(0,0)” for nodes at level 1, “hash(hash(0,0),hash(0,0))” for nodes at level 2, and so on. These zero-hashes are constant.

Now we describe the algorithm. To represent a Merkle tree of height  $h$ , the algorithm maintains only two arrays of length  $h$ , called **branch** and **zero\_hashes** respectively, that store the left and right siblings of a path from a new leaf node to the root. When inserting a new data hash, the algorithm computes the path from the new leaf node to the root. Each node of the path can be computed in a constant time, by retrieving only its left or right sibling from the **branch** or **zero\_hashes** array. After the path computation, the **branch** array is updated to contain all the left siblings of a next new path that will be computed in the next run of the algorithm. Here the **branch** array update is done in a constant time, since only a single element of the array needs to be updated, and the element has already been computed as part of the path computation.<sup>7</sup> Note that the **zero\_hashes** array is computed once at the very beginning when all the leaves are empty, and never be updated during the lifetime of the Merkle tree.

*Complexity* Both the time and space complexity of the algorithm is linear in the tree height  $h$ . The space complexity is linear, because the size of the **branch** and **zero\_hashes** arrays is  $h$ , and no other nodes are stored by the algorithm. The time complexity is also linear. For the path computation, the length of the path is  $h$ , and each node can be computed in a constant time by using the two arrays. The **branch** array update can be also done in a constant time as explained earlier.

*Implementation and optimization* The incremental Merkle tree algorithm implemented in the deposit contract consists of two main functions: **deposit** and **get\_deposit\_root**. The **deposit** function takes as input a new deposit hash, and inserts it into the Merkle tree. The **get\_deposit\_root** function computes and returns the root of the current partial Merkle tree whose leaves are filled with the deposit hashes received up to that point.

Specifically, the **deposit** function fills the first (leftmost) empty leaf node with a given deposit hash, and updates a single element of the **branch** array. The **get\_deposit\_root** function computes the tree root by traversing a path from the last (rightmost) non-empty leaf to the root.

As an optimization, the **deposit** function does not fully compute the path from the leaf to the root, but computes only a smaller partial path from the leaf to the node that is needed to update the **branch** array. Indeed, for all odd-numbered deposits (i.e., 1<sup>st</sup> deposit, 3<sup>rd</sup> deposit,  $\dots$ ), such a partial path becomes empty, because the leaf node is the one needed for the **branch** array update. In that case, the **deposit** function returns immediately in a constant

<sup>7</sup> See Appendix A for more details about updating the **branch** array.

time. For even-numbered deposits, the partial path is not empty but still much smaller than the full path in most cases. This optimization is useful when the tree root computation is not needed for every single partial Merkle tree. Indeed, in many cases, multiple deposit hashes are inserted at once, for which only the root of the last partial Merkle tree is needed.

*Correctness* Consider a Merkle tree of height  $h$  employed in the deposit contract. Suppose that a sequence of `deposit` function calls are made, say `deposit( $v_1$ )`, `deposit( $v_2$ )`,  $\dots$ , and `deposit( $v_m$ )`, where  $m < 2^h$ . Then, the function call `get_deposit_root()` will return the root of the Merkle tree whose leaves are filled with the deposit data hashes  $v_1, v_2, \dots, v_m$ , respectively, in order from left to right, starting from the leftmost one.

Note that the correctness statement requires the condition  $m < 2^h$ , that is, the rightmost leaf must be kept empty, which means that the maximum number of deposits that can be stored in the tree using this incremental algorithm is  $2^h - 1$  instead of  $2^h$ . See Section 4.1 for more details.

The proof of the correctness is presented in Appendix A.

### 3 Bytecode Verification of Deposit Contract

Now we present the formal verification of the compiled bytecode of the deposit contract. The bytecode verification ensures that the compiled bytecode is a sound refinement of the source code. This rules out the need to trust the compiler. We used the KEVM verifier [45] to formally specify the desired bytecode behavior, and verify the compiled bytecode against the formal specification. We adopted the KEVM verifier to reason about all possible corner-case behaviors of the compiled bytecode, especially those introduced by certain unintuitive and questionable aspects of the underlying Ethereum Virtual Machine (EVM) [30]. This was possible because the KEVM verifier is derived from a complete and thoroughly tested formal semantics of the EVM, called KEVM [34]. Our formal specification and verification artifacts are publicly available at [48].

First, we verified the functional correctness of the bytecode. For each function of the contract, we verified that its return value and its storage state update, if any, are correct at the bytecode level. In addition to executing the incremental Merkle tree algorithm, most of the functions perform certain additional low-level tasks, and we verified that such tasks are correctly performed. Specifically, for example, given deposit data,<sup>8</sup> the `deposit` function computes its 32-byte hash (called Merkleization) according to the SimpleSerialize (SSZ) specification [27]. The leaves of the Merkle tree store only the computed hashes instead of the original deposit data. The `deposit` function also emits a `DepositEvent` log that contains the original deposit data, where the log message needs to be encoded as a byte sequence following the contract event ABI specification [22]. Other low-level

<sup>8</sup> Each deposit data consists of the public key, the withdrawal credentials, the deposit amount, and the signature of the deposit owner.

operations performed by those functions that we verified include: correct zero-padding for the 32-byte alignment, correct conversion from big-endian to little-endian, input bytes of the SHA2-256 hash function being correctly constructed, and return values being correctly serialized to byte sequences according to the contract ABI specification [22].

We also verified a liveness property that the contract is always able to accept a new (valid) deposit as long as a sufficient amount of gas is provided. This liveness is not trivial since it needs to hold even in any future hard-fork where the gas fee schedule is changed. Indeed, we found a bug of the Vyper compiler that a hard-coded amount of gas is attached when calling to the `memcpy` builtin function (more precisely, the ID precompiled contract). This bug could make the deposit contract non-functional in a certain future hard-fork where the gas fee schedule for the builtin function is increased, because the contract will always fail due to the out-of-gas exception no matter how much gas users supply. This bug has been reported and fixed [21].

Our formal specification includes both positive and negative behaviors. The positive behaviors describe the desired behaviors of the contracts in a legitimate input state. The negative behaviors, on the other hand, describe how the contracts handle exceptional cases (e.g., when benign users feed invalid inputs by mistake, or malicious users feed crafted inputs to take advantage of the contracts). The negative behaviors are mostly related to security properties.

For example, the specification says that the `deposit` function increments the `deposit_count` global variable, and updates the `branch` global array as follows: `branch[k] ← ND(k)`, where  $k$  is the smallest integer less than `TREE_HEIGHT` such that  $\lfloor \text{deposit\_count} / 2^k \rfloor$  is odd,<sup>9</sup> and  $ND(k)$  is a 32-byte word that is recursively defined as follows:

$$ND(i + 1) = \text{hash}(\text{branch}[i] ++ ND(i)) \quad \text{for } 0 \leq i < \text{TREE\_HEIGHT}$$

where  $ND(0)$  denotes the deposit data hash to be stored in a Merkle tree leaf. The `deposit` function reverts if either a call-value (i.e., `msg.value`) or a call-data (i.e., `msg.data`) is invalid, the tree is full, the deposit amount is less than the required minimum amount, or the call-data is not well-formed.

For the full specification of the verified bytecode behaviors, refer to [47].

## 4 Findings and Lessons Learned

In the course of our formal verification effort, we found subtle bugs [14,12,13] of the deposit contract, as well as a couple of refactoring suggestions [15,16,17] that can improve the code readability and reduce the gas cost. The subtle bugs of the deposit contract are partly due to another hidden bugs of the Vyper compiler [18,19,20,21] that we revealed in the verification process.

<sup>9</sup> Note that such  $k$  always exists since we have `deposit_count` <  $2^{\text{TREE\_HEIGHT}}$  by the assertion at the beginning of the function.

Below we elaborate on the bugs we found and lessons we learned along the way. We note that all the bugs of the deposit contract have been reported, confirmed, and properly fixed in the latest version (v0.10.0).

#### 4.1 Maximum Number of Deposits

In the original version of the contract that we were asked to verify, the bug is triggered when all of the leaf nodes of a Merkle tree are filled with deposit data, in which case the contract (specifically, the `get_deposit_root` function) incorrectly computes the root hash of a tree, returning the zero root hash (i.e., the root hash of an empty Merkle tree) regardless of the content of leaf nodes. For example, suppose that we have a Merkle tree of height 2, which has four leaf nodes, and every leaf node is filled with certain deposit data, say  $v_1$ ,  $v_2$ ,  $v_3$ , and  $v_4$ , respectively. Then, while the correct root hash of the tree is  $\text{hash}(\text{hash}(v_1, v_2), \text{hash}(v_3, v_4))$ , the `get_deposit_root` function returns  $\text{hash}(\text{hash}(0, 0), \text{hash}(0, 0))$ , which is incorrect.

Due to the complex logic of the code, it is non-trivial to properly fix this bug without significantly rewriting the code, and thus we suggested a workaround that simply forces to never fill the last leaf node, i.e., accepting only  $2^h - 1$  deposits at most, where  $h$  is the height of a tree. We note that, however, it is infeasible in practice to trigger this buggy behavior in the current setting, since the minimum deposit amount is 1 Ether and the total supply of Ether is less than 130M which is much smaller than  $2^{32}$ , thus it is not feasible to fill all the leaves of a tree of height 32. Nevertheless, this bug has been fixed by the contract developers as we suggested, since the contract may be used in other settings in which the buggy behavior can be triggered and an exploit may be possible. Refer to [14] for more details.

We also want to note that this bug was quite subtle to catch. Indeed, we had initially thought that the original code was correct until we failed to write a formal proof of the correctness theorem. The failure of our initial attempt to prove the correctness led us to identify a missing premise (i.e., the correctness condition  $m < 2^h$  in Section 2) that was needed for the theorem to hold, from which we could find the above buggy behavior scenario, and suggested the bugfix. This experience reconfirms the importance of formal verification. Although we were not “lucky” to find this bug when we had eyeball-reviewed the code, which is all traditional security auditors do, the formal verification process thoroughly guided and even “forced” us to find it eventually.

#### 4.2 ABI Standard Conformance of `get_deposit_count` Function

In the previous version, the `get_deposit_count` function does not conform to the ABI standard [22], where its return value contains incorrect zero-padding [12], due to a Vyper compiler bug [18]. Specifically, in the buggy version of the compiled bytecode, the `get_deposit_count` function, whose return type is `bytes` [8], returns a byte sequence of length 96, where the last byte is `0x20` while it should be `0x00`. According to the ABI specification [22], the last 24 bytes must be all

zero, serving as zero-pad for the 32-byte alignment. Thus the return value does not conform to the ABI standard. This is problematic because any contract (written in either Solidity or Vyper) that calls to (the buggy version of) the deposit contract, expecting that the `deposit_count` function conforms to the ABI standard, could have misbehaved.

This buggy behavior is mainly due to a subtle Vyper compiler bug [18] that fails to correctly compile a function whose return type is `bytes[n]` where  $n < 16$ . This leads to the compiled function returning a byte sequence with insufficient zero-padding as mentioned above, failing to conform to the ABI standard.

We note that this bug could not have been detected if we did not take the bytecode as the verification target. This reconfirms that the bytecode-level verification is critical to ensure the ultimate correctness (unless we formally verify the underlying compiler), because we cannot (and should not) trust the compiler.

### 4.3 Checking Well-Formedness of Calldata

The calldata decoding process in the previous version of the compiled bytecode does not have sufficient runtime-checks for the well-formedness of calldata. As such, it fails to detect certain ill-formed calldata, causing invalid deposit data to be put into the Merkle tree. This is problematic especially when clients make mistakes and send deposit transactions with incorrectly encoded calldata, which may result in losing their deposit fund.

Specifically, we found a counter-example ill-formed calldata whose size (196 bytes) is much less than that of well-formed calldata (356 bytes). The problem, however, is that the `deposit` function does *not* reject the ill-formed calldata, but simply inserts certain invalid (garbage) deposit data in the Merkle tree. Since the invalid deposit data cannot pass the signature validation later, no one can claim the deposited fund associated with this, and the deposit owner loses the fund. Note that this happens even though the `deposit` function employs assertions at the beginning of the function that ensures the size of each of the arguments is correct, which turned out to not work as expected.

This problem would not exist if the Vyper compiler thoroughly generated runtime checks to ensure the well-formedness of calldata. However, since it was not trivial to fix the compiler to generate such runtime checks, we suggested several ways to improve the deposit contract to prevent this behavior without fixing the compiler. After careful discussion with the deposit contract development team, we together decided to employ a checksum-based approach where the `deposit` function takes as an additional input a checksum for the deposit data, and rejects any ill-formed calldata using the checksum. The checksum-based approach is the most non-intrusive and the most gas-efficient of all the suggested fixes. For more details of other suggested fixes, refer to [13].

We note that this issue was found when we were verifying the negative behaviors of the deposit contract. This shows the importance of having the formal specification to include not only positive but also negative behaviors.



#### 4.4 Liveness

As mentioned in Section 3, the previous version of the deposit contract fails to satisfy a liveness property in that it may not be able to accept a new deposit, even if it is valid, in a certain future hard-fork that updates the gas fee schedule. This was mainly due to another subtle Vyper compiler bug [21] that generates bytecode where a hard-coded amount of gas is supplied when calling to certain precompiled contracts. Although this hard-coded amount of gas is sufficient in the current hard-fork (code-named Istanbul [26]), it may not be sufficient in a certain future hard-fork that increases the gas fee schedule of the precompiled contracts. In such a future hard-fork, the previous version of the deposit contract will always fail due to the out-of-gas exception, regardless of how much amount of gas is initially supplied. Refer to [21] for more details.

We admit that we could not find this issue until the deposit contract development team carefully reviewed and discussed with us about the formal specification [47] of the bytecode. Initially, we considered only the behaviors of the bytecode in the current hard-fork, without identifying the requirement that the contract bytecode should work in any future hard-fork. We identified the missing requirement, and found this liveness issue, at a very late stage of the formal verification process, which delayed the completion of formal verification.

This experience essentially illustrates the well-known problem caused by the gap between the intended behaviors (that typically exists only informally) by developers, and the formal specification written by verification engineers. To reduce this gap, the two groups should work closely together, or ideally, developers should write their own specifications in the first place. For the former, the formal verification process should involve developers more frequently. For the latter, the formal verification tools should become much easier to use without requiring advanced knowledge of formal methods. We leave both as future work.

#### 4.5 Discussion

*Verification effort* The net effort for formal verification took 7 person-weeks (excluding various discussions with developers, reporting bugs and following-up, especially for compiler bugs, etc.), where the algorithm correctness proof took 2 person-weeks, and the bytecode verification took 5 person-weeks. The size of the bytecode specification is  $\sim 10$  times larger than that of the source code, while the number of instructions in the bytecode is  $\sim 30$  times larger than the number of lines of the source code.

*Trust base* The validity of the bytecode verification result assumes the correctness of the bytecode specification and the KEVM verifier. The algorithm correctness proof is partially mechanized—only the proof of major lemmas are mechanized in the K framework. The non-mechanized proofs are included in our trust base. The Vyper compiler is *not* in the trust base.

*Continuous verification* The verification target contract was a moving target. Even if the contract code had been frozen before starting the formal verification process, the code (both source code or bytecode) was updated in the middle of the verification process, to fix bugs found during the process. Indeed, we found several bugs in both the contract and the compiler, and each time we found a bug, we had to re-verify the newly compiled bytecode that fixes the bug. Here the problem was the overhead of re-verification. About 20% of the bytecode verification effort was spent on re-verification.

The re-verification overhead could have been reduced by automatically adjusting formal specifications to updated bytecode, and/or making specifications as independent of the specific details of the bytecode as possible. For example, the current bytecode specification employs specific program-counter (PC) values to refer to some specific positions of the bytecode, especially when specifying loop invariants. Most of such PC values need to be updated whenever the bytecode is modified. The re-verification overhead could have been reduced by automatically updating such PC values, or even having the specification refer to specific positions without using PC values. We leave this as future work.

## 5 Related Work

*Static analysis and verification of smart contracts* There have been proposed many static analysis tools [38,35,5,54,42,39,29,53,9] that are designed to automatically detect a certain fixed set of bugs and vulnerabilities of smart contracts, at the cost of generality and expressiveness. VerX [46] can verify past-time linear temporal properties over multiple runs of smart contracts, but it requires the target contracts to be effectively loop-free.

There also have been proposed verification tools that allow us to specify and verify arbitrary functional correctness and/or security properties, such as [3,32] based on the F\* proof assistant [52], [1] based on Isabelle/HOL [43], the KEVM verifier [45] based on the K framework [50], and VeriSol [37] based on Boogie [2]. The KEVM verifier has also been used to verify high-profile and challenging smart contracts [49], including a multi-signature wallet called Gnosis Safe [31], a decentralized token exchange called Uniswap [55], and a partial consensus mechanism called Casper FFG [6].

*Verification of systems software* There have been reported formal verification of various systems software, from OS kernels [36,33,41], to file systems [7,51], to cryptographic code [4]. While most of the verified systems code is either synthesized from specifications, or implemented (or adjusted) to be verification-friendly, there also exist efforts [11,8] to verify actual production code as it is. Such efforts are necessary especially when production code is highly performance-critical and/or existing development processes are hard to change to help produce verification-friendly code. The deposit contract we verified was given to us at the code-frozen stage, and also performance-critical (especially in terms of the gas cost), and thus we took and verified the given production-ready code as it is, without any modification except for fixing bugs.

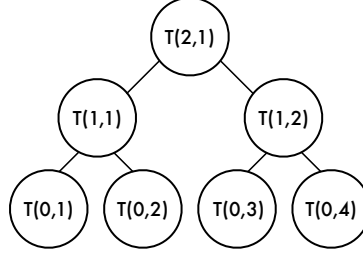
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**Fig. 2.** A Merkle tree of height 2. We write  $T(l, i)$  to denote the node of a tree  $T$  at the level  $l$  and the index  $i$ , where the level of leafs is 0, and the index of the left-most node is 1.

## A Formalization and Correctness Proof of Incremental Merkle Tree Algorithm

We formalize the incremental Merkle tree algorithm [56], especially the one employed in the deposit contract [23], and prove its correctness w.r.t. the original full-construction Merkle tree algorithm [40].

*Notations* Let  $T$  be a perfect binary tree [44] (i.e., every node has exactly two child nodes) of height  $h$ , and  $T(l, i)$  denote its node at level  $l$  and index  $i$ , where the level of leafs is 0, and the index of the left-most node is 1. For example, if  $h = 2$ , then  $T(2, 1)$  denotes the root whose children are  $T(1, 1)$  and  $T(1, 2)$ , and the leafs are denoted by  $T(0, 1)$ ,  $T(0, 2)$ ,  $T(0, 3)$ , and  $T(0, 4)$ , as shown in Figure 2. We write  $\llbracket T(l, i) \rrbracket$  to denote the value of the node  $T(l, i)$ , but we omit  $\llbracket \cdot \rrbracket$  when the meaning is clear in the context.

Let us define two functions,  $\uparrow$  and  $\downarrow$ , as follows:

$$\uparrow x = \lceil x/2 \rceil \quad (1)$$

$$\downarrow x = \lfloor x/2 \rfloor \quad (2)$$

Moreover, let us define  $\uparrow^k x = \uparrow(\uparrow^{k-1} x)$  for  $k \geq 2$ ,  $\uparrow^1 x = \uparrow x$ , and  $\uparrow^0 x = x$ . Let  $\{T(k, \uparrow^k x)\}_{k=0}^h$  be a path  $\{T(0, \uparrow^0 x), T(1, \uparrow^1 x), T(2, \uparrow^2 x), \dots, T(h, \uparrow^h x)\}$ . We write  $\{T(k, \uparrow^k x)\}_k$  if  $h$  is clear in the context. Let us define  $\downarrow^k$  and  $\{T(k, \downarrow^k x)\}_k$  similarly. For the presentation purpose, let  $T(l, 0)$  denote a dummy node which has the parent  $T(l+1, 0)$  and the children  $T(l-1, 0)$  and  $T(l-1, 1)$ . Note that, however, these dummy nodes are only conceptual, allowing the aforementioned paths to be well-defined, but *not* part of the tree at all.

In this notation, for a non-leaf, non-root node of index  $i$ , its left child index is  $2i - 1$ , its right child index is  $2i$ , and its parent index is  $\uparrow i$ . Also, note that  $\{T(k, \uparrow^k m)\}_k$  is the path starting from the  $m$ -th leaf going all the way up to the root.

First, we show that two paths  $\{T(k, \uparrow^k x)\}_k$  and  $\{T(k, \downarrow^k (x - 1))\}_k$  are parallel with a “distance” of 1.

**Lemma 1.** *For all  $x \geq 1$ , and  $k \geq 0$ , we have:*

$$(\uparrow^k x) - 1 = \uparrow^k (x - 1) \quad (3)$$

*Proof.* Let us prove by induction on  $k$ . When  $k = 0$ , we have  $(\uparrow^0 x) - 1 = x - 1 = \uparrow^0 (x - 1)$ . When  $k = 1$ , we have two cases:

– When  $x$  is odd, that is,  $x = 2y + 1$  for some  $y \geq 0$ :

$$(\uparrow x) - 1 = (\uparrow (2y + 1)) - 1 = \left\lceil \frac{2y + 1}{2} \right\rceil - 1 = y = \left\lfloor \frac{2y}{2} \right\rfloor = \uparrow 2y = \uparrow (x - 1)$$

– When  $x$  is even, that is,  $x = 2y$  for some  $y \geq 1$ :

$$(\uparrow x) - 1 = (\uparrow 2y) - 1 = \left\lceil \frac{2y}{2} \right\rceil - 1 = y - 1 = \left\lfloor \frac{2y - 1}{2} \right\rfloor = \uparrow (2y - 1) = \uparrow (x - 1)$$

Thus, we have:

$$(\uparrow x) - 1 = \uparrow (x - 1) \quad (4)$$

Now, assume that (3) holds for some  $k = l \geq 1$ . Then,

$$\begin{aligned} \uparrow^{l+1} x &= \uparrow (\uparrow^l x) && \text{(By the definition of } \uparrow^k) \\ &= \uparrow ((\uparrow^l (x - 1)) + 1) && \text{(By the assumption)} \\ &= (\uparrow (\uparrow^l (x - 1))) + 1 && \text{(By the equation 4)} \\ &= \uparrow^{l+1} (x - 1) + 1 && \text{(By the definition of } \uparrow^k) \end{aligned}$$

which concludes.

Now let us define the Merkle tree.

**Definition 1.** *A perfect binary tree  $T$  of height  $h$  is a Merkle tree [40], if the leaf node contains data, and the non-leaf node's value is the hash of its children's, i.e.,*

$$\forall 0 < l \leq h. \forall 0 < i \leq 2^{h-l}. T(l, i) = \text{hash}(T(l - 1, 2i - 1), T(l - 1, 2i)) \quad (5)$$

*Let  $T_m$  be a partial Merkle tree up-to  $m$  whose first  $m$  leafs contain data and the other leafs are zero, i.e.,*

$$T_m(0, i) = 0 \quad \text{for all } m < i \leq 2^h \quad (6)$$

*Let  $Z$  be the zero Merkle tree whose leafs are all zero, i.e.,  $Z(0, i) = 0$  for all  $0 < i \leq 2^h$ . That is,  $Z = T_0$ . Since all nodes at the same level have the same value in  $Z$ , we write  $Z(l)$  to denote the value at the level  $l$ , i.e.,  $Z(l) = Z(l, i)$  for any  $0 < i \leq 2^{h-l}$ .*

Now we formulate the relationship between the partial Merkle trees. Given two partial Merkle trees  $T_{m-1}$  and  $T_m$ , if their leaves agree up-to  $m - 1$ , then they only differ on the path  $\{T_m(k, \uparrow^k m)\}_k$ . This is formalized in Lemma 2.



**Lemma 2.** Let  $T_m$  be a partial Merkle tree up-to  $m > 0$  of height  $h$ , and let  $T_{m-1}$  be another partial Merkle tree up-to  $m - 1$  of the same height. Suppose their leafs agree up to  $m - 1$ , that is,  $T_{m-1}(0, i) = T_m(0, i)$  for all  $1 \leq i \leq m - 1$ . Then, for all  $0 \leq l \leq h$ , and  $1 \leq i \leq 2^{h-l}$ ,

$$T_{m-1}(l, i) = T_m(l, i) \quad \text{when } i \neq \uparrow^l m \quad (7)$$

*Proof.* Let us prove by induction on  $l$ . When  $l = 0$ , we immediately have  $T_{m-1}(0, i) = T_m(0, i)$  for any  $i \neq m$  by the premise and the equation (6). Now, assume that (7) holds for some  $l = k$ . Then by the equation 5, we have  $T_{m-1}(k + 1, i) = T_m(k + 1, i)$  for any  $i \neq \uparrow(\uparrow^k m) = \uparrow^{k+1} m$ , which concludes.

Corollary 1 induces a *linear-time* incremental Merkle tree insertion algorithm [56].

**Corollary 1.**  $T_m$  can be constructed from  $T_{m-1}$  by computing only  $\{T_m(k, \uparrow^k m)\}_k$ , the path from the new leaf,  $T_m(0, m)$ , to the root.

*Proof.* By Lemma 2.

Let us formulate more properties of partial Merkle trees.

**Lemma 3.** Let  $T_m$  be a partial Merkle tree up-to  $m$  of height  $h$ , and  $Z$  be the zero Merkle tree of the same height. Then, for all  $0 \leq l \leq h$ , and  $1 \leq i \leq 2^{h-l}$ ,

$$T_m(l, i) = Z(l) \quad \text{when } i > \uparrow^l m \quad (8)$$

*Proof.* Let us prove by induction on  $l$ . When  $l = 0$ , we immediately have  $T_m(0, i) = Z(0) = 0$  for any  $m < i \leq 2^h$  by the equation (6). Now, assume that (8) holds for some  $0 \leq l = k < h$ . First, for any  $i \geq (\uparrow^{k+1} m) + 1$ , we have:

$$2i - 1 \geq (2 \uparrow^{k+1} m) + 1 = 2 \left\lceil \frac{\uparrow^k m}{2} \right\rceil + 1 \geq 2 \frac{\uparrow^k m}{2} + 1 = (\uparrow^k m) + 1 \quad (9)$$

Then, for any  $\uparrow^{k+1} m < i \leq 2^{h-(k+1)}$ , we have:

$$\begin{aligned} T_m(k + 1, i) &= \text{hash}(T_m(k, 2i - 1), T_m(k, 2i)) && \text{(By the equation 5)} \\ &= \text{hash}(Z(k), Z(k)) && \text{(By the equations 8 and 9)} \\ &= Z(k + 1) && \text{(By the definition of } Z) \end{aligned}$$

which concludes.

Lemma 4 induces a *linear-space* incremental Merkle tree insertion algorithm.

**Lemma 4.** A path  $\{T_m(k, \uparrow^k m)\}_k$  can be computed by using only two other paths,  $\{T_{m-1}(k, \uparrow^k (m - 1))\}_k$  and  $\{Z(k)\}_k$ .

*Proof.* We will construct the path from the leaf,  $T_m(0, m)$ , which is given. Suppose we have constructed the path up to  $T_m(q, \uparrow^q m)$  for some  $q > 0$  by using only two other sub-paths,  $\{T_{m-1}(k, \uparrow^k (m - 1))\}_{k=0}^{q-1}$  and  $\{Z(k)\}_{k=0}^{q-1}$ . Then, to construct  $T_m(q + 1, \uparrow^{q+1} m)$ , we need the sibling of  $T_m(q, \uparrow^q m)$ , where we have two cases:

- Case  $(\uparrow^q m)$  is odd. Then, we need the right-sibling  $T_m(q, (\uparrow^q m) + 1)$ , which is  $Z(q)$  by Lemma 3.
- Case  $(\uparrow^q m)$  is even. Then, we need the left-sibling  $T_m(q, (\uparrow^q m) - 1)$ , which is  $T_m(q, \uparrow^q(m - 1))$  by Lemma 1, which is in turn  $T_{m-1}(q, \uparrow^q(m - 1))$  by Lemma 2.

By the mathematical induction on  $k$ , we conclude.

**Lemma 5.** *Let  $h = \text{TREE\_HEIGHT}$ . For any integer  $0 \leq m < 2^h$ , the two paths  $\{T_m(k, \uparrow^k m)\}_k$  and  $\{T_{m+1}(k, \uparrow^k(m+1))\}_k$  always converge, that is, there exists unique  $0 \leq l \leq h$  such that:*

$$(\uparrow^k m) + 1 = \uparrow^k(m + 1) \text{ is even for all } 0 \leq k < l \quad (10)$$

$$(\uparrow^k m) + 1 = \uparrow^k(m + 1) \text{ is odd for } k = l \quad (11)$$

$$\uparrow^k m = \uparrow^k(m + 1) \text{ for all } l < k \leq h \quad (12)$$

$$T_m(k, \uparrow^k m) = T_{m+1}(k, \uparrow^k(m + 1)) \text{ for all } l < k \leq h \quad (13)$$

*Proof.* The equation 12 follows from the equation 11, since for an odd integer  $x$ ,  $\uparrow(x - 1) = \uparrow x$ . Also, the equation 13 follows from Lemma 2, since  $\uparrow^k(m + 1) = (\uparrow^k m) + 1 \neq \uparrow^k m = \uparrow^k(m + 1)$  by Lemma 1 and the equation 12. Thus, we only need to prove the unique existence of  $l$  satisfying (10) and (11). The existence of  $l$  is obvious since  $1 \leq m + 1 \leq 2^h$ , and one can find the smallest  $l$  satisfying (10) and (11). Now, suppose there exist two different  $l_1 < l_2$  satisfying (10) and (11). Then,  $\uparrow^{l_1}(m + 1)$  is odd since  $l_1$  satisfies (11), while  $\uparrow^{l_1}(m + 1)$  is even since  $l_2$  satisfies (10), which is contradiction, thus  $l$  is unique, and we conclude.

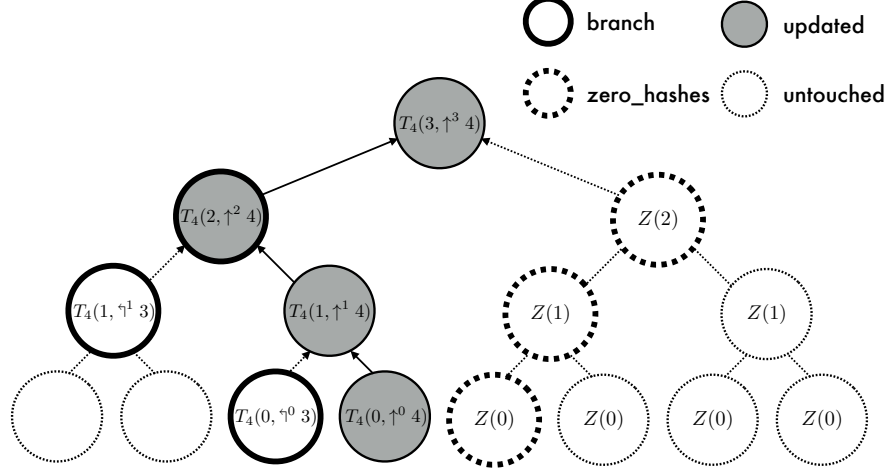
### A.1 Pseudocode

Figure 4 shows the pseudocode of the incremental Merkle tree algorithm [56] that is employed in the deposit contract [23]. It maintains a global counter `deposit_count` to keep track of the number of deposits made, and two global arrays `zero_hashes` and `branch`, which corresponds to  $Z$  (Definition 1) and a certain part of  $\{T_m(k, \uparrow^k m)\}_k$ , where  $m$  denotes the value of `deposit_count`. The `init` function is called once at the beginning to initialize `zero_hashes` which is never updated later. The `deposit` function inserts a given new leaf value in the tree by incrementing `deposit_count` and updating only a single element of `branch`. The `get_deposit_root` function computes the root of the current partial Merkle tree  $T_m$ .

Since the loops are bounded to the tree height and the size of global arrays is equal to the tree height, it is clear that both time and space complexities of the algorithm are linear.

### A.2 Correctness Proof

Now we prove the correctness of the incremental Merkle tree algorithm shown in Figure 4.



**Fig. 3.** A partial Merkle tree  $T_4$  of height 3, illustrating the incremental Merkle tree algorithm shown in Figure 4, where  $TREE\_HEIGHT = 3$ . The bold-lined nodes correspond to the **branch** array. The bold-dotted-lined nodes correspond to the **zero\_hashes** array. The **get\_deposit\_root** function computes the gray nodes by using only the bold-lined nodes (i.e., **branch**) and the bold-dotted-lined nodes (i.e., **zero\_hashes**), where  $deposit\_count = 4$ .

**Theorem 1 (Correctness of Incremental Merkle Tree Algorithm).** *Suppose that the **init** function is executed at the beginning, followed by a sequence of **deposit** function calls, say  $deposit(v_1)$ ,  $deposit(v_2)$ ,  $\dots$ , and  $deposit(v_m)$ , where  $m < 2^{TREE\_HEIGHT}$ . Then, the function call **get\_deposit\_root**() will return the root of the partial Merkle tree  $T_m$  such that  $T_m(0, i) = v_i$  for all  $1 \leq i \leq m$ .*

*Proof.* By Lemmas 6, 7, 8, and 9.

Note that the correctness theorem requires the condition  $m < 2^h$ , where  $h$  is the tree height, that is, the rightmost leaf must be kept empty, which means that the maximum number of deposits that can be stored in the tree using this incremental algorithm is  $2^h - 1$  instead of  $2^h$ . See Section 4.1 for more details.

**Lemma 6 (init).** *Once **init** is executed, **zero\_hashes** denotes  $Z$ , that is,*

$$zero\_hashes[k] = Z(k) \quad (14)$$

for  $0 \leq k < TREE\_HEIGHT$ .

*Proof.* By the implementation of **init** and the definition of  $Z$  in Definition 1.

**Lemma 7 (deposit).** *Suppose that, before executing **deposit**, we have:*

$$deposit\_count = m < 2^{TREE\_HEIGHT} - 1 \quad (15)$$

$$branch[k] = T_m(k, \uparrow^k m) \quad \text{if } \uparrow^k m \text{ is odd} \quad (16)$$

```

1  # globals
2  zero_hashes: int[TREE_HEIGHT] = {0} # zero array
3  branch:      int[TREE_HEIGHT] = {0} # zero array
4  deposit_count: int = 0 # max: 2^TREE_HEIGHT - 1
5
6  fun init() -> unit:
7      i: int = 0
8      while i < TREE_HEIGHT - 1:
9          zero_hashes[i+1] = hash(zero_hashes[i], zero_hashes[i])
10         i += 1
11
12  fun deposit(value: int) -> unit:
13      assert deposit_count < 2^TREE_HEIGHT - 1
14      deposit_count += 1
15      size: int = deposit_count
16      i: int = 0
17      while i < TREE_HEIGHT:
18          if size % 2 == 1:
19              break
20          value = hash(branch[i], value)
21          size /= 2
22          i += 1
23      branch[i] = value
24
25  fun get_deposit_root() -> int:
26      root: int = 0
27      size: int = deposit_count
28      h: int = 0
29      while h < TREE_HEIGHT:
30          if size % 2 == 1: # size is odd
31              root = hash(branch[h], root)
32          else:             # size is even
33              root = hash(root, zero_hashes[h])
34          size /= 2
35          h += 1
36      return root

```

**Fig. 4.** Pseudocode implementation of the incremental Merkle tree algorithm employed in the deposit contract [23].

Then, after executing **deposit**( $v$ ), we have:

$$\mathbf{deposit\_count}' = m + 1 \leq 2^{\mathbf{TREE\_HEIGHT}} - 1 \quad (17)$$

$$\mathbf{branch}'[k] = T_{m+1}(k, \mathfrak{r}^k(m+1)) \quad \text{if } \mathfrak{r}^k(m+1) \text{ is odd} \quad (18)$$

for any  $0 \leq k < \mathbf{TREE\_HEIGHT}$ , where:

$$T_{m+1}(0, m+1) = v \quad (19)$$

*Proof.* Let  $h = \mathbf{TREE\_HEIGHT}$ . The equation 17 is obvious by the implementation of **deposit**. Let us prove the equation 18. Let  $l$  be the unique integer described in Lemma 5. We claim that **deposit** updates only **branch**[ $l$ ] to be  $T_{m+1}(l, \mathfrak{r}^l(m+1))$ . Then, for all  $0 \leq k < l$ ,  $\mathfrak{r}^k(m+1)$  is not odd. For  $k = l$ , we conclude by the aforementioned claim. For  $l < k \leq h$ , we conclude by the equation 13 and the fact that **branch**[ $k$ ] is not modified (by the aforementioned claim).

Now, let us prove the aforementioned claim. Since **branch** is updated only at line 23, we only need to prove  $i = l$  and **value** =  $T_{m+1}(l, \mathfrak{r}^l(m+1))$  at that point. We claim the following loop invariant at line 17:

$$i = i < \mathbf{TREE\_HEIGHT} \quad (20)$$

$$\mathbf{value} = T_{m+1}(i, \mathfrak{r}^i(m+1)) \quad (21)$$

$$\mathbf{size} = \mathfrak{r}^i(m+1) \quad (22)$$

$$\mathfrak{r}^k(m+1) \text{ is even for any } 0 \leq k < i \quad (23)$$

Note that  $i$  cannot reach  $\mathbf{TREE\_HEIGHT}$ , since  $(m+1) < 2^{\mathbf{TREE\_HEIGHT}}$ . Thus, by the loop invariant, we have the following after the loop at line 23:

$$i = i < \mathbf{TREE\_HEIGHT} \quad (24)$$

$$\mathbf{value} = T_{m+1}(i, \mathfrak{r}^i(m+1)) \quad (25)$$

$$\mathbf{size} = \mathfrak{r}^i(m+1) \text{ is odd} \quad (26)$$

$$\mathfrak{r}^k(m+1) \text{ is even for any } 0 \leq k < i \quad (27)$$

Moreover, by Lemma 5, we have  $i = l$ , which suffices to conclude the aforementioned claim.

Now we only need to prove the loop invariant. First, at the beginning of the first iteration, we have  $i = 0$ , **value** =  $v = T_{m+1}(0, m+1)$  by (19), and **size** =  $(m+1)$ , which satisfies the loop invariant. Now, assume that the invariant holds at the beginning of the  $i^{\text{th}}$  iteration that does not reach the **break** statement at line 19 (i.e., **size** =  $\mathfrak{r}^i(m+1)$  is even). Then,  $i' = i + 1$ , **size**' =  $\mathfrak{r}^{i+1}(m+1)$ , and:

$$\begin{aligned} T_{m+1}(i+1, \mathfrak{r}^{i+1}(m+1)) &= \text{hash}(T_{m+1}(i, \mathfrak{r}^i(m)), T_{m+1}(i, \mathfrak{r}^i(m+1))) \\ &\quad \text{(by Equation 10)} \\ &= \text{hash}(T_m(i, \mathfrak{r}^i(m)), \mathbf{value}) \\ &\quad \text{(by Lemmas 1 \& 2 and Equation 21)} \\ &= \text{hash}(\mathbf{branch}[i], \mathbf{value}) \quad \text{(by Equations 16 \& 10)} \\ &= \mathbf{value}' \end{aligned}$$

Thus, the loop invariant holds at the beginning of the  $(i + 1)^{\text{th}}$  iteration as well, and we conclude.

**Lemma 8 (Contract Invariant).** *Let  $m = \text{deposit\_count}$ . Then, once `init` is executed, the following contract invariant holds. For all  $0 \leq k < \text{TREE\_HEIGHT}$ ,*

1.  $\text{zero\_hashes}[k] = Z(k)$
2.  $\text{branch}[k] = T_m(k, \uparrow^k m)$  if  $\uparrow^k m$  is odd
3.  $\text{deposit\_count} \leq 2^{\text{TREE\_HEIGHT}} - 1$

*Proof.* Let us prove each invariant item.

1. By Lemma 6, and the fact that `zero_hashes` is updated by only `init`.
2. By Lemma 7, and the fact that `branch` is updated by only `deposit`.
3. By the assertion of `deposit` (at line 13 of Figure 4), and the fact that `deposit_count` is updated by only `deposit`.

**Lemma 9 (`get_deposit_root`).** *The `get_deposit_root` function computes the path  $\{T_m(k, \uparrow^k(m+1))\}_k$  and returns the root  $T_m(h, 1)$ , given a Merkle tree  $T_m$  of height  $h$ , that is,  $\text{deposit\_count} = m < 2^h$  and  $\text{TREE\_HEIGHT} = h$  when `get_deposit_root` is invoked.*

*Proof.* We claim the following loop invariant at line 29, which suffices to conclude the main claim.

$$\begin{aligned} \mathbf{h} &= k \quad \text{where } 0 \leq k \leq h \\ \mathbf{size} &= \uparrow^k m \\ \mathbf{root} &= T_m(k, \uparrow^k(m+1)) \end{aligned}$$

Now let us prove the above loop invariant claim by the mathematical induction on  $k$ . The base case ( $k = 0$ ) is trivial, since  $\uparrow^0 m = m$ ,  $\uparrow^0(m+1) = m+1$ , and  $T_m(0, m+1) = 0$  by Definition 1. Assume that the loop invariant holds for some  $k = l$ . Let  $\mathbf{h}'$ ,  $\mathbf{size}'$ , and  $\mathbf{root}'$  denote the values at the next iteration  $k = l + 1$ . Obviously, we have  $\mathbf{h}' = l + 1$  and  $\mathbf{size}' = \uparrow^{l+1} m$ . Also, we have  $(\uparrow^l m) + 1 = \uparrow^l(m+1)$  by Lemma 1. Now, we have two cases:

- Case  $\mathbf{size} = \uparrow^l m$  is odd. Then,  $\uparrow^l(m+1)$  is even. Thus,

$$\begin{aligned} T_m(l+1, \uparrow^{l+1}(m+1)) &= \text{hash}(T_m(l, \uparrow^l m), T_m(l, \uparrow^l(m+1))) \\ &= \text{hash}(\text{branch}[l], \mathbf{root}) \quad (\text{by Lemma 8}) \\ &= \mathbf{root}' \end{aligned}$$

- Case  $\mathbf{size} = \uparrow^l m$  is even. Then,  $\uparrow^l(m+1)$  is odd. Thus,

$$\begin{aligned} T_m(l+1, \uparrow^{l+1}(m+1)) &= \text{hash}(T_m(l, \uparrow^l(m+1)), T_m(l, (\uparrow^l(m+1)) + 1)) \\ &= \text{hash}(\mathbf{root}, Z(l)) \quad (\text{by Lemma 3}) \\ &= \text{hash}(\mathbf{root}, \text{zero\_hashes}[l]) \quad (\text{by Lemma 8}) \\ &= \mathbf{root}' \end{aligned}$$

Thus, we have  $\mathbf{root}' = T_m(l+1, \uparrow^{l+1}(m+1))$ , which concludes.

*Mechanized Proofs* The loop invariant proofs of Lemma 7 and Lemma 9 are mechanized in the K framework, which can be found at [48].

*Remark* Since the `deposit` function reverts when `deposit_count`  $\geq 2^{\text{TREE\_HEIGHT}} - 1$ , the loop in the `deposit` function cannot reach the last iteration, thus the loop bound (in line 17 of Figure 4) can be safely decreased to `TREE_HEIGHT - 1`.