

# Cache-Oblivious Data Structures and Algorithms for Undirected Breadth-First Search and Shortest Paths

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**Abstract.** We present improved cache-oblivious data structures and algorithms for breadth-first search and the single-source shortest path problem on undirected graphs with non-negative edge weights. Our results removes the performance gap between the currently best *cache-aware* algorithms for these problems and their *cache-oblivious* counterparts. Our shortest-path algorithm relies on a new data structure, called *bucket heap*, which is the first cache-oblivious priority queue to efficiently support a weak DECREASEKEY operation.

## 1 Introduction

*Breadth-first search* (BFS) and the *single-source shortest path* (SSSP) problem are fundamental combinatorial optimization problems with numerous applications. SSSP is defined as follows: Let  $G = (V, E)$  be a graph with  $V$  vertices and  $E$  edges,<sup>1</sup> let  $s$  be a distinguished vertex of  $G$ , and let  $\omega$  be an assignment of non-negative real *weights* to the edges of  $G$ . The weight of a path is the sum of the weights of its edges. We want to find for every vertex  $v$  that is reachable from  $s$ , the weight  $\text{dist}(s, v)$  of a minimum-weight (“shortest”) path from  $s$  to  $v$ . BFS can be seen as the unweighted version of SSSP.

Both problems are well understood in the RAM model, where the cost of a memory access is assumed to be independent of the accessed memory location. However, modern computers contain a hierarchy of memory levels; the cost of a memory access depends on the currently lowest memory level that contains

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<sup>1</sup> For convenience, we use the name of a set to denote both the set and its cardinality. Furthermore, we will assume that  $E = \Omega(V)$ , in order to simplify notation.

the accessed element. This is not accounted for in the RAM model, and current BFS and SSSP-algorithms, when run in memory hierarchies, turn out to be notoriously inefficient for sparse input graphs. The purpose of this paper is to provide improved data structures and algorithms for BFS and SSSP under the currently most powerful model for multi-level memory hierarchies.

*Models for memory hierarchies.* The most widely used model for the design of cache-aware algorithms is the *I/O-model* of Aggarwal and Vitter [2]. This model assumes a memory hierarchy consisting of two levels; the lower level has size  $M$ ; data is transferred between the two levels in blocks of  $B$  consecutive data items. The complexity of an algorithm is the number of blocks transferred (I/Os). The parameters  $M$  and  $B$  are assumed to be known to the algorithm. The strength of the I/O-model is its simplicity, while it still adequately models the situation when the I/Os between two levels of the memory hierarchy dominate the running time of the algorithm; this is often the case when the size of the data significantly exceeds the size of main memory. *Cache-oblivious* algorithms are designed to be I/O-efficient without knowing  $M$  or  $B$ ; that is, they are formulated in the RAM model and analyzed in the I/O-model, assuming that the memory transfers are performed by an optimal offline paging algorithm. Since the analysis holds for any block and memory sizes, it holds for *all* levels of a multi-level memory hierarchy (see [16] for details). Thus, the cache-oblivious model elegantly combines the simplicity of the I/O-model with a coverage of the entire memory hierarchy.

A comprehensive list of results for the I/O-model have been obtained—see [3,19,22] and the references therein. One of the fundamental facts is that, in the I/O-model, comparison-based sorting of  $N$  elements takes  $\Theta(\text{Sort}(N))$  I/Os in the worst case, where  $\text{Sort}(N) = \frac{N}{B} \log_{M/B} \frac{N}{B}$ .

For the cache-oblivious model, Frigo et al. developed optimal cache-oblivious algorithms for matrix multiplication, matrix transposition, fast Fourier transform, and sorting [16]. The cache-oblivious sorting bound matches that for the I/O-model:  $\mathcal{O}(\text{Sort}(N))$  I/Os. After the publication of [16], a number of results for the cache-oblivious model have appeared; see [13,19] for recent surveys.

Some results in the cache-oblivious model, in particular those concerning sorting and algorithms and data structures that can be used to sort, such as priority queues, are proved under the assumption that  $M \geq B^2$ . This is also known as the *tall-cache assumption*. In particular, this assumption is made in the FUNNELSORT algorithm of Frigo et al. [16]. A variant termed LAZY-FUNNELSORT [6] works under the weaker tall-cache assumption that  $M \geq B^{1+\varepsilon}$ , for any fixed  $\varepsilon > 0$ . Recently, it has been shown [8] that a tall-cache assumption is necessary for cache-oblivious comparison-based sorting algorithms.

*Previous and related work.* Graph algorithms for the I/O-model have received considerable attention in recent years. Many efficient cache-aware algorithms do have a cache-oblivious counterpart that achieves the same performance; see Table 1. Despite these efforts, only little progress has been made on the solution of the SSSP-problem with general non-negative edge weights using either cache-aware or cache-oblivious algorithms: The best known lower bound is

**Table 1.** I/O-bounds for some fundamental graph problems.

Problem	Best cache-oblivious result	Best cache-aware result
List ranking	$\mathcal{O}(\text{Sort}(V))$ [4]	$\mathcal{O}(\text{Sort}(V))$ [11]
Euler Tour	$\mathcal{O}(\text{Sort}(V))$ [4]	$\mathcal{O}(\text{Sort}(V))$ [11]
Spanning tree/MST	$\mathcal{O}(\text{Sort}(E) \cdot \log \log V)$ [4]	$\mathcal{O}(\text{Sort}(E) \cdot \log \log(VB/E))$ [5]
	$\mathcal{O}(\text{Sort}(E))$ (randomized) [1]	$\mathcal{O}(\text{Sort}(E))$ (randomized) [1]
Undirected BFS	$\mathcal{O}(V + \text{Sort}(E))$ [21]	$\mathcal{O}(\text{ST}(E) + \text{Sort}(E) + \sqrt{VE/B})$ [18]
	$\mathcal{O}(\text{ST}(E) + \text{Sort}(E) + \frac{E}{B} \cdot \log V + \sqrt{VE/B})$ <b>New</b>	
	$\mathcal{O}(\text{ST}(E) + \text{Sort}(E) + \frac{E}{B} \cdot \frac{1}{\epsilon} \cdot \log \log V + \sqrt{VE/B} \cdot \sqrt{VB/E^\epsilon})$ <b>New</b>	
Directed BFS & DFS	$\mathcal{O}((V + E/B) \cdot \log V + \text{Sort}(E))$ [4]	$\mathcal{O}((V + E/B) \cdot \log V + \text{Sort}(E))$ [10]
Undirected SSSP	$\mathcal{O}(V + (E/B) \cdot \log(E/B))$ <b>New</b>	$\mathcal{O}(V + (E/B) \cdot \log(E/B))$ [17]

$\Omega(\text{Sort}(E))$  I/Os, which can be obtained through a reduction from list ranking; but the currently best algorithm [17] performs  $\mathcal{O}(V + (E/B) \log_2(E/B))$  I/Os on undirected graphs. For  $E = \mathcal{O}(V)$ , this is hardly better than naïvely running Dijkstra’s internal-memory algorithm [14,15] in external memory, which would take  $\mathcal{O}(V \log_2 V + E)$  I/Os. On dense graphs, however, the algorithm is efficient. The algorithm of [17] is not cache-oblivious, because the applied external-memory priority queue based on the tournament tree is not cache-oblivious. Cache-oblivious priority queues exist [4,7]; but none of them efficiently supports a DECREASEKEY operation. Indeed, the tournament tree is also the only cache-aware priority queue that supports at least a weak form of this operation.

For bounded edge weights, an improved external-memory SSSP-algorithm has been developed recently [20]. This algorithm is an extension of the currently best external-memory BFS-algorithm [18], FAST-BFS, which performs  $\mathcal{O}(\sqrt{VE/B} + \text{Sort}(E) + \text{ST}(E))$  I/Os, where  $\text{ST}(E)$  is the number of I/Os required to compute a spanning tree (see Table 1). Again, the key data structure used in FAST-BFS is not cache-oblivious, which is why the currently best cache-oblivious BFS-algorithm is that of [21].

*Our results.* In Section 2, we develop the first cache-oblivious priority queue, called *bucket heap*, that supports an UPDATE operation, which is a combined INSERT and DECREASEKEY operation. The amortized cost of operations UPDATE, DELETE, and DELETEMIN is  $\mathcal{O}((1/B) \log_2(N/B))$  where  $N$  is the number of distinct elements in the priority-queue. Using the bucket heap, we obtain a cache-oblivious shortest-path algorithm for undirected graphs with non-negative edge weights that matches the performance of the best cache-aware algorithm for this problem:  $\mathcal{O}(V + (E/B) \log_2(E/B))$  I/Os. Independently of our work, the bucket heap as well as a cache-oblivious version of the tournament tree have simultaneously been developed by Chowdhury and Ramachandran [12].

In Section 3, we develop a new cache-oblivious algorithm for undirected BFS. The algorithm comes in two variants: The first variant performs  $\mathcal{O}(\text{ST}(E) + \text{Sort}(E) + \frac{E}{B} \log V + \sqrt{VE/B})$  I/Os; the second variant performs  $\mathcal{O}(\text{ST}(E) + \text{Sort}(E) + \frac{E}{B} \cdot \frac{1}{\varepsilon} \cdot \log \log V + \sqrt{VE/B} \cdot \sqrt{VB/E^\varepsilon})$  I/Os, for any  $\varepsilon > 0$ . Here,  $\text{ST}(E)$  denotes the cost of cache-obliviously finding a spanning tree.

## 2 The Bucket Heap and Undirected Shortest Paths

In this section, we describe the *bucket heap*, which is a priority queue that supports an UPDATE (a weak DECREASEKEY) operation and does so in the same I/O-bound as the tournament tree of [17]. Using the bucket heap, the SSSP-algorithm of [17] becomes cache-oblivious. Similar to the tournament tree, the bucket heap supports the following three operations, where we refer to an element  $x$  with priority  $p$  as element  $(x, p)$ :

**Update** $(x, p)$  inserts element  $(x, p)$  into the priority queue if  $x$  is not in the priority queue; otherwise, it replaces the current element  $(x, p')$  in the priority queue with  $(x, \min(p, p'))$ .

**Delete** $(x)$  removes element  $x$  from the priority queue.

**DeleteMin** removes and reports the minimal element in the priority queue.

The bucket heap consists of  $q$  buckets  $\mathcal{B}_1, \mathcal{B}_2, \dots, \mathcal{B}_q$  and  $q + 1$  signal buffers  $\mathcal{S}_1, \mathcal{S}_2, \dots, \mathcal{S}_{q+1}$ , where  $q$  varies over time, but is always at most  $\lceil \log_4 N \rceil$ . The capacity of bucket  $\mathcal{B}_i$  is  $2^{2i}$ ; buffer  $\mathcal{S}_i$  has capacity  $2^{2i-1}$ . In order to allow for temporary overflow, we allocate  $2^{2i+1}$  memory locations for bucket  $\mathcal{B}_i$  and  $2^{2i}$  memory locations for buffer  $\mathcal{S}_i$ . We store all buckets and buffers consecutively in memory, in the following order:  $\mathcal{S}_1, \mathcal{B}_1, \mathcal{S}_2, \mathcal{B}_2, \dots, \mathcal{S}_q, \mathcal{B}_q, \mathcal{S}_{q+1}$ .

Buckets  $\mathcal{B}_1, \mathcal{B}_2, \dots, \mathcal{B}_q$  store the elements currently in the priority queue. We maintain the invariant that for any two buckets  $\mathcal{B}_i$  and  $\mathcal{B}_j$  with  $i < j$  and any two elements  $(x, p) \in \mathcal{B}_i$  and  $(y, q) \in \mathcal{B}_j$ ,  $p \leq q$ .

Buffers  $\mathcal{S}_1, \mathcal{S}_2, \dots, \mathcal{S}_{q+1}$  store three types of signals, which we use to update the bucket contents in a lazy manner: UPDATE $(x, p)$  and DELETE $(x)$  signals are used to implement UPDATE $(x, p)$  and DELETE $(x)$  operations. A PUSH $(x, p)$  signal is used to push elements from a bucket  $\mathcal{B}_i$  to a bucket  $\mathcal{B}_{i+1}$  when  $\mathcal{B}_i$  overflows. Every signal has a time stamp corresponding to the time when the operation posting this signal was performed. The time stamp of an element in a bucket is the time stamp of the UPDATE signal that led to its insertion.

The three priority queue operations are implemented as follows: A DELETE-MIN operation uses the FILL operation below to make sure that bucket  $\mathcal{B}_1$  is non-empty and, hence, contains the element with lowest priority. This element is removed and returned. An UPDATE $(x, p)$  or DELETE $(x)$  operation inserts the corresponding signal into  $\mathcal{S}_1$  and empties  $\mathcal{S}_1$  using the EMPTY operation below. Essentially, all the work to update the contents of the bucket heap is delegated to two auxiliary procedures: Procedure EMPTY $(\mathcal{S}_i)$  empties the signal buffer  $\mathcal{S}_i$ , applies these signals to bucket  $\mathcal{B}_i$ , and inserts appropriate signals into buffer  $\mathcal{S}_{i+1}$ . If this leads to an overflow of buffer  $\mathcal{S}_{i+1}$ , the procedure is applied recursively

to  $\mathcal{S}_{i+1}$ . Procedure  $\text{FILL}(\mathcal{B}_i)$  fills an underfull bucket  $\mathcal{B}_i$  with the smallest  $2^{2i}$  elements in buckets  $\mathcal{B}_i, \dots, \mathcal{B}_q$ . The details of these procedures are as follows:

**EMPTY( $\mathcal{S}_i$ )**

- 1 If  $i = q + 1$ , then increase  $q$  by one and create two new arrays  $\mathcal{B}_q$  and  $\mathcal{S}_{q+1}$ .
- 2 Scan bucket  $\mathcal{B}_i$  to determine the maximal priority  $p'$  of the elements in  $\mathcal{B}_i$ . (If  $i = q$  and  $\mathcal{S}_{q+1} = \emptyset$ , then  $p' = \infty$ . Otherwise, if  $\mathcal{B}_i = \emptyset$ , then  $p' = -\infty$ .)
- 3 Scan buckets  $\mathcal{S}_i$  and  $\mathcal{B}_i$  simultaneously and perform the following operations for each signal in  $\mathcal{S}_i$ :
  - UPDATE( $x, p$ ): If  $\mathcal{B}_i$  contains an element  $(x, p'')$ , replace this element with  $(x, \min(p, p''))$  and mark the UPDATE( $x, p$ ) signal in  $\mathcal{S}_i$  as handled. If  $x$  is not in  $\mathcal{B}_i$ , but  $p \leq p'$ , insert  $(x, p)$  into  $\mathcal{B}_i$  and replace the UPDATE( $x, p$ ) signal with a DELETE( $x$ ) signal. If  $x$  is not in  $\mathcal{B}_i$  and  $p > p'$ , do nothing.
  - PUSH( $x, p$ ): If there is an element  $(x, p'')$  in  $\mathcal{B}_i$ , replace it with  $(x, p)$ . Otherwise, insert  $(x, p)$  into  $\mathcal{B}_i$ . Mark the PUSH( $x, p$ ) signal as handled.
  - DELETE( $x$ ): If element  $x$  is in  $\mathcal{B}_i$ , delete it.
- 4 If  $i < q$  or  $\mathcal{S}_{i+1}$  is non-empty, then scan buffers  $\mathcal{S}_i$  and  $\mathcal{S}_{i+1}$  and insert all unhandled signals in  $\mathcal{S}_i$  into  $\mathcal{S}_{i+1}$ .  $\mathcal{S}_i \leftarrow \emptyset$
- 5 If  $|\mathcal{B}_i| > 2^{2i}$ , then find the  $2^{2i}$ -th smallest priority  $p$  in  $\mathcal{B}_i$ . Scan bucket  $\mathcal{B}_i$  and buffer  $\mathcal{S}_{i+1}$  twice: The first scan removes all elements with priority greater than  $p$  from  $\mathcal{B}_i$  and inserts corresponding PUSH signals into  $\mathcal{S}_{i+1}$ . The second scan removes  $|\mathcal{B}_i| - 2^{2i}$  elements with priority  $p$  from  $\mathcal{B}_i$  and inserts corresponding PUSH signals into  $\mathcal{S}_{i+1}$ .
- 6 If  $|\mathcal{S}_{i+1}| > 2^{2i+1}$ , then EMPTY( $\mathcal{S}_{i+1}$ )

**FILL( $\mathcal{B}_i$ )**

- 1 EMPTY( $\mathcal{S}_i$ )
- 2 If  $|\mathcal{B}_{i+1}| < 2^{2i}$  and  $i < q$ , then FILL( $\mathcal{B}_{i+1}$ )
- 3 Find the  $(2^{2i} - |\mathcal{B}_i|)$ -th smallest priority  $p$  in  $\mathcal{B}_{i+1}$ . Scan  $\mathcal{B}_i$  and  $\mathcal{B}_{i+1}$  twice. The first scan moves all elements with priority less than  $p$  from  $\mathcal{B}_{i+1}$  to  $\mathcal{B}_i$ . The second scan moves the correct number of elements with priority  $p$  from  $\mathcal{B}_{i+1}$  to  $\mathcal{B}_i$  so that  $\mathcal{B}_i$  contains  $2^{2i}$  elements or  $\mathcal{B}_{i+1}$  is empty at the end.
- 4  $q \leftarrow \max\{j : \mathcal{B}_j \text{ or } \mathcal{S}_{j+1} \text{ is non-empty}\}$

**2.1 Correctness**

A priority queue is *correct* if, given a sequence  $o_1, o_2, \dots, o_t$  of priority queue operations, every DELETEMIN operation  $o_i$  returns the smallest element in the set  $\mathcal{O}_{i-1}$  constructed by operations  $o_1, \dots, o_{i-1}$  according to their definitions at the beginning of this section. In the following we use the term “element at level  $j$ ” to refer to an element in bucket  $\mathcal{B}_j$  or to an UPDATE signal in buffer  $\mathcal{S}_j$ . We say that a DELETE( $x$ ) signal in a buffer  $\mathcal{S}_i$  *hides* an element  $(x, p)$  at level  $j$  if  $i \leq j$  and the time stamp of the DELETE( $x$ ) signal is greater than the time stamp of element  $(x, p)$ . An element  $(x, p')$  *hides* an element  $(x, p)$  if it is not hidden by a DELETE( $x$ ) signal and  $p' < p$ . An element that is not hidden is *visible*.

Observe that a hidden element can never be returned by a DELETEMIN operation. Hence, it suffices to show that the set  $\mathcal{V}_i$  of elements that are visible after applying operations  $o_1, o_2, \dots, o_i$  equals the set  $\mathcal{O}_i$  and that every DELETEMIN operation returns the minimal element in the current set of visible elements.

**Lemma 1.** *A DELETEMIN operation  $o_i$  returns the minimal element in  $\mathcal{V}_{i-1}$ .*

*Proof.* We have already observed that the returned element  $(y, q)$  is in  $\mathcal{V}_{i-1}$ . If  $(x, p)$  is the smallest visible element and  $q > p$ , we distinguish a number of cases: Let  $i$  be the current level of element  $(x, p)$ , and let  $j$  be the current level of element  $(y, q)$ . If  $i \leq j$ , then element  $(x, p)$  will move to lower buckets before or at the same time as  $(y, q)$ . Hence,  $(x, p)$  would have to be returned before  $(y, q)$ , a contradiction. If  $j < i$ , we observe that element  $(y, q)$  can only be represented by an UPDATE( $y, q$ ) signal in  $\mathcal{S}_j$  because neither bucket  $\mathcal{B}_i$  nor buffer  $\mathcal{S}_i$  can contain elements with priorities less than those of the elements in  $\mathcal{B}_j$ . Hence, before  $(y, q)$  can be moved to a bucket and ultimately returned, we must reach the case  $i \leq j$ , in which case we would return  $(x, p)$  first, as argued above.  $\square$

**Lemma 2.** *For any sequence  $o_1, o_2, \dots, o_t$  and any  $1 \leq i \leq t$ ,  $\mathcal{V}_i = \mathcal{O}_i$ .*

*Proof.* The proof is by induction on  $i$ . For  $i = 0$ , the claim holds because  $\mathcal{O}_i$  and  $\mathcal{V}_i$  are empty. So assume that  $i > 0$  and that  $\mathcal{V}_{i-1} = \mathcal{O}_{i-1}$ . If  $o_i$  is a DELETEMIN operation, it removes and returns the minimum element  $(x, p)$  in  $\mathcal{V}_{i-1}$ , so that  $\mathcal{V}_i = \mathcal{V}_{i-1} \setminus \{(x, p)\} = \mathcal{O}_{i-1} \setminus \{(x, p)\} = \mathcal{O}_i$ . If  $o_i$  is a DELETE( $x$ ) operation, its insertion into  $\mathcal{S}_1$  hides all copies of  $x$  in the priority queue. Hence,  $\mathcal{V}_i = \mathcal{V}_{i-1} \setminus \{x\} = \mathcal{O}_{i-1} \setminus \{x\} = \mathcal{O}_i$ . If  $o_i$  is an UPDATE( $x, p$ ) operation, we distinguish three cases: If  $x$  is not in  $\mathcal{O}_{i-1}$ , there is no element  $(x, p')$  that hides the UPDATE( $x, p$ ) signal. Hence,  $\mathcal{V}_i = \mathcal{V}_{i-1} \cup \{(x, p)\} = \mathcal{O}_{i-1} \cup \{(x, p)\} = \mathcal{O}_i$ . If there is an element  $(x, p')$  in  $\mathcal{O}_{i-1}$  and  $p' < p$ , element  $(x, p')$  hides the UPDATE( $x, p$ ) signal, and  $\mathcal{V}_i = \mathcal{V}_{i-1} = \mathcal{O}_{i-1} = \mathcal{O}_i$ . If  $p' > p$ , the UPDATE( $x, p$ ) signal hides element  $(x, p')$ , and  $\mathcal{V}_i = (\mathcal{V}_{i-1} \setminus \{(x, p')\}) \cup \{(x, p)\} = (\mathcal{O}_{i-1} \setminus \{(x, p')\}) \cup \{(x, p)\} = \mathcal{O}_i$ .  $\square$

## 2.2 Analysis

We assume that every element has a unique ID drawn from a total order and keep the elements in each bucket or buffer sorted by their IDs. This invariant allows us to perform updates by scanning buckets and buffers as in the description of procedures EMPTY and FILL. The amortized cost per scanned element is hence  $\mathcal{O}(1/B)$ . In our analysis of the amortized complexity of the priority queue operations, we assume that  $M = \Omega(B)$ , large enough to hold the first  $\log_4 B$  buckets and buffers plus one cache block per stream that we scan. Under this assumption, operations UPDATE, DELETE, and DELETEMIN, excluding the calls to EMPTY and FILL, do not cause any I/Os because bucket  $\mathcal{B}_1$  and buffer  $\mathcal{S}_1$  are always in cache. We have to charge the I/Os incurred by EMPTY and FILL operations to UPDATE and DELETE operations in such a manner that no operation is charged for more than  $\mathcal{O}((1/B) \log_2(N/B))$  I/Os. To achieve this,

we define the following potential function, where  $U$ ,  $D$ , and  $P$  are the numbers of UPDATE, DELETE, and PUSH signals in buffers  $\mathcal{S}_1, \mathcal{S}_2, \dots, \mathcal{S}_q$ :

$$\Phi = (3U + D + 2P)(\log_4(N/B) + 3) + \sum_{i=\log_4 B}^q ((|\mathcal{B}_i| - |\mathcal{S}_i|) \cdot (i - \log_4 B) + 2^{2i})$$

Since the actual cost of an UPDATE or DELETE operation is 0 and each of them increases the potential by  $\mathcal{O}(\log_2(N/B))$ , the amortized cost of these operations is  $\mathcal{O}((1/B) \log_2(N/B))$  if we can show that all I/Os incurred by FILL and EMPTY operations can be paid by a sufficient potential decrease, where a potential decrease of  $\Omega(B)$  is necessary to pay for a single I/O.

We distinguish two types of EMPTY operations: A *regular*  $\text{EMPTY}(\mathcal{S}_i)$  operation is one with  $|\mathcal{S}_i| > 2^{2i-1}$ . If  $|\mathcal{S}_i| \leq 2^{2i-1}$ , the operation is *early*. The latter type of  $\text{EMPTY}(\mathcal{S}_i)$  operation may be triggered by a  $\text{FILL}(\mathcal{B}_i)$  operation.

First consider a regular  $\text{EMPTY}(\mathcal{S}_i)$  operation, where  $i \leq q$ . If  $i < \log_4 B$ , the operation causes no I/Os—because  $\mathcal{S}_i, \mathcal{S}_{i+1}$ , and  $\mathcal{B}_i$  are in cache—and the potential does not increase. If  $i \geq \log_4 B$ , the cost is bounded by  $\mathcal{O}(2^{2i-1}/B)$  because only buffers  $\mathcal{S}_i$  and  $\mathcal{S}_{i+1}$  and bucket  $\mathcal{B}_i$  are scanned. Let  $k$  be the increase of the size of bucket  $\mathcal{B}_i$ , let  $u, p$ , and  $d$  be the number of UPDATE, PUSH, and DELETE operations in  $\mathcal{S}_i$ , and let  $u', p'$ , and  $d'$  be the number of such operations inserted into  $\mathcal{S}_{i+1}$ . Then we have  $u + d + p = |\mathcal{S}_i| > 2^{2i-1}$ . From the description of the  $\text{EMPTY}$  operation, we obtain that  $u + d = u' + d'$  and  $k + u' + p' \leq u + p$ . The change of potential is  $\Delta\Phi \leq (3u' + d' + 2p' - 3u - d - 2p)(\log_4(N/B) + 3) + (u + d + p + k)(i - \log_4 B) - (u' + d' + p')(i + 1 - \log_4 B)$ . Using elementary transformations, this gives  $\Delta\Phi \leq -2^{2i-1}$ .

If  $i = q + 1$ , the actual cost of a regular  $\text{EMPTY}(\mathcal{S}_i)$  operation remains the same, but the change of potential is  $\Delta\Phi \leq -(3u + d + 2p)(\log_4(N/B) + 3) + (u + d + p + k)(i - \log_4 B) + 2^{2i}$ . Again, this can be bounded by  $\Delta\Phi \leq -2^{2i-1}$ .

Next we show that the cost of FILL and early  $\text{EMPTY}$  operations can be paid by a sufficient decrease of the potential  $\Phi$ . Consider a  $\text{FILL}(\mathcal{B}_1)$  operation, and let  $j$  be the highest index such that a  $\text{FILL}(\mathcal{B}_j)$  operation is triggered by this  $\text{FILL}(\mathcal{B}_1)$  operation. Then the cost of all FILL and early  $\text{EMPTY}$  operations triggered by this  $\text{FILL}(\mathcal{B}_1)$  operation is  $\mathcal{O}(2^{2j}/B)$ . If there are new elements inserted into the buckets during the  $\text{EMPTY}$  operations, a similar analysis as for regular  $\text{EMPTY}$  operations shows that the resulting potential change is zero or negative. Hence, it suffices to show that, excluding these insertions, the potential decreases by  $\Omega(2^{2j})$ . We distinguish two cases. If  $q$  does not change, then the  $\text{FILL}(\mathcal{B}_j)$  operation moves at least  $3 \cdot 2^{2j-2}$  elements from  $\mathcal{B}_{j+1}$  to  $\mathcal{B}_j$ , which results in the desired potential decrease. If  $q$  decreases, then  $q > j$  before the  $\text{FILL}(\mathcal{B}_1)$  operation and  $q$  decreases by at least one. This results in a potential decrease of at least  $2^{2q} \geq 2^{2j}$ . Hence, we obtain the following result.

**Theorem 1.** *The bucket heap supports the operations UPDATE, DELETE, and DELETEMIN at an amortized cost of  $\mathcal{O}((1/B) \log_2(N/B))$  I/Os.*

The shortest path algorithm of [17] is cache-oblivious, except for its use of a cache-aware priority queue: the tournament tree. Since the bucket heap is cache-

oblivious and achieves the same I/O-bound as the tournament tree, we obtain the following result by replacing the tournament tree with the bucket heap.

**Corollary 1.** *There exists a cache-oblivious algorithm that solves the single-source shortest path problem on an undirected graph  $G = (V, E)$  with non-negative edge weights and incurs at most  $\mathcal{O}(V + (E/B) \log_2(E/B))$  I/Os.*

### 3 Cache-Oblivious Breadth-First Search

In this section, we develop a cache-oblivious version of the undirected BFS-algorithm from [18]. As in [18], the actual BFS-algorithm is the one from [21], which generates the BFS levels one by one, using that, in an undirected graph,  $L_{i+1} = \mathcal{N}(L_i) \setminus (L_i \cup L_{i-1})$ , where  $\mathcal{N}(S)$  is the set of nodes<sup>2</sup> that are neighbours of nodes in  $S$ , and  $L_i$  is the set of nodes of the  $i$ 'th level of the BFS tree with root  $s$ . The algorithm from [21] relies only on sorting and scanning and, hence, can be implemented cache-obliviously; this gives the cache-oblivious  $\mathcal{O}(V + \text{Sort}(E))$  result from Table 1. The speed-up in [18] over [21] is due to a data structure which, for a query set  $S$ , returns  $\mathcal{N}(S)$ . The data structure does this in an I/O-efficient manner by exploiting that the query sets are the levels  $L_0, L_1, L_2, \dots$  of a BFS traversal. We provide a cache-obliviously version of this data structure.

#### 3.1 The Data Structure

To construct the data structure, we first build a spanning tree for  $G$  and then construct an Euler tour  $\mathcal{T}$  for the tree (using [4]). Next, we assign (by scanning and sorting) to each node  $v$  the rank in  $\mathcal{T}$  of the first occurrence of  $v$ , and denote this value  $r(v)$ . As  $\mathcal{T}$  has length  $2V - 1$ , we have  $r(v) \in [0; 2V - 2]$ .

**Observation 1 ([18]).** *If for two nodes  $u$  and  $v$  the values  $r(v)$  and  $r(u)$  differ by  $d$ , then a section of the Euler tour constitute a path in  $G$  of length  $d$  connecting  $u$  and  $v$ ; hence,  $d$  is an upper bound on the distance between their BFS levels.*

Let  $g_0 < g_1 < g_2 < \dots < g_h$  be an increasing sequence of  $h + 1$  integers where  $g_0 = 1$ ,  $g_{h-1} < 2V - 2 \leq g_h$ , and  $g_i$  divides  $g_{i+1}$ . We will later consider two specific sequences, namely  $g_i = 2^i$  and one for which  $g_i = \Theta(2^{(1+\varepsilon)^i})$ . For each integer  $g_i$ , we can partition the nodes into groups of at most  $g_i$  nodes each by letting the  $k$ 'th group  $V_{ki}$  be all nodes  $v$  for which  $kg_i \leq r(v) < (k+1)g_i$ . We call a group  $V_{ki}$  of nodes a  $g_i$ -node-group and call its set of adjacency lists  $\mathcal{N}(V_{ki})$  a  $g_i$ -edge-group. Since  $g_i$  divides  $g_{i+1}$ , the groups form a hierarchy of  $h + 1$  levels, with level  $h$  containing one group with all nodes and level 0 containing  $2V - 1$  groups of at most one node.

The data structure consists of  $h$  levels  $G_1, \dots, G_h$ , where each level stores a subset of the adjacency lists of the graph  $G$ . Each adjacency list  $\mathcal{N}(v)$  will appear in exactly one of the levels, unless it has been removed from the structure.

<sup>2</sup> As shorthand for  $\mathcal{N}(\{v\})$  we will use  $\mathcal{N}(v)$ .



Since the query sets of the BFS-algorithm are the BFS-levels  $L_0, L_1, L_2, \dots$ , each node  $v$  is part of a query set  $S$  exactly once. Its adjacency list  $\mathcal{N}(v)$  will leave the data structure when this happens.

Initially, all adjacency lists are in level  $h$ . Over time, the query procedure GETEDGELISTS moves the adjacency list of each node from higher numbered to lower numbered levels, until the adjacency list eventually reaches level  $G_1$  and is removed. GETEDGELISTS is a recursive procedure that takes as input a query set  $S$  of nodes and a level number  $i$  to query. The output consists of the  $g_{i-1}$ -edge-groups stored at level  $G_i$  for which the corresponding  $g_{i-1}$ -node-group contains one or more nodes in  $S$ . The BFS-algorithm will query the data structure by calling GETEDGELISTS( $S, 1$ ), which will return  $\mathcal{N}(v)$ , for all  $v$  in  $S$ .

```

GETEDGELISTS( $S, i$ )
1   $S' \leftarrow \{v \in S \mid \mathcal{N}(v) \text{ is not stored in level } G_i\}$ 
2  if  $S' \neq \emptyset$ :
3       $X \leftarrow \text{GETEDGELISTS}(S', i + 1)$ 
4      for each  $g_i$ -edge-group  $g$  in  $X$ 
5          insert  $g$  in  $G_i$ 
6  for each  $g_{i-1}$ -edge-group  $\gamma$  in  $G_i$  containing  $\mathcal{N}(v)$  for some  $v \in S$ 
7      remove  $\gamma$  from  $G_i$ 
8      include  $\gamma$  in the output set
    
```

Next we describe how we represent a level  $G_i$  so that GETEDGELISTS can be performed efficiently. By induction on time, it is clear that the edges stored in level  $G_i$  always constitute a set of  $g_i$ -edge-groups from each of which zero or more  $g_{i-1}$ -edge-groups have been removed. Since  $g_{i-1}$  divides  $g_i$ , the part of a  $g_i$ -edge-group residing at level  $G_i$  is a collection of  $g_{i-1}$ -edge-groups. We store the adjacency lists of level  $G_i$  in an array  $B_i$ . Each  $g_{i-1}$ -edge-group is stored in consecutive locations of  $B_i$ , and the adjacency lists  $\mathcal{N}(v)$  of a  $g_{i-1}$ -edge-group occupy these locations in order of increasing ranks  $r(v)$ . The  $g_{i-1}$ -edge-groups of each  $g_i$ -edge-group are also stored in order of increasing ranks of the nodes involved, but empty locations may exist between the  $g_{i-1}$ -edge-groups. However, the entire array  $B_i$  will have a number of locations which is at most a constant times the number of edges it contains. This will require  $B_i$  to shrink and grow appropriately. The arrays  $B_1, B_2, \dots, B_h$  will be laid out in  $\mathcal{O}(E)$  consecutive memory locations. Due to space restrictions, we refer to the full version [9] of the paper for a description of how to maintain this layout at sufficiently low cost.

In order to keep track of the  $g_i$ -edge-groups within  $B_i$  we maintain an index  $A_i$ , which is an array of entries  $(k, p)$ , one for every  $g_i$ -edge-group present in  $G_i$ . Here  $k$  is the number of the corresponding  $g_i$ -node-group  $V_{ki}$ , and  $p$  is a pointer to the start of the  $g_i$ -edge-group in  $B_i$ . The entries of  $A_i$  are sorted by their first components. The indexes  $A_1, A_2, \dots, A_h$  occupy consecutive locations of one of two arrays  $A'$  and  $A''$  of size  $\mathcal{O}(V)$ . Finally, every  $g_i$ -edge-group  $g$  of a level  $G_i$  will contain an index of the  $g_{i-1}$ -edge-groups it presently contains. This index consists of the first and last edge of each  $g_{i-1}$ -edge-group  $\gamma$  together with

pointers to the first and last locations of the rest of  $\gamma$ . These edges are kept at the front of  $g$ , in the same order as the  $g_{i-1}$ -edge-groups to which they belong.

We now describe how each step of GETEDGELISTS is performed. We assume that every query set  $S$  of nodes is sorted by assigned rank  $r(v)$ , which can be ensured by sorting the initial query set before the first call. In line 1 of the algorithm, we find  $S'$  by simultaneously scanning  $S$  and  $A_i$ , using that, if  $(k, p)$  is an entry of  $A_i$ , all nodes  $v \in S$  for which  $kg_i \leq r(v) < (k+1)g_i$  will have  $\mathcal{N}(v)$  residing in the  $g_i$ -edge-group pointed to by  $p$  (otherwise,  $\mathcal{N}(v)$  would have been found earlier in the recursion, i.e. for a smaller  $i$ , and  $v$  would have been removed from  $S$ ). In short,  $S'$  is the subset of  $S$  not covered by the entries in  $A_i$ .

In line 5, when a  $g_i$ -edge-group  $g$  is to be inserted into level  $G_i$ , the index of the  $g_{i-1}$ -edge-groups of  $g$  is generated by scanning  $g$ , and  $g$  (now with the index) is appended to  $B_i$ . An entry for  $A_i$  is generated. When the for-loop in line 4 is finished, the set of new  $A_i$  entries are sorted by their first components and merged with the current  $A_i$ . Specifically, the merging writes  $A_i$  to  $A''$  if  $A_i$  currently occupies  $A'$ , and vice versa, implying that the location of the entire set of  $A_i$ 's alternates between  $A'$  and  $A''$  for each call GETEDGELISTS( $S$ , 1).

In line 6, we scan  $S$  and the updated  $A_i$  to find the entries  $(k, p)$  pointing to the relevant  $g_i$ -edge-groups of the updated  $B_i$ . During the scan of a group  $g$ , we generate a pair  $(v, p)$  for each of the  $g_{i-1}$ -edge-groups  $\gamma$  inside  $g$  that contains one or more nodes from  $S$ , where  $v$  is the first node in  $\gamma$  and  $p$  is the pointer to  $g$ . These pairs are now sorted in reverse lexicographic order (the second component is most significant), so that the  $g_i$ -edge-groups can be accessed in the same order as they are located in  $B_i$ . For each such group  $g$ , we scan its index to find the relevant  $g_{i-1}$ -edge-groups and access these in the order of the index. Each  $g_{i-1}$ -edge-group is removed from its location in  $B_i$  (leaving empty positions) and placed in the output set. We also remove its entry in the index of  $g$ . The I/O-bound of this process is the minimum I/O-bound of a scan of  $B_i$  and a scan of each of the moved  $g_{i-1}$ -edge-groups.

### 3.2 Analysis

In the following we analyze the number of I/Os performed by our cache-oblivious BFS-algorithm, assuming that the management of the layout of the  $B_i$ 's can be done efficiently (for this, see [9]). The underlying BFS-algorithm from [21] scans each BFS-level  $L_i$  twice: once while constructing  $L_{i+1}$  and once while constructing  $L_{i+2}$ , causing a total of  $\mathcal{O}(V/B)$  I/Os for all lists  $L_i$ . Edges extracted from the data structure storing the adjacency lists are sorted and scanned for filtering out duplicates and already discovered nodes, causing a total of  $\mathcal{O}(\text{Sort}(E))$  I/Os.

We now turn to the I/Os performed during queries of the data structure storing the adjacency lists. The cost for constructing the initial spanning tree is  $\mathcal{O}(\text{ST}(E))$ ; the Euler tour can be constructed in  $\mathcal{O}(\text{Sort}(V))$  I/Os [4]. Assigning ranks to nodes and labeling the edges with the assigned ranks requires further  $\mathcal{O}(\text{Sort}(E))$  I/Os. The total preprocessing of the data structure hence costs  $\mathcal{O}(\text{ST}(E) + \text{Sort}(E))$  I/Os.

For each query from the basic BFS-algorithm, the query algorithm for the data structure accesses the  $A_i$  and  $B_i$  lists. We first consider the number of I/Os for handling the  $A_i$  lists. During a query, the algorithm scans each  $A_i$  list at most a constant number of times: to identify which  $g_i$ -edge-groups to extract recursively from  $B_{i+1}$ ; to merge  $A_i$  with new entries extracted recursively; and to identify the  $g_{i-1}$ -edge-groups to extract from  $B_i$ . The number of distinct  $g_i$ -edge-groups is  $2V/g_i$ . Each group is inserted into level  $G_i$  at most once. By Observation 1, when a  $g_i$ -edge-group is inserted into level  $G_i$ , it will become part of an initial query set  $S$  within  $g_i$  queries from the basic BFS-algorithm, that is, within the next  $g_i$  BFS-levels; at this time, it will be removed from the structure. In particular, it will reside in level  $G_i$  for at most  $g_i$  queries. We conclude that the total cost of scanning  $A_i$  during the complete run of the algorithm is  $\mathcal{O}((2V/g_i) \cdot g_i/B)$ , implying a total number of  $\mathcal{O}(h \cdot V/B)$  I/Os for scanning all  $A_i$  lists. This bound holds because the  $A_i$ 's are stored in consecutive memory locations, which can be considered to be scanned in a single scan during a query from the basic BFS-algorithm. Since each node is part of exactly one query set of the basic BFS-algorithm, the total I/O cost for scanning the  $S$  sets during all recursive calls is also  $\mathcal{O}(h \cdot V/B)$ .

We now bound the sorting cost caused during the recursive extraction of groups. The pointer to each  $g_i$ -edge-group participates in two sorting steps: When the group is moved from level  $i + 1$  to level  $i$ , the pairs generated when scanning  $A_{i+1}$  are sorted before accessing  $B_{i+1}$ ; when the  $g_i$ -edge-group has been extracted from  $B_{i+1}$ , the pointers to extracted groups are sorted before they are merged into  $A_i$ . We conclude that the total sorting cost is bounded by  $\mathcal{O}(\sum_{i=0}^h \text{Sort}(2V/g_i))$  which is  $\mathcal{O}(\text{Sort}(V))$ , since  $g_i$  is at least exponentially increasing for both of the two sequences considered.

Finally, we need to bound the I/O cost of accessing the  $B_i$  lists. For each query of the basic BFS-algorithm, these will be accessed in the order  $B_h, B_{h-1}, \dots, B_1$ . Let  $t$  be any integer for which  $1 \leq t \leq h$ . The cost of accessing  $B_t, \dots, B_1$  during a query is bounded by the cost of scanning  $B_t, \dots, B_1$ . Since an edge in  $B_i$  can only remain in  $B_i$  for  $g_i$  queries from the basic BFS-algorithm, we get a bound on the total I/O cost for  $B_1, \dots, B_t$  of  $\mathcal{O}(\sum_{i=1}^t g_i \cdot E/B)$ , which is  $\mathcal{O}(g_t \cdot E/B)$  since  $g_i$  is at least exponentially increasing. To bound the cost of accessing  $B_h, \dots, B_{t+1}$ , we note that the number of I/Os for moving a  $g_i$ -edge-group list containing  $k$  edges from  $B_{i+1}$  to  $B_i$  is bounded by  $\mathcal{O}(1 + k/B + g_{i+1}/(g_i B))$ , where  $g_{i+1}/g_i$  is the bound of the size of the index of a  $g_{i+1}$ -edge-group. Since the number of  $g_i$ -edge-groups is bounded by  $2V/g_i$ , the I/O cost for accessing  $B_h, \dots, B_{t+1}$  is bounded by  $\mathcal{O}(\sum_{i=t}^{h-1} (2V/g_i + E/B + (2V/g_i) \cdot g_{i+1}/(g_i B))) = \mathcal{O}(V/g_t + h \cdot E/B)$ , since  $g_{i+1} \leq g_i^2$  holds for both of the two sequences considered (when  $0 < \varepsilon \leq 1$ ). The total cost of accessing all  $B_i$  is, hence,  $\mathcal{O}(g_t \cdot E/B + V/g_t + h \cdot E/B)$ , for all  $1 \leq t \leq h$ . Adding all the bounds above gives a bound of  $\mathcal{O}(\text{ST}(E) + \text{Sort}(E) + g_t \cdot E/B + V/g_t + h \cdot E/B)$  on the total number of I/Os incurred by the query algorithm, for all  $1 \leq t \leq h$ .

For  $g_i = 2^i$ , we select  $g_t = \Theta(\sqrt{VB/E})$  and have  $h = \Theta(\log V)$ , so the I/O-bound becomes  $\mathcal{O}(\text{ST}(E) + \text{Sort}(E) + \frac{E}{B} \log V + \sqrt{VE/B})$ . For  $g_i = \Theta(2^{(1+\varepsilon)^i})$ ,

we select the smallest  $g_t \geq \sqrt{VB/E}$ , i.e.  $g_t \leq \sqrt{VB/E}^{1+\varepsilon}$ , and have  $h = \Theta(\frac{1}{\varepsilon} \log \log V)$ , so the I/O-bound becomes  $\mathcal{O}(\text{ST}(E) + \text{Sort}(E) + \frac{E}{B} \cdot \frac{1}{\varepsilon} \cdot \log \log V + \sqrt{VE/B} \cdot \sqrt{VB/E}^\varepsilon)$ .

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