Improved external memory BFS implementations

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Abstract
Breadth first search (BFS) traversal on massive graphs in external memory was considered non-viable until recently, because of the large number of I/Os it incurs. Ajwani et al. [3] showed that the randomized variant of the $o(n)$ I/O algorithm of Mehlhorn and Meyer [24] (MM$_{BFS}$) can compute the BFS level decomposition for large graphs (around a billion edges) in a few hours for small diameter graphs and a few days for large diameter graphs. We improve upon their implementation of this algorithm by reducing the overhead associated with each BFS level, thereby improving the results for large diameter graphs which are more difficult for BFS traversal in external memory. Also, we present the implementation of the deterministic variant of MM$_{BFS}$ and show that in most cases, it outperforms the randomized variant. The running time for BFS traversal is further improved with a heuristic that preserves the worst case guarantees of MM$_{BFS}$. Together, they reduce the time for BFS on large diameter graphs from days shown in [3] to hours. In particular, on line graphs with random layout on disks, our implementation of the deterministic variant of MM$_{BFS}$ with the proposed heuristic is more than 75 times faster than the previous best result for the randomized variant of MM$_{BFS}$ in [3].

1 Introduction
Large graphs arise naturally in many applications and very often we need to traverse these graphs for solving optimization problems. Breadth first search (BFS) is a fundamental graph traversal strategy. It decomposes the input graph $G = (V, E)$ of $n$ nodes and $m$ edges into at most $n$ levels where level $i$ comprises all nodes that can be reached from a designated source $s$ via a path of $i$ edges, but cannot be reached using less than $i$ edges. Typical real-world applications of BFS on large graphs (and some of its generalizations like shortest paths or A*) include crawling and analyzing the WWW [26, 27], route planning using small navigation devices with flash memory cards [19], state space exploration [17], etc.

While modern processor speeds are measured in GHz, average hard disk latencies are in the range of a few milliseconds [28]. Hence, the cost of accessing a data element from the hard-disk (an I/O) is around a million times more than the cost of an instruction. Therefore, it comes as no surprise that the I/Os dominate the runtimes of even basic graph traversal strategies like BFS on large graphs, making their standard implementations non-viable. One way to ease this problem can be to represent the graph [7, 8] in a more compact way that minimizes the I/Os required by the standard algorithms. However, such approaches work only for graphs with good separators. The other approach that we consider in this paper relies on new algorithmic ideas capturing the I/Os into the performance metric of the computation model. In order to do so, we need to look beyond the traditional RAM model which assumes an unbounded amount of memory with unit cost access to any location.

1.1 Computation models. We consider the commonly accepted external memory model of Aggarwal and Vitter [2] and the cache oblivious model [18]. They both assume a two level memory hierarchy with faster internal memory having a capacity to store $M$ vertices/edges. In an I/O operation, one block of data, which can have $B$ vertices/edges is transferred between disk and internal memory. The measure of performance of an algorithm is the number of I/Os it performs. The number of I/Os needed to read $N$ contiguous items from disk is $\text{scan}(N) = \Theta(N/B)$. The number of I/Os required to sort $N$ items is $\text{sort}(N) = \Theta((N/B) \log_{M/B}(N/B))$. Here $A$ is the block length, $M$ is the memory size, and $B$ is the disk block size. For all realistic values of $N$, $M/R$, and $M$, $\text{scan}(N) < \text{sort}(N) \ll N$. The difference between the two models is that the values of $B$ and $M$ are not known to the algorithm in the cache oblivious model, allowing the algorithms designed under this model to be simultaneously efficient on all levels of the memory hierarchy.

1.2 Algorithms. BFS is well-understood in the RAM model. There exists a simple linear time algorithm [15] (hereafter referred as IM$_{BFS}$) for the BFS traversal in a graph. IM$_{BFS}$ keeps a set of appropriate candidate nodes for the next vertex to be visited in a
FIFO queue $Q$. Furthermore, in order to find out the unvisited neighbours of a node from its adjacency list, it marks the nodes as either visited or unvisited. Unfortunately as reported in [3], even when half of the graph fits in the main memory, the running time of this algorithm deviates significantly from the predicted RAM performance (hours as compared to minutes) and for massive graphs, such approaches are simply non-viable. As discussed before, the main cause for such a poor performance of this algorithm on massive graphs is the number of I/Os it incurs. Remembering visited nodes needs $\Theta(m)$ I/Os in the worst case and the unstructured indexed access to adjacency lists may result in $\Theta(n)$ I/Os.

The algorithm by Munagala and Ranade [25] (referred as MR_BFS) ignores the second problem but addresses the first by exploiting the fact that the neighbours of a node in BFS level $i$ are all in BFS levels $i+1$, $i$ or $i-1$. Thus, the set of nodes in level $i+1$ can be computed by removing all nodes in level $i$ and $i-1$ from the neighbours of nodes in level $i$. The resulting worst-case I/O-bound is $O(n + sort(n+m))$.

Mehlhorn and Meyer suggested another approach [24] (MM_BFS) which involves a preprocessing phase to restructure the adjacency lists of the graph representation. It groups the vertices of the input graph into disjoint clusters of small diameter and stores the adjacency lists of the nodes in a cluster contiguously on the disk. Thereafter, an appropriately modified version of MR_BFS is run. MM_BFS exploits the fact that whenever the first node of a cluster is visited then the remaining nodes of this cluster will be reached soon after. By spending only one random access (and possibly, some sequential accesses depending on cluster size) in order to load the whole cluster and then keeping the cluster data in some efficiently accessible data structure (pool) until it is all used up, on sparse graphs the total amount of I/O can be reduced by a factor of up to $\sqrt{B}$. The neighbouring nodes of a BFS level can be computed simply by scanning the pool and not the whole graph. Though some edges may be scanned more often in the pool, unstructured I/O in order to fetch adjacency lists is considerably reduced, thereby saving the total number of I/Os. The preprocessing of MM_BFS comes in two variants: randomized and deterministic (referred as MM_BFS_R and MM_BFS_D, respectively). In the randomized variant, the input graph is partitioned by choosing master nodes independently and uniformly at random with a probability $\mu$ and running a BFS like routine with joint adjacency list queries from these master nodes “in parallel”.

The deterministic variant first builds a spanning tree for $G$ and then constructs an Euler tour $T$ for the tree. Next, each node $v$ is assigned the rank in $T$ of the first occurrence of the node (by scanning $T$ and a sorting step). We denote this value as $r(v)$. $T$ has length $2V - 1$; so $r(v) \in [0; 2V - 2]$. Note that if for two nodes $u$ and $v$, the values $r(u)$ and $r(v)$ differ by $d$, then $d$ is an upper bound on the distance between their BFS level. Therefore, we chop the Euler tour into chunks of $\sqrt{B}$ nodes and store the adjacency lists of the nodes in the chunk consecutively as a cluster.

The randomized variant incurs an expected number of $O(\sqrt{n \cdot (n + m)} \cdot \log(n \cdot \sqrt{B} + sort(n+m))$ I/Os, while the deterministic variant incurs $O(\sqrt{n \cdot (n + m)} \cdot B + sort(n + m) + ST(n,m))$ I/Os, where $ST(n,m)$ is the number of I/Os required for computing a spanning tree of a graph with $n$ nodes and $m$ edges. Arge et al. [4] show an upper bound of $O((1 + \log \log (D \cdot B \cdot n/m)) \cdot sort(n+m))$ I/Os for computing such a spanning tree.

Brodal et al. [9] gave a cache oblivious algorithm for BFS achieving the same worst case I/O bounds as MM_BFS_D. Their preprocessing is similar to that in MM_BFS_D, except that it produces a hierarchical clustering using the cache oblivious algorithms for sorting, spanning tree, Euler tour and list ranking. The BFS phase uses a data-structure that maintains a hierarchy of pools and provides the set of neighbours of the nodes in a BFS level efficiently.

The other external memory algorithms for BFS are restricted to special graphs classes like trees [12], grid graphs [5], planar graphs [23], outer-planar graphs [21], and graphs of bounded tree width [22].

1.3 Related Work. Ajwani et al. [3] showed that the usage of the two external memory algorithms MR_BFS and MM_BFS_R along with disk parallelism and pipelining can alleviate the I/O bottleneck of BFS on many large sparse graph classes, thereby making the BFS viable for these graphs. Even with just a single disk, they computed a BFS level decomposition of small diameter large graphs (around 256 million nodes and a billion edges) in a few hours and moderate and large diameter graphs in a few days, which otherwise would have taken a few months with IM_BFS. As for their relative comparison, MR_BFS performs better than MM_BFS_R on small-diameter random graphs saving a few hours. However, the better asymptotic worst-case I/O complexity of MM_BFS helps it to outperform MR_BFS for large diameter sparse graphs (computing in a few days versus a few months), where MR_BFS incurs close to its worst case of $\Omega(n)$ I/Os.

Independently, Christiani [14] gave a prototypical implementation of MR_BFS, MM_BFS_R as well as MM_BFS_D and reached similar conclusions regarding the comparative performance between MR_BFS and
MM_BFS_R. Though their implementation of MR_BFS and MM_BFS_R is competitive and on some graph classes even better than [3], their experiments were mainly carried out on smaller graphs (up to 50 million nodes). Since their main goal was to design cache oblivious BFS, they used cache oblivious algorithms for sorting, minimum spanning tree and list ranking even for MM_BFS_D. As we discuss later, these algorithms slow down the deterministic preprocessing in practice, even though they have the same asymptotic I/O complexity as their external memory counterparts.

1.4 Our Contribution. Our contributions in this paper are the following:

- We improve upon the MR_BFS and MM_BFS_R implementation described in [3] by reducing the computational overhead associated with each BFS level, thereby improving the results for large diameter graphs.

- We discuss the various choices made for a fast MM_BFS_D implementation. This involved experimenting with various available external memory connected component and minimum spanning tree algorithms. Our partial re-implementation of the list ranking algorithm of [28] adapting it to the STXXL framework outperforms the other list ranking algorithms for the sizes of our interest. As for the Euler tour in the deterministic preprocessing, we compute the cyclic order of edges around the nodes using the STXXL sorting.

- We conduct a comparative study of MM_BFS_D with other external memory BFS algorithms and show that for most graph classes, MM_BFS_D outperforms MM_BFS_R. Also, we compared our BFS implementations with Christiani’s implementations [14], which have some cache-oblivious subroutines. This gives us some idea of the loss factor that we will have to face for the performance of cache-oblivious BFS.

- We propose a heuristic for maintaining the pool in the BFS phase of MM_BFS. This heuristic improves the runtime of MM_BFS in practice, while preserving the worst case I/O bounds of MM_BFS.

- Putting everything together, we show that the BFS traversal can also be done on moderate and large diameter graphs in a few hours, which would have taken the implementations of [3] and [14] several days and IM_BFS several months. Also, on low diameter graphs, the time taken by our improved MR_BFS is around one-third of that in [3]. Towards the end, we summarize our results (Table 13) by giving the state of the art implementations of external memory BFS on different graph classes.

2 Improvements in the previous implementations of MR_BFS and MM_BFS_R

The computation of each level of MR_BFS involves sorting and scanning of neighbours of the nodes in the previous level. Even if there are very few elements to be sorted, there is a certain overhead associated with initializing the external sorters. In particular, while the STXXL stream sorter (with the flag DSTXXL_SMALL_INPUT_PSORT_OPT) does not incur an I/O for sorting less than $B$ elements, it still requires to allocate some memory and does some computation for initialization. This overhead accumulates over all levels and for large diameter graphs, it dominates the running time. This problem is also inherited by the BFS phase of MM_BFS. Since in the pipelined implementation of [3], we do not know in advance the exact number of elements to be sorted, we can’t switch between the external and the internal sorter so easily. In order to get around this problem, we first buffer the first $B$ elements and initialize the external sorter only when the buffer is full. Otherwise, we sort it internally.

In addition to this, we make the graph representation for MR_BFS more compact. Except the source and the destination node pair, no other information is stored with the edges.

3 Designing MM_BFS_D

There are three main components for the deterministic variant of MM_BFS - Sorting, Connected Component/ Minimum Spanning Tree, and List Ranking. The MM_BFS_D implementation of Christiani [14] uses the cache-oblivious lazy funnel-sort algorithm [11] (CO_sort). As Table 1 shows, the STXXL stream sort (STXXL_sort) proved to be much faster on external data. This is in line with the observations of Brodal et al. [10], where it is shown that an external memory sorting algorithm in the library TPIE [6] is better than their carefully implemented cache-oblivious sorting algorithm, when run on disk.

Regarding connected components and minimum spanning forest, Christiani’s implementations [14] use the cache oblivious algorithm given in [1] (CO_MST). Empirically, we found that the external memory implementation of [16] (EM_MST) performs better than the one in [1]. Table 2 shows the total time required for their deterministic preprocessing using CO_MST and EM_MST on low diameter random graphs and on high diameter line graphs.

As for list ranking, we found Sibeyn’s algorithm
<table>
<thead>
<tr>
<th>$n$</th>
<th>CO_sort</th>
<th>STXXL_sort</th>
</tr>
</thead>
<tbody>
<tr>
<td>$256 \times 10^6$</td>
<td>21</td>
<td>8</td>
</tr>
<tr>
<td>$512 \times 10^6$</td>
<td>46</td>
<td>13</td>
</tr>
<tr>
<td>$1024 \times 10^6$</td>
<td>96</td>
<td>25</td>
</tr>
</tbody>
</table>

Table 1: Timing in minutes for sorting $n$ elements using CO_sort and with using STXXL_sort

<table>
<thead>
<tr>
<th>Graph class</th>
<th>CO_MST</th>
<th>EM_MST</th>
</tr>
</thead>
<tbody>
<tr>
<td>Random graph; $n = 2^{28}, m = 2^{30}$</td>
<td>107</td>
<td>35</td>
</tr>
<tr>
<td>Line graph with contiguous disk layout; (Simple Line) $n = 2^{28}$</td>
<td>38</td>
<td>16</td>
</tr>
<tr>
<td>Line graph with random disk layout (Random Line); $n = 2^{28}$</td>
<td>47</td>
<td>22</td>
</tr>
</tbody>
</table>

Table 2: Timing in hours required by deterministic preprocessing by Christiani’s implementation using CO_MST and EM_MST.

<table>
<thead>
<tr>
<th>Graph class</th>
<th>$n$</th>
<th>$m$</th>
<th>Long clusters</th>
<th>Random clusters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grid($2^{14} \times 2^{14}$)</td>
<td>$2^{28}$</td>
<td>$2^{28}$</td>
<td>51</td>
<td>28</td>
</tr>
</tbody>
</table>

Table 3: Time taken (in hours) by the BFS phase of MM_BFS_D with long and random clustering.

in [28] promising as it has low constant factors in its I/O complexity. Sibeyn’s implementation relies on the operating system for I/Os and does not guarantee that the top blocks of all the stacks remain in the internal memory, which is a necessary assumption for the asymptotic analysis of the algorithm. Besides, its reliance on internal arrays and swap space puts a restriction on the size of the lists it can rank. The deeper integration of the algorithm in the STXXL framework, using the STXXL stacks and vectors in particular, made it possible to obtain a scalable solution, which could handle graph instances of the size we require while keeping the theoretical worst case bounds.

Christiani uses the algorithm in [13] for list ranking the Euler tour. While Christiani’s cache oblivious list ranking implementation takes around 14.3 hours for ranking $2^{29}$ element random list using 3 GB RAM, our adaptation of Sibeyn’s algorithm takes less than 40 minutes in the same setting.

To summarize, our STXXL based implementation of MM_BFS_D uses our adaptation of [28] for list ranking the Euler tour around the minimum spanning tree computed by EM_MST. The Euler tour is then chopped into sets of $\sqrt{B}$ consecutive nodes which after duplicate removal gives the requisite graph partitioning. The BFS phase remains similar to MM_BFS_R.

Quality of the spanning tree The quality of the spanning tree computed can have a significant impact on the clustering and the disk layout of the adjacency list after the deterministic preprocessing, and consequently on the BFS phase. For instance, in the case of grid graph, a spanning tree containing a list with elements in a snake-like row major order produces long and narrow clusters, while a “random” spanning tree is likely to result in clusters with low diameters. Such a “random” spanning tree can be attained by assigning random weights to the edges of the graph and then computing a minimum spanning tree or by randomly permuting the indices of the nodes. The nodes in the long and narrow clusters tend to stay longer in the pool and therefore, their adjacency lists are scanned more often. This causes the pool to grow external and results in larger I/O volume. On the other hand, low diameter clusters are evicted from the pool sooner and are scanned less often reducing the I/O volume of the BFS phase. Consequently as Table 3 shows, the BFS phase of MM_BFS_D takes only 28 hours with clusters produced by “random” spanning tree, while it takes 51 hours with long and narrow clusters.

4 A Heuristic for maintaining the pool

As noted in Section 1.2, the asymptotic improvement and the performance gain in MM_BFS over MR_BFS is obtained by decomposing the graph into low diameter
clusters and maintaining an efficiently accessible pool of adjacency lists which will be required in the next few levels. Whenever the first node of a cluster is visited during the BFS, the remaining nodes of this cluster will be reached soon after and hence, this cluster is loaded into the pool. For computing the neighbours of the nodes in the current level, we just need to scan the pool and not the entire graph. Efficient management of this pool is thus, crucial for the performance of MM BFS. In this section, we propose a heuristic for efficient management of the pool, while keeping the worst case I/O bounds of MM BFS.

For many large diameter graphs, the pool fits into the internal memory most of the time. However, even if the number of edges in the pool is not so large, scanning all the edges in the pool for each level can be computationally quite expensive. Hence, we keep a portion of the pool that fits in the internal memory as a multi-map hash table. Given a node as a key, it returns all the nodes adjacent to the current node. Thus, to get the neighbours of a set of nodes we just query the hash function for those nodes and delete them from the hash table. For loading the cluster, we just insert all the adjacency lists of the cluster in the hash table, unless the hash table has already $O(M)$ elements.

Recall that after the deterministic preprocessing, the elements are stored on the disk in the order in which they appear on the Euler tour around a spanning tree of the input graph. The Euler tour is then chopped into clusters with $\sqrt{B}$ elements (before the duplicate removal) ensuring that the maximum distance between any two nodes in the cluster is at most $\sqrt{B} - 1$. However, the fact that the contiguous elements on the disk are also closer in terms of BFS levels is not restricted to intra-cluster adjacency lists. The adjacency lists that come alongside the requisite cluster will also be required soon and by caching these other adjacency lists, we can save the I/Os in the future. This caching is particularly beneficial when the pool fits in the internal memory. Note that we still load the $\sqrt{B}$ node clusters in the pool, but keep the remaining elements of the block in the pool-cache. For the line graphs, this means that we load the $\sqrt{B}$ nodes in the internal pool, while keeping the remaining $O(B)$ adjacency lists which we get in the same block, in the pool-cache, thereby reducing the I/O complexity for the BFS traversal on line graphs to the computation of a spanning tree.

We represent the adjacency lists of nodes in the graph as a STXXL vector. STXXL already provides a fully associative vector-cache with every vector. Before doing an I/O for loading a block of elements from the vector, it first checks if the block is already there in the vector-cache. If so, it avoids the I/O loading the elements from the cache instead. Increasing the vector-cache size of the adjacency list vector with a layout computed by the deterministic preprocessing and choosing the replacement policy to be LRU provides us with an implementation of the pool-cache. Figure 1 depicts the implementation of our heuristic.

5 Experiments

Configuration. We have implemented the algorithms in C++ using the g++ 4.02 compiler (optimization level -O3) on the GNU/Linux distribution with a 2.6 kernel and the external memory library STXXL version 0.77. Our experimental platform has two 2.0 GHz Opteron processors, 3 GB of RAM, 1 MB cache and 250 GB Seagate Baracuda hard-disks [29]. These hard-disks have 8 MB buffer cache. The average seek time for read and write is 8.0 and 9.0 msec, respectively, while the sustained data transfer rate for outer zone (maximum) is 65 MByte/s. This means that for graphs with $2^{28}$ nodes, $n$ random read and write I/Os will take around 600 and 675 hours, respectively. In order to compare better with the results of [3], we restrict the available memory to 1 GB for our experiments and use only one processor and one disk.

First, we show the comparison between improved MM BFS_R and MR BFS with the corresponding implementations in [3]. Then we compare our implementation of MM BFS_D (without our heuristic) with Christiani’s implementation based on cache-oblivious routines. Finally, we look at the relative performance of improved versions of MR BFS, MM BFS_R and MM BFS_D. We summarize this section by highlighting the best algorithms for each graph class and its run-time. Note that some of the results shown in this section have been interpolated using the symmetry in the graph structure.

Graph classes. We consider the same graph classes as in [3] - Random, Grid, MR_worst graph, MM_worst graph, line graphs with different layouts and the webgraph. They covers a broad spectrum of different performances of external memory BFS algorithms.
<table>
<thead>
<tr>
<th>Graph class</th>
<th>n</th>
<th>m</th>
<th>MM_BFS_R of</th>
<th>Improved MM_BFS_R</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>[3] Phase 1</td>
<td>Phase 2</td>
</tr>
<tr>
<td>Random</td>
<td>$2^{28}$</td>
<td>$2^{30}$</td>
<td>5.1</td>
<td>4.5</td>
</tr>
<tr>
<td>MM_worst</td>
<td>$4.3 \cdot 10^7$</td>
<td>$4.3 \cdot 10^7$</td>
<td>6.7</td>
<td>26</td>
</tr>
<tr>
<td>MR_worst</td>
<td>$2^{28}$</td>
<td>$2^{30}$</td>
<td>5.1</td>
<td>45</td>
</tr>
<tr>
<td>Grid (2$^{28} \times 2^{14}$)</td>
<td>$2^{28}$</td>
<td>$2^{29}$</td>
<td>7.3</td>
<td>47</td>
</tr>
<tr>
<td>Simple Line</td>
<td>$2^{28}$</td>
<td>$2^{28} - 1$</td>
<td>85</td>
<td>191</td>
</tr>
<tr>
<td>Random Line</td>
<td>$2^{28}$</td>
<td>$2^{28} - 1$</td>
<td>81</td>
<td>203</td>
</tr>
<tr>
<td>Webgraph</td>
<td>$1.4 \cdot 10^8$</td>
<td>$1.2 \cdot 10^8$</td>
<td>6.2</td>
<td>3.2</td>
</tr>
</tbody>
</table>

Table 4: Timing in hours taken for BFS by the two MM_BFS_R implementations

Random graph: On a $n$ node graph, we randomly select $m$ edges with replacement (i.e., $m$ times selecting a source and target node such that source $\neq$ target) and remove the duplicate edges to obtain random graphs.

MR_worst graph: This graph consists of $B$ levels, each having $\frac{n}{2}$ nodes, except the level 0 which contains only the source node. The edges are randomly distributed between consecutive levels, such that these $B$ levels approximate the BFS levels. The initial layout of the nodes on the disk is random. This graph causes MR_BFS to incur its worst case of $\Omega(n)$ I/Os.

Grid graph ($x \times y$): It consists of a $x \times y$ grid, with edges joining the neighboring nodes in the grid.

MM BFS worst graph: This graph causes MM_BFS_R to incur its worst case of $\Theta(n \cdot \sqrt{\frac{\log n}{B}} + \text{sort}(n))$ I/Os.

Line graphs: A line graph consists of $n$ nodes and $n - 1$ edges such that there exists two nodes $u$ and $v$, with the path from $u$ to $v$ consisting of all the $n - 1$ edges. We took two different initial layouts - simple, in which all blocks consists of $B$ consecutively lined nodes and the random in which the arrangement of nodes on disk is given by a random permutation.

Web graph: As an instance of a real world graph, we consider an actual crawl of the world wide web [30], where an edge represents a hyperlink between two sites. This graph has around 130 million nodes and 1.4 billion edges. It has a core which consists of most of its nodes and behaves like random graph.

Comparing MM_BFS_R. Table 4 shows the improvement that we achieved in MM_BFS_R. As Table 5 shows, these improvements are achieved by reducing the computation time per level in the BFS phase. On I/O bound random graphs, the improvement is just around 15%, while on computation bound line graphs with random disk layout, we improve the running time of the BFS phase from around 200 hours to 25 hours. Our implementation of the randomized preprocessing in the case of the simple line graphs additionally benefits from the way clusters are laid out on the disk as this layout reflects the order in which the nodes are visited by the BFS. This reduces the total running time for the BFS phase of MM_BFS_R on simple line graphs from around 190 hours to 2.9 hours. The effects of caching are also seen in the I/O bound BFS phase on the grid ($2^{14} \times 2^{14}$) graphs, where the I/O wait time decreases from 46 hours to 24 hours.

Comparing MR_BFS. Improvements in MR_BFS are shown in the Table 6. On random graphs where MR_BFS performs better than the other algorithms, we improve the runtime from 3.4 hours to 1.4 hours. Similarly for the web-crawl based graph, the running time reduces from 4.0 hours to 2.6 hours. The other graph class where MR_BFS outperforms MM_BFS_R is the MM_worst graph and here again, we improve the performance from around 25 hours to 13 hours.

Penalty for cache obliviousness. We compared the performance of our implementation of MM_BFS_D (without the heuristic) with Christiani’s implementation [14] based on cache-oblivious subroutines. Table 7 and 8 show the results of the comparison on the two extreme graph classes - random graphs and line graphs with random layout on disk - for the preprocessing and the BFS phase respectively. We observed that on both graph classes, the preprocessing time required by our implementation is significantly less than the one by Christiani. While pipelining helps the BFS phase of our implementation on random graphs, it becomes a liability on line graphs as it brings extra computation cost per level.

We suspect that these performance losses are inherent in cache-oblivious algorithms to a certain extent and will be carried over to the cache-oblivious BFS implementation.

Comparing MM_BFS_D with other external memory BFS algorithm implementations. Table 9 shows the performance of our implementations
Table 5: I/O wait time and the total time in hours for the BFS phase of the two MM_BFS_R implementations on moderate to large diameter graphs

<table>
<thead>
<tr>
<th>Graph class</th>
<th>n</th>
<th>m</th>
<th>MM_BFS_R of [3]</th>
<th>Improved MM_BFS_R</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>I/O wait</td>
<td>Total</td>
<td>I/O wait</td>
<td>Total</td>
</tr>
<tr>
<td>MM_worst</td>
<td>2^{28}</td>
<td>2^{29}</td>
<td>13</td>
<td>26</td>
</tr>
<tr>
<td>Grid (2^{14} × 2^{14})</td>
<td>2^{28}</td>
<td>2^{28} - 1</td>
<td>0.5</td>
<td>191</td>
</tr>
<tr>
<td>Simple Line</td>
<td>2^{28}</td>
<td>2^{28} - 1</td>
<td>21</td>
<td>203</td>
</tr>
</tbody>
</table>

Table 6: Timing in hours taken for BFS by the two MR_BFS implementations

<table>
<thead>
<tr>
<th>Graph class</th>
<th>n</th>
<th>m</th>
<th>MR_BFS of [3]</th>
<th>Improved MR_BFS</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>I/O wait time</td>
<td>Total time</td>
<td>I/O wait time</td>
<td>Total time</td>
</tr>
<tr>
<td>Random</td>
<td>2^{28}</td>
<td>2^{30}</td>
<td>2.4</td>
<td>3.4</td>
</tr>
<tr>
<td>Webgraph</td>
<td>135 × 10^6</td>
<td>1.18 × 10^9</td>
<td>3.7</td>
<td>4.0</td>
</tr>
<tr>
<td>MM_worst</td>
<td>42.6 × 10^6</td>
<td>42.6 × 10^6</td>
<td>25</td>
<td>25</td>
</tr>
<tr>
<td>Simple line</td>
<td>2^{28}</td>
<td>2^{28} - 1</td>
<td>0.6</td>
<td>10.2</td>
</tr>
</tbody>
</table>

Table 7: Timing in hours for computing the deterministic preprocessing of MM_BFS by the two implementations of MM_BFS_D

<table>
<thead>
<tr>
<th>Graph class</th>
<th>n</th>
<th>m</th>
<th>Christiani’s implementation</th>
<th>Our implementation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Random graph</td>
<td>2^{28}</td>
<td>2^{30}</td>
<td>107</td>
<td>5.2</td>
</tr>
<tr>
<td>Random Line</td>
<td>2^{28}</td>
<td>2^{28} - 1</td>
<td>47</td>
<td>3.2</td>
</tr>
</tbody>
</table>

Table 8: Timing in hours for the BFS phase of MM_BFS by the two implementations of MM_BFS_D (without heuristic)

<table>
<thead>
<tr>
<th>Graph class</th>
<th>MR_BFS</th>
<th>MM_BFS_R</th>
<th>MM_BFS_D</th>
</tr>
</thead>
<tbody>
<tr>
<td>Random graph</td>
<td>1.4</td>
<td>8.9</td>
<td>8.7</td>
</tr>
<tr>
<td>Random Line</td>
<td>4756</td>
<td>89</td>
<td>3.6</td>
</tr>
</tbody>
</table>

Table 9: Timing in hours taken by our implementations of different external memory BFS algorithms.

<table>
<thead>
<tr>
<th>Graph class</th>
<th>n</th>
<th>m</th>
<th>Randomized</th>
<th>Deterministic</th>
</tr>
</thead>
<tbody>
<tr>
<td>Random graph</td>
<td>2^{28}</td>
<td>2^{30}</td>
<td>500</td>
<td>630</td>
</tr>
<tr>
<td>Random Line</td>
<td>2^{28}</td>
<td>2^{28} - 1</td>
<td>10500</td>
<td>480</td>
</tr>
</tbody>
</table>

Table 10: I/O volume (in GB) required in the preprocessing phase by the two variants of MM_BFS
of different external memory BFS algorithms with the heuristic. While MR\textsubscript{BFS} performs better than the other two on random graphs saving a few hours, our implementation of MM\textsubscript{BFS\_D} with the heuristic outperforms MR\textsubscript{BFS} and MM\textsubscript{BFS\_R} on line graphs with random layout on disk saving a few months and a few days, respectively. Random line graphs are an example of a tough input for external memory BFS as they not only have a large number of BFS levels, but also their layout on the disk makes the random accesses to adjacency lists very costly. Also, on moderate diameter grid graph, MM\textsubscript{BFS\_D} which takes 21 hours outperforms MM\textsubscript{BFS\_R} and MR\textsubscript{BFS}. It is interesting to note that Christiani [14] reached a different conclusion regarding the relative performance of MM\textsubscript{BFS\_D} and MM\textsubscript{BFS\_R}. As noted before, this is because of the cache oblivious routines used in their implementation.

On large diameter sparse graphs such as line graphs, the randomized preprocessing scans the graph $\Omega(\sqrt{B})$ times, incurring an expected number of $O(\sqrt{n} \cdot (n + m) \cdot \log(n)/B)$ I/Os. On the other hand, the I/O complexity of the deterministic preprocessing is $O((1 + \log \log (D \cdot B \cdot n/m)) \cdot \text{sort}(n + m))$, dominated by the spanning tree computation. Note that the Euler tour computation followed by list ranking only requires $O(\text{sort}(m))$ I/Os. This asymptotic difference shows in the I/O volume of the two preprocessing variants (Table 11), thereby explaining the better performance of the deterministic preprocessing over the randomized one (Table 11). On low diameter random graphs, the diameter of the clusters is small and consequently, the randomized variant scans the graph fewer times leading to less I/O volume.

As compared to MM\textsubscript{BFS\_R}, MM\textsubscript{BFS\_D} provides dual advantages: First, the preprocessing itself is faster and second, for most graph classes, the partitioning is also more robust, thus leading to better worst-case runtimes in the BFS phase. The later is because the clusters generated by the deterministic preprocessing are of diameter at most $\sqrt{B}$, while the ones by randomized preprocessing can have a larger diameter causing adjacency lists to be scanned more often. Also, MM\textsubscript{BFS\_D} benefits much more from our caching heuristic than MM\textsubscript{BFS\_R} as the deterministic preprocessing gathers neighbouring clusters of the graph on contiguous locations in the disk.

### 5.1 Results with heuristic.

Table 12 shows the results of MM\textsubscript{BFS\_D} with our heuristic on different graph classes. On moderate diameter grid graphs as well as large diameter random line graphs, MM\textsubscript{BFS\_D} with our heuristic provides the fastest implementation of BFS in the external memory.

### 5.2 Summary.

Table 13 gives the current state of the art implementations of external memory BFS on different graph classes.

Our improved MR\textsubscript{BFS} implementation outperforms the other external memory BFS implementations on low diameter graphs or when the nodes of a graph are arranged on the disk in the order required for BFS traversal. For random graphs with 256 million nodes and a billion edges, our improved MR\textsubscript{BFS} performs BFS in just 1.4 hours. Similarly, improved MR\textsubscript{BFS} takes only 2.6 hours on webgraphs (whose runtime is dominated by the short diameter core) and 0.4 hours on line graph with contiguous layout on disk. On moderate diameter square grid graphs, the total time for BFS is brought down from 54.3 hours for MM\textsubscript{BFS\_R} implementation in [3] to 21 hours for our implementation of MM\textsubscript{BFS\_D} with heuristics, an improvement of more than 60%. For large diameter graphs like random line graphs, MM\textsubscript{BFS\_D} along with our heuristic computes the BFS in just about 3.6 hours, which would have taken the MM\textsubscript{BFS\_R} implementation in [3] around 12 days and MR\textsubscript{BFS} and IM\textsubscript{BFS} a few months, an improvement by a factor of more than 75 and 1300, respectively.

### 6 Discussion

We implemented the deterministic variant of MM\textsubscript{BFS} and showed its comparative analysis with other external memory BFS algorithms. Together with the improved implementations of MR\textsubscript{BFS} and MM\textsubscript{BFS\_R} and our heuristic for maintaining the pool, it provides viable BFS traversal on different classes of massive sparse graphs. In particular, we obtain an improvement factor between 75 and 1300 for line graphs with random disk layout over the previous external memory implementations of BFS.
Graph class | n | m | MM_BFS_D
---|---|---|---
| | | | Phases
Random | $2^{28}$ | $2^{30}$ | 5.2 | 3.4
Webgraph | $\sim 1.4 \cdot 10^8$ | $\sim 1.2 \cdot 10^9$ | 3.3 | 2.4
Grid ($2^{21} \times 2^7$) | $2^{28}$ | $2^{29}$ | 3.6 | 0.4
Grid ($2^{27} \times 2$) | $2^{28}$ | $2^{28} + 2^{27}$ | 3.2 | 0.6
Simple Line | $2^{28}$ | $2^{28} - 1$ | 2.6 | 0.4
Random Line | $2^{28}$ | $2^{28} - 1$ | 3.2 | 0.5

Table 12: Time taken (in hours) by the two phases of MM_BFS_D with our heuristic

<table>
<thead>
<tr>
<th>Graph class</th>
<th>n</th>
<th>m</th>
<th>Current best results</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Total time</td>
</tr>
</tbody>
</table>
Random | $2^{28}$ | $2^{30}$ | 1.4 | Improved MR_BFS
Webgraph | $\sim 1.4 \cdot 10^8$ | $\sim 1.2 \cdot 10^9$ | 2.6 | Improved MR_BFS
Grid ($2^{21} \times 2^7$) | $2^{28}$ | $2^{29}$ | 21 | MM_BFS_D w/ heuristic
Grid ($2^{27} \times 2$) | $2^{28}$ | $2^{28} + 2^{27}$ | 3.8 | MM_BFS_D w/ heuristic
Simple Line | $2^{28}$ | $2^{28} - 1$ | 0.4 | Improved MR_BFS
Random Line | $2^{28}$ | $2^{28} - 1$ | 3.6 | MM_BFS_D w/ heuristic

Table 13: The best total running time (in hours) for BFS traversal on different graphs with the best external memory BFS implementations

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We are grateful to Rolf Fagerberg and Frederik Juul Christiani for providing us their code. Also thanks are due to Dominik Schultes and Roman Dementiev for their help in using the external MST implementation and STXXL, respectively. The authors also acknowledge the usage of the computing resources of the University of Karlsruhe.

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