# Scalable Distributed-Memory External Sorting

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Abstract—We engineer algorithms for sorting huge data sets on massively parallel machines. The algorithms are based on the multiway merging paradigm. We first outline an algorithm whose I/O requirement is close to a lower bound. Thus, in contrast to naive implementations of multiway merging and all other approaches known to us, the algorithm works with just two passes over the data even for the largest conceivable inputs. A second algorithm reduces communication overhead and uses more conventional specifications of the result at the cost of slightly increased I/O requirements. An implementation wins the well known sorting benchmark in several categories and by a large margin over its competitors.

# I. INTRODUCTION

There are currently two main ways to handle huge inputs in a cost-efficient manner: keeping most data externally on low cost hard disks, and clustering many inexpensive machines. The combination of both approaches allows relatively cheap machines to handle huge inputs that would otherwise require high-end, power hungry super-computers with lots of internal memory. On high-end machines equipped with sufficient disk bandwidth, one could handle inputs of unprecedented size. For example, a mid-size cluster with 1024 Terabyte disks which cost about 100 KEuro, can scan a Petabyte of data in a few hours.

Perhaps the most important nontrivial operation needed for processing such huge data sets is sorting. For example, sorting (or similar computations) can be used to build index data structures or to arrange geometrical data such that closeby data can be processed together (e.g., using space filling curves). Fundamental lower bounds [4] basically tell us that in order to process inputs significantly larger than the *cumulative* main memory size  $M^{-1}$ , at least two passes<sup>2</sup> over the data are needed. More precisely, up to  $M^2/B$  elements can be processed in two passes (refer to Table I for explanations of the symbols P, M, D, B, N, R used in this paper).

Although there is a lot of previous work on parallel external sorting, the problem is not solved yet. In particular, algorithms used in practice can have very bad behavior for worst-case inputs, whereas all previous theoretical results lead to algorithms

that need more than two passes even for easy inputs. Section II gives more details.

In Section III, we outline a conceptually simple variant of multiway mergesort that needs two passes even for inputs whose size is close to the theoretical limit for being sorted with two passes. However, this algorithm has relatively large communication overhead and outputs the data in a globally striped fashion, i.e., subsequent blocks of output are allocated on subsequent PEs (processing elements). Therefore, in Section IV, we refine the algorithm so that it needs very little communication and outputs the data in a format more conventional in parallel computing, and more convenient for further processing: PE i gets the elements of ranks (i-1)N/P +  $1, \ldots, iN/P$  where N is the total number of elements and P is the number of PEs<sup>3</sup>. At least on the average, and up to small "clean up" costs, this CANONICALMERGESORT algorithm needs only two passes and communicates elements only once. Section VI gives experimental results on a careful implementation described in Section V. These experiments show that the algorithm performs very well in practice An inplace implementation sorts about 564 GB/min with 195 8-core nodes and 780 disks, leading the "Indy GraySort" category of the SortBenchmark [2] in 2009. We summarize the results and outline possible future work in Section VII.

# II. RELATED WORK

Since sorting is an essential ingredient of most external memory algorithms, considerable work has been invested in finding I/O-optimal parallel disk sorting algorithms (e. g., [27], [19], [6], [13]) that approach the lower bound of  $2N/DB(1+\lceil\log_{M/B}N/M\rceil)$  I/O operations for sorting N elements on a

TABLE I

Symbols used in this paper. We generally omit trivial rounding issues when dividing these quantities.

Resource/Number	Symbol
#PEs	P
internal memory (in #elements)	M
#disks	D
block size (in #elements) in the EM model	В
#elements	N
#runs	R

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 $<sup>^{1}</sup>$ To avoid cumbersome notation, we will also use M to denote the size of a run in external mergesort algorithms. Depending on details of the implementation, the run size might be a factor around two smaller or larger [14]. However, this difference has little effect on the overall performance.

<sup>&</sup>lt;sup>2</sup>One pass comprises reading and writing the data once.

 $<sup>^3</sup>$ Depending on the implementation, P might denote the number of nodes, each of which could have several cores.

machine with D disks, fast memory size<sup>4</sup> M and block size B. The challenge is to avoid getting a base M/DB for the logarithm that spoils performance for very large systems. An important motivation for this paper is the observation that a large D only makes sense in a system with many processors. Although [27], [18], [3] develop sophisticated asymptotically optimal parallel algorithms, these algorithms imply considerable constant factors of overhead with respect to both I/Os and communication compared to the best randomized sequential algorithms [6], [13], [11].

We only note in passing that there is also considerable work on parallel disk sorting with shared-memory parallel processors, e. g., [20]. This is an easier problem since communication overhead is less of an issue.

Many external memory algorithms for distributed-memory machines have been proposed (e. g., see the references in [25]). One of the most successful ones is NOW-Sort [5] which is somewhat similar to our algorithm CANONICALMERGESORT, i. e., it sorts up to  $M^2/(PB)$  elements in two passes. However, it only works efficiently for random inputs. In the worst case, it deteriorates to a sequential algorithm since all the data ends up in a single processor. This problem can be repaired by finding appropriate splitter keys in a preprocessing step [15]. However, this costs an additional scan of the data and still does not result in exact partitioning.

In [24], a merge-based parallel external sorting algorithm is proposed that is inspired by parallel mesh algorithms. This algorithm needs at least four passes over the data.<sup>5</sup>

In [7] an algorithm based on column-sort is proposed that sorts up to  $(M/P)^{3/2}/\sqrt{2}$  elements using three passes over the data. Using one additional pass, the input size can be increased to  $\max(\mathcal{O}(M^{3/2},(M/P)^{5/3}))$  elements. It is instructive to use some realistic numbers. On current machines it is quite realistic to assume about 2 GiB of RAM per core. Using this number, the amount of data that can be sorted with the three pass algorithm is limited to inputs of size around  $2^{31^{3/2}}/\sqrt{2}=2^{46}$ , i.e. about 64 TiB regardless of the number of available PEs.

In [9], a general emulation technique for emulating parallel algorithms on a parallel external memory machine is developed. It is proposed to apply this technique to a variant of sample sort. This results in an algorithm that needs five passes over the data for sorting  $\mathcal{O}(M^2/(PB))$  elements.

Our exact partitioning algorithm for parallel multiway merging owes a lot to [12] where multiway merging is used for shared-memory parallel sorting.

## III. MERGESORT WITH GLOBAL STRIPING

Since multiway mergesort is a good algorithm for parallel disk external sorting and parallel internal sorting, it is a natural idea to use it also for parallel external sorting. Here we outline how to do this in a scalable way: The first phase is run formation where initial runs of size M are loaded into the

cumulative memory of the parallel machine, sorted in parallel, and written back to disk.

Next follow one or more merging phases<sup>6</sup> where up to  $k = \mathcal{O}(M/B)$  sorted runs are merged in a single pass. The challenge is that we are only allowed a constant number of buffer blocks for each run. In particular, we may not be able to afford k buffer blocks on every PE. We solve this by fetching a batch of  $\Theta(M/B)$  blocks at a time into the internal memory (those blocks that will be needed next in the merging process), extracting the  $\Theta(M)$  smallest unmerged elements using internal parallel merging, and writing them to the disks. Fetched elements that are larger than the smallest unfetched elements are kept in internal memory until the next batch. Note that this is possible since by definition of the blocks to be fetched, for each run, at most B elements remain unmerged. Note that we could even afford to replace batch merging by fully-fledged parallel sorting of batches without performing more work than during run formation.

The difficult part is how to do the disk accesses efficiently. However, this can be done in an analogous fashion to previous (sequential) parallel disk sorting algorithms [6], [11], [13]. The runs and the final output are *striped* over all disks, i.e., subsequent blocks are allocated on subsequent disks. This way, writing becomes easy: We maintain D buffer blocks. Whenever they are full, we output them to the disks in parallel. Efficiently fetching the data is more complicated. A prediction sequence consisting of the smallest element in each data block can be used to predict in which order the data blocks are needed during merging [14], [11]. Using randomization, some buffer space, and appropriate prefetching algorithms, it is then possible to make good use of all disks at once. The only part of this algorithm that is not straight-forward to parallelize is the prefetching algorithm. In Appendix A, we outline an efficient prefetching algorithm for the cases  $B = \Omega(\log P)$ and  $M = \Omega(DB \log D)$ .

We believe that the above algorithm could be implemented efficiently. However, it requires a substantial amount of communication: During run formation, all the data has to be communicated in the parallel sorting routine and again for writing it in a striped fashion. Similarly, during a merging pass, the data has to be communicated during internal memory multiway merging and for outputting it in a striped fashion. Moreover, globally striped output is often not what is needed for further processing so that we need 4–5 communications for two passes of sorting. In the next section we want to bring this down to a single communication at least in the best case.

## IV. CANONICALMERGESORT

In the following, we describe a variant of parallel external mergesort that produces its output in way more canonical for parallel processing – PE i gets the elements of ranks  $(i-1)N/P+1,\ldots,iN/P$  and this data is striped over the local disk. This is not only more useful for some applications but

<sup>&</sup>lt;sup>4</sup>All sizes are given in number of elements.

<sup>&</sup>lt;sup>5</sup>This bound is derived from the bounds in the paper assuming that logarithms with fractional values have to be rounded up.

<sup>&</sup>lt;sup>6</sup>In general we need  $\lceil \log_{\Theta(M/B)} \frac{N}{M} \rceil$  merging phases.

it also reduces the amount of communication to a minimum at the price of some additional I/Os.

In the first phase, R=N/M global runs of size M (the last run might be smaller) are created. Section IV-B gives more details. This is similar to the algorithm of Section III but now the output is not striped globally over the disks but output locally, which saves communication. Moreover, if all runs have a similar input distribution, most elements will already end up on the PE where they are needed for a globally sorted final output. In order to make this assumption approximately true, each PE chooses its participating blocks for the run randomly. This is implemented by randomly shuffling the IDs of the local input blocks in a preprocessing step.

In the second phase, multiway selection operations are performed on all runs. In general, a multiway selection operation finds the element e with global rank r from R sorted sequences, and returns R splitter positions which partition the sequences with respect to e. For external parallel mergesort, each PE i selects for each run the first element it is supposed to contain in the final result, resulting in P-1 splitter elements per run. After communicating the splitter positions to PEs i and i-1, every PE knows the elements it has to merge (see Section IV-A for more details).

The data is then redistributed accordingly using a global external all-to-all operation described in Section IV-C. If the input is uniformly distributed, or if global randomization is applied, most of the data will already be in the right place, so the all-to-all operation takes only little time.

In the third phase, the data is merged locally. Each element is read and written once, no communication is involved in this phase. The internal computation amounts to  $\mathcal{O}(N/P\log R) = \mathcal{O}(N/P\log N/M)$ . Overall, we need  $\mathcal{O}(N/P\log N)$  internal computation, with a very low constant factor.

An overview of CANONICALMERGESORT can be found in Figure 1.

# A. Multiway Selection

As stated before, a multiway selection finds out the element e with global rank r among R sorted sequences, plus the splitter positions that partition the sequences with respect to e. Let the length of the sequences M be a power of two, rounded up and (conceptually) fill up with  $\infty$  otherwise.

We maintain approximate splitter positions that are moved in steps of size s. The basic algorithm uses initial splitter positions 0 and step size s=M. Within a round, the splitter corresponding to the smallest element is increased by s until the number of elements to the left of the splitters becomes larger than r. Then, s is halved and the splitters corresponding to the largest element are decreased by s while the number of elements to the left of the splitters is still larger than r. This process is repeated until s=1. After at most  $\lceil \log_2 M \rceil$  rounds, the process terminates. Since in each half round every splitter is touched at most once, the overall number of sequence elements touched is  $\mathcal{O}(R\log M)$  and the total execution time is  $\mathcal{O}(R\log R\log M)$  using a priority queue for identifying the sequences to be touched.

In phase two of our algorithm, processor i runs multiway selection for rank r = iN/P. Although these selections can run in parallel, they have to request data from remote disks and thus the worst case number of I/O steps is  $\mathcal{O}(RP \log M)$ when a constant fraction of request is directed to a single disk. This could be a bottleneck for large P. This problem is greatly reduced by the randomization used during run formation. Furthermore, during run formation, we store every K-th element of the sorted run as a sample (for some parameter K). During multiway selection, this sample is used to find initial values for the approximate splitters. As a third optimization, we cache the most recently accessed disk blocks to eliminate the  $R \log B$  last disk accesses of a multiway selection. In our implementation, we keep the sample in main memory. In our experiments, the resulting selection algorithm takes negligible time. In Appendix B we analyze a slightly more complicated variant that provably scales to very large machines, still using only very little time.

# B. Internal Memory Parallel Sorting

We essentially use a distributed-memory implementation of the parallel multiway merging approach already used in [12], [26]. We therefore only outline the algorithm. Each node sorts its local data. Then, the internal memory variant of the multiway selection algorithm from Section IV-A is used to split the P sorted sequences into P pieces of equal size. An all-to-all communication is used to move the pieces to the right PE. Note that in the best case, this is the only time when the data is actually communicated.

# C. External All-to-All

In an all-to-all operation, each PE sends and receives different amounts of data to/from all other PEs. Compared to the ordinary all-to-all operation provided by MPI we are facing two problems. First, each PE might have to communicate more data than fits into its local memory. We solve this problem by splitting the external all-to-all into k internal memory suboperations by logically splitting the data sent to a receiver into k (almost) equally-sized parts. The choice of k depends on the available internal memory but will be at most  $\mathcal{O}(R)$ . The second problem is that the data has to be collected from R different runs. We therefore assemble the submessages by consuming all the participating data of run i before switching to run i + 1. This way, each PE j needs only a single buffer block for each PE that it sends data to. Note that due to randomization, the number P' of required blocks will grow much more slowly than the worst case of P-1 communication partners. The total number of I/O steps for data volume V will be  $\frac{2V}{PB} + \mathcal{O}(RP')$ .

## D. Summary of the Analysis

The most easy summary of the analysis is that CANON-ICALMERGESORT needs I/O volume  $4N + \mathrm{o}(N)$ , communication volume  $N + \mathrm{o}(N)$ , and local work similar to a fast sequential internal algorithm. Here, the " $\mathrm{o}(\cdot)$ "-notation expresses that the overheads are independent of the input size

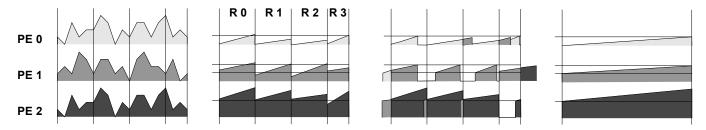


Fig. 1. CANONICALMERGESORT: On the very left the initial input situation, going to the right the results of the three phases: run formation, redistribution (hopefully negligible), local merging. The y-axis denotes the element rank, the horizontal lines illustrate the global splitters.

N or only grow sublinearly. A little more care must be taken however, since these bounds only hold under a number of assumptions on the values of the other machine parameters, namely  $P,\,M,\,B,\,$  and D. To simplify matters a little bit, we assume that  $D=\Theta(P).$  We also introduce the shorthand m for the local memory size M/P. For example, on our machine, we have  $P\in 1...200$  nodes (with 8 cores each),  $D=4P,\,$   $m=2^{34}$  byte, and  $B=2^{23}$  byte.

The theoretically most important restriction is that the maximal amount of data that can be sorted is  $\mathcal{O}(M \cdot \frac{M}{PB}) = \mathcal{O}\left(P\frac{m^2}{B}\right)$ . This is a factor  $\Theta(P)$  less than the globally striped algorithm from Section III can sort since *every* PE must be able to hold one buffer block from each run in the merging phase. However,  $P\frac{m^2}{B}$  is P times the amount that can be sorted by a single PE, which sounds very reasonable. In particular, any single PE equipped with a *reasonable* amount of RAM and disks can sort the complete content of these disks in two passes since for technological reasons the price ratio between one byte of disk space and one byte of RAM has always been bounded by a few hundred. In this sense, the CANONICALMERGESORT is sufficiently scalable.

The second most important restriction is that even the randomized algorithm cannot move all the data to the right PE already during run formation. In Appendix C, we show that this amount of data remains small if  $m\gg PB\log P$  (and the factor  $\log P$  may be an artifact of the analysis), i.e., each PE must be able to store some number of blocks for each other PE. This assumption is reasonable for the medium-sized machine we have used, and for average case inputs, the B disappears from the restriction, leading to an algorithm that scales even to very large machines with many thousands of PEs. For very large machines and worst case inputs, our algorithm degrades to a three-pass algorithm which is still a good result.

A similar restriction on the local memory size applies to the external all-to-all algorithm from Section IV-C – each local memory must be able to hold a constant number of blocks for each other PE. However, randomization will mitigate this problem so that this part of the algorithm will scale to very large machines.

Another similar restriction applies to the multiway selection algorithm described in Section IV-A whose naive implementation is only efficient if  $m \gg PB \log M$ . Here, our more clever implementation with sampling and caching basically

eliminates the problem.

#### E. Further Issues

Hierarchical Parallelism.: In our terms, a PE is defined with respect to communication. Data has to be communicated if and only if it resides on different PEs. In practice, a PE can have multiple processors/cores and multiple disks. We exploit this *local* parallelism also. The blocks on a PE are striped over the local disks. For complex operations like internal sorting and merging, shared-memory parallel algorithms are used. Thus, we exploit hierarchical parallelism.

Taking each processor core as a PE would lead to a larger number P, negatively influencing some of the stated properties of the algorithm.

(Nearly) In-Place Operation.: In the following, we analyze the additional external memory needed per node during the course of the algorithm.

The run formation in phase 1 can be done in-place easily. The data is written back to the blocks where it was read from.

In phase 2, the multiway selection does not need considerable extra space. The subsequent external all-to-all operation has a certain overhead since in each suboperation it receives P' pieces of data, which may lead to partially filled blocks. Since there is not sufficient internal memory to buffer all this data, these partially filled blocks have to be written out to disk. Also, the in-place global external all-to-all needs P+1 more blocks, leading to a total temporary overhead of RP' blocks per PE.

For merging in phase 3, blocks that are read to internal buffers are deallocated from disk immediately, so there are always blocks available for writing the output.

Overlapping.: For run formation, we overlap internal computation and communication with I/O. While run i is globally sorted internally, we first write the (already sorted) run i-1 before fetching the data for run i+1.

As a special optimization for inputs that fit into internal memory, we also overlap for this single-run case: Immediately after a block is read from disk, it is sorted, while the disk is busy with subsequent blocks. When all blocks are read and sorted, the algorithm only has to merge the blocks instead of still sorting everything.

We could also use overlapping of internal computation and communication in the internal global sort, splitting up the internal sort into three phases: local internal sort, global distribution, local internal merge. However, our current implementation does not yet support this. It is questionable whether this would help the performance, since all three operations still share the memory bandwidth.

#### V. IMPLEMENTATION

We have implemented CANONICALMERGESORT in C++. We used the STXXL, the standard template library for XXL data sets [10], for handling asynchronous block-wise access to the multiple disks highly efficiently. To sort and to merge data internally we used the parallel mode of the STL implementation of GCC 4.3.1, which exploits multi-core parallelism, and is based on the Multi-Core Standard Template Library [26]. Communication between nodes is done using the message passing interface MPI [17], we used MVAPICH 1.1 here. Unfortunately, in MPI, data volumes are specified using 32-bit signed integers. This means that no data volume greater than 2 GiB can be passed to MPI routines. We have re-implemented MPI\_Alltoallv to break this barrier.

# VI. EXPERIMENTAL RESULTS

The testing machine was a 200-node Intel Xeon cluster running Linux kernel 2.6.22. Each node consists of two Quad-Core Intel Xeon X5355 processors clocked at 2 667 MHz with 16 GiB main memory and 2×4 MiB cache. The nodes are connected by a 288-port InfiniBand 4xDDR switch, the resulting point-to-point peak bandwidth between two nodes is more than 1 300 MB/s. However, this value decreases when most nodes are used because the fabric gets overloaded (we have measured bandwidths as low as 400 MB/s). On every compute node, the 4 disks were configured as RAID-0 (striping)<sup>7</sup>. Each node contains 4 Seagate Barracuda 7200.10 hard drives with a capacity of 250 GB each. We have measured peak I/O rates between 60 and 71 MiB/s, in average 67 MiB/s, on an XFS file system. If not stated otherwise, we used a block size of 8 MiB. One cluster node corresponds to one PE in the following.

We tested scalability by sorting 100 GiB of data per PE, with an increasing number of PEs, up to 64. The element size is (only) 16 bytes with 64-bit keys. This makes internal computation efficiency as important as high I/O throughput. As shown in Figure 2, the scalability is very good for random input data. For worst-case input, a penalty of up to 50% in running time can appear (Figure 6), as expected by the additional I/O performed by the all-to-all phase. This overhead can be diminished by using randomization (Figure 4), which reduces the I/O volume greatly. Figure 5 shows that a smaller block size of 2 MiB can further improve the effect of randomization, but usually at the cost of a little worse I/O performance.

As expected, run formation takes about the same time as the final merging. The average I/O bandwidth per disk is about 50 MiB/s, which is more than 2/3 of the maximum. The reasons for this overhead are worse performance of tracks closer to the center of a disk (when disks fill up), file

system overhead, natural spreading of disk performance, and startup/finalization overhead. Multiway selection takes in fact only negligible time.

Figure 3 shows the time consumption across the nodes for a 32-node run. The work is very well balanced, but there is some variance in disk speed.

We have not compared our program to implementations of other algorithms directly. However, we made experiments on the well-established SortBenchmark, initiated by Jim Gray in 1984, and continuously adapted to the changing circumstances [2]. This setting considers 100-byte elements with a 10-byte key. The results [23] using 195 nodes show that we can sort  $10^{12}$  bytes in less than 64 seconds, which is about a third of the time needed by the 2007 winner TokuSampleSort. This is despite the fact the we use the same number of cores<sup>8</sup>, but only a third of the hard disks. We also slightly improve on a recent result for the Terabyte category published informally by Google [8], where 12 000 disks<sup>9</sup> were used instead of 780 as in our case.

In the MinuteSort category, a time limit of one minute is given, the processed amount of the data is the metric. We have beaten the former record of TokuSampleSort by a factor of 3.6, processing 955 GB of data, which rendered the TerabyteSort category obsolete. Yahoo achieved a result half as high using the Hadoop framework [21], [1], but with a machine 7 times as large.

However, for the results mentioned so far, N < M, so the sort is merely internal and only 2 I/Os per block of elements are needed.

Concerning the newly established GraySort category, we can sort  $10^{14}$  bytes (close to  $100\,\mathrm{TiB}$ ) in slightly less than three hours on 195 nodes, resulting in about 564 GB Bytes of sorted data per minute. The Google program in this case takes only twice the time for ten times the amount of data, but they use an even larger machine than before, featuring 48 000 disks, which is a factor of 61 larger. The better performance of a factor of 5 is thus reduced to less than 0.1 in terms of relative efficiency. Yahoo's official result of 578 GB/min is only 2.5% faster than us, but its efficiency is even worse, since they used 17 times the number of nodes. Those nodes were very similar to the ones used by us, except having only half the memory. They also had a worse communication bandwidth. However, this would not have been a limiting factor for our algorithm.

# VII. CONCLUSION

We explored some of the design space for merging based parallel external sorting. Our globally striped algorithm minimizes the required I/Os. Our CANONICALMERGESORT algorithm is theoretically a bit less scalable but it has close to minimal communication overhead, and a more useful output format. Moreover, it sorts any technologically reasonable inputs in two to three passes. For medium-sized machines or

<sup>&</sup>lt;sup>7</sup>Parallel disks are also directly supported by the program and could lead to even better timings, but we could not configure the machine accordingly at the time of testing.

<sup>&</sup>lt;sup>8</sup>For such large elements, the algorithm is not compute-bound at all.

<sup>&</sup>lt;sup>9</sup>Google used 3-fold redundancy, but still, at least the performance of 4 000 disks could be achieved. Also, for a machine like ours, redundancy is not that desperately needed.

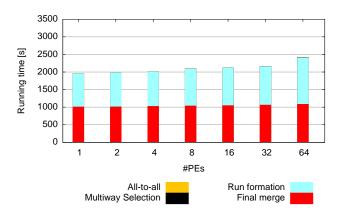
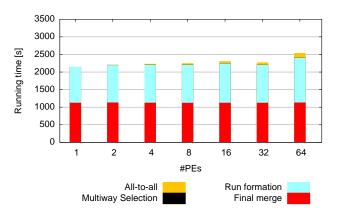
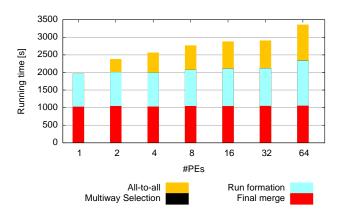


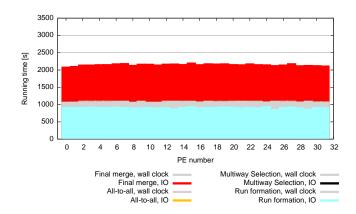
Fig. 2. Running times for random input, split up by the phases of the algorithm. Please note that the order of the phases is different from the order in the algorithm, to allow for better visual comparison.



 ${\rm Fig.~4.}$  Running times for worst-case input with randomization applied.



 ${\rm Fig.\,6.}\,$  Running times for worst-case input without randomization applied.



 ${
m Fig.~3.}$  Running times of the different phases on 32 nodes for random input. For each phase, both the I/O time and the wall clock time are shown. If there is a grey gap, the phase is not fully I/O-bound, as is the case for the run formation.

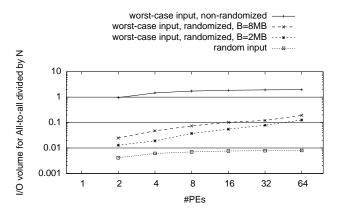


Fig. 5. I/O volume for the all-to-all phase for different inputs with/without randomization.

average case inputs, the I/O requirement remains closer to two passes than three passes.

A number of interesting questions remain for the future, in particular, a stronger analysis. Run formation could perhaps be improved to allow longer runs [14, Section 5.4.1]. The main effect is that by decreasing the number of runs, we can further increase the block size. For the very largest inputs this could yield a slight improvement in performance. An interesting question is whether on large machines that have considerably higher communication bandwidth than I/O bandwidth, the globally striped algorithm could indeed be the better choice. This algorithm could also be useful for pipelined sorting where the run formation does not fetch the data but obtains it from some data generator (no randomization possible for CANONICALMERGESORT) and where the output is not written to disk but fed into a postprocessor that requires its input in sorted order (e.g., variants of Kruskal's algorithm [22]). When scaling to very large machines, fault tolerance will play a bigger role. An interesting question is whether this can be achieved with lower overhead than in [8].

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# A. Prefetching with Global Striping

Perhaps the easiest way to do prefetching is to simply use the order in which the blocks are needed for merging, which is determined by the order of the smallest<sup>10</sup> keys in the data blocks. Unfortunately, it is open whether this leads to optimal I/O rates unless  $\Omega(D \log D)$  prefetch buffer blocks are available [6]. However, in [11], very good performance is observed for random inputs. In [11], [13], an optimal prefetching algorithm is used that is efficient already for  $\Omega(D)$  buffer blocks. This algorithm is based on simulating a buffered writing process which iteratively fills a shared write buffer and then simulates the output of one block on each disk whose queue contains a write request. We can use the sequential algorithm from [13] as long as  $B = \Omega(P)$ since we only perform constant work for each data block. Parallelizing this algorithm is possible but requires relatively fine-grained coordination: Allocating  $\mathcal{O}(D)$  blocks to disk queues can be implemented using plain message passing since randomization ensures that the number of blocks per queue is at most  $\mathcal{O}(\log D/\log\log D)$ . Simulating the outputs can be done locally on each PE. But then we have to count how many write queues are nonempty, which requires a global sumreduction. This is possible in time  $\mathcal{O}(\log P)$  on distributedmemory parallel machines.

#### B. Scalable Multiway Selection

Recall that during run formation, we sample every K-th element from each run together with its run number and position. For this analysis, we choose K = B, sample the smallest element of each block, and store it in a sample sequence together with its original position. Note that this approach is similar to the prediction sequences already mentioned in Section III. To initialize multiway selection of the element of rank global r, we sort (in parallel) the sample, and extract the element x of sample-local rank |r/B|. By scanning the sorted sample backwards, we also find the predecessor of x in each run. These elements are the initial values for the approximate splitter positions and B is the initial step size. This initialization can be done for all P desired ranks using a parallel sorting step and a single parallel scan of the sorted sample and thus takes only a factor  $\mathcal{O}(1/B)$  of the total work performed for sorting the full input. Subsequently, the remaining selection work for PE i only depends on one block in each run, i.e., overall, we have to access RP blocks and deliver them to the PEs that have to process them. Randomization ensures that the number of blocks to be accessed and communicated on each PE is well balanced, i. e., close to the expectation R. The final phase of multiway selection can work locally and in parallel and needs time  $\mathcal{O}(R \log R \log B)$ .

#### C. Analysis of Data Redistribution

We use the bounded difference inequality [16] which bounds how any function f of independent random variables is concentrated around its mean, provided that changing a single variable does not change the function value by too much. In our case we have M/B random variables that are used to determine the blocks sorted by a particular run j. The function f we consider is the global rank of the smallest element of run j that is stored on PE i. The expectation of f is iN/P. The deviation from this rank is proportional to the amount of data from run j to be moved to PE i. By changing a single random variable, the value of f changes by at most the block size B. We get

$$\mathbb{P}\left[f - \mathbb{E}[f] \ge t\right] \le \exp\left(-\frac{t^2}{2\frac{N}{B}B^2}\right) = \exp\left(-\frac{t^2}{2MB}\right),\tag{1}$$

i. e., it is unlikely that the more than  $\mathcal{O}\!\left(\sqrt{MB}\right)$  elements have to be moved per run. However, we have to be a bit careful since the running time of a parallel algorithm depends on the PE where things are worst. Equation (1) also shows that it is unlikely that any PE has to move more than  $\mathcal{O}(\sqrt{MB\log P})$ elements for run j. Since we are really interested in the worst sum of data movements over all runs, the truth lies somewhere in the middle. Anyway,  $\mathcal{O}(R\sqrt{MB\log P})$  is an upper bound for the expected amount of data movement to/from any PE. This is small compared to the total per PE amount of data movement of N/P if  $M/P \gg PB \log P$ , i.e., each PE must be able to store  $\Omega(P \log P)$  data blocks (and the  $\log P$ factor is probably overly conservative). This is a reasonable assumption for small and medium P but does not hold for very large machines. 12 We also see that the reorganization overhead grows with the square-root of B (Figure 5 supports this claim). Hence, on large machines, it might pay to use a smaller block size for reading blocks during run formation. Note that this affects only one fourth of the I/Os and we will furthermore not see the worst-case behavior of fully random accesses here since during run formation, we can use offline disk scheduling techniques to reduce seek times and rotational delays.

Average Case.: By setting B=1, we get a bound on the data movement for random inputs, i.e., for a random permutation of distinct elements. For low data movement, we need the condition that  $M/P\gg P\log P$ , i.e., every PE must be able to hold a logarithmic amount of data for every other PE in its local memory. This is a very mild condition. Indeed, internal memory parallel sorting algorithms that work with a single communication of the data have a similar condition.

<sup>&</sup>lt;sup>10</sup>In [14] and a lot of subsequent work, the *largest* key in the *previous block* is used. Here we use the approach from [11] which is arguably more elegant and allows the merger to proceed for slightly longer without having to wait for a block from disk.

 $<sup>^{11} \</sup>rm Note$  that these block indices are *not independent*. However, if we determine the blocks to be used by generating local random permutations the standard algorithm for determining random permutations uses M/B independent random values for determining the blocks used in a single run.

 $<sup>^{12}\</sup>mbox{For example, our nodes can hold only about 2\,000 of the very large blocks we are using.$