A massively parallel algorithm for constructing the BWT of large string sets

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Abstract

We present a new scalable, lightweight algorithm to incrementally construct the BWT and FM-index of large string sets such as those produced by Next Generation Sequencing. The algorithm is designed for massive parallelism and can effectively exploit the combination of low capacity high-bandwidth memory and slower external system memory typical of GPU accelerated systems. Particularly, for a string set of \( n \) characters from an alphabet with \( \sigma \) symbols, it uses a constant amount of high-bandwidth memory and at most \( 3n \log(\sigma) \) bits of system memory. Given that deep memory hierarchies are becoming a pervasive trait of high performance computing architectures, we believe this to be a relevant feature. The implementation can handle reads of arbitrary length and is up to 2 and respectively 6.5 times faster than state-of-the-art for short and long genomic reads.

1 Introduction

Recently, BWT and FM-index construction of very large string sets has become an important building block for bioinformatics applications such as de novo assembly [Simpson and Durbin 2011] and compression of large genomic databases [Cox et al. 2012]. In this context, a few novel lightweight algorithms have been developed to work specifically with very large collections of relatively short DNA strings, substantially outperforming previously known general purpose algorithms [Bauer et al. 2011; Li 2014]. However, these algorithms are either serial or offer very limited parallelism. Liu et al. [2014] has recently provided a new massively parallel algorithm that exploits the excellent sorting speed of modern GPUs for blockwise suffix sorting [Kärkkäinen 2007] but the algorithm’s speed is strongly limited by the speed at which suffixes can be gathered from the CPU’s memory subsystem, which is several times slower than high bandwidth GPU memory. Moreover, Liu et al’s [2014] algorithm is not incremental. This work provides a novel algorithm, set-bwte, that drastically reduces the impact of the external memory speed bottleneck while allowing to incrementally add new strings to pre-existing indices. The algorithm can be seen as extending and adapting the bwte algorithm by Ferragina et al [2012] to string sets and modern parallel architectures with deep memory hierarchies.

2 Overview

Let \( \Sigma = \{c_1, \ldots, c_\sigma\} \) be an ordered alphabet, with \( c_1 < c_2 < \cdots < c_\sigma \). For a string \( T = T[0 \ldots n-1] \), we denote its \( i \)-th symbol with \( T[i] \), and its \( i \)-th suffix with \( T^i = T[i \ldots n-1] \).

The suffix array of \( T \) is an array \( SA[0 \ldots n-1] \) such that \( SA[i] \) is the index of the \( i \)-th smallest suffix of \( T \), i.e. \( T[SA[i]] \leq \cdots \leq T[SA[n-1]] \). The Burrows-Wheeler Transform, or BWT of \( T \) is a string \( B \) defined as:

\[
B[i] = T[(SA[i] - 1) \mod n]
\]

(1)

The BWT of a string set \( (S_i)_{0 \leq i < m} \) is defined as the BWT of the string \( T = S_0 S_1 \ldots S_{m-1} S_{m-1} \ldots S_0 \), where we define the special terminator symbols \( (S_i)_{0 \leq i < m} \) such that \( S_0 < \cdots < S_{m-1} < c_1 \).

As typical in the treatment of the FM-index [Ferragina and Manzini 2005], we define the following string ranking operation:

\[
rank(c, k, B) = |\{i < k : B[i] = c\}|
\]

(2)

counting the occurrences of a character \( c \) in the prefix \( B[0 \ldots k-1] \).

Similarly to the bwte algorithm, set-bwte partitions the input set of strings in \( K \) blocks \( 0 = j_0 < \cdots < j_K = m \), such that each block \( S_{j_k} = S[j_k, j_{k+1}) \) contains roughly the same amount of suffixes \( M \) and adds each block in turn to the partial BWT of the previously added blocks, \( B_{ext} \). This is done by first computing the SA of the new block to sort the suffixes relative to each other, then ranking the new, sorted suffixes relative to \( B_{ext} \), and finally inserting the corresponding BWT symbols in sorted order. Pseudo-code is given in Algorithm 1.

for each block \( S_{j_k} \) do

\[
\begin{align*}
\text{n} &:= j_{k+1} - j_k; \\
\text{n}_{\text{sufl}} &:= \sum_{P \in S_{j_k}} (1 + |P|) - 1; \\
\text{// build the suffix array of the block } S_{j_k} \\
\text{SA}_{\text{int}}[0 \ldots n_{\text{sufl}}] &:= \text{ConstructSA}(S_{j_k}); \\
\text{// extract the BWT symbols given the SA} \\
\text{B}_{\text{int}}[0 \ldots n_{\text{sufl}}] &:= \text{B}(S_{j_k}, \text{SA}_{\text{int}}); \\
\text{// rank the suffixes of } S_{j_k} \text{ in } B_{\text{ext}} \\
\text{g}[0 \ldots n_{\text{sufl}}] &:= \text{ComputeRanks}(S_{j_k}, B_{\text{ext}}); \\
\text{// reorder } g \text{ by the suffix order} \\
\text{g}_{\text{sa}}[0 \ldots n_{\text{sufl}}] &:= \{g[\text{SA}_{\text{int}}[0]] \ldots g[\text{SA}_{\text{int}}[n_{\text{sufl}}]]\}; \\
\text{// insert the symbols of } B_{\text{int}} \text{ in } B_{\text{ext}} \text{ at } g_{\text{sa}} \\
\text{B}_{\text{ext}} &:= \text{Insert}(B_{\text{int}}, g_{\text{sa}}, B_{\text{ext}}); \\
\end{align*}
\]

Algorithm 1: set-bwte

Notice that the algorithm differs from bwte for some relevant aspects: the first is that, unlike the single-string algorithm which proceeded backwards from the end of the string, in set-bwte the strings are added in a forward loop, starting from the beginning of the string set (though reversal is also possible). This is a crucial difference, allowing the algorithm to be used for adding new strings at any time. This is possible because suffixes have limited length and don’t propagate across block boundaries. The second is that rather than computing the ranks of the old suffixes into the new block, we do the opposite, ranking the new ones relative to the external BWT: this allows to perform only \( O(|B_{ext}|) \) work at each step, as opposed to \( O(|B_{ext}|) \).

3 Suffix Array Construction

Construction of the suffix array of a block of strings can be done with any suffix sorting algorithm. Our implementation uses a massively parallel GPU based MSD radix-sort algorithm that treats strings as long integer keys made of multiple 32-bit words, and sieves unique keys at each iteration in a spirit similar to that of the method described by Larsson and Sadakane [2007]. The algorithm runs entirely...
in GPU memory as the blocks are limited in size. On a Tesla K40, we use blocks of about 250 million symbols.

4 Computing Ranks

Computing the ranks of the suffixes of a string $P$ with respect to the external BWT can be done with an adaptation of Lemma 1 of Ferragina et al. 2012.

Lemma 1 : Let $C[c]$ denote the number of symbols in $B_{ext}$ that are smaller than $c$, and suppose that suffix $P^h$ is lexicographically larger than precisely $i$ suffixes in $B_{ext}$. Then, $P^{k-1}$ is lexicographically larger than precisely $j = C[c] + \text{rank}(c, i, B_{ext})$ suffixes, where $c = P[k - 1]$.

This gives us a simple recipe for a massively parallel implementation of ComputeRanks, in Algorithm 2. Notice that as anticipated this is reversing the roles of the new and old suffixes ($B_{int}$ and $B_{ext}$) in the single-string version of the lemma provided by Ferragina et al. 2012.

Data: a block of $M$ strings $(P_i)_{0 \leq i < M}$; $B_{ext}$
Result: $g[0] + \sum (|P_i| + 1)$
 offsets: $[0..M-1] := \text{prefixsum}(|P_i| + 1)$;
forall the $j$ in $[0..M-1]$
do
\begin{align*}
    k &:= |P_j|; \\
    i &:= n_{ext}; \\
    offset &:= offsets[j]; \\
    g[offset + j + k] &:= i;
\end{align*}
while $k > 0$
do
\begin{align*}
    k &:= k - 1; \\
    c &:= P[k]; \\
    i &:= C[c] + \text{rank}(c, i, B_{ext}); \\
    g[offset + j + k] &:= i;
\end{align*}
end

Algorithm 2: ComputeRanks

5 Insertion

The last step of Algorithm 1 involves inserting the symbols $B_{int}[i]$ at the positions $g[n][i]$ in $B_{ext}$. Unlike Ferragina et al. 2012, who kept $B_{ext}$ on disk and used serial scans to perform the insertions, we keep $B_{ext}$ in system memory (i.e. the most external layer in the random access memory hierarchy of a GPU accelerated system), and employ a new data structure allowing highly parallel insertion.

| Data          | Algorithm   | RAM  | Time  | Throughput |
|---------------|-------------|------|-------|------------|
| NA12878       | beetl-bcr   | 1.8G | 11.2h | 3.1 Mbp/s  |
| NA12878       | ropebw-bcr  | 39.3G| 3.3h  | 10.5 Mbp/s |
| NA12878       | ropebw2     | 34.0G| 5.0h  | 6.9 Mbp/s  |
| NA12878       | nvSetBWT    | 63.8G| 4.1h  | 8.4 Mbp/s  |
| NA12878       | set-bwte    | 78.0G| 1.7h  | 20.4 Mbp/s |
| Venter        | ropebw2     | 22.2G| 1.4h  | 5.4 Mbp/s  |
| Venter        | set-bwte    | 28.6G| 780s  | 35.5 Mbp/s |

Table 1: Benchmarks. Results have been generated on the following hardware: CPU: 24-core Xeon E5-2597-v2 at 2.7Ghz, GPU: NVIDIA Tesla K40, RAM: 128GB.

The data structure is essentially a paged array, with pages containing, at any time, between $p/2$ and $p$ symbols. Together with the actual page storage (allocated from a pool) we keep an index of the pages $P$, and an offset vector $O$ specifying the global offset of the first symbol of each page. The latter allows to efficiently locate all the pages containing all the insertion points with a vectorized binary search. Once such pages are located, they can be assigned to different threads in a pool which take care of inserting the new symbols at the proper place and eventually split them if overflowing. This data structure can be thought of as a flattened B+ tree, where the hierarchy has been removed and replaced by a flat index in order to allow more memory-efficient parallel searches. In our experiments, this provided tenfold speedups on modern multi-core architectures.

In order to facilitate ranking, we incorporate symbol occurrence counters in this paged array. Specifically, we maintain a set of $\sigma$ 64-bit global counters for each page, and a sampled set of relative 32-bit counters within each page. For DNA we use a spacing of 128 symbols (resulting in 1 bit per symbol).

6 Complexity Analysis

In the following, we assume a set of $m$ strings totalling $n$ characters; we further denote with $l$ the average blockwise LCP length, i.e. $l = \text{avg}_{jk}(\text{LCP}(S_{jk}))$; notice that $l$ can be much smaller than the global LCP $L$ if the input is divided in many blocks. Our parallel suffix sorting algorithm has a worst case complexity of $O(ml)$, though typically the average runtime is much better due to our suffix filtering strategy (which prunes sorted suffixes at an exponential rate on random input). Ranking has complexity $O(n)$ and insertion has an asymptotic complexity of $O(n \log(n))$. Hence, the algorithm has a total complexity of $O(ml + n\log(n))$. This is asymptotically lower than the $O(ml + n^2/M)$ limit of Liu et al.’s approach 2014.

In practice, for genomic datasets the $ml$ dependence is rather weak, and the algorithm seems fairly insensitive to the average read length. It has also to be noted that these limits are only asymptotic: for finite $n$ and large block sizes $M$ (i.e. when $K = n/M$ is relatively small), the random bulk insertions touch each page, so that the complexity of insertion is initially proportional to $n^2/M$. The actual cost of ranking is also superlinear in $n$, due to the fact that the memory accesses in $B_{ext}$ become sparser and sparser as $n$ grows. These factors typically dominate the runtime.

The algorithm uses a constant amount of high speed memory, and at most $3n \log(\sigma)$ bits of system memory: $2n \log(\sigma)$ bits for the paged array, and up to $n \log(\sigma)$ bits for the occurrence counters.

7 Results and Discussion

We implemented the algorithm and evaluated its performance on the previously published NA12878 dataset containing 1.2 billion x 101bp human reads DePristo et al. 2011, and the Venter dataset containing 32 million x 875bp Sanger reads. In Table 1 we compared the results to those published by Li 2014 on similar hardware, including four other algorithms: Illumina’s beetle-bcr, implementing 1 for fixed $n$ the quantity $n^2/M$ is in fact an improvement over $pn \log(n)$, if the page size $p$ is larger than $n/M$; this also applies to other paged data structures, such as rope and B+ trees.
For short reads set-bwte is almost 2 times faster than the previously fastest non-incremental algorithm, ropebwt-bcr, and almost 3 times faster than the state-of-the-art incremental algorithm, ropebwt2. For longer reads the gap is even larger, reaching a speedup of 6.5x.

In our implementation, we perform suffix array construction on the GPU and ranking and insertion on the CPU. The three steps plus I/O are performed as stages in a pipeline, where separate CPU threads execute each stage while performing multiple buffering of the outputs (see Figure 1). Thus, I/O, GPU and CPU computations are carefully overlapped. Table 2 reports the average throughputs of the individual stages. For large sets of short reads, on the Xeon E5-2597-v2 system we ran on, ranking was the bottleneck, and overall CPU processing took almost three times as long as the GPU portion. In other words a system with the same GPU and a faster CPU providing higher memory bandwidth could theoretically run almost 3 times as fast.

![Figure 1: Our parallel pipeline visualized as a DAG. The blue boxes are stages performed by the CPU, the green box is performed on the GPU.](image)

| Stage   | Venter  | NA12878 |
|---------|---------|---------|
| Suffix Sorting | 43 Mbp/s | 77 Mbp/s |
| Ranking   | 57 Mbp/s | 37 Mbp/s |
| Insertion | 98 Mbp/s | 44 Mbp/s |

Table 2: Breakdown of the throughputs of the various stages of our pipeline for the NA12878 and Venter datasets.

We would now like to draw the reader’s attention on the fundamental primitives employed by our and other external memory BWT construction algorithms. From a high-level perspective, set-bwte can be thought of as a special form of insertion sort. Specifically, at each iteration the algorithm scatters partially sorted symbols into an external BWT to avoid having to explicitly maintain a full sorting index, which would demand impractical amounts of memory. BCR [Bauer et al. 2011] falls into the same category and could be parallelized in a similar manner (except it requires working with a core dataset of exactly \( m \) suffixes, whereas our algorithm allows for an arbitrary block size). This can be thought of as the dual of the blockwise suffix sorting [Kärkkäinen 2007] skeleton employed by Liu et al. [2014], which gathers sparse input suffixes from system memory. Besides granting a lower asymptotic bound, we empirically observed that the former can be performed more efficiently on contemporary shared memory multi-core architectures, where all cores share the overall memory system’s bandwidth. It has to be pointed out, however, that the latter is more scalable to small clusters, where each node can keep a copy of the entire input string-set and perform gathers independently - whereas scattered insertion in a shared database would necessarily involve inter-node communication. We believe the superior single-node performance and the incremental capability of our algorithm to be interesting tradeoffs against the better inter-node scalability of the slower, non-incremental blockwise suffix sorting algorithms.

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