# External Memory BWT and LCP Computation for Sequence Collections with Applications

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# The problem

Given a collection of strings $S_1$ , $S_2$ , $S_3$ ... $S_k$ compute the BWT and LCP array of the collection.

Mainly interested in the case of many (relatively) short strings, but no limitations on the number of strings and their lengths

# Single string BWT/LCP

$S_1$ = abcab$

| LCP | BWT | suffixes |
|---|---|---|
| | b | $ |
| 0 | c | ab$ |
| 2 | $ | abcab$ |
| 0 | a | b$ |
| 1 | a | bcab$ |
| 0 | b | cab$ |

$S_2$ = aabcabc#

| LCP | BWT | suffixes |
|---|---|---|
| | c | # |
| 0 | # | aabcabc |
| 1 | c | abc# |
| 3 | a | abcabc# |
| 0 | a | bc# |
| 2 | a | bcabc# |
| 0 | b | c# |
| 1 | b | cabc# |

# Multi-String BWT/LCP

$S_1$ = abcab$

$S_2$ = aabcabc#

| LCP | BWT | suffixes |
|---|---|---|
| | b | $ |
| 0 | c | # |
| 0 | # | aabcabc |
| 1 | c | ab$ |
| 2 | c | abc# |
| 3 | $ | abcab$ |
| 5 | a | abcabc# |
| 0 | a | b$ |
| 1 | a | bc# |
| 2 | a | bcab$ |
| 4 | a | bcabc# |
| 0 | b | c# |
| 1 | b | cab$ |
| 3 | b | cabc# |

# The Terminator problem

We cannot use distinct terminators otherwise the alphabet size would blow up. We use the same symbol and keep track of its origin.

Eg: $\$_1 < \$_2 < \$_3 \cdots$

# State of the art

- gSACA+Φ optimal O(n) RAM algorithm: builds Suffix Array, LCP array, uses only 10KB working space [Louza et al 2017]
- BCR+LCP external memory algorithm from BEETL library. Disk I/Os: O(n Maxlen/(B log n)) [Cox et al 2011-2016].

# Our contribution

External memory algorithm taking $O(n \text{ MaxLCP}/(B \log n))$ I/Os

For DNA reads the actual running time is $O(n \text{ AveLCP}/(B \log n))$. In our tests we are faster than BCR+LCP for average length $\geq 300$

# Applications

- Multi-string BWT are used to build a compressed Suffix Array supporting counting queries and more..
- LCP values are used to emulate a Suffix Tree and solve a host of interesting problems:
  - ✔ Mutation detection (previous talk)
  - ✔ Maximal repeats
  - ✔ Suffix-Prefix Overlaps
  - ✔ Many others...

We propose external memory algorithms for computing Maximal repeats, All pairs suffix-prefix overlaps, and succinct De Bruijn graphs.

The challenge was to transform internal memory Suffix Tree algorithms into external memory algorithms working on BWT and LCP arrays.

# Algorithm outline

- Split the input into chunks that fit in RAM and compute BWT of each chunk using Louza et al. optimal algorithm
- Merge the BWTs in external memory and compute the LCP values using a modified H&M algorithm.
- Sort the LCP values in external memory using standard multiway merge

# Merging BWTs

| BWT | suffixes |
|---|---|
| b | $ |
| c | ab$ |
| $ | abcab$ |
| a | b$ |
| a | bcab$ |
| b | cab$ |

$S_1$ = abcab$

+

| BWT | suffixes |
|---|---|
| c | # |
| # | aabcabc |
| c | abc# |
| a | abcabc# |
| a | bc# |
| a | bcabc# |
| b | c# |
| b | cabc# |

$S_2$ = aabcabc#

=

| BWT | suffixes |
|---|---|
| b | $ |
| c | # |
| # | aabcabc |
| c | ab$ |
| c | abc# |
| $ | abcab$ |
| a | abcabc# |
| a | b$ |
| a | bc# |
| a | bcab$ |
| a | bcabc# |
| b | c# |
| b | cab$ |
| b | cabc# |

# The H&M algorithm

Holt and McMillan [Bioinformatics 2014] proposed a simple and elegant algorithm to merge BWTs in small space

The idea is to compute the bounded context BWT for context size 0,1,2,…

# Context size: 0

| | |
|---|---|
| b | $ |
| c | ab$ |
| $ | abcab$ |
| a | b$ |
| a | bcab$ |
| b | cab$ |

+

| | |
|---|---|
| c | # |
| # | aabcabc |
| c | abc# |
| a | abcabc# |
| a | bc# |
| a | bcabc# |
| b | c# |
| b | cabc# |

=

| Z | BWT | |
|---|---|---|
| 0 | b | $ |
| 0 | c | ab$ |
| 0 | $ | abcab$ |
| 0 | a | b$ |
| 0 | a | bcab$ |
| 0 | b | cab$ |
| 1 | c | # |
| 1 | # | aabcabc |
| 1 | c | aabc# |
| 1 | a | abcabc# |
| 1 | a | bc# |
| 1 | a | bcabc# |
| 1 | b | c# |
| 1 | b | cabc# |

We represent the merged BWT
with the array Z

# Context size: 1

| | |
|---|---|
| b | $ |
| c | ab$ |
| $ | abcab$ |
| a | b$ |
| a | bcab$ |
| b | cab$ |

+

| | |
|---|---|
| c | # |
| # | aabcabc |
| c | abc# |
| a | abcabc# |
| a | bc# |
| a | bcabc# |
| b | c# |
| b | cabc# |

=

| Z | BWT | |
|---|---|---|
| 0 | b | $ |
| 1 | c | # |
| 0 | c | ab$ |
| 0 | $ | abcab$ |
| 1 | # | aabcabc |
| 1 | c | aabc# |
| 1 | a | abcabc# |
| 0 | a | b$ |
| 0 | a | bcab$ |
| 1 | a | bc# |
| 1 | a | bcabc# |
| 0 | b | cab$ |
| 1 | b | c# |
| 1 | b | cabc# |

We represent the merged BWT
with the array Z

# Context size: 2

| | |
|---|---|
| b | $ |
| c | ab$ |
| $ | abcab$ |
| a | b$ |
| a | bcab$ |
| b | cab$ |

+

| | |
|---|---|
| c | # |
| # | aabcabc |
| c | abc# |
| a | abcabc# |
| a | bc# |
| a | bcabc# |
| b | c# |
| b | cabc# |

=

| Z | BWT | |
|---|---|---|
| 0 | b | $ |
| 1 | c | # |
| 1 | # | aabcabc |
| 1 | c | aabc# |
| 0 | c | ab$ |
| 0 | $ | abcab$ |
| 1 | a | abcabc# |
| 0 | a | b$ |
| 0 | a | bcab$ |
| 1 | a | bc# |
| 1 | a | bcabc# |
| 1 | b | c# |
| 0 | b | cab$ |
| 1 | b | cabc# |

We represent the merged BWT with the array Z

# Context size: 2

| | |
|---|---|
| b | $ |
| c | ab$ |
| $ | abcab$ |
| a | b$ |
| a | bcab$ |
| b | cab$ |

+

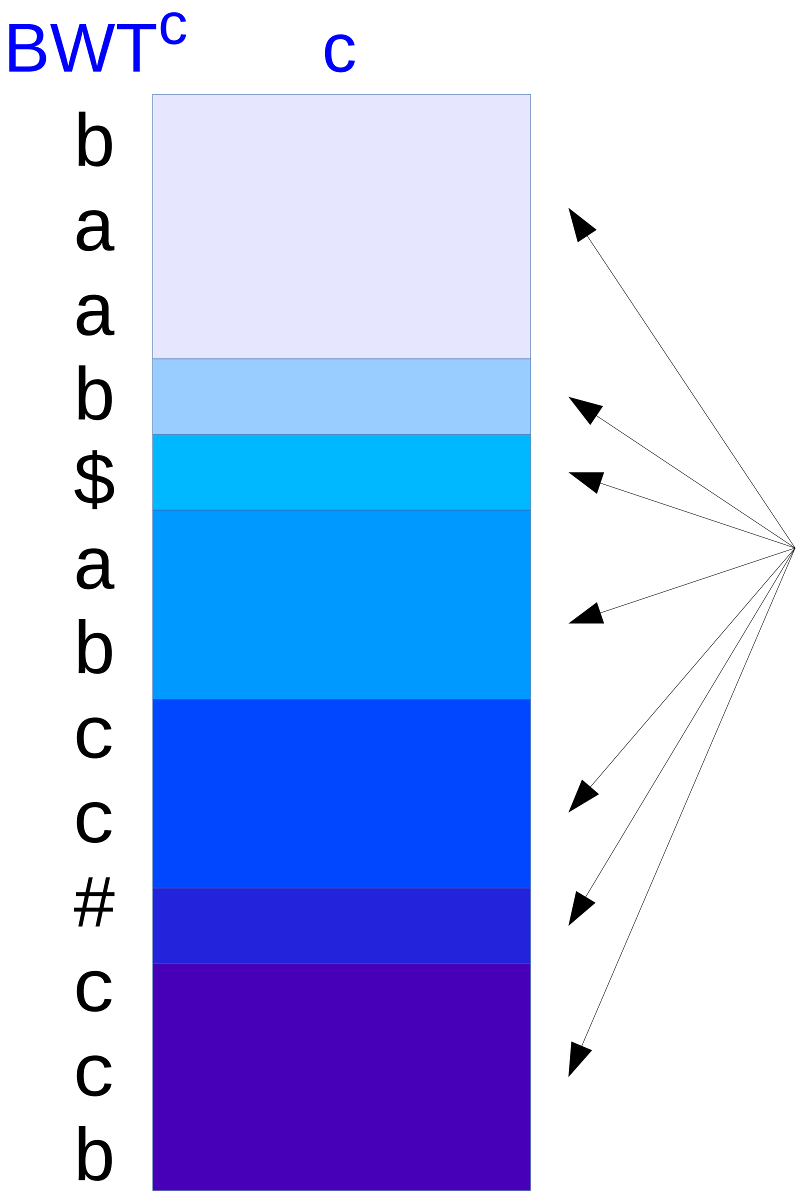
| | |
|---|---|
| c | # |
| # | aabcabc |
| c | abc# |
| a | abcabc# |
| a | bc# |
| a | bcabc# |
| b | c# |
| b | cabc# |

=

| Z | BWT | |
|---|---|---|
| 0 | b | $ |
| 1 | c | # |
| 1 | # | aabcabc |
| 1 | c | aabc# |
| 0 | c | ab$ |
| 0 | $ | abcab$ |
| 1 | a | abcabc# |
| 0 | a | b$ |
| 0 | a | bcab$ |
| 1 | a | bc# |
| 1 | a | bcabc# |
| 1 | b | c# |
| 0 | b | cab$ |
| 1 | b | cabc# |

The H&M algorithm only uses $BWT_0$ $BWT_1$ and Z

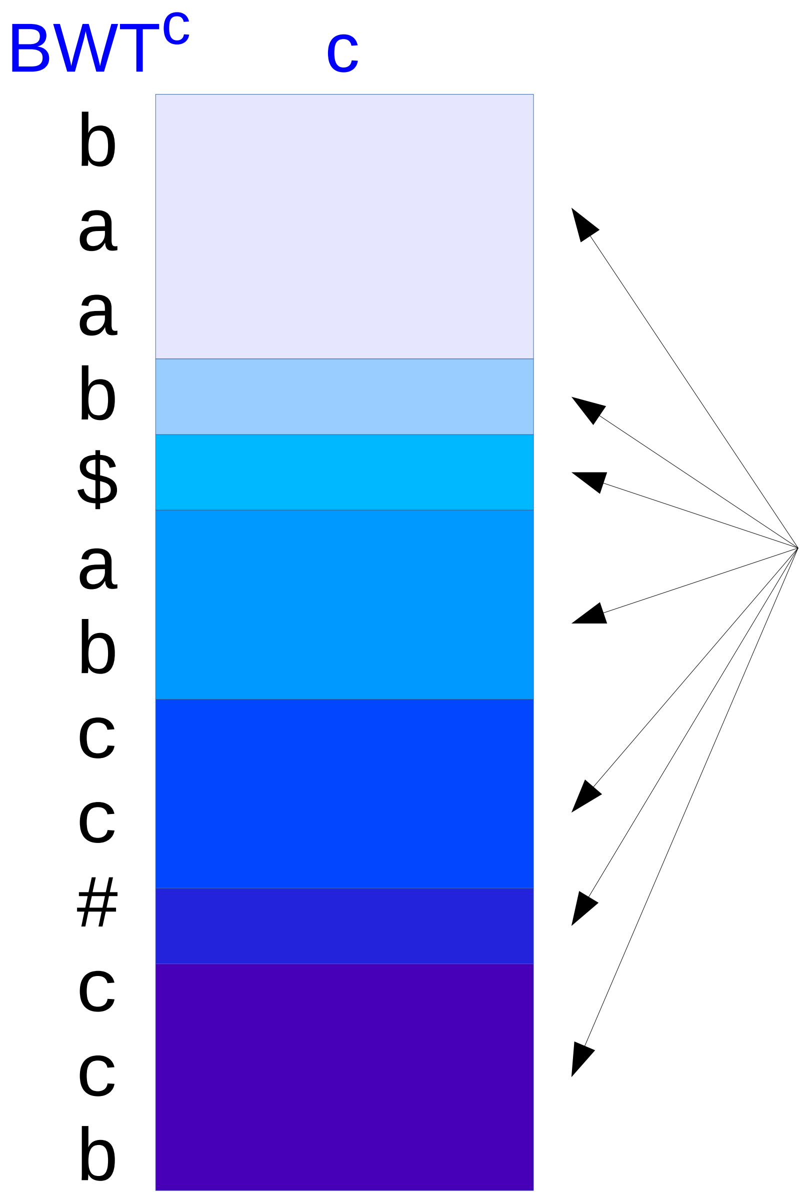
# Computing LCP values




At iteration c a block is a set of suffixes sharing a length-c prefix

Each iteration reorders suffixes within a block and creates new blocks splitting old ones

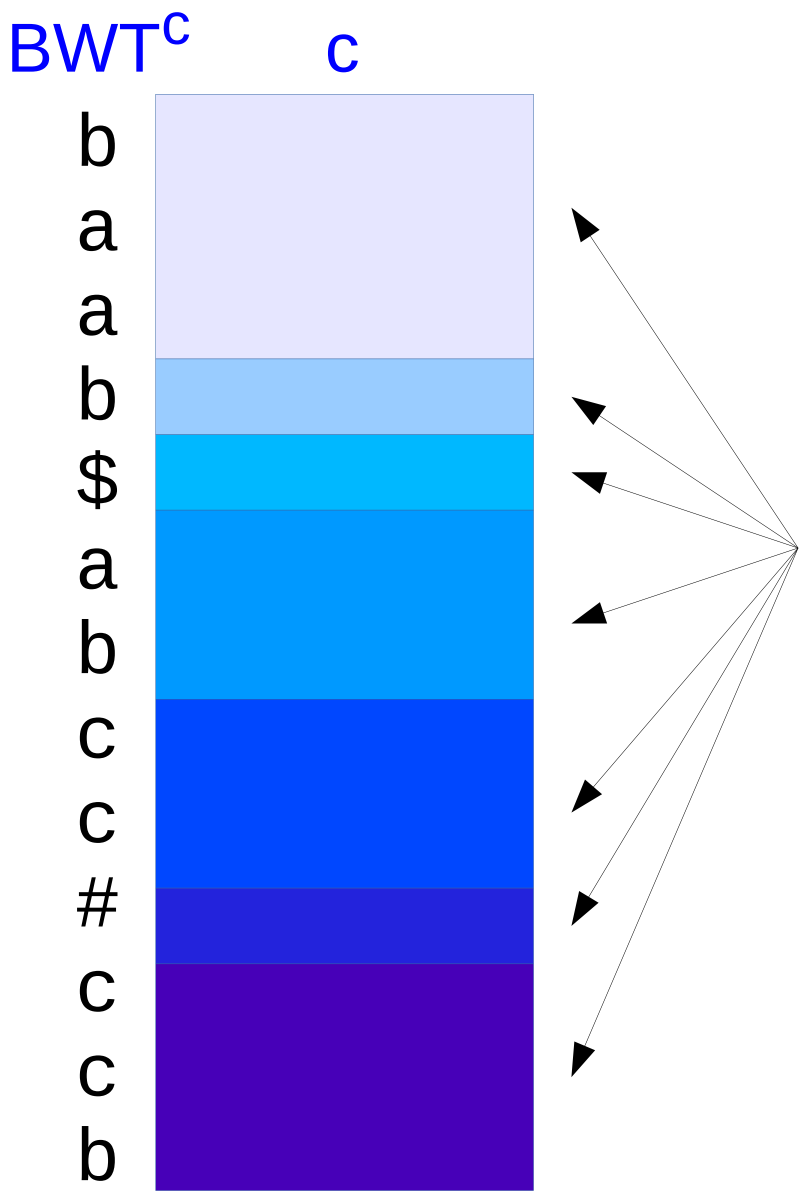
# Computing LCP values




We can prove that if we split a block at iteration c+1 the LCP value for the position where the splitting occurs is c.

- During the merging we “discover” larger and larger LCP values
- Each time a LCP value is discovered we write to file the pair <position, LCP>
- When the merging is done, we sort the pairs by position and save the resulting LCP values

# When to stop?




At iteration c a block is a set of suffixes sharing a length-c prefix

Each iteration reorders suffixes within a block and creates new blocks splitting old ones

# Running time

- When all the blocks have size 1 the merging is done and all LCP values have been computed
- The resulting algorithm takes O(n MaxLCP) time and O(n MaxLCP/(B log n)) I/Os
- A simple heuristic (skipping ranges of size-1 blocks) makes the I/O complexity in practice closer to O(n AveLCP/(B log n)) I/Os

# Experimental results

- External memory algorithms should be tested using RAM much smaller than input size
- The RAM should be limited at boot time, otherwise the OS will use the extra RAM to avoid disk transfers
- We have compared our algorithm (eGap) with the state of the art for external memory (BCR+LCP)

| Name | Size GB | $\sigma$ | N. of strings | Max Len | Ave Len | Max LCP | Ave LCP |
|---|---|---|---|---|---|---|---|
| shortreads | 8.0 | 6 | 85,899,345 | 100 | 100 | 99 | 27.90 |
| longreads | 8.0 | 5 | 28,633,115 | 300 | 300 | 299 | 90.28 |
| pacbio.1000 | 8.0 | 5 | 8,589,934 | 1,000 | 1,000 | 876 | 18.05 |
| pacbio | 8.0 | 5 | 942,248 | 71,561 | 9,116 | 3,084 | 18.32 |

Collections

| Name | eGap | | | BCR+LCP | | |
|---|---|---|---|---|---|---|
| | 1GB | 8GB | 32GB | 1GB | 8GB | 32GB |
| shortreads | 17.19 | 3.76 | 2.87 | $\times$ | 5.65 | 3.96 |
| longreads | 52.39 | 9.75 | 6.76 | 18.54 | 16.01 | 10.88 |
| pacbio.1000 | 24.88 | 3.54 | 1.81 | $\times$ | 54.00 | 36.96 |
| pacbio | 23.43 | 3.42 | 1.82 | $> 70$ | $> 50$ | $> 50$ |

Running time in µsecs x symb

# Observations

- eGap is faster for datasets with longer reads
- eGap running time appears to be related to AveLCP rather than MaxLCP
- eGap is better at exploiting all the available RAM
- More experiments required ...

# Summing Up

- We propose an external memory algorithm which is faster than the state of the art for long reads
- In addition to BWT and LCP our algorithm can produce the Document Array and the useful xlcp bit array (see paper)
- Using these additional arrays we can compute maximal repeats, suffix-prefix overlaps and compact DB-graphs efficiently in external memory