A Framework for Reproducible Parallel DNA String Matching

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Abstract: In this paper, we propose an output reproducible framework that executes parallel sequence comparison algorithms, computing the edit distance. The framework generates tables/graphics and linear regressions that can be used to predict the execution times. We also propose parallel OpenMP versions of serial algorithms (DP and UK) used to compute the edit distance. Our parallel DP is antidiagonal block-based, where the blocks that belong to the same set of antidiagonals are assigned to different threads, which compute them simultaneously. Due to data dependencies presented by UK, we opted to compute each antidiagonal in parallel. Our results with synthetic and real sequences show that the parallel UK version presents the best execution times in most cases. We also show that the linear regressions generated by our tool have errors below 10%, on average.

1 INTRODUCTION

Even though reproducibility is a key concept in science, it is often neglected. According to (Gundersen, 2021), there are three different types of reproducibility: (a) outcome: the outcome of the reproducibility experiment is the same as the output of the original experiment; (b) analysis: the outputs are not the same but the same analysis can be made; (c) interpretation: neither the outputs nor the analyses are the same but the same conclusion can be reached. Recently, a lot of effort has been made in reproducibility, since it has a direct impact on the results' reliability. Besides being able to reproduce results, other functionalities are important, such as expressiveness and prediction (Wratten et al., 2021). We claim that scientific experiments should be at least outcome reproducible, with tools that provide ease of use and expressiveness.

The growth of massive amounts of biological data has created an increasing demand for tools to assist researchers in analyzing these data. The use of these computational tools can improve confidence in published results, allow double-checking them by other researchers, and facilitate redoing the entire experiment. Therefore, in order to ease replication efforts, there is a need for more openly available tools.

There are many bioinformatics frameworks available, such as Bioconductor (Huber et al., 2015), Galaxy (Price et al., 2024), and Biopython (Cock et al., 2009). Although these frameworks have a set of features like maturity, extensibility and high modularity, they are not focused on parallel algorithms. In particular, Bioconductor is a widely used framework for the analysis of high-throughput genomic data and it is based on the R programming language. Galaxy is a web-based platform for managing bioinformatics workflows with great focus on training and education. Biopython is a set of tools for biological computation written in Python to interact with biological databases and integrate with other bioinformatics tools.

In order to generate results easily and make the execution of experiments reproducible, we designed a reproducible framework that executes a given algorithm multiple times, varying the parameters required by the execution scenarios. At the end of the execution, the framework generates several graphics and presents them to the user. Besides that, the tool has a module that generates linear regressions, which can be used for execution time prediction.

As a case study, we chose the Approximate String Matching (ASM) problem. ASM computes the similarity degree between two strings, where a high similarity degree means very few differences (Hall and Dowling, 1980). For ASM, the most widely used metric is the edit distance or Levenshtein distance (Levenshtein, 1966), which determines the minimum number of operations needed to transform one string into another. Since the 1970s, the ASM problem is formulated as dynamic programming (DP) (Wagner and Fischer, 1974; Sellers, 1974) and this is the most used

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approach (Berger et al., 2021). In this case, a DP matrix is computed with size $n \times m$, where n and m are the lengths of the sequences.

In this paper, we deal with unrestricted ASM algorithms, which do not restrict the problem to a maximum error k nor do not limit the size of one of the strings. The algorithms considered are DP (Wagner and Fischer, 1974) and UK (Ukkonen, 1983). In particular, UK is an algorithm with pruning, i.e., it does not compute the entire DP matrix in most cases. In practice, string matching has many applications beyond text search such as: computational biology, pattern recognition, computer vision, among others. In this paper, we will focus on computational biology.

Sequence alignment algorithms, such as Smith-Waterman and Needleman-Wunsch, are also used in many tools (Figueiredo et al., 2021; Schmidt et al., 2024) and they compute differently the DP matrix. Even though there are widely used, they are outside the scope of this paper.

We propose a reproducibility framework and parallel implementations for the algorithms DP and UK, using the OpenMP programming interface. Parallel DP is a block-based approach which always computes the entire DP matrix. Parallel UK has pruning capabilities computing, on the average case, much less than DP.

Our results show that, depending on the dissimilarity between the sequences and their lengths, one algorithm performs better than the other. For the synthetic sequences compared, Parallel UK performed better in most cases. For the real SARS-CoV-2 DNA sequences case study, Parallel UK also performed better than DP in most comparisons. This happened because the sequences have low dissimilarity and are considerably long.

The remainder of this paper is organized as follows. Section 2 presents the ASM problem and the DP and UK algorithms used to solve it. Section 3 presents the design of our reproducible framework and the parallel algorithms integrated to it. Section 4, experimental results are presented for synthetic sequences and real SARS-CoV-2 DNA sequences. Finally, Section 5 concludes the paper.

2 APPROXIMATE STRING MATCHING (ASM)

2.1 Overview

String matching is a classical problem involving strings that searches for occurrences of a pattern P in a text T (Navarro, 2001). Exact string matching finds the exact pattern P in text T whereas Approximate String Matching is an approach of finding strings that match P approximately, i.e., allowing errors.

For ASM, the alphabet is defined as a finite set of symbols (characters) and represented by Σ, where $|\Sigma|$ denotes the length of the alphabet. For comparing DNA sequences, the alphabet is $\Sigma = \{A, T, G, C\}$ and $|\Sigma| = 4$. For computational biology ASM applications, the term *sequence* is used instead of *string* and the character that occurs in position i of T (or P) is denoted by T_i (or P_i).

The goal of ASM is to find approximate occurrences (matchings) of P (called P') in T when a certain tolerance is allowed and a degree of similarity is enough to satisfy the match ($P \approx P'$).

ASM algorithms use a distance function $d(T,P)$, for measuring the similarity of two strings (Navarro, 2001). One of the most widely used distance functions is the edit distance or Levenshtein distance (Levenshtein, 1966). The metric $ed(T,P)$ computes the minimal number of operations that are executed in P in order to obtain $P = P'$. The operations are: (i) insertion, when P'_i has an extra character, i.e. $P_i = \varepsilon$, where ε corresponds to the empty string; (ii) deletion, when P has an extra character, i.e. $P'_i = \varepsilon$; (iii) substitution, when P_i and P'_i have different characters.

		C	T	T	A	G	T
	0	0	0	0	0	0	0
C	1	0	1	1	1	1	1
T	2	1	0	1	2	2	1
A	3	2	1	1	1	2	2
C	4	3	2	2	2	2	3
T	5	4	3	2	3	3	2

(a)

$d \downarrow$ / $e \rightarrow$	-2	-1	0	1	2	3
-4	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	3
-3	$-\infty$	$-\infty$	$-\infty$	$-\infty$	2	
-2	$-\infty$	$-\infty$	$-\infty$	1	5	
-1	$-\infty$	$-\infty$	0	3	4	
0	$-\infty$	-1	2	3	4	
1	$-\infty$	$-\infty$	-1	3	5	
2	$-\infty$	$-\infty$	$-\infty$	-1	3	
3	$-\infty$	$-\infty$	$-\infty$	$-\infty$	-1	
4	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	-1

(b)

Figure 1: (a) DP matrix with edit distance highlighted at bottom-right corner and (b) UK matrix with edit distance highlighted at row $n - m$.

2.2 Algorithm DP (Wagner & Fischer 1974)

The DP algorithm (Wagner and Fischer, 1974) is based on dynamic programming (DP). It compares two strings T and P with m and n characters, respectively, by computing a DP matrix C of size $(m+1, n+1)$. To create the DP matrix, the first DP cell is set to zero ($C_{0,0} = 0$). Then, the cells which belong to the first row are initialized with column index (j) and the cells belonging to the first column are initialized with (i). The remaining values are calculated with Equation 1. Time complexity of DP is $O(mn)$. In the case of a match (i.e., the characters T_i and P_j, are the same) $\delta(x_i, y_i) = 0$; and $\delta(x_i, y_i) = 1$, otherwise.

$$C_{i,j} = \min \begin{cases} C_{i-1,j-1} + \delta(x_i, y_i), \\ C_{i-1,j} + 1 \\ C_{i,j-1} + 1 \end{cases} \tag{1}$$

Figure 1(a) presents matrix C produced by Algorithm DP when comparing strings $T = CTTAGT$ and $P = CTACT$. In this case, the edit distance is 2.

2.3 Algorithm UK (Ukkonen, 1983)

Ukkonen's algorithm (Ukkonen, 1983) (UK) is based on theoretical properties of the DP matrix computation when the metric used is edit distance. Ukkonen noticed that the diagonals values of the DP matrix increase monotonically from the upper-left to the lower-right cells, i.e., the values of adjacent cells can differ at most by one: $0 \leq C_{i,j} - C_{i-1,j-1} \leq 1$.

Hence, in his algorithm a new matrix L is build based on this property since it is only necessary to store the information about the position of the diagonal where the value is incremented. $L(d,e)$ is calculated, where d corresponds to the diagonal and e is the edit distance computed so far, i. e., the maximum row number of the DP matrix where the value e occurs in a given diagonal d. In the initialization step, $L(d,|d|-1) = |d|-1$ when $d < 0$, $L(d,|d|-1) = -1$ when $d \geq 0$ and $L(d,e) = -\infty$ when $e < d$. The remaining values of L are calculated after obtaining the maximum of the three previously defined values (upper-left diagonal, left and bottom-left diagonal elements) and then increasing the value while a match occurs between T_i and P_j. Time complexity of UK is $O(ed(T,P).min(m,n))$, where ed is the edit distance between T and P.

Figure 1(b) presents the L matrix for comparing strings $T = CTTAGT$ and $P = CTACT$. In this case, the edit distance is 2, i.e., the row where the maximum value (5) occurs in matrix C.

3 REPRODUCIBILITY FRAMEWORK

In Section 3.1 we propose our reproducibility framework to execute the parallel algorithms. Sections 3.2 and 3.3 describe the parallel versions.

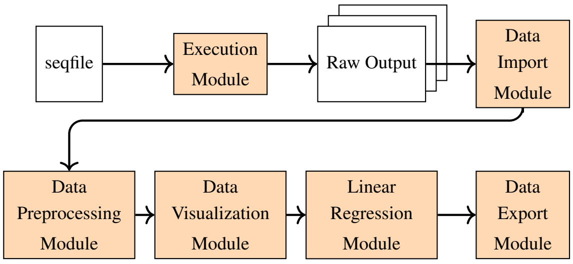


Figure 2: Reproducibility Framework.

3.1 Reproducibility Framework

We designed a reproducibility framework that automatically executes the experiments, collects the results and runs statistical analysis. The framework was developed using IPython Notebook (Pérez and Granger, 2007), a computational workbook environment for running Python. Furthermore, it provides features such as the ability to run code in a cell-by-cell basis and a collection of libraries. In particular, we make use of the Numerical Python library (NumPy) and the Matplotlib library.

In order to start the framework execution (Figure 2), a text file containing a list of FASTA files to be compared (seqfile) and a set of parameters should be provided as input for the execution module.

As input parameters, the Execution Module (Algorithm 1) receives (a) the names of files containing all pairs of sequences to be compared (seqfile); (b) the algorithm (DP, UK or both); (c) the number of threads (may be a range); (d) the number of repetitions for each execution; and (e) the block size, needed for running parallel DP. Every time the execution module runs the algorithm, the output is appended to an output file. The details of how the algorithms are executed are shown in Algorithm 1 and a sample seqfile can be seen in Table 1.

Algorithm 1: Execution module pseudocode.

```
for 1 to THREAD_QUANTITY do
    for each SEQFILE do
        Create temporary output directory
        for each SEQUENCE_PAIR do
            for each ALGORITHM do
                Create the output file
                for 1 to REPEATS do
                    Execute algorithm
                    Append the output to file
                end for
            end for
        end for
    end for
end for
```

The Data Import Module reads the output files in

Table 1: A seqfile consists of a list of pairs of FASTA files containning the sequences to be compared.

"./data/NC_045512.2.fasta" , "./data/OP537480.1.fasta"
"./data/NC_045512.2.fasta" , "./data/OP809597.1.fasta"
"./data/NC_045512.2.fasta" , "./data/OP883605.1.fasta"
"./data/NC_045512.2.fasta" , "./data/OQ026463.1.fasta"
"./data/NC_045512.2.fasta" , "./data/OQ050253.1.fasta"

raw format from the Execution Module and parses them to a structured format. This module is also responsible to detect errors in the output files such as missing values or inconsistent data due possible file corruption, i.e., it is important to ensure the correctness of the data before proceeding to the next steps.

In the Data Preprocessing Module, the framework performs operations such as: filtering, to remove data that is not relevant for the analysis; splitting, to separate the data in different categories; and grouping, to organize and summarize sets of data. These operations are necessary to help the user to identify patterns and trends in the data.

The Data Visualization Module generates comparison tables and heatmaps from the processed data. Heatmaps are useful to visualize the execution times of the algorithms, where the color intensity is proportional to the execution time. A table can be constructed using colors to identify and categorize data with particular properties.

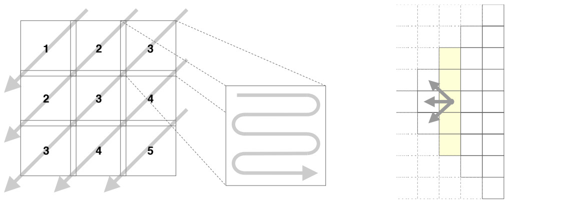
The linear regression models calculated with the data collected in the experiments can help to predict the execution times of future experiments. Besides the regression equation, it also outputs other statistical measures, such as the p-value, the standard error of the estimate, and the R^2 coefficient of determination.

The Data Export Module saves the processed data in human friendly formats. In addition to CVS, it is also possible to export in LaTex and Excel formats. These formats can be easily imported into other tools for further analysis.

3.2 Parallel DP Design

In the DP algorithm (Section 2.2), the dependencies for cell (i, j) are $(i-1, j-1)$, $(i, j-1)$ and $(i-1, j)$ (Equation 1). So, all elements of antidiagonal d may be computed in parallel, as soon as antidiagonal $d-1$ is computed. However, depending on the size of the matrix, the parallelism obtained when computing the antidiagonalis in parallel may be small. In order to increase the parallelism, we use a block-based approach, which considers blocks of antidiagonals. In this case, each thread computes a block sequentially, in parallel with the other threads (Figure 3a).

The DP matrix is divided into blocks of cells and each block is assigned to a thread. When a thread finishes to compute a blocked antidiagonal, the last row and the last column of each block are used as initial values to the computation of the next antidiagonal. Since the blocks are computed in an antidiagonal fashion, the first block to be computed is the one in the upper-left corner of the matrix (antidiagonal 1) and the last one is the one in the lower-right corner (antidiagonal 5).



(a) Parallel DP (b) Parallel UK

Figure 3: (a) Parallel DP: blocks are computed by antidiagonal, but each block submatrix is computed sequentially. (b) Parallel UK: the cells of each column are computed in parallel.

Algorithm 2: Parallel DP pseudocode.

1: **do in parallel** num_threads
2: initialize DP matrix
3: split DP matrix in blocks
4: **do in parallel** num_threads
5: **for each** tile **do**
6: execute dp in block
7: **end for**
8: **return** score

Algorithm 2 presents Parallel DP. In the initialization phase (lines 1-2), the OpenMP directive PARALLEL FOR is used to parallelize the loops that initialize the DP matrix. In the execution phase (lines 3-7), the DP matrix is divided into square blocks of specified size and then the inner loop (lines 5-6) is responsible to compute each block among the threads using the recurrence relation shown in Equation 1.

3.3 Parallel UK Design

In Parallel UK, we opted to compute each row in the L matrix in parallel, since cells ranging from $-e \leq d \leq +e$ can be calculated independently. This happens because, in UK, the computation of each cell depends on the values of three cells from the previous column: upper-left cell, left cell and bottom-left cell (Figure 3b).

Algorithm 3 presents Parallel UK. Lines 1-2 initialize the UK matrix in parallel by filling the upper and lower diagonals of the triangular shaped matrix. Lines 3-11 show the execution loop, executed in parallel with *num_threads* until the algorithm reaches a

Algorithm 3: Parallel UK pseudocode.

```
1:  do in parallel num_threads
2:      initialize UK matrix
3:  do in parallel num_threads
4:      for each column e do
5:          for each row d do
6:              calculate column d,e
7:              if score is found then break
8:          end for
9:      end for
10: return score
```

stop condition (line 7). Line 10 returns the calculated score.

4 EXPERIMENTAL RESULTS

Parallel DP (Section 3.2) and Parallel UK (Sections 3.3) were implemented in C++ and OpenMP 5.3, compiled with the GNU g++ compiler version 11.3.0 with no optmization flag. The reproducibility framework was implemented in Python. Our experiments were collected in a desktop with an Intel Core i5-8400 Coffee Lake 2.8GHz (6 cores) with 32GB of RAM running Ubuntu Linux 22.04. In the experiments, we used synthetic and real DNA sequences.

Table 2: Execution times (ms) for synthetic sequences (serial).

SERIAL EXEC TIME (ms)								
SIZE	1000		5000		10000		30000	
DISS	DP	UK	DP	UK	DP	UK	DP	UK
0	16.35	0.03	401.70	0.22	1606.58	0.46	14469.48	2.44
10	18.16	0.97	443.95	23.33	1763.24	93.47	15864.51	945.74
20	19.71	2.50	482.17	61.64	1917.30	263.00	17374.97	2633.44
30	21.05	4.48	519.32	119.76	2075.56	499.06	18674.96	5081.58
40	23.08	7.00	569.53	190.72	2244.12	793.45	20205.88	8291.49
50	25.10	10.02	595.86	285.13	2394.99	1154.82	21417.63	12258.71
60	26.64	13.59	608.32	391.16	2401.68	1608.85	21651.17	17578.00
70	25.20	17.94	589.80	513.59	2358.90	2116.55	21421.84	25229.88
80	23.38	21.99	581.76	639.51	2323.62	2642.07	20930.05	33539.03
90	24.46	26.31	573.97	750.47	2296.81	3130.46	20650.92	44322.13
100	23.35	31.92	567.29	874.63	2269.18	3697.26	20419.64	56972.07

Table 3: Execution times (ms) for synthetic sequences using 6 threads.

PARALLEL EXEC TIME (ms)								
SIZE	1000		5000		10000		30000	
DISS	DP	UK	DP	UK	DP	UK	DP	UK
0	4.22	0.19	79.65	0.41	307.39	0.65	2732.26	1.36
10	4.59	0.59	86.80	7.59	335.41	27.34	2990.96	238.81
20	4.97	1.07	93.82	16.58	363.25	63.09	3239.56	578.72
30	5.31	1.63	100.42	27.48	388.80	106.05	3474.35	1080.48
40	5.58	2.19	106.04	39.89	411.19	157.17	3690.27	1695.99
50	5.83	3.14	110.58	62.48	429.37	252.04	3838.69	2893.79
60	5.98	3.89	113.86	76.36	441.89	312.80	3962.96	3591.24
70	6.14	4.76	115.74	98.63	448.95	418.16	4032.16	5153.66
80	6.10	5.58	116.14	117.35	451.16	508.86	4057.45	6837.91
90	6.96	6.11	116.07	129.09	450.75	562.42	4065.38	8749.73
100	6.21	7.09	115.98	148.71	449.58	643.70	4060.20	11281.79

4.1 Results with Synthetic Sequences

The synthetic sequences were generated using 'A' characters as the reference text and sequences with random replacements by the character '.', depending on the chosen dissimilarity. We generated sequences of the following lengths: 1000, 2000, 5000, 10000, and 30000 characters, increasing the dissimilarity between them varying from 0% (identical sequences) to 100% (totally different sequences). Each experiment was executed n times, depending in the value provided in for the script's input parameter (Section 3.1).

The results from the experiments conducted using synthetic sequences can be seen in Tables 2 and 3, with the heatmaps generated by our reproducibility tool. The tables present (a) the dissimilarity between the sequences, and (b) the total time (sum of initialization time and execution time) for each comparison as a result of running serial and parallel versions, respectively.

In this case, by analyzing the execution times, we were able to split them into two zones where the colors indicate the performance of one algorithm in relation to the other: (a) the green zone, where UK had better performance than DP; and (b) the yellow zone, where DP had better performance than UK. Considering the comparison between DP and UK, the serial and parallel versions present similar behavior. It can be seen that UK outperforms DP in most of the comparisons, achieving the best execution time for sequences with dissimilarity $\leq 60\%$.

Figure 4 presents the graphic of execution time generated by our framework.

The speedup achieved by parallel DP and parallel UK is shown in Table 4. The speedup is calculated as the ratio between the execution time of the serial implementation and the parallel one, with 6 threads (one thread running on each CPU core). It can be seen that Parallel UK has low speedup with 0% dissimilarity. This happens because the serial execution time is very low (e.g. 0.03ms for sequences of size 1000). On the other cases, very good speedups are obtained for both Parallel DP and Parallel UK.

4.2 Linear Regression Analysis

The prediction of the execution time of parallel sequence comparison applications is very important, specially when a great number of comparisons need to be made. In this context, our reproducible tool generates linear regressions that can be used for execution time prediction.

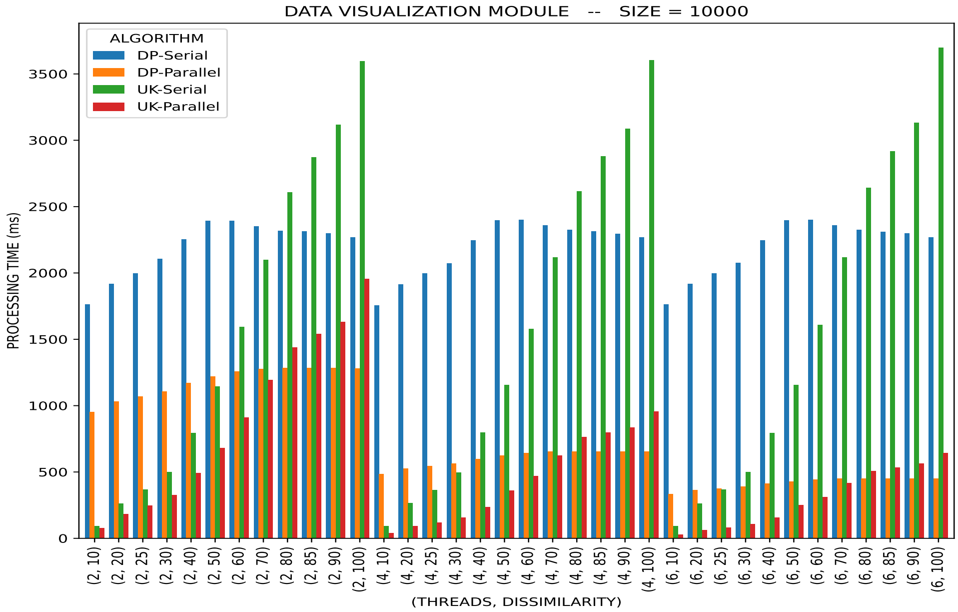


Figure 4: Execution times (ms) for comparing sequences of size 10000.

Table 4: Speedups for synthetic sequences.

SPEED-UP (SERIAL/PARALLEL)								
SIZE	1000		5000		10000		30000	
DISS	DP	UK	DP	UK	DP	UK	DP	UK
0	3.87×	0.16×	5.04×	0.54×	5.23×	0.71×	5.30×	1.79×
10	3.96×	1.64×	5.11×	3.07×	5.26×	3.42×	5.30×	3.96×
20	3.97×	2.34×	5.14×	3.72×	5.28×	4.17×	5.36×	4.55×
30	3.96×	2.75×	5.17×	4.36×	5.34×	4.71×	5.38×	4.70×
40	4.14×	3.20×	5.37×	4.78×	5.46×	5.05×	5.48×	4.89×
50	4.31×	3.19×	5.39×	4.56×	5.58×	4.58×	5.58×	4.24×
60	4.45×	3.49×	5.34×	5.12×	5.44×	5.14×	5.46×	4.89×
70	4.10×	3.77×	5.10×	5.21×	5.25×	5.06×	5.31×	4.90×
80	3.83×	3.94×	5.01×	5.45×	5.15×	5.19×	5.16×	4.90×
90	3.51×	4.31×	4.95×	5.81×	5.10×	5.57×	5.08×	5.07×
100	3.76×	4.50×	4.89×	5.88×	5.05×	5.74×	5.03×	5.05×

We opted to use multilinear regression models to empirically estimate the execution time for different input sizes, dissimilarity values and number of threads, as shown in Equation 2.

$$\begin{aligned}\ln(\mathrm{TIME}) = a \; & + \; b_1 \times \ln(\mathrm{SIZE}) \\ & + \; b_2 \times \mathrm{DISS} \\ & + \; b_3 \times \mathrm{THREADS}\end{aligned} \tag{2}$$

where TIME is the dependent variable that corresponds to the execution time (ms), a is the y-intersect, b_i are the regression coefficients, and the independent variables are the SIZE (input size), DISS (dissimilarity value in percentage), and THREADS (number of threads used in the execution).

This linear regression model was used for the serial and parallel versions of DP and UK. In each case, the training used 77% of the data and the testing was made with the remaining 23%. For training, we have used pre-defined lengths for input sizes (1000, 2000, 10000, 30000), dissimilarity values (10%, 20%, 30%, 40%, 50%, 60%, 70%, 80%, 90%, 100%), and number of threads (2, 4, 6). For prediction, we have used the same values for number of threads (2, 4, 6), with lengths 2500, 7500, 15000, 25000 for for input sizes and values 25%, 45% and 85% for dissimilarity.

For the DP algorithm, the execution time was predicted using the following linear regression equations:

- Serial DP linear regression:

$$\begin{aligned}\ln(y) &= 2.97 + 1.99 \times \ln(\mathrm{SIZE}) + 0.25 \times \mathrm{DISS}; \\ R^2 &= 0.999\end{aligned}$$

- Parallel DP linear regression:

$$\begin{aligned}\ln(y) &= 2.85 + 1.94 \times \ln(\mathrm{SIZE}) + 0.32 \times \mathrm{DISS} \\ &\quad -0.24 \times \mathrm{THREADS}; \\ R^2 &= 0.998\end{aligned}$$

Table 5 presents the DP prediction results for 2, 4, 6 threads (TH), with sequence lengths 2500 and 15000 and dissimilarities 25%, 45% and 85%. In the table, the lowest error is marked in bold and the highest error is underlined. It can be seen that our equations provide a quite accurate prediction, with all errors below 15%. For the serial DP, most of the errors are below 5% whereas most errors for parallel DP are below 10%.

The execution time of the UK algorithm was predicted using the following linear regression equations:

- Serial UK linear regression:

$$\begin{aligned}\ln(y) &= 0.05 + 2.10 \times \ln(\mathrm{SIZE}) + 3.81 \times \mathrm{DISS}; \\ R^2 &= 0.987\end{aligned}$$

- Parallel UK linear regression:

$$\begin{aligned}\ln(y) &= 0.45 + 2.02 \times \ln(\mathrm{SIZE}) + 3.30 \times \mathrm{DISS} \\ &\quad -0.25 \times \mathrm{THREADS}; \\ R^2 &= 0.987\end{aligned}$$

Table 5: Execution time prediction (ms) for DP.

TH.	SIZE	DISS	SERIAL Real	Predicted	Error	PARALLEL Real	Predicted	Error
2	2500	25%	125.08	126.92	1.47%	68.08	67.41	-0.98%
2	2500	45%	145.98	133.97	-8.23%	76.17	72.00	-5.47%
2	2500	85%	144.33	149.27	3.42%	81.26	82.13	1.07%
2	15000	25%	4485.88	4526.52	0.91%	2405.02	2241.57	-6.80%
2	15000	45%	5236.91	4778.10	-8.76%	2693.74	2394.09	-11.12%
2	15000	85%	5195.09	5323.97	2.48%	2912.31	2730.98	-6.23%
4	2500	25%	125.18	126.96	1.42%	36.25	40.88	12.77%
4	2500	45%	145.38	134.02	-7.81%	40.59	43.66	7.56%
4	2500	85%	144.28	149.33	3.50%	43.38	49.80	14.80%
4	15000	25%	4490.28	4528.18	0.84%	1222.05	1359.22	11.22%
4	15000	45%	5230.59	4779.85	-8.62%	1369.06	1451.71	6.04%
4	15000	85%	5256.54	5325.93	1.32%	1477.64	1655.99	12.07%
6	2500	25%	125.22	127.01	1.43%	26.25	24.79	-5.56%
6	2500	45%	145.48	134.07	-7.84%	29.29	26.47	-9.63%
6	2500	85%	144.43	149.38	3.43%	31.25	30.20	-3.36%
6	15000	25%	4540.56	4529.84	**-0.24%**	838.69	824.19	-1.73%
6	15000	45%	5231.09	4781.60	-8.59%	939.34	880.27	-6.29%
6	15000	85%	5230.48	5327.88	1.86%	1010.59	1004.14	**-0.64%**

Table 6: Execution time prediction (ms) for UK.

TH.	SIZE	DISS	SERIAL Real	Predicted	Error	PARALLEL Real	Predicted	Error
2	2500	25%	21.22	18.09	-14.75%	15.27	13.16	-13.82%
2	2500	45%	55.73	39.06	-29.91%	33.39	25.78	-22.79%
2	2500	85%	166.35	182.16	9.50%	86.49	98.97	14.43%
2	15000	25%	843.43	774.32	**-8.19%**	582.23	503.82	-13.47%
2	15000	45%	2203.47	1672.17	-24.11%	1339.80	987.14	-26.32%
2	15000	85%	6544.81	7798.35	19.15%	3522.62	3789.56	7.58%
4	2500	25%	20.87	18.09	-13.32%	8.17	7.95	-2.69%
4	2500	45%	53.78	39.06	-27.37%	17.45	15.57	-10.77%
4	2500	85%	168.21	182.15	8.29%	44.72	59.78	33.68%
4	15000	25%	845.73	774.28	-8.45%	276.61	304.32	10.02%
4	15000	45%	2239.91	1672.09	-25.35%	660.38	596.26	-9.71%
4	15000	85%	6513.57	7797.98	19.72%	1847.55	2288.98	23.89%
6	2500	25%	20.71	18.09	-12.65%	5.97	4.80	-19.60%
6	2500	45%	53.65	39.06	-27.19%	12.56	9.41	-25.08%
6	2500	85%	165.15	182.14	10.29%	31.94	36.11	13.06%
6	15000	25%	848.75	774.24	-8.78%	183.68	183.81	**0.07%**
6	15000	45%	2191.20	1672.01	-23.69%	431.14	360.15	-16.47%
6	15000	85%	6677.75	7797.61	16.77%	1264.54	1382.59	9.34%

Table 6 presents the prediction results for UK using 2, 4, 6 threads, with sequence lengths 2500 and 15000 and dissimilarities 25%, 45% and 85%. It can be seen that, on average, the prediction errors are higher for UK than DP, both in the serial and in the parallel versions. This happens because UK has pruning capability and the number of cells computed depends on the dissimilarity between the sequences, leading to a more complex behavior. For this reason, we consider that a maximum error of 33.68% is a good result, considering that most errors for UK are below 20%.

4.3 Real DNA Sequences: Covid-19 Case Study

We also conducted a set of experiments using real DNA sequences publicly available at the National Center for Biotechnology Information (NCBI), *https://www.ncbi.nlm.nih.gov/*. For the first set of experiments, we chose sequences from variants of SARS-CoV-2 (lengths $\sim$ 29900) all over the world were compared to the reference sequence SARS-CoV-2 isolate Wuhan-Hu-1 (length = 29903) using parallel DP and Parallel UK. The dissimilarity is obtained by dividing the edit distance by the length of the sequence. Values in bold highlight the best execution time for each comparison (Table 7).

Table 7: Execution times (ms) for the SARS-CoV-2 case study. The dissimilarity is the result of dividing edit distance value by the length of the sequence.

COUNTRY	DISS	EDIT DIST.	TIME(ms) DP SERIAL	DP PARAL.	UK SERIAL	UK PARAL.
Japan	7.11%	2082	20490.47	3992.93	224.02	**40.03**
Chile	0.64%	192	20768.15	4042.56	3.99	**1.90**
Australia	0.52%	156	20916.51	4036.69	3.34	**1.76**
France	0.7%	208	20749.34	4031.12	4.23	**2.01**
UK	0.44%	130	20786.62	4038.58	3.11	**1.67**
Canada	17.44%	5184	20659.38	4056.76	1311.57	**231.02**
Russia	0.83%	246	20724.72	4032.93	4.81	**2.20**
South Africa	0.54%	161	20732.42	4057.27	3.48	**1.79**
Libya	0.81%	242	20747.39	4043.30	4.68	**2.18**
India	1.02%	305	20779.65	4073.30	6.11	**2.51**
USA	0.76%	226	20808.56	4039.60	4.72	**2.08**

The results in Table 7 show Serial DP as the algorithm with the worst performance among all SARS-CoV-2 comparisons while Serial UK is noticeably better. The high values of some edit distances – the case of Canada (OQ305820.1) and Japan (LC753266.1) – is due to the presence of some long chains of 'N' characters in their DNA sequences indicating the impossibility of a correct identification of some parts of it. In all cases, Parallel UK performed much better than Parallel DP.

It is possible to make a linking between the real DNA sequences with the 30K-character-length synthetic sequences from Tables 2 and 3. For the covid-19 case study, the sequence sizes are about 30000. We can see that all dissimilarities are below 20% and that Serial and Parallel UK behaved much better than Serial and Parallel DP. This is consistent with the result obtained with the comparison of synthetic sequences with length equal to 30000. Therefore, for SARS-CoV-2 sequence comparisons, Parallel UK is the best choice, particularly because hundreds or even thousands of those sequences of SARS-Cov-2 are compared in a unique biological study (Uraki, 2023; Teylo et al., 2021; Hidalgo et al., 2022).

5 CONCLUSION

In this paper, we proposed a reproducible framework to execute parallel sequence comparison algorithms. Besides producing reproducible outputs, our framework also generates linear regressions with the output data, which are able to estimate the execution time of future executions.

The use of the framework allowed us to automate several repeatable tasks that are time consuming and prone to errors, such as executing the algorithms with correct parameters (Execution Module), collecting results from each execution (Data Import Module), processing these results (Data Preprocessing Module), generation of graphics (Data Visualization Module), statistical analysis and linear regressions (Linear Regression Module), and the data exporting to other formats (Data Export Module). Furthermore, the modular design of the framework also allowed an easy integration of new algorithms.

Hence, OpenMP versions of two dynamic programming algorithms (DP and UK) to compute the edit distance between strings were also proposed and evaluated. These algorithms were implemented in C++ and executed in a multicore machine using the proposed framework.

Our results with synthetic and real DNA sequences whose sizes ranged from 1000 to 30000 show that our parallel versions are able to obtain very good speedups (up to 5.88x, with 6 threads). Also, we show that Parallel UK is the best choice for the majority of the tests, producing the smallest execution time for the synthetic and real sequences. Moreover, we show that our framework generates automatically graphics, simplifying the task of running experiments, and that the linear regressions obtained with the framework have very good statistical relevance ($R^2 \geq 9.87$), generating accurate execution time predictions.

As future work, we want to expand the linear regression module of our framework, including additional plugins with machine learning strategies. In addition, we want to incorporate other parallel versions of biological sequence comparison algorithms for local and global alignment, such as MASA-OpenCL (de Figueiredo Jr. et al., 2019), to our framework. Finally, we intend to create a new module, that will connect to the Data Export Module and use the alignments produced by the executions in more complex problems, such as Multiple Sequence Alignment.

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