SMITH-WATERMAN ALGORITHM

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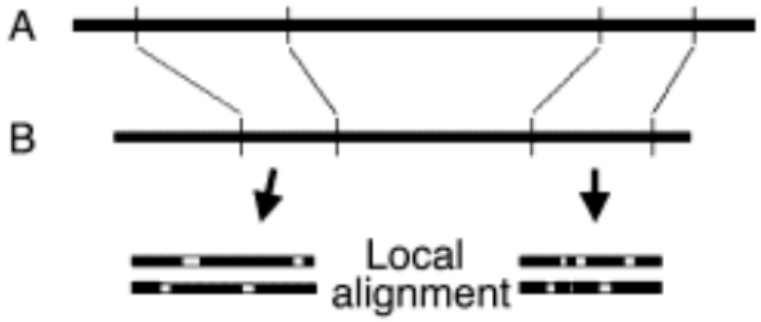
Smith-Waterman Algorithm

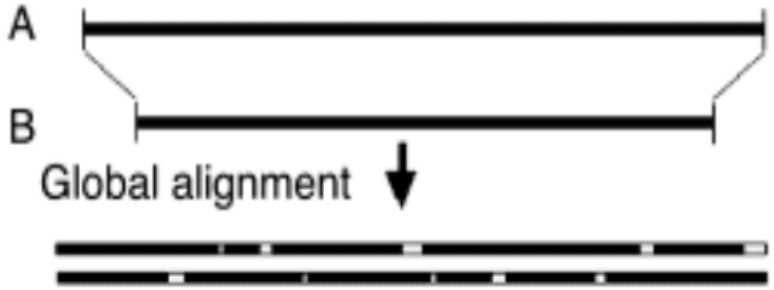
- The Smith-Waterman algorithm is a well-known method used in bioinformatics for local sequence alignment; that is, for aligning subsequences of proteins or nucleic acids.
- The Smith-Waterman algorithm is a dynamic programming algorithm used for local sequence alignment.
- It compares segments of all possible lengths and optimizes the measure of similarity.
- The goal is to identify regions of similarity that may be a consequence of functional, structural, or evolutionary relationships between the sequences

SMITH WATERMAN



		T	G	T	T	A	C	G	G
	0	0	0	0	0	0	0	0	0
G	0	0	3	1	0	0	0	3	3
G	0	0	3	1	0	0	0	3	6
T	0	3	1	6	4	2	0	1	4
T	0	3	1	4	9	7	5	3	2
G	0	1	6	4	7	6	4	8	6
A	0	0	4	3	5	10	8	6	5
C	0	0	2	1	3	8	13	11	9
T	0	3	1	5	4	6	11	10	8
A	0	1	0	3	2	7	9	8	7

NEEDLEMAN–WUNSCH



		G	C	A	T	G	C	G
	0	-1	-2	-3	-4	-5	-6	-7
G	-1	1	0	-1	-2	-3	-4	-5
A	-2	0	0	1	0	-1	-2	-3
T	-3	-1	-1	0	2	1	0	-1
T	-4	-2	-2	-1	1	1	0	-1
A	-5	-3	-3	-1	0	0	0	-1
C	-6	-4	-2	-2	-1	-1	1	0
A	-7	-5	-3	-1	-2	-2	0	0

Algorithm

- Consider the maximum value from 4 cases
- Apply Gap penalty to top and left
- Match/Mismatch score to the diagonal value
- Set the score to zero if it negative

Match/Mismatch: +3/-3

Gap penalty: -2

$$H_{ij} = \max \begin{cases} H_{i-1,j-1} + s(a_i, b_j), \\ \max_{k \geq 1}\{H_{i-k,j} - W_k\}, \\ \max_{l \geq 1}\{H_{i,j-l} - W_l\}, \\ 0 \end{cases} \qquad (1 \leq i \leq n, 1 \leq j \leq m)$$

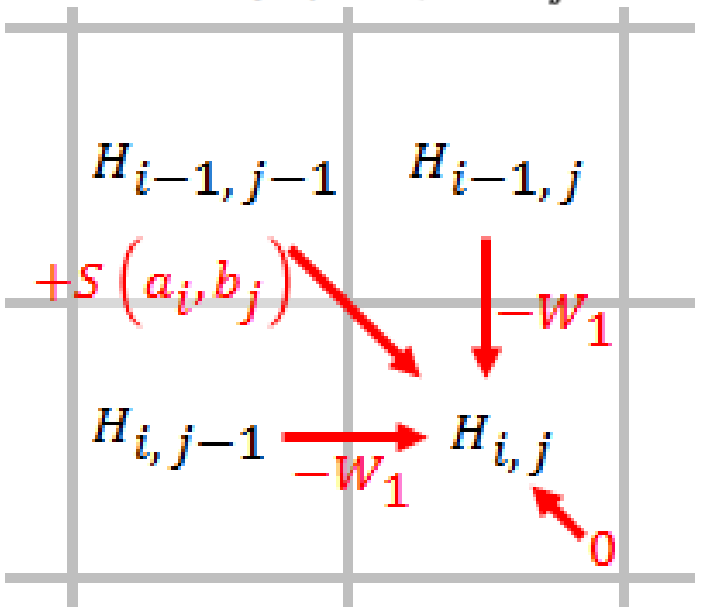
where

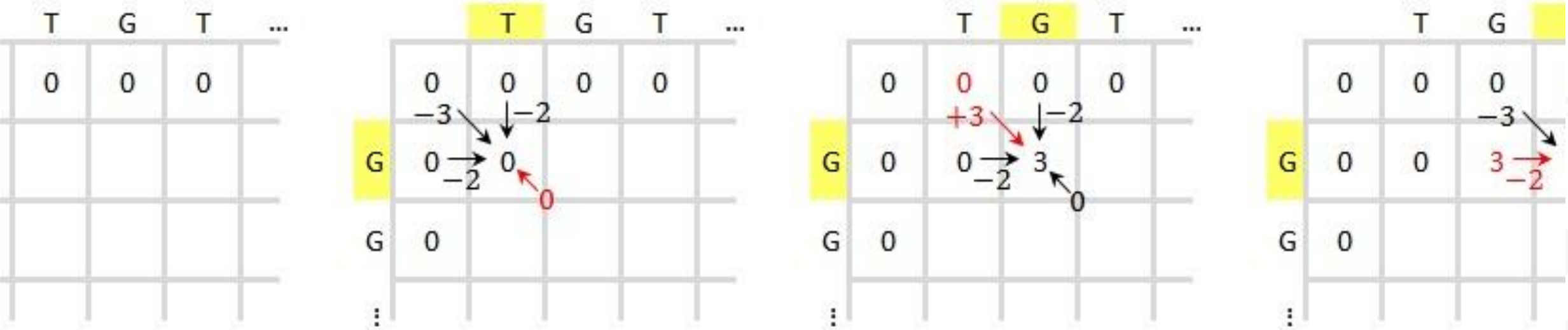
$H_{i-1,j-1} + s(a_i, b_j)$ is the score of aligning a_i and b_j,

$H_{i-k,j} - W_k$ is the score if a_i is at the end of a gap of length k,

$H_{i,j-l} - W_l$ is the score if b_j is at the end of a gap of length l,

0 means there is no similarity up to a_i and b_j.





		T	G	T	T	A	C	G	G
	0	0	0	0	0	0	0	0	0
G	0	0	3	1	0	0	0	3	3
G	0	0	3	1	0	0	0	3	6
T	0	3	1	6	4	2	0	1	4
T	0	3	1	4	9	7	5	3	2
G	0	1	6	4	7	6	4	8	6
A	0	0	4	3	5	10	8	6	5
C	0	0	2	1	3	8	13	11	9
T	0	3	1	5	4	6	11	10	8
A	0	1	0	3	2	7	9	8	7

		T	G	T	T	A	C	G	G
	0	0	0	0	0	0	0	0	0
G	0	0	3	1	0	0	0	3	3
G	0	0	3	1	0	0	0	3	6
T	0	3	1	6	4	2	0	1	4
T	0	3	1	4	9	7	5	3	2
G	0	1	6	4	7	6	4	8	6
A	0	0	4	3	5	10	8	6	5
C	0	0	2	1	3	8	13	11	9
T	0	3	1	5	4	6	11	10	8
A	0	1	0	3	2	7	9	8	7

The Alignment result is:

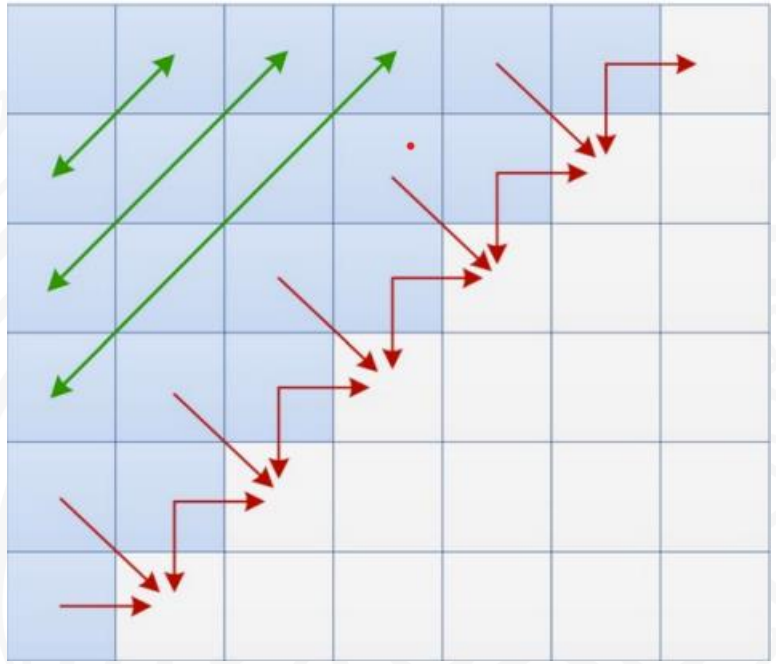
G T T – A C
G T T G A C

Need for Parallel

- Sequence alignment is a highly time-consuming task as it takes quadratic time which is O(mn), m,n are the lengths of the protein sequences
- Let’s take an example of (COVID-19), scientists identified its common features by aligning it against other viruses

Parallel Implementation

- Each cell in the computation matrix depends on the calculations of three other cells, as indicated by red arrows in the document.
- Diagonal elements doesn't depend on the other diagonal elements so they can be computed parallelly



Parallel Implementation

	-	C	G	G	G	T	A	T	C
-	0	0	0	0	0	0	0	0	0
C	0	T1	T2	T3	T4	T5	T6	T7	T8
C	0	T2	T3	T4	T5	T6	T7	T8	T9
C	0	T3	T4	T5	T6	T7	T8	T9	T10
T	0	T4	T5	T6	T7	T8	T9	T10	T11
A	0	T5	T6	T7	T8	T9	T10	T11	T12
G	0	T6	T7	T8	T9	T10	T11	T12	T13
G	0	T7	T8	T9	T10	T11	T12	T13	T14
T	0	T8	T9	T10	T11	T12	T13	T14	T15

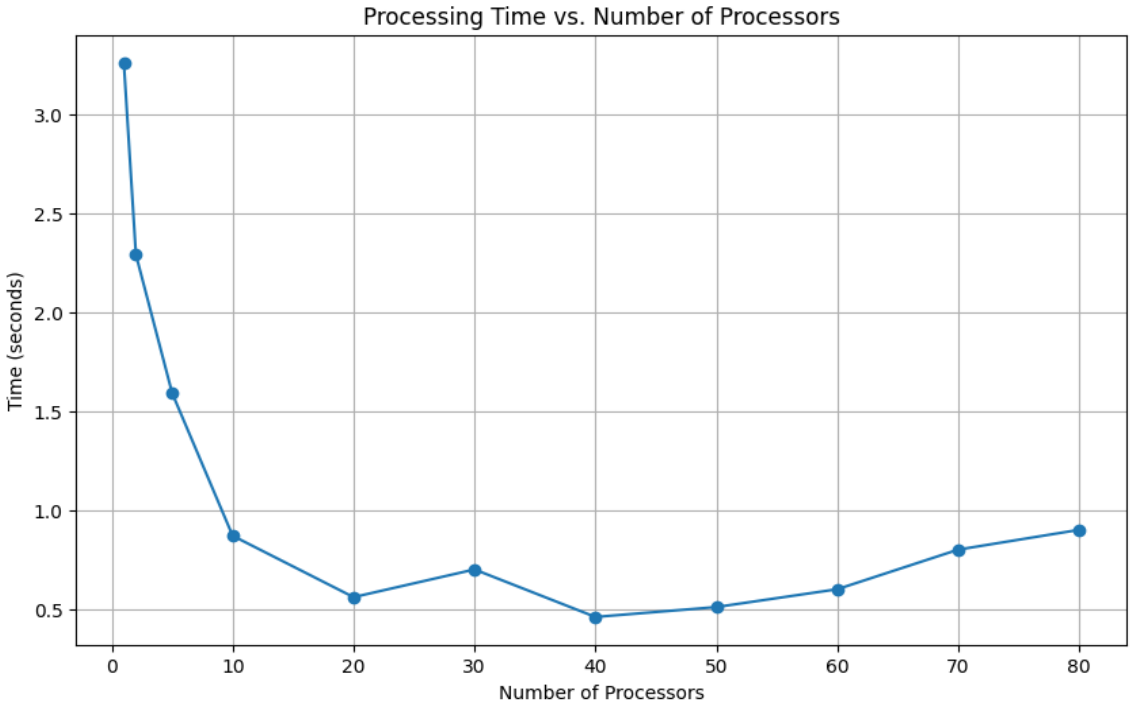
Figure 2. Cases calculable at the same time T_i.

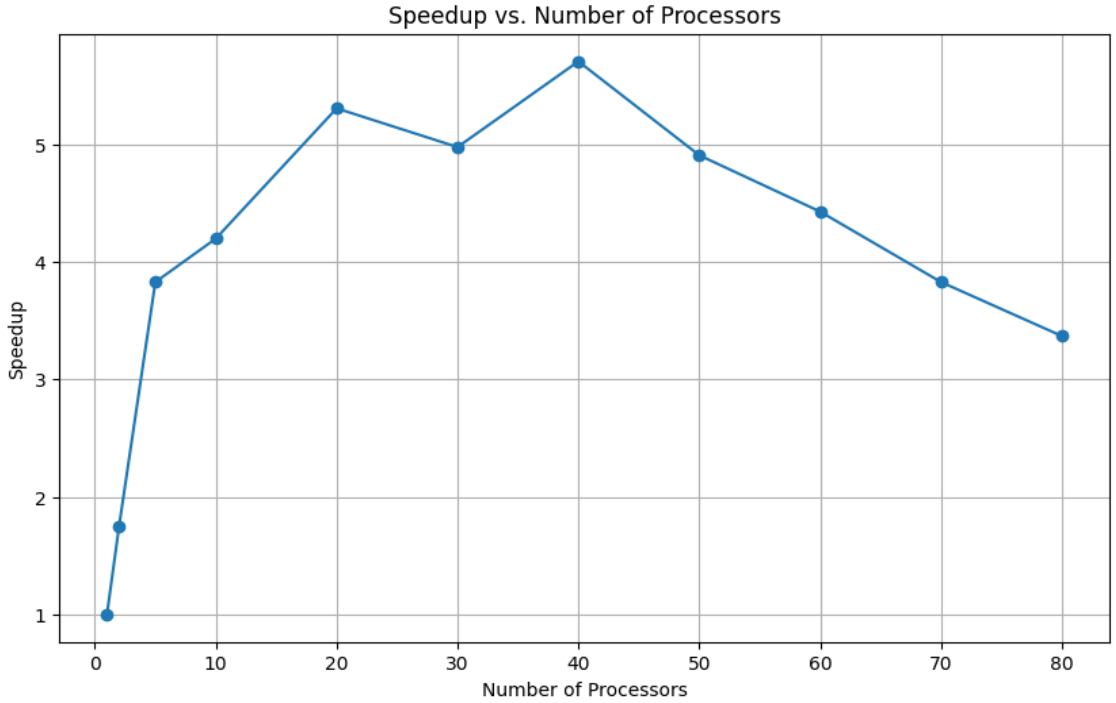
-	C	G	G	G	T	A	T	C								
0	0	0	0	0	0	0	0	0								
-	0	T1	T2	T3	T4	T5	T6	T7	T8							
	C	0	T2	T3	T4	T5	T6	T7	T8	T9						
		C	0	T3	T4	T5	T6	T7	T8	T9	T10					
			C	0	T4	T5	T6	T7	T8	T9	T10	T11				
				T	0	T5	T6	T7	T8	T9	T10	T11	T12			
					A	0	T6	T7	T8	T9	T10	T11	T12	T13		
						G	0	T7	T8	T9	T10	T11	T12	T13	T14	
							G	0	T8	T9	T10	T11	T12	T13	T14	T15
								T	0							

Figure 3. Linear representation of the parallelizable boxes.

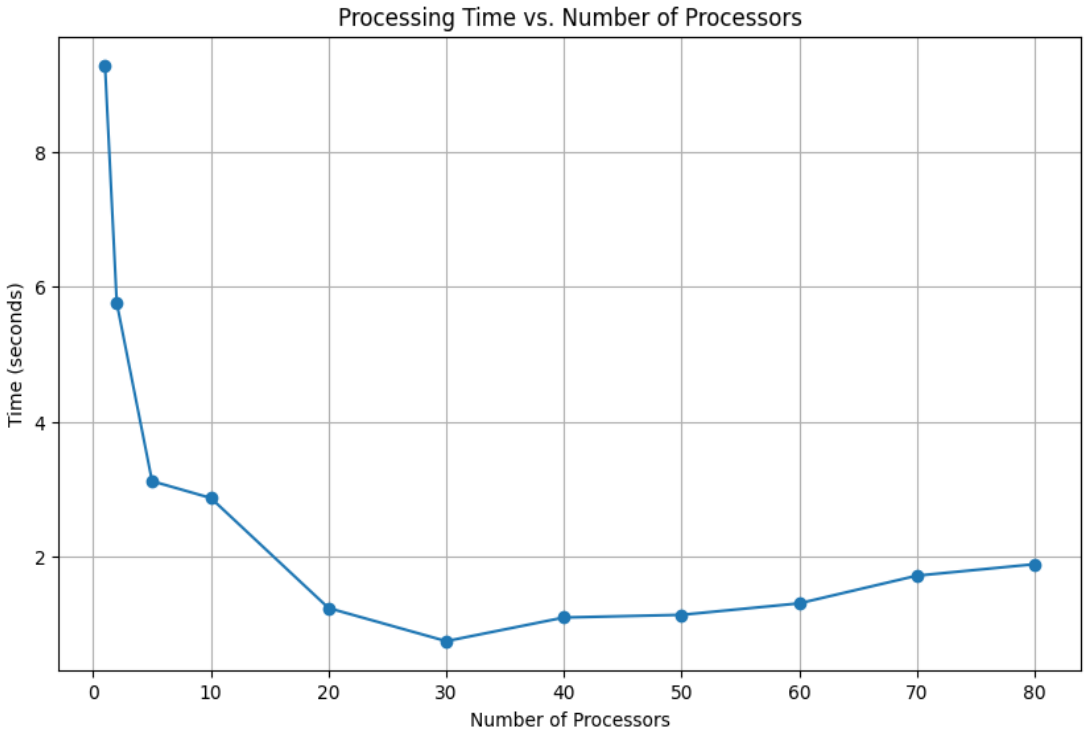
Results

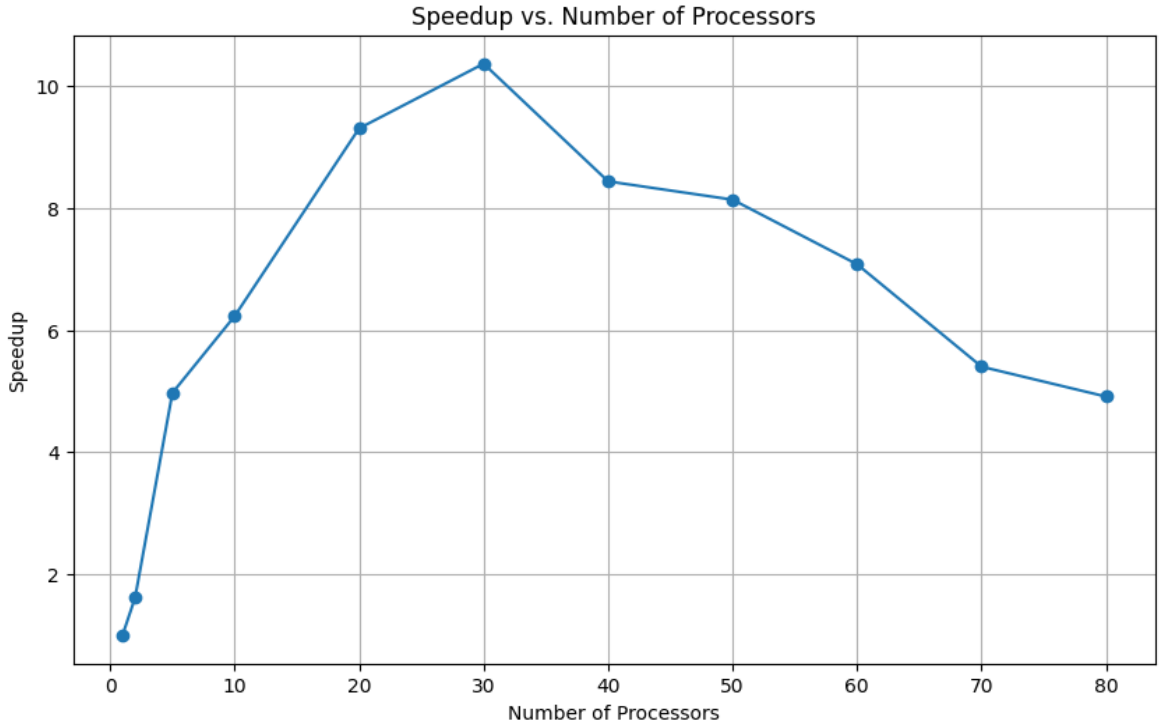
For dataset N = 1000



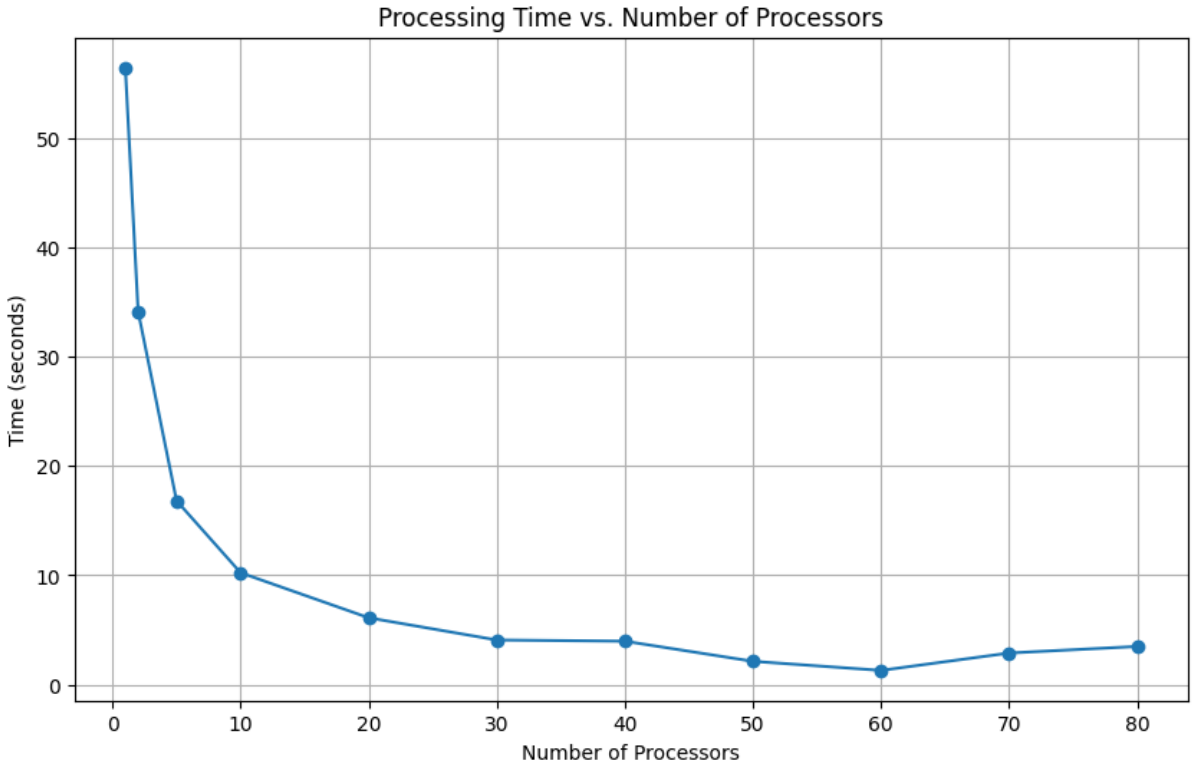


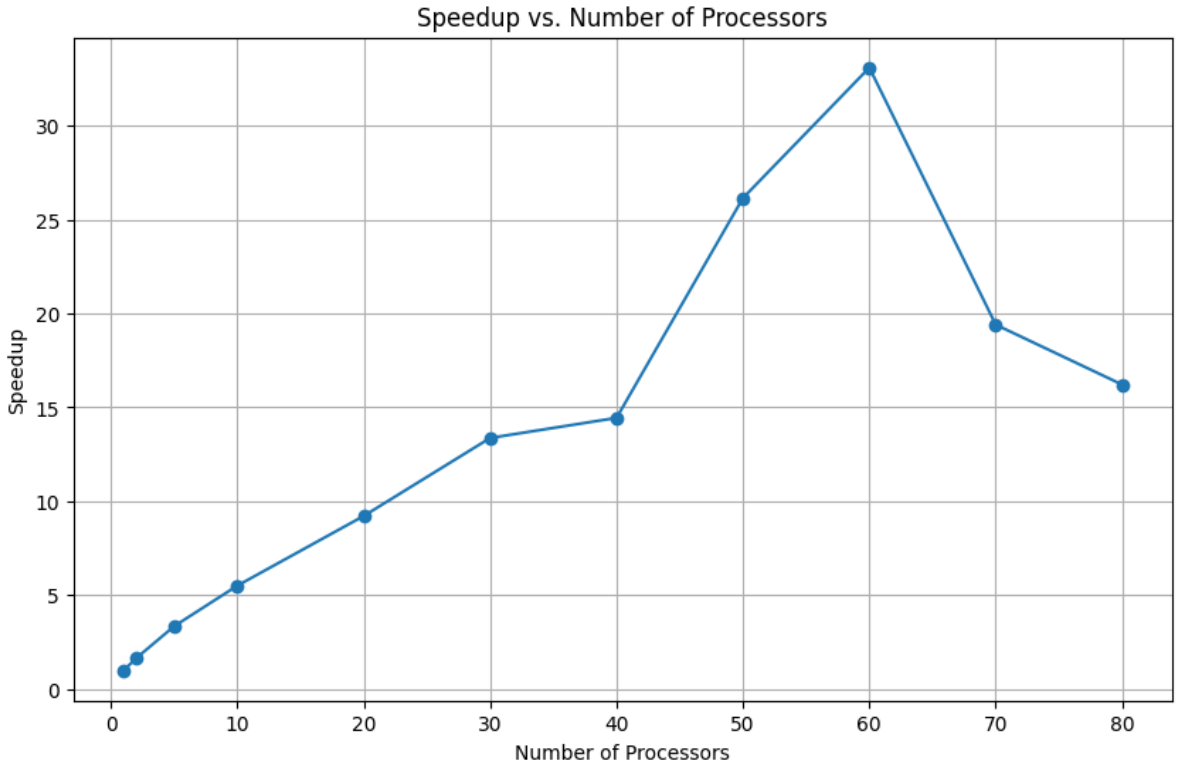
For N = 2000


Processing Time vs. Number of Processors
Time (seconds)
Number of Processors
0
10
20
30
40
50
60
70
80
2
4
6
8

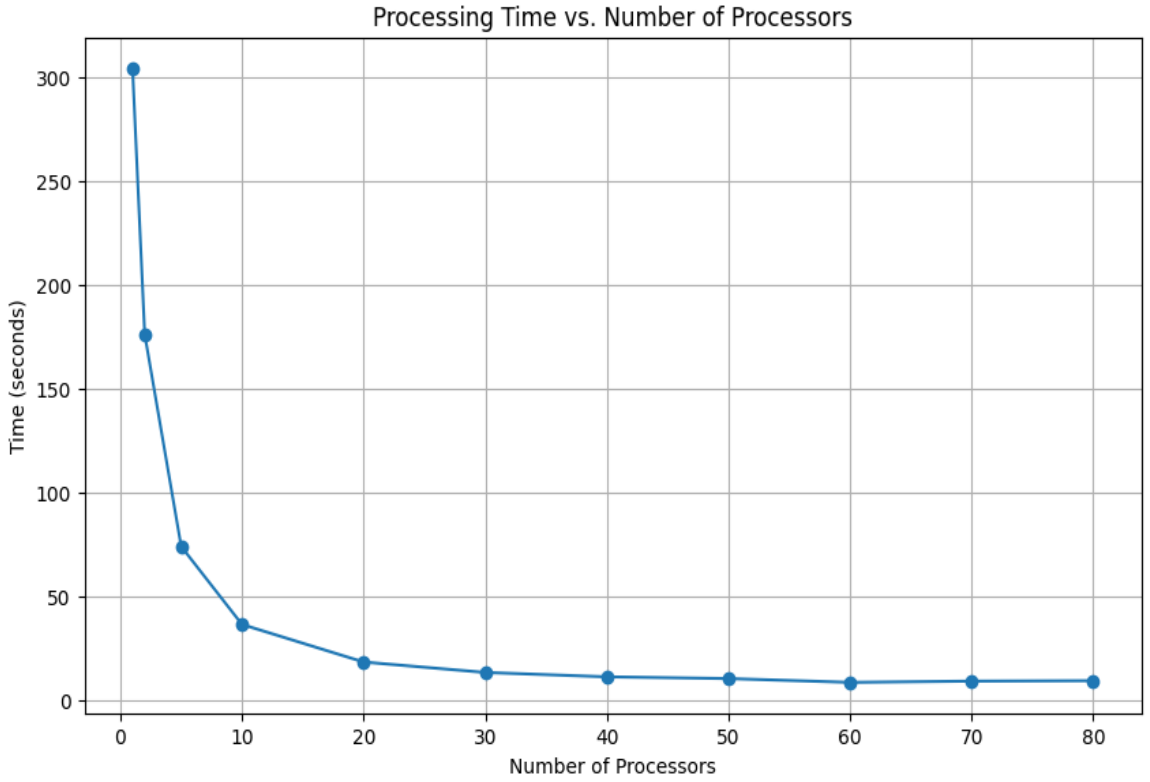

Speedup vs. Number of Processors
Speedup
Number of Processors
0
10
20
30
40
50
60
70
80
2
4
6
8
10

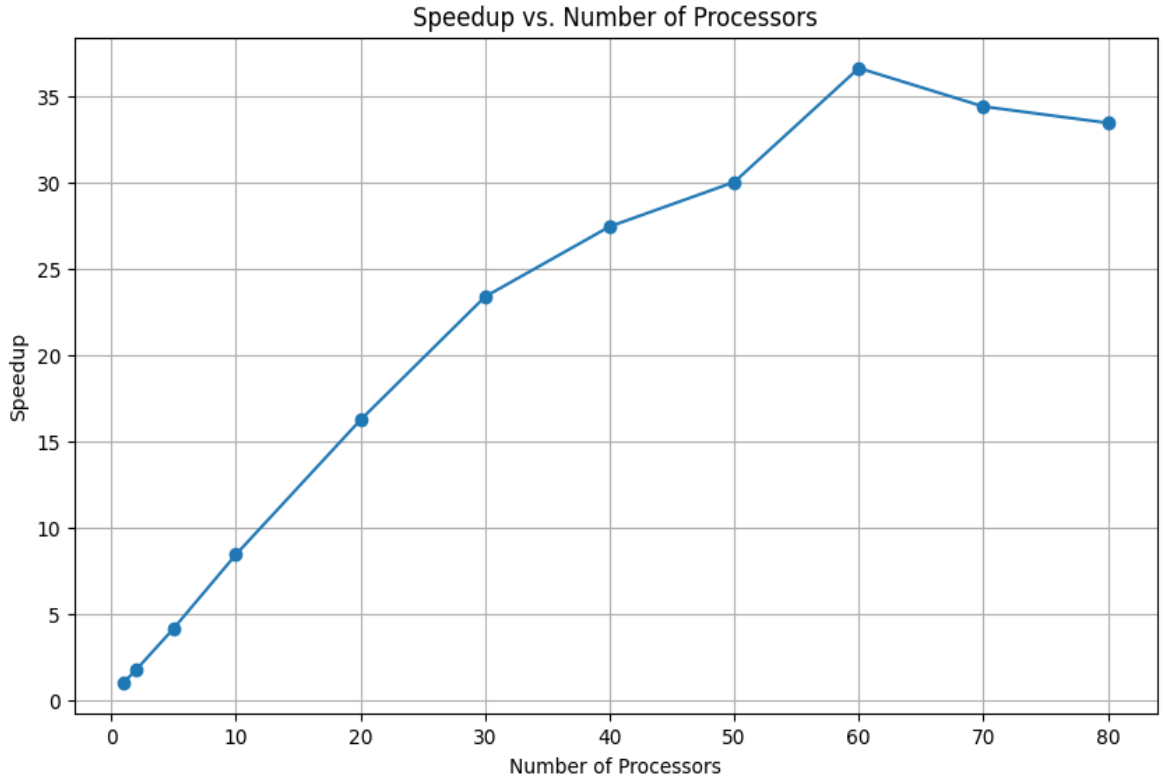
For N = 5000


Processing Time vs. Number of Processors
Time (seconds)
Number of Processors
0
10
20
30
40
50
60
70
80


Speedup vs. Number of Processors
Speedup
Number of Processors
0
5
10
15
20
25
30
40
50
60
70
80

For N = 10000


Processing Time vs. Number of Processors
Time (seconds)
Number of Processors
0
50
100
150
200
250
300
0
10
20
30
40
50
60
70
80


Speedup vs. Number of Processors
Speedup
Number of Processors
0
5
10
15
20
25
30
35
0
10
20
30
40
50
60
70
80

References

- Chaibou, Amadou, and Oumarou Sie. "Comparative study of the parallelization of the Smith-Waterman algorithm on OpenMP and Cuda C." Journal of Computer and Communications 3.06 (2015): 107.
- https://en.wikipedia.org/wiki/Smith%E2%80%93Waterman_algorithm
- Parallelizing the Smith-Waterman Algorithm using OpenSHMEM and MPI-3 One-Sided Interfaces - Matthew Baker, Aaron Welch, Manjunath Gorentla Venkata.

Thank You