4005-735 Parallel Computing I Project Report: Longest Common Subsequence Length Calculation

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1 Abstract

The Longest Common Subsequence (LCS) problem is common to bioinformatics and a classic in computer science, generally considered NP-hard. The problem is commonly encountered in bioinformatics in the comparison of DNA which results in strings that are a combination of DNA base pairs representing an organism's DNA sequence. These sequences are typically very long in length resulting in a computationally intensive problem. By determining the longest common subsequence of DNA, biologists can determine the relative closeness of two organisms. The goal of this project was to research methods by which one could parallelize the LCS length calculation problem to speed up string comparison. Currently, the most common methods used in bioinformatics are the BLAST and FASTA heuristics. Both algorithms emphasize speed of comparison at the expense of sensitivity of determining optimal alignments of sequences. Algorithms like Smith-Waterman provide exactness at the expense of speed. This project aims to inspect and evaluate means of calculating the length of the longest common subsequence, a value useful for calculating the similarity in two strings, where the longest common subsequence string is not needed.

2 Computational Problem

The Longest Common Subsequence (LCS) problem is common to bioinformatics and a classic in computer science. The problem is one in which given two sequences $X=< x_1, x_2, \cdots, x_m >$ and $Y=< y_1, y_2, \cdots, y_n >$ we attempt to find the maximum-length common subsequences of X and Y. A subsequence is not the same as a substring (subsequences do not need to be consecutive in the string). Given the string $X=< x_1, x_2, \cdots, x_m >$, string $Z=< z_1, z_2, \cdots, z_k >$ is then a subsequence of X if there is a strictly increasing sequence $< i_1, i_2, \cdots, i_k >$ of indices of X such that for all $j=1,2,\cdots,k$ we have $x_{i_j}=z_j$ [2].

This problem is commonly encountered in bioinformatics in the comparison of DNA which is represented by the four DNA bases adenine, guanine, cytosine, and thymine represented relatively by the letters A, C, G, T. This results in strings that are a combination of these letters representing an organism's DNA sequence. These sequences are typically very long in length resulting in a computationally intensive problem.

A subset of the LCS problem is the longest common subsequence length problem, where the length of the longest common subsequence is determined, and not the actual sequence string. The length of the longest common subsequence string is used as a metric for determining the similarity between two sequences.

Parallelizing the LCS length problem results in great increases in speed, as well as decreased memory requirements. For short sequences, the network overhead causes the total execution time to be far greater than the execution time of the sequential version. For longer sequences, the parallel version greatly increases the processing speed.

The goal of this project is to determine the speed-up of this problem when using parallelization techniques and compare these performance metrics with a sequential single-CPU experiment.

3 Paper Analysis: Liu et al

3.1 Problem Description

With it being one of the primary tasks in bioinformatics, finding the LCS of a biosequence efficiently is imperative. Currently, there are various paralleled LCS implementations that vary in space and time complexity. They all seek to produce exact, correct results that sequential algorithms like Smith-Waterman and Needleman-Wunsch have been producing since the early 1980s. This paper presents an algorithm called $FAST_LCS$ that promises better performance over other parallel LCS algorithms.

3.2 Contributions

Their contribution is their $FAST_LCS$ algorithm which works in max8*(n+1)+8*(m+1), L space, and O(|LCS(X,Y)|) time, where m and n are the lengths of strings X and Y respectively, L is the number of identical character pairs and |LCS(X,Y)| is the length of the LCS of X,Y [6]. A primary data structure for the algorithm builds a successor table TX and TY for the strings X and Y respectively, where each entry in these tables lists the successor of character CH(i) in the string.

$$TX(i,j) = \begin{cases} min\{k|k \in SX(i,j)\} & SX(i,j) \neq \phi \\ - & otherwise \end{cases}$$

[6]

Using the successor tables, a second table categorizing identical character pairs of X and Y is called S(X) and S(Y) respectively. A parallel computation, and the basic operation of the algorithm is producing the direct successors of each identical pair at each time step.

3.3 Investigative Use

The research into LCS algorithms, especially parallelizable ones is an ongoing area of active research; unfortunately it was clear that a unique solution, even a naive one was not approachable withing the context of this project. This paper helped us understand the need for a dynamic table-based solution. It was decided to choose an algorithm focused in this area, similar to [6] and implement it in Parallel Java. We choose the algorithms discussed in [1] and [?].

4 Paper Analysis: Boukerche et al

4.1 Problem Description

This paper approaches the problem of finding an efficient means of finding all longest common subsequences between two input strings. While many algorithms use heuristics in order to estimate the longest common subsequence (BLAST, FASTA), the algorithm described in "An exact parallel algorithm to compare very long biological sequences in clusters of workstations"

determines the exact length of the longest common subsequences, as well as all instances of longest common subsequences [1].

4.2 Contributions

"And exact parallel algorithm to compare very long biological sequences in clusters of workstations" provides a very concise description of a parallel algorithm that calculates the longest common subsequence instances in two phases - the first pass, that calculates the coordinates in the similarity matrix of all longest common subsequences, and the second pass that takes the list of all coordinates and backtracks the longest common subsequence.

The first phase, the only one required to calculate the length of the longest common subsequence, uses the *wavefront* method of parallelizing the calculation of the similarity table. By calculating blocks of the table in parallel, the wavefront method calculates the LCS length with minimal size and time requirements. The exact algorithm used to calculate the LCS length in parallel is described under the heading "Dynamic-Programming-LCS-Length-Clu".

Additionally, this paper provided the second phase. During the second phase, a list of the end locations of the LCSs is gathered from each processor. Once the global LCS length is calculated, coordinates are distributed to workers who then use the backtracking algorithm used in Hirschberg's algorithm to calculate the actual LCS.

4.3 Investigative Use

The first pass of "An exact parallel algorithm..." describes the *wavefront* method, a means of parallelizing the calculation of the similarity table, and additionally, the length of the longest common subsequence. The algorithm described in this paper was used to calculate the longest common subsequence length.

5 Problem Solution

This project involves two sets of deliverables, a sequential version utilizing the Dynamic algorithm for LCS, and a parallel LCS algorithm developed by [6].

5.1 Sequential

We investigated the single-processor, single-threaded version of an LCS algorithm using the common Dynamic table generation algorithm. Refer to section 6 for benchmarks recorded for this sequential algorithm, compared against our parallelized algorithm. This code was written in Java using the Parallel Java libraries [3].

The dynamic table generation algorithm is a quadratic-time linear-space algorithm for the calculation of the length of the longest common subsequence. The dynamic programming LCS algorithm computes with O(2 * min(n, m)) space and time complexity of O(mn) time, where X and Y are two input strings and |x| = n and |y| = m.

Algorithm Description

The Dynamic programming algorithm operates by constructing a table, where each cell contains the length of the longest common subsequence up until the indices of that cell in the input sequences. As the value of a cell solely depends on the cells above, to the left, and diagonally from the cell, only two rows of the table need to be maintained at any given time. The value of the cell in the last row and column contains the length of the longest common subsequence.

DYNAMIC-PROGRAMMING-LCS-LENGTH(m, n, A, B)

```
▶ Initialization
     K[1][j] \leftarrow 0[j = 0 \dots n]
 3
     for i \leftarrow 1 to m
 4
             do
                  K[0][j] \leftarrow K[1][j](j = 0..n)
 5
 6
                  for j \leftarrow 1 to n
 7
                        do
 8
                            if A[i] = B[j]
 9
                                then
                                        K[1][j] \leftarrow K[0][j-1] + 1
10
11
                                        K[1][j] \leftarrow \max(K[1][j-1], K[0][j])
12
     LL[j] \leftarrow K[1][j](j = 0 \dots n)
13
```

5.2 Parallelized

The parallel algorithm uses a technique called $wavefront\ parallelism$. The shorter sequence is initially broken into k chunks, and each processor is made responsible for a series of columns. Each processor is tasked with computing the values for its column in blocks of h rows. As a processor finishes computing a block, it sends the data overlapping with its neighbor, the "passage band", to the next processor, who is then able to compute a block of values itself. Once the entire table is calculated, the answer remains in the final processor's computation block. Refer to 6 for the computation time, speedup, efficiency, and experimentally determined sequential fraction values for a number of test cases.

While this technique does provide a good amount of parallelism, it does not achieve load balancing when calculating the first k blocks and the last k blocks. This does not significantly effect the result; however, as the block size is so small that the unbalanced computation time is insignificant.

```
Dynamic-Programming-LCS-Length-Clu(m, n, A, B)

→ Allocate block

    data\_block[width][height] \leftarrow 0(width = 0...(m/k) + 1)
 2
 3
    while rows < total\_rows
 4
           do
 5
              if not process 0
 6
                 then
 7
                        \triangleright read passing band
 8
              for i \leftarrow 1 to height
 9
                    do
10
                        for j \leftarrow 1 to width
11
                        if A[j] == B[i]
12
                          then
                                 data\_block[i][j] = data\_block[i-1][j-1] + 1
13
14
                          else
                                 data\_block[i][j] \leftarrow max(data\_block[i-1][j], data\_block[i][j-1])
15
16
    > Send passing band to neighbor
17
    > Copy bottom row of block to top row
```

6 Performance Metrics

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The following table provides reported metrics for various test conditions. The variables are the length of input strings A and B, resulting in increasing memory and time requirements. All test cases were run on the RIT paranoia cluster, which consists of 32 back end computers (named thug01 through thug32 each an UltraSPARC-IIe CPU, 650 MHz clock, 1 GB main memory. They are connected by a 100-Mbps switched Ethernet back end interconnection network and aggregate 21 GHz clock, 32 GB main memory [4]. Tables 1 through 9 list the trial runs of two data strings increasing in size by a power of two from 512 bytes up to 128 kilobytes. The sequential, 1 processor trial runs for the 128 kilobyte test case could not be done due to default settings on the paranoia CS cluster preventing jobs from running longer than 1 hour, instead these trial time values were extrapolated by applying a power function curve fitting as described in Appendix C in [5].

7 Conclusion

The results of the testing the dynamic sequential and the dynamic solutions to the LCS length problem were very mixed.

The best example of the functionality of the parallel version can be seen in the calculations for two 8192 byte strings. In the 8 kilobyte test cases, the parallel version with one processor and the sequential version operate in approximately equal time. The parallel version, with additional processors, shows moderate speedup, increasing slowly as the number of processors increases.

| A (bytes) | B (bytes) | K | T (msec) | Speedup | Eff | EDSF |
|-----------|-----------|-----|----------|---------|-------|-------|
| 512 | 512 | seq | 808 | XXX | XXX | XXX |
| 512 | 512 | 1 | 961 | 0.841 | 0.841 | XXX |
| 512 | 512 | 2 | 1275 | 0.634 | 0.317 | 1.653 |
| 512 | 512 | 4 | 1557 | 0.519 | 0.130 | 1.827 |
| 512 | 512 | 8 | 2014 | 0.401 | 0.050 | 2.252 |
| 512 | 512 | 16 | 2168 | 0.373 | 0.023 | 2.340 |

Table 1: Two 512-byte strings compared on 1,2,4,8,16 processors. Times are the average of five trial runs.

| A (bytes) | B (bytes) | K | T (msec) | Speedup | Eff | EDSF |
|-----------|-----------|-----|----------|---------|-------|-------|
| 1024 | 1024 | seq | 956 | XXX | XXX | XXX |
| 1024 | 1024 | 1 | 854 | 1.119 | 1.119 | XXX |
| 1024 | 1024 | 2 | 1340 | 0.713 | 0.357 | 2.138 |
| 1024 | 1024 | 4 | 1616 | 0.592 | 0.148 | 2.190 |
| 1024 | 1024 | 8 | 1687 | 0.567 | 0.071 | 2.115 |
| 1024 | 1024 | 16 | 2660 | 0.359 | 0.022 | 3.256 |

Table 2: Two 1-kilobyte strings compared on 1,2,4,8,16 processors. Times are the average of five trial runs.

In the test cases of less than 8 kilobytes of data, the network overhead of peer to peer communication lead to increasing computation times as more processors were added. This caused the parallel version to operate slower in almost all instances.

In the cases of more than 8 kilobytes of data, the network overhead was no longer the limiting factor for time, rather, it was the actual table calculation. As more data was used the comparisons, the parallel version became extremely super-linear, and showed remarkable speedup. This can be attributed to the JIT compiler effect. In the calculation of the 128 kilobyte sequence similarities, the sequential and single processor parallel versions were extrapolated, as the Paranoia cluster only runs parallel software for an hour before terminating execution. While the sequential version was unable to calculate the similarity of two 128 kilobyte sequences within an hour, the parallel version with 16 processors was able to calculate the length of the longest common sequence in 3.65 minutes.

| A (bytes) | B (bytes) | K | T (msec) | Speedup | Eff | EDSF |
|-----------|-----------|-----|----------|---------|-------|-------|
| 2048 | 2048 | seq | 1276 | XXX | XXX | XXX |
| 2048 | 2048 | 1 | 1204 | 1.060 | 1.060 | XXX |
| 2048 | 2048 | 2 | 1848 | 0.690 | 0.345 | 2.070 |
| 2048 | 2048 | 4 | 1834 | 0.696 | 0.174 | 1.698 |
| 2048 | 2048 | 8 | 2257 | 0.565 | 0.071 | 2.000 |
| 2048 | 2048 | 16 | 2553 | 0.500 | 0.031 | 2.195 |

Table 3: Two 2-kilobyte strings compared on 1,2,4,8,16 processors. Times are the average of five trial runs.

| A (bytes) | B (bytes) | K | T (msec) | Speedup | Eff | EDSF |
|-----------|-----------|-----|----------|---------|-------|-------|
| 4096 | 4096 | seq | 3066 | XXX | XXX | XXX |
| 4096 | 4096 | 1 | 2567 | 1.194 | 1.194 | XXX |
| 4096 | 4096 | 2 | 2737 | 1.120 | 0.560 | 1.132 |
| 4096 | 4096 | 4 | 2720 | 1.127 | 0.282 | 1.079 |
| 4096 | 4096 | 8 | 2641 | 1.161 | 0.145 | 1.033 |
| 4096 | 4096 | 16 | 3206 | 0.956 | 0.060 | 1.266 |

Table 4: Two 4-kilobyte strings compared on 1,2,4,8,16 processors. Times are the average of five trial runs.

| A (bytes) | B (bytes) | K | T (msec) | Speedup | Eff | EDSF |
|-----------|-----------|-----|----------|---------|-------|-------|
| 8192 | 8192 | seq | 10408 | XXX | XXX | XXX |
| 8192 | 8192 | 1 | 10365 | 1.004 | 1.004 | XXX |
| 8192 | 8192 | 2 | 6883 | 1.512 | 0.756 | 0.328 |
| 8192 | 8192 | 4 | 4783 | 2.176 | 0.544 | 0.282 |
| 8192 | 8192 | 8 | 4191 | 2.483 | 0.310 | 0.319 |
| 8192 | 8192 | 16 | 4227 | 2.462 | 0.154 | 0.368 |

Table 5: Two 8-kilobyte strings compared on 1,2,4,8,16 processors. Times are the average of five trial runs.

| A (bytes) | B (bytes) | K | T (msec) | Speedup | Eff | EDSF |
|-----------|-----------|-----|----------|---------|-------|--------|
| 16384 | 16384 | seq | 49159 | XXX | XXX | XXX |
| 16384 | 16384 | 1 | 86032 | 0.571 | 0.571 | XXX |
| 16384 | 16384 | 2 | 27481 | 1.789 | 0.894 | -0.361 |
| 16384 | 16384 | 4 | 13932 | 3.528 | 0.882 | -0.117 |
| 16384 | 16384 | 8 | 8609 | 5.710 | 0.714 | -0.028 |
| 16384 | 16384 | 16 | 8154 | 6.029 | 0.377 | 0.034 |

Table 6: Two 16-kilobyte strings compared on 1,2,4,8,16 processors. Times are the average of five trial runs.

| A (bytes) | B (bytes) | K | T (msec) | Speedup | Eff | EDSF |
|-----------|-----------|-----|----------|---------|-------|--------|
| 32768 | 32768 | seq | 321322 | XXX | XXX | XXX |
| 32768 | 32768 | 1 | 398561 | 0.806 | 0.806 | XXX |
| 32768 | 32768 | 2 | 177135 | 1.814 | 0.907 | -0.111 |
| 32768 | 32768 | 4 | 61540 | 5.221 | 1.305 | -0.127 |
| 32768 | 32768 | 8 | 28503 | 11.273 | 1.409 | -0.061 |
| 32768 | 32768 | 16 | 16645 | 19.304 | 1.207 | -0.022 |

Table 7: Two 32-kilobyte strings compared on 1,2,4,8,16 processors. Times are the average of five trial runs.

| | A (bytes) | B (bytes) | K | T (msec) | Speedup | Eff | EDSF |
|---|-----------|-----------|-----|----------|---------|-------|--------|
| ſ | 65536 | 65536 | seq | 1451538 | XXX | XXX | XXX |
| | 65536 | 65536 | 1 | 1604761 | 0.905 | 0.905 | XXX |
| | 65536 | 65536 | 2 | 813422 | 1.784 | 0.892 | 0.014 |
| | 65536 | 65536 | 4 | 372594 | 3.896 | 0.974 | -0.024 |
| | 65536 | 65536 | 8 | 117537 | 12.350 | 1.544 | -0.059 |
| | 65536 | 65536 | 16 | 56647 | 25.624 | 1.602 | -0.029 |

Table 8: Two 64-kilobyte strings compared on 1,2,4,8,16 processors. Times are the average of five trial runs.

| A (bytes) | B (bytes) | K | T (msec) | Speedup | Eff | EDSF |
|-----------|-----------|-----|----------|---------|-------|--------|
| 131072 | 131072 | seq | 5183648* | XXX | XXX | XXX |
| 131072 | 131072 | 1 | 5925532* | 0.875 | 0.875 | XXX |
| 131072 | 131072 | 2 | 3208530 | 1.616 | 0.808 | 0.083 |
| 131072 | 131072 | 4 | 1635557 | 3.169 | 0.792 | 0.035 |
| 131072 | 131072 | 8 | 721019 | 7.189 | 0.899 | -0.004 |
| 131072 | 131072 | 16 | 219387 | 23.628 | 1.477 | -0.027 |

Table 9: Two 128-kilobyte strings compared on 1,2,4,8,16 processors. Times are the average of five trial runs.

^{*} This value was extrapolated from the previous data points due to constraints on the paranoia cluster.

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