HIGH PERFORMANCE AND PARALLEL COMPUTING REPORT

CAB401: High Performance and Parallel Computing

OCTOBER 27, 2017

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1 Introduction

The application chosen to be parallelised was the Bioinformatics – Genome Similarity Using Frequency Vectors. This application's purpose is to compare different types of bacteria to each other by calculating the correlation between two different bacteria.

1.1 Software Architecture

Figure 1 below shows the basic process of Bioinformatics – Genome Similarity Using Frequency Vectors' architecture. The detailed software architecture can be found in full in section 6.3 of the Appendix of this report.

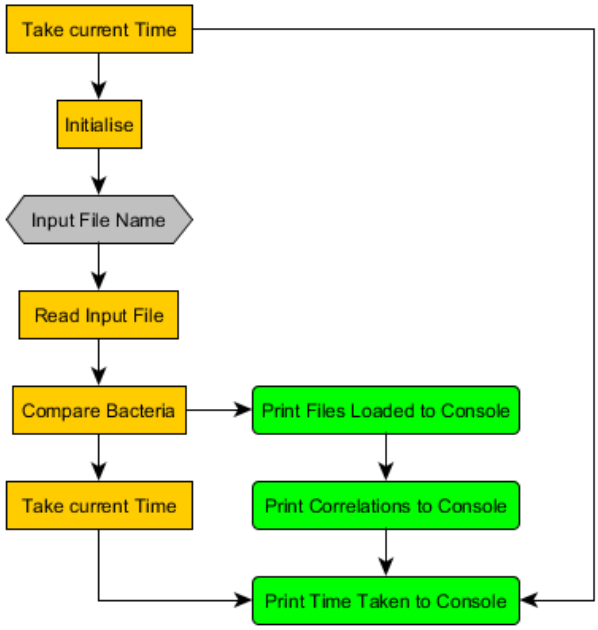


Figure 1: Basic View of Software Architecture

1.1.1 Time

The application takes the time before and after the application and the difference is calculated. This is printed to the console to notify the user how long the program took to complete the Bioinformatics – Genome Similarity Using Frequency Vectors application.

1.1.2 Initialise

This method initialises long variables M1 and M, based on the predefined value for AA_NUMBER and LEN, for the class Bacteria.

1.1.3 Input Filename and Read Input File

The program takes a users' input argument. This argument is the filename for a text file. This text file contains the number of bacteria and the names of the associated bacteria files. The first line contains the number of bacteria. From the second line down, these lines contain the name of each *.faa file. The extension *.faa is used by the NCBI for FASTA animo acids. In this application, forty-one protein FASTA files are being used. Figure 2, on the next page, shows the detail view software architecture for this function.

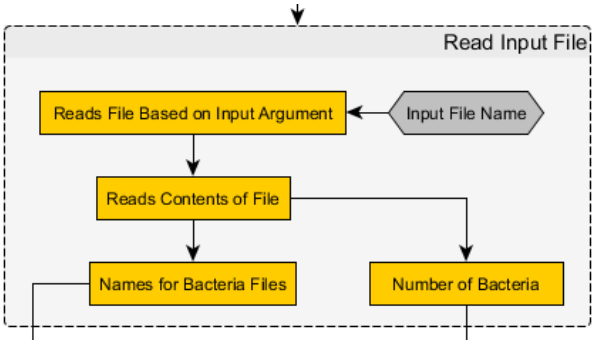


Figure 2: Read Input File Software Architecture

1.1.4 Compare All Bacteria

This component of the application is where most of the runtime and computational work in located. This function does three things. The first creates the number of classes of bacteria based on the number of bacteria to be read. The second component is made of two parts. The first part is printing to the console which file is being loaded. The second part is loading the *.faa files and loading the data into their respective bacteria class. The third calls for the compare bacteria function which calculates the correlation between two pairs of different bacteria and then printing the result to the console. Figure 3 on the next page shows a detailed view of the CompareAllBacteria function.

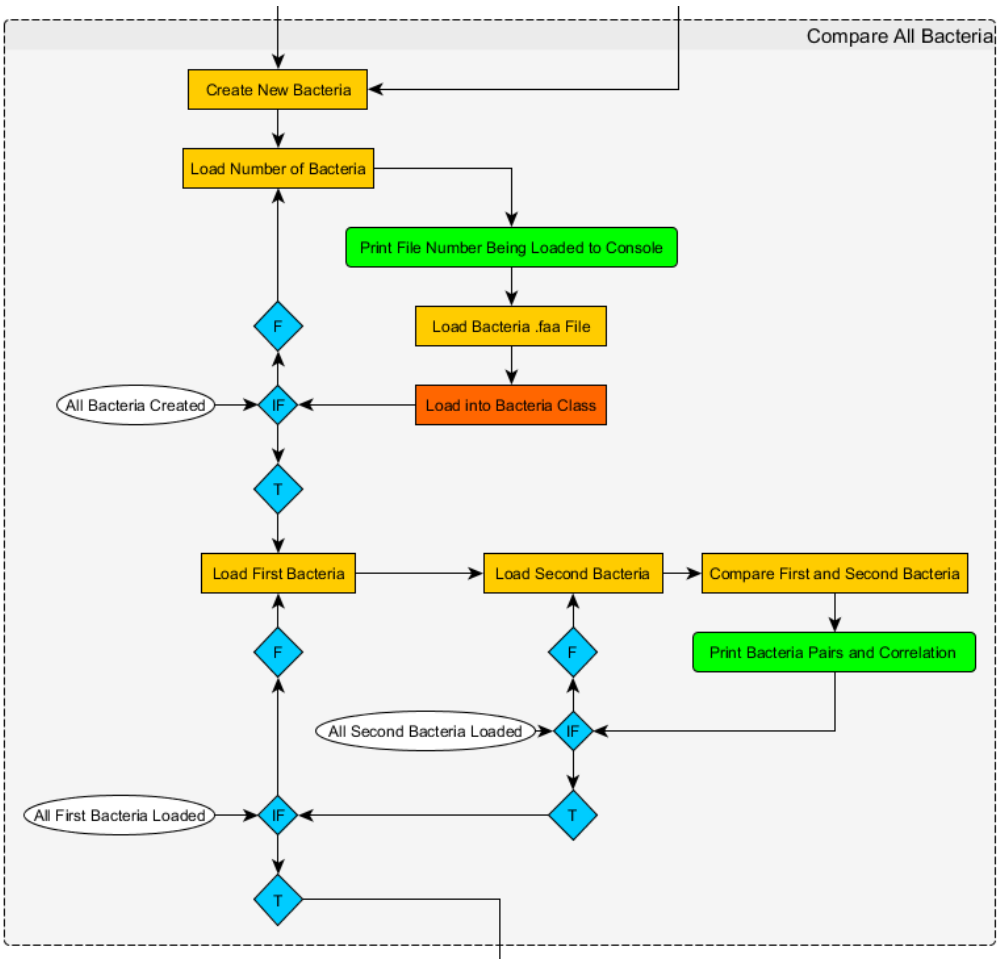


Figure 3: Compare All Bacteria Software Architecture

1.1.5 Bacteria Class

The bacteria files are opened and vectors are initialised. The bacteria class holds data based on the contents in the *.faa files. The class obtains the necessary characters from the respective *.faa file. Figure 4, shown below, shows some of the contents of file AcMNPV.faa.

```
1  >gi|9627743|ref|NP_054030.1| protein tyrosine phosphatase [Autographa californica nucleopolyhedrovirus]
2  MFPARWHNYLQCGQVIKDSNLICFKTPLRPELFAYVTSEEDVWTAEQIVKQNPSIGAIIDLTNTSKYYDG
3  VHFLRAGLLYKKIQVPGQTLPPESIVQEFIDTVKEFTEKCPGMLVGVHCTHGINRTGYMVCRYLMHTLGI
4  APQEAIDRFEKARGHKIERQNYVQDLLI
5  >gi|9627744|ref|NP_054031.1| baculovirus repeated ORF [Autographa californica nucleopolyhedrovirus]
6  MARVKIGEFKFGEDTFNLRYVLERDQQVRFVAKDVANSLKYTVCDKAIRVHVDNKYKSLFEQTIQNGGPT
7  SNSVVKRGDPLYLQPHTVLITKSGVIQLIMKSKLPYAIELQEWLLEEVIPQVLCTGKYDPAIKQREEESK
8  QLVTKLIATFTEHTNALQAVVAQKTEELVKKQEFIERIVAIKDKQIEAKDLQVTRVMTDLNRMYTGFQET
9  MQKKDEIMQKKDAQVTDLVAKVVDLSDRAVQYPADKRKHPVLCVTRDGTTFTAITGQKTYVENQKHKRNI
10 NVANIVVENIRPNPTVDWNNATDRLQAKRSKRSIVLVRWKKRNNLKIG
```

Figure 4: AcMNPV Animo Acid File Content Example

The first stage of the bacteria class is obtaining the data in the respective *.faa file. In this process there are three parts. The first part is whether the end of the file has been met. If so, the search to get the characters for the bacteria class ends. If not, then the second part comes into effect. If the character identified is a '>', then that line is skipped. This line is skipped because the line does not contain the data required, rather just the name and reference of the amino acid. This can be seen in lines one and five in Figure 4 above. When the line is skipped the characters are read initialise buffer is called. The last part is whether a '\n', or space, character is identified. If not, the process continues to get a character. If a '\n' is identified, then continue buffer is called. This section of the bacteria class can be seen below in Figure 5

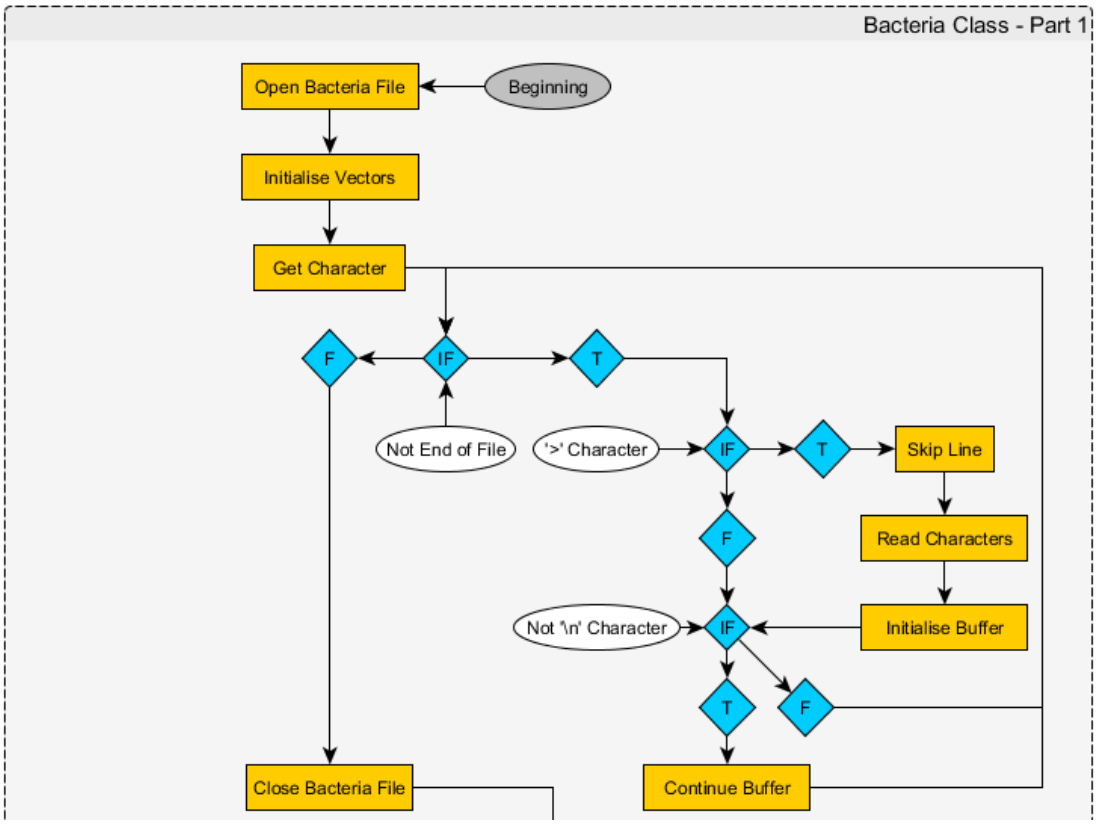


Figure 5: Get Data from *.faa File

When the end of the file has been confirmed the respective file is closed. From here the calculations are performed. Figure 6, shown below, shows the software architecture for this stage up to the point where stochastic is calculated.

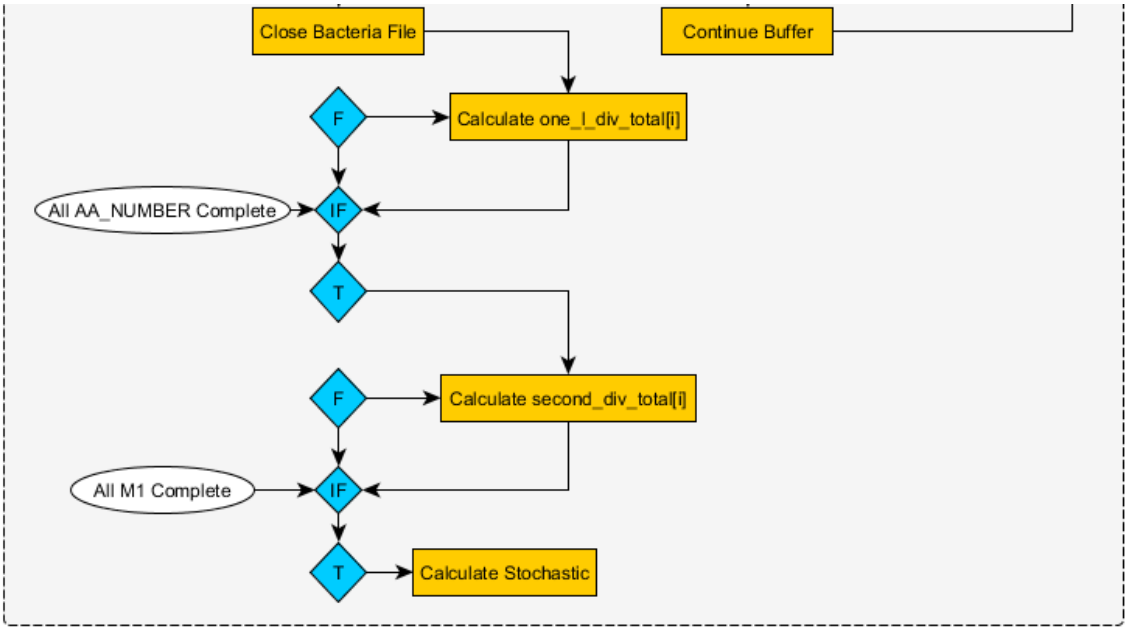


Figure 6: Calculate Variables in Bacteria Class – Part 1

The bacteria class proceeds to calculate other variables which can be seen below in Figure 7.

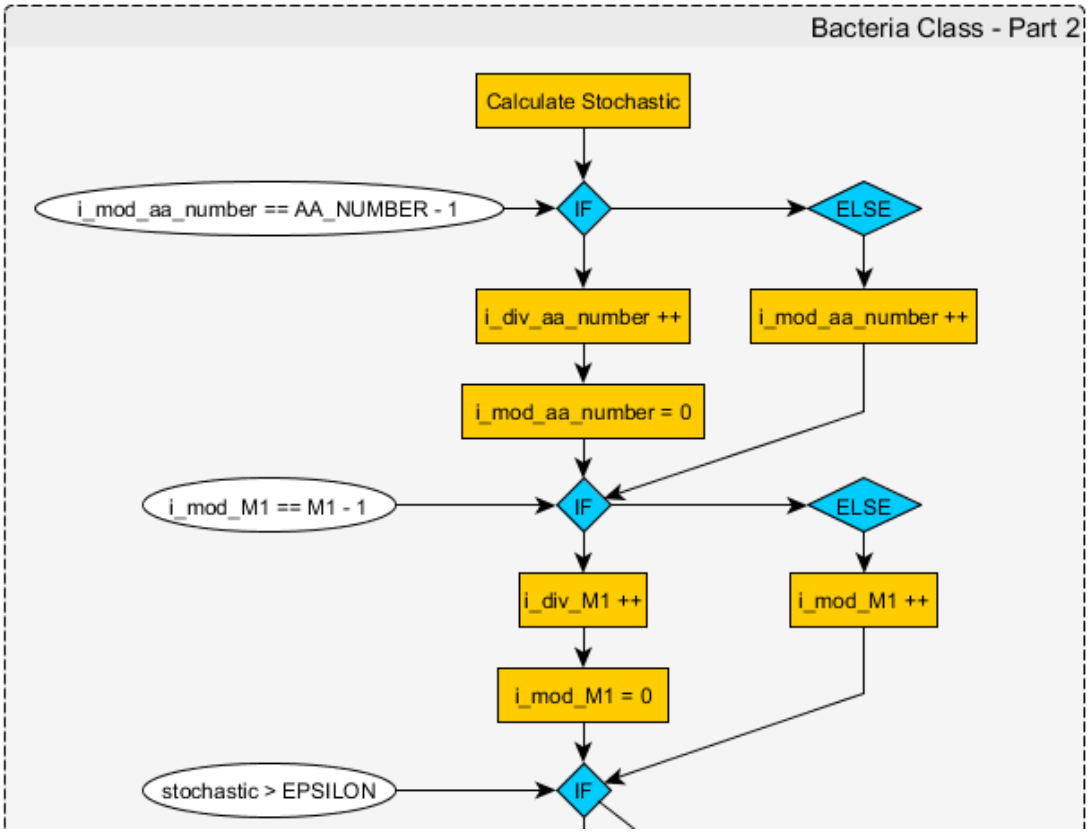


Figure 7: Other Values Calculated in Bacteria Class

The main importance of the bacteria class is the calculated values for tv[] and ti[]. These variables are used when comparing two different bacteria. Figure 8 below shows the software architecture for the rest of the bacteria class. The full software architecture diagram for the bacteria class can be found in the appendices. Bacteria Class – Part 1 software architecture can be found in section 6.4 of this report. Bacteria Class – Part 2 software architecture can be found in section 6.5 of this report.

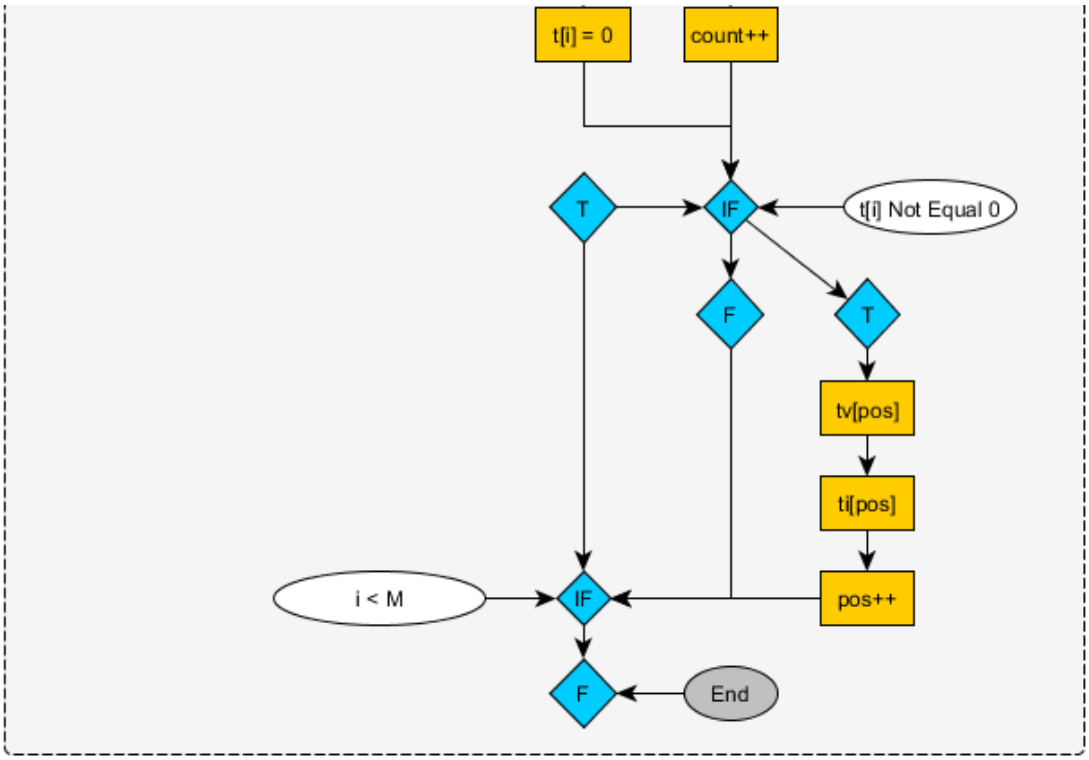


Figure 8: Bacteria Class Ending

1.1.6 Compare Bacteria

The compare bacteria function takes two bacteria as inputs and proceeds to calculate the correlation between the two bacteria based on their vectors, ti and tv variables. In this application, the two bacteria that are taken are two different bacteria. This occurs in the CompareAllBacteria function which includes a nested loop to ensure that every possible unique pair of bacteria are compared. The detail software architecture for the CompareBacteria function can be seen in Figure 9 on the next page and in section 6.6 of the appendices in this report.

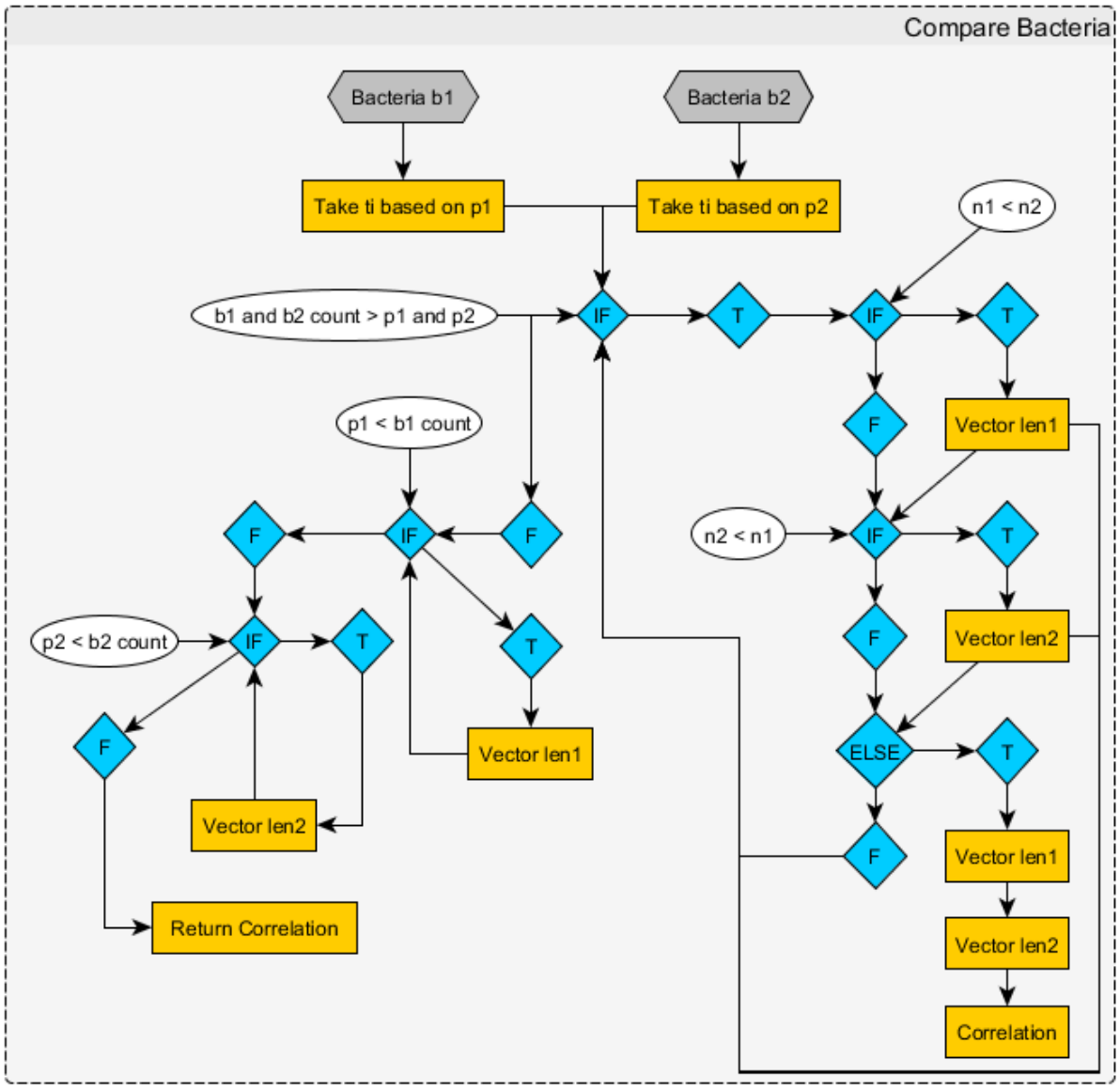


Figure 9: Detail View of Compare Bacteria

2 Bioinformatics – Genome Similarity Using Frequency Vectors

This section of the report discusses what parts of the original code that were analysed. This includes sections of code that resulted in success and failure to be parallelised and what parts of the application can be scalable. This section also discusses the software used and techniques during this analysis.

2.1 Software, Compiler, Hardware and Techniques

2.1.1 Software

The integrated development environment (IDE) used when analysing the application and its code was Microsoft's Visual Studio 2017. This IDE's diagnostic tools were used to identify which section of code took the most amount of time to process. Furthermore, the diagnostic tools show the memory and CPU usage that is being used by the application is real-time. This assisted in analysing for-loop parallelisation as to how much memory was being used and the difference between the original and parallelised version of code's CPU usage.

OpenMP 2.0 is included as part of Visual Studio 2017. This was enabled and chosen for the following reasons. Its simplicity, ease of use and integration in the IDE makes it a wonderful choice when parallelising for-loops and multi-threading other components of the application. The second reason is that I have not used the OpenMP API before. The third reason, OpenMP performed faster results than using POSIX threads. Unfortunately, OpenMP does not perform while-loop parallelisation. While-loops can be parallelised using OpenMP tasks, but this was found to provide no further performance gain and all while loops did not benefit from this.

2.1.2 Compiler

The compiler used was the default compiler that Microsoft has included in Visual Studio 2017. This version of the compiler was Visual C++ 14.1.

2.1.3 Hardware

In this report two machines were used. Both machines use the Windows 10 OS and are running on High Performance mode.

The machine used, named miniTOP, has an i7-4710MQ Intel processor operating at 2.50GHz to 3.50GHz with 16.0 GB of DDR3 RAM. This CPU has four physical cores and eight threads. This machine does not overclock the CPU. This machine's RAM clock rate is at 1600 MHz.

2.1.4 Techniques

OpenMP's sections, parallel and for techniques were used make the program complete within a faster time frame during testing. Sections to perform two different tasks at the same time or splitting sections of work. Parallel and for were used to parallelise for-loops. Other techniques attempted were removing a nested for-loop for a while loop. Utilising an array to store the correlation variables before printing to the console in order.

2.2 Analysis of Code and Parallelisation Process

2.2.1 Successful Parallelisation

Most of the processing time and memory being used in this application is when the CompareAllBacteria function is called from main. This function contains one for-loop and a nested for-loop. These for-loops call the bacteria class to be filled with *.faa file data and compare bacteria calculates the correlation of the two bacteria. This can be seen in Figure 10 below.

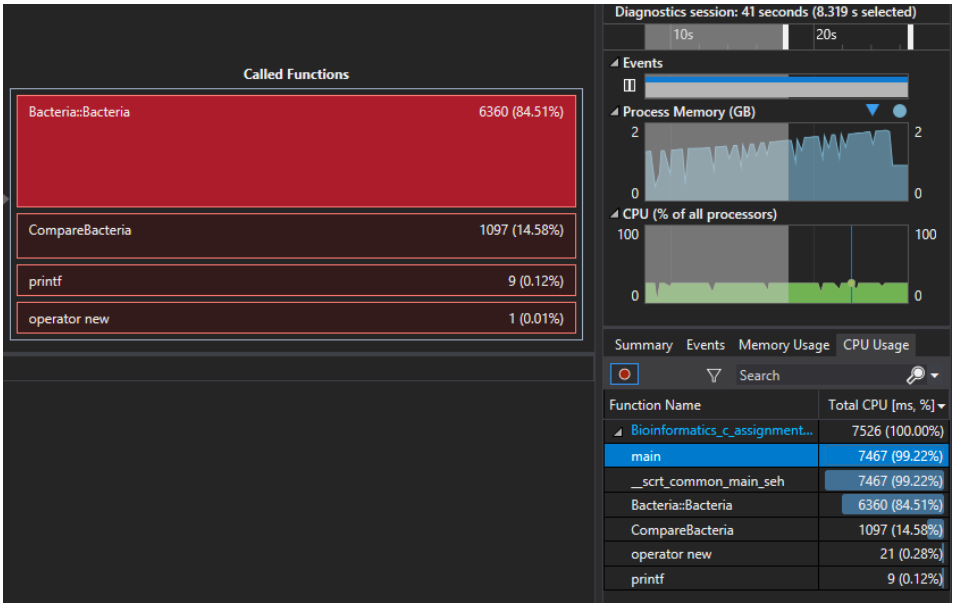


Figure 10: Total CPU (ms, %) of Functions in Bioinformatics – Genome Similarity Using Frequency Vectors Application

The largest components are the bacteria class when files are being loaded and when two bacteria are being compared.

The first for-loop loads each *.faa file into its respective bacteria class. The original code loads each of these files sequentially, one at a time, when there are forty-one files to be loaded. This also fills data into each bacteria class sequentially as well for the respective bacteria file loaded. This for-loop could be parallelised to load multiple bacteria files on numerous threads. This section of code can be found in section 6.1 of the appendix, lines 239 to 243.

The nested for-loop inputs which two bacteria should be compared. This then calculates the correlation between two different bacteria. This nested loop then prints the result of the two bacteria to the console. This nested-loop sequentially calculates and prints each result to the console. This nested-for loop could be parallelised by calculating the correlation of two different bacteria over numerous threads and having them print to the console. However, this could be printed out of order which would lead to a disorganised console output. This section of code can be found in section 6.1 of the appendix, lines 245 to 252.

A solution to keep order but keeping parallelisation would be to load the correlated results into an array and then use the array to print the correlated results in sequential order. This will require changing of the code.

These for-loops should be scalable based on the number of bacteria to be loaded and compared. This will be shown further in section 4 of this report.

2.2.2 Further Analysed Parallelisation Attempts

While most of the run-time is performed in the CompareAllBacteria function, there are other for-loops, while-loops and other sections of code that were analysed to see if there would be any performance increase. However, this was not the case for the following.

2.2.2.1 Two Functions at the Same Time in Main

In the main function of the application, there are two functions that are called. Both functions were found to have a low, if negligible, computational time. However, the ReadInputFile function does not have any variables that are dependant of the previous called Init function. It would be interesting to see if there is a time reduction when running both functions at the same time on two different threads instead of the sequential process of Init being called then ReadInputData. However, this did not provide any faster computation. This is because the code in Init and ReadInputFile proved to have insignificant computation time.

2.2.2.2 Parallelising Bacteria Class

In the bacteria class there are four for-loops. The first for-loop, at lines 108 to 109 at section 6.1 of this report, parallelisation resulted with no additional performance gain. The second for-loop, at lines 112 to 113 at section 6.1 of this report, parallelisation resulted with no additional performance gain.

The third for-loop, at lines 117 to 118 at section 6.1 of this report, OpenMP's parallel and for techniques resulted in different outcomes. The parallel for (combined) parallelisation technique resulted in a memory access violation for the variable p2 calculation. The for parallelisation technique resulted in an infinite loop where nothing is being processed according to Visual Studio's diagnostic tools. The parallel parallelisation technique resulted the application printing the correct results to the console, but at no reduce time.

The fourth for-loop, at lines 158 to 166 at section 6.1 of this report, also had different outcomes when using the OpenMP for-loop parallelisation techniques. Parallel and for combined resulted with incorrect correlation values being printed to the console. The for technique caused a never-ending loop where the processor did no computational work. The parallel technique resulted with a working application printing the correct results, but this did not lower the time spent.

After further analysis with the calculations and variable dependency in the bacteria class, OpenMP sections were utilised to split up the work load over numerous threads. However, this continued to cause a memory access violation at locations at the second for-loop, lines 112 to 113 section 6.1 of this report. This resulted in accepting that the bacteria class could not have its work load split into pieces to reduce to time taken for the application.

2.2.2.3 Parallelising Comparing Two Bacteria

In the CompareBacteria function there is a while-loop at lines 195 to 219 in section 6.1 in the appendices of this report. This while-loop was tested with OpenMP's parallel technique and resulted in a worse performance time for the application. OpenMP's parallel technique was also used on the while-loops from lines 220 to 231 in section 6.1 of this report. The result had no changes to the time taken for the application. These while loops were then split into OpenMP sections as they do not have any related variable or data dependencies with the exception to the variable count. This resulted in the application to crash while running the Debug model. No warnings displayed, or exceptions caught. In the Release model, an infinite loop occurs.

3 Code Implemented

This section of the report includes the code from the original Bioinformatics – Genome Similarity Using Frequency Vectors application in comparison to the final parallelised version. These code changes will start from the top most changes down to the bottom of the code.

3.1 Code Changes in Compare All Bacteria Function

The original version of code for the CompareAllBacteria function can be seen below in Figure 11. Below Figure 11, Figure 12 can be seen which includes the code in the high-performance version.

```
236   void CompareAllBacteria()
237   {
238         Bacteria** b = new Bacteria*[number_bacteria];
239         for (int i = 0; i<number_bacteria; i++)
240         {
241               printf("load %d of %d\n", i + 1, number_bacteria);
242               b[i] = new Bacteria(bacteria_name[i]);
243         }
244
245         for (int i = 0; i<number_bacteria - 1; i++)
246               for (int j = i + 1; j<number_bacteria; j++)
247               {
248                     printf("%2d %2d -> ", i, j);
249                     double correlation = CompareBacteria(b[i], b[j]);
250                     printf("%.20lf\n", correlation);
251               }
252   }
```

Figure 11: Original Code for Compare All Bacteria Function

```
280   void CompareAllBacteria() {
281         Bacteria** b = new Bacteria*[number_bacteria];
282         /*
283         [8] Success with major improvement
288         */
289         #pragma omp parallel for
290         for (int i = 0; i < number_bacteria; i++) {
291               printf("load %d of %d\n", i + 1, number_bacteria);
292               b[i] = new Bacteria(bacteria_name[i]);
293         }
294
295         /*
296         [9]
336         */
337         #pragma omp parallel for
338         for (int i = 0; i < number_bacteria - 1; i++) {
339               /*
340               [10]
341               */
342               for (int j = i + 1; j < number_bacteria; j++) {
343                     double correlation = CompareBacteria(b[i], b[j]);
344                     printf("%2d %2d -> %.20lf\n", i, j, correlation);
345               }
346         }
347   }
```

Figure 12: Parallelised Code for Compare All Bacteria Function

The complete version of the code for the original version of the application can be found in section 6.1 of the appendices. The complete version of the code for the parallelised version of the application can be found in section 6.2 of the appendices. In Figure 12, there are missing lines of code. These lines were removed as they are commented notes taken during the analysis and parallelisation process.

The lines of code in Figure 12, lines 289 and 337, are the OpenMP parallel and for functionality that OpenMP can perform. OpenMP parallel spawns a group of threads. OpenMP for divides the loop iterations between the spawned threads. Both the 'parallel' and 'for' techniques offered by OpenMP were combined. Through testing they provided the quickest time to achieving that all the *.faa files were loaded, all respective data was used to create each respective bacteria class, all bacteria comparisons were calculated, and those results are printed to the console.

Below in Figures 13 and 14 it can be seen what happens in the first second of the two versions of the application when it starts. In Figure 13, the first file is being loaded. In Figure 14, four bacteria *.faa files are being read and those classes are being created for bacteria one, twelve, thirty-two and twenty-two. This is because the test was running on a four core, four read capable CPU so only a maximum of four files can be read at any one time when using this machine. However, on a four core, eight thread capable CPU, a maximum of eight files can be read. This can be seen in Figure 15 on the next page.

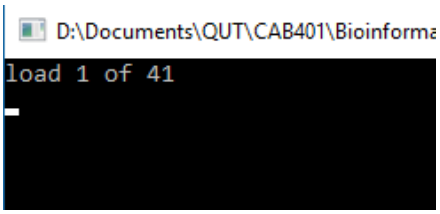


Figure 13: Original Loading Bacteria

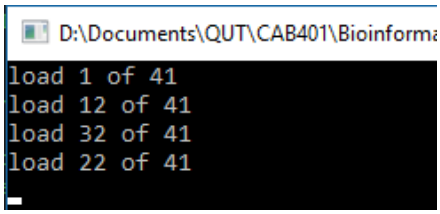


Figure 14: Parallel Loading Bacteria Four Threads Max

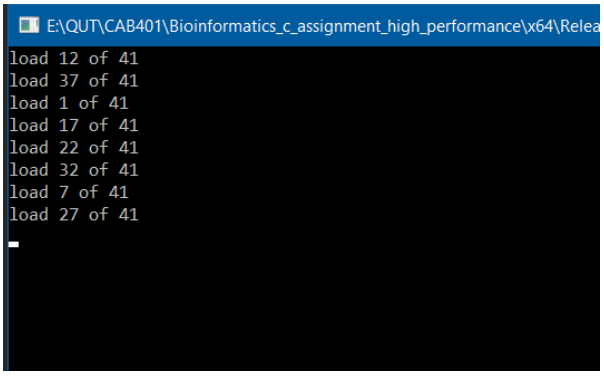


Figure 15: Parallel Loading Bacteria Eight Threads Max

Using OpenMP's parallel and for techniques for the for-loop at lines 289 to 293, shown at Figure 12, multiple files can be read, and bacteria classes created at the same time. The obvious limitation here is the read speed of the disc that the files are stored on. However, the use of OpenMP allows for the application to be scalable. This scalability is dependent of the

maximum number of threads of a CPU, the clock rate of the CPU, enough memory and the number of bacteria being compared. Below, in Figures 16 and 17, the amount of memory being used increases with each bacteria file being read and class created.

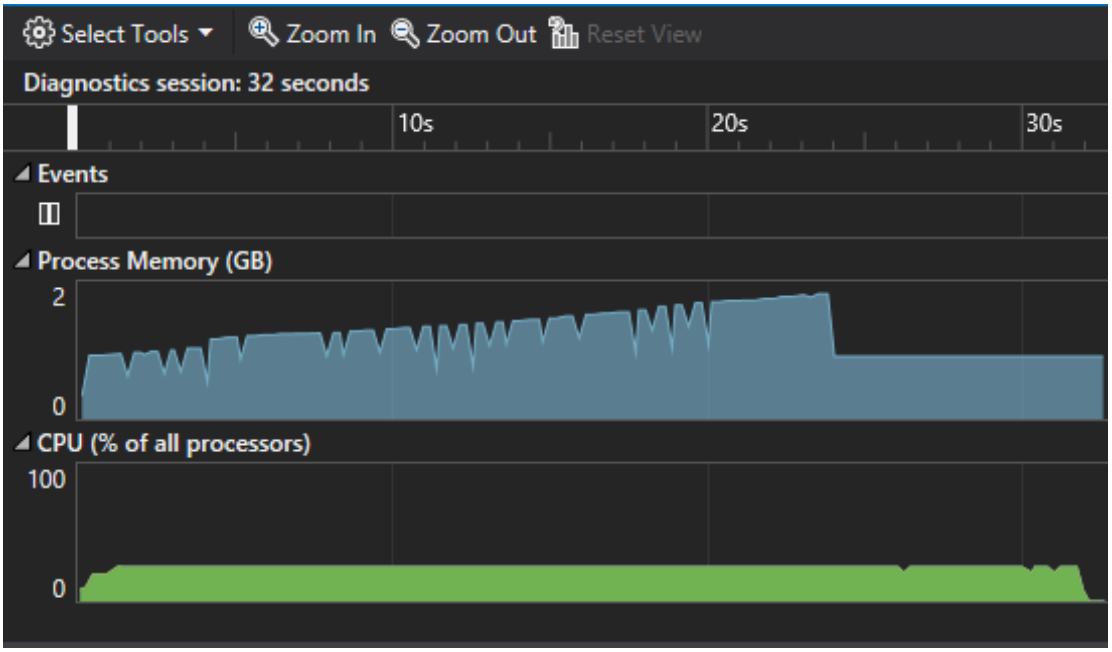


Figure 16: Sequential Application Memory and CPU Usage

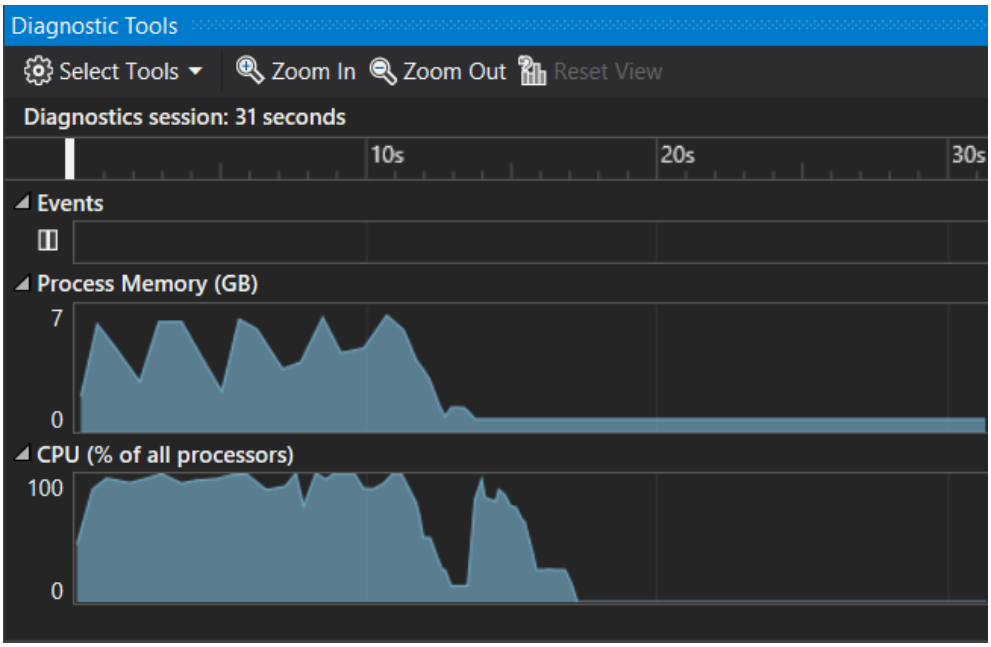


Figure 17: Parallelised Application Memory and CPU Usage

For the parallelisation of the nested for-loop, from lines 337 to 346 in Figure 12, the correlation printed will be in a mixed order. While, the results are still the same, only the order of the printed results are different. If the user wished to have the correlation printed in numerical order, bacteria 0 and bacteria 1 to bacteria 39 and bacteria 40, but still wish for a faster performance time using OpenMP then Figure 18 on the next page can be used instead.

```
295           /*
296           [9]
336           */
337           #pragma omp for
338           for (int i = 0; i < number_bacteria - 1; i++) {
339                 /*
340                 [10]
341                 */
342                 for (int j = i + 1; j < number_bacteria; j++) {
343                       double correlation = CompareBacteria(b[i], b[j]);
344                       printf("%2d %2d -> %.20lf\n", i, j, correlation);
345                 }
346           }
347     }
```

Figure 18: Parallelised Nested For-Loop in Order

The difference between Figure 12 and Figure 18 is that the OpenMP statement removed the parallel functionality. This added a few seconds of extra time computational time to the application, but the printed correlation and bacteria pairs are printed to the console in order. This order difference can be seen in Figures 19 and 20 below.

```
3 32 -> 0.00173857472560830185
3 33 -> 0.00119861580795493547
3 34 -> 0.00132066757407171918
3 35 -> 0.00115326991777306800
3 36 -> 0.00126922941777803675
3 37 -> 0.00155134347347462751
```

Figure 19: Correlation in Order

```
 3 32 -> 0.00173857472560830185
28 30 -> 0.00208711780367286511
 3 33 -> 0.00119861580795493547
28 31 -> 0.00126214769015896462
17 20 -> 0.00174925382121538398
28 32 -> 0.00192751640765809564
```

Figure 20: Correlation not in Order

This version of the code was not taken though as the purpose of this assignment was to take a sequential program that could be parallelised and then parallelised to create the same results but in a shorter time frame that still produces the same results.

4 Results

In this section of the report, the correlation and times taken to run the application, both the original and high-performance models, on two different machines are discussed.

4.1 Time Taken for Execution of Sequential and Parallelised Applications

The systems specification for this machine can be found in section 2.1.3 of this report.

Table 1 below shows the time to complete the original and the parallelised versions of the Bioinformatics – Genome similarity using Frequency Vectors application. The application was executed five times and the average mean time was calculated. The parallelised version had each OpenMP line of code set to the specified number of threads below.

	Time Taken (Seconds)					
Application Version	1st	2nd	3rd	4th	5th	**Average**
Original	28 secs	29 secs	28 secs	28 secs	28 secs	**28.2 secs**
High Performance (1 Thread)	29 secs	29 secs	29 secs	29 secs	29 secs	**29.0 secs**
High Performance (2 Threads)	20 secs	20 secs	20 secs	20 secs	20 secs	**20.0 secs**
High Performance (3 Threads)	18 secs	17 secs	17 secs	17 secs	17 secs	**16.2 secs**
High Performance (4 Threads)	16 secs	17 secs	17 secs	17 secs	17 secs	**16.8 secs**
High Performance (5 Threads)	16 secs	16 secs	16 secs	16 secs	16 secs	**16.0 secs**
High Performance (6 Threads)	16 secs	16 secs	16 secs	16 secs	16 secs	**16.0 secs**
High Performance (7 Threads)	16 secs	16 secs	16 secs	16 secs	16 secs	**16.0 secs**
High Performance (8 Threads)	16 secs	16 secs	16 secs	16 secs	16 secs	**16.0 secs**

Table 1: Sequential and Different Thread Count for Parallelised Application Run-Time

From the results shown above I cannot state whether the application is limited to four threads or if the test results were limited due to the number of physical cores available on the hardware used. A machine with more than four physical cores is required to prove the previous statement.

4.2 Profiling Reports

Figure 21 below is a CPU profiling report created in Visual Studio 2017 showing the CPU usage of the sequential application and percentage of work for functions during run-time.

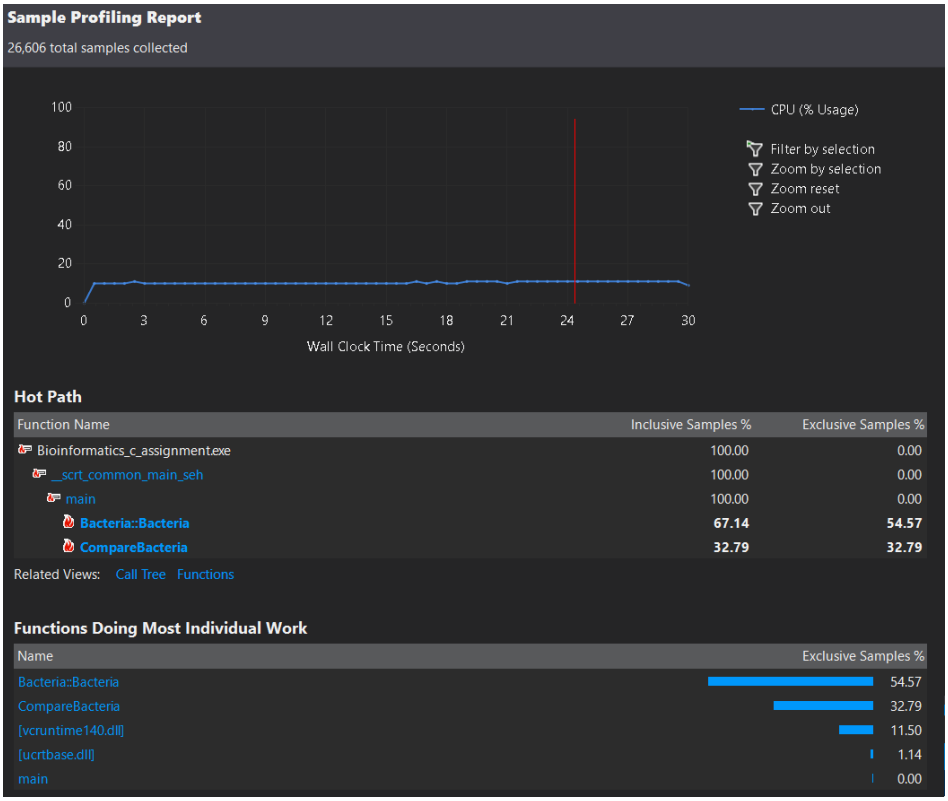


Figure 21: Sequential CPU Profiler

Figure 22 below is a CPU profiling report created in Visual Studio 2017 showing the CPU usage of the parallelised application and percentage of work for functions during run-time.

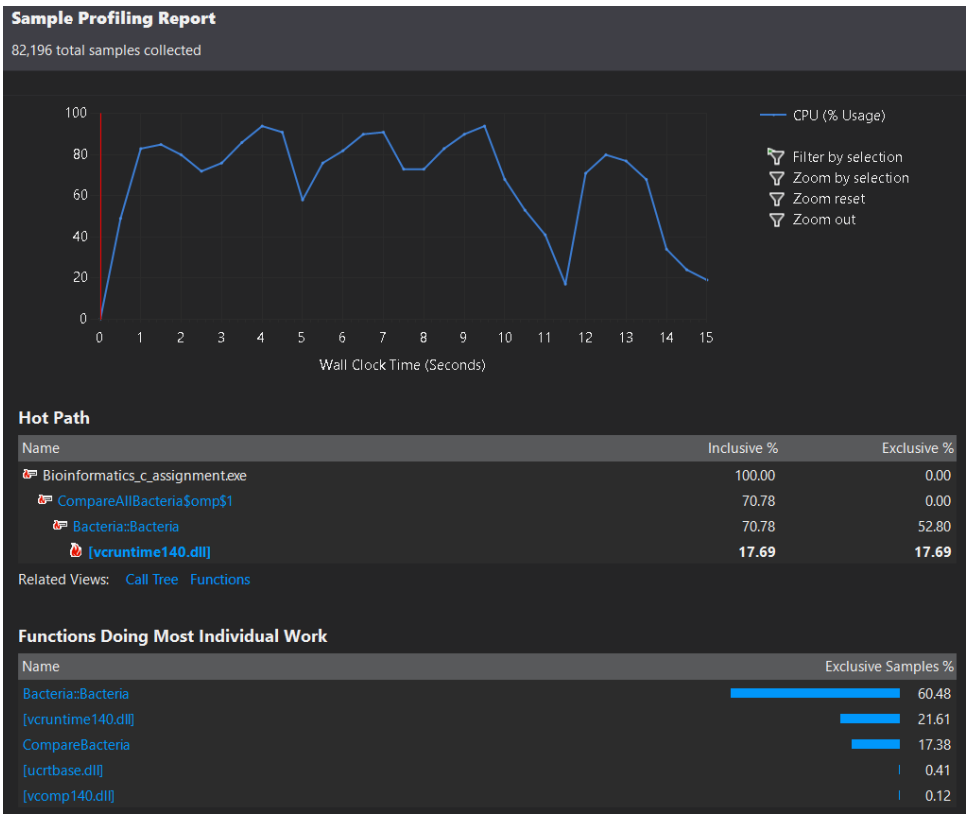


Figure 22: Parallelised CPU Profiler

4.3 Speed Up Graph

The graph below shows the speed up of the parallelised version of the application compared to the sequential application based on the time difference and the number of threads being used.

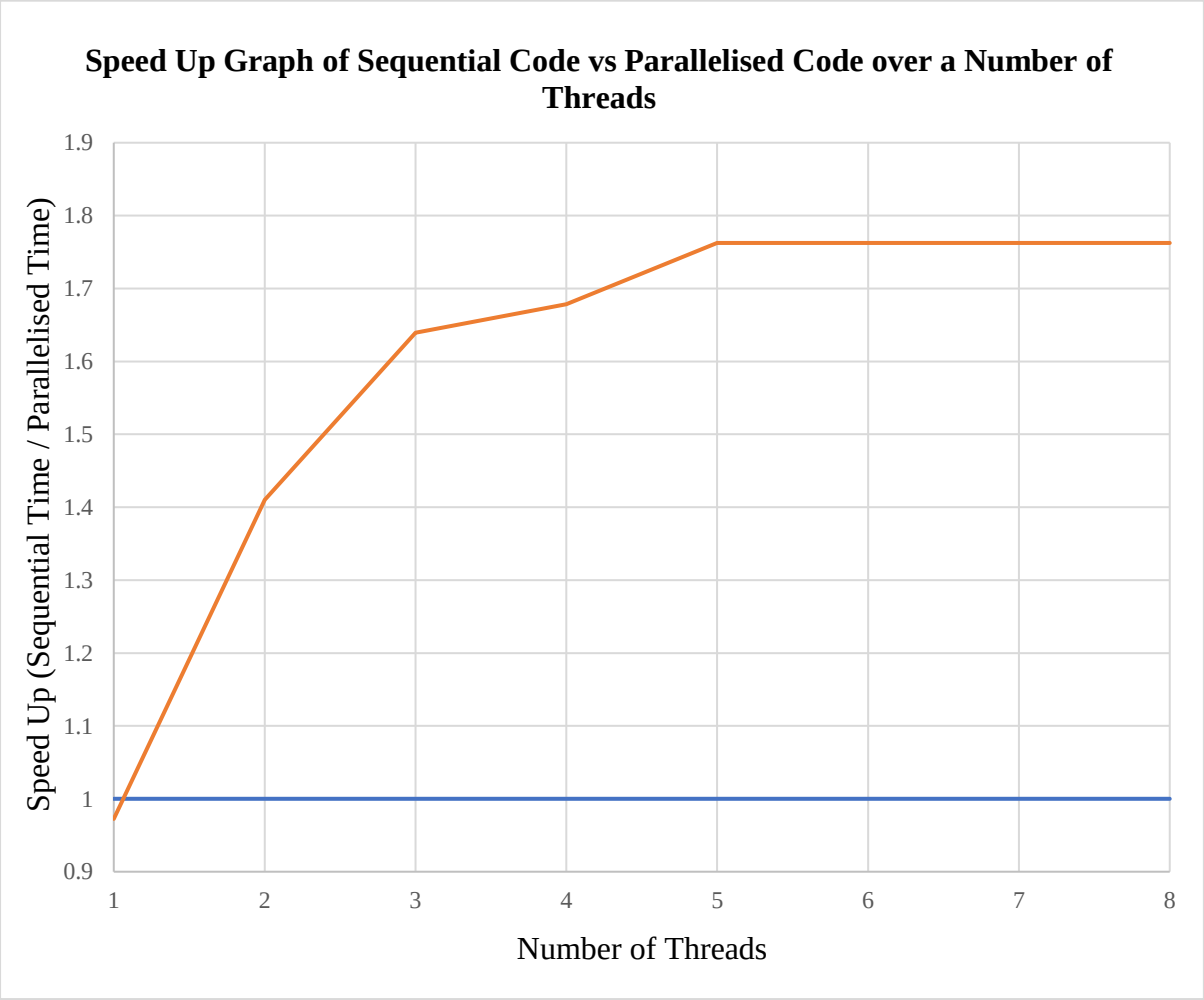


Figure 23: Speed Up Graph of Sequential vs Parallelised Over Threads

5 Reflection

Originally the Bioinformatics – Genome similarity using Frequency Vectors application was supposed to be parallelised using MPI, mpich3 or openMP, on my Raspberry Pi Beowulf cluster. This was scrapped because the application immediately gets a segmentation fault. Instead of fiddling around to get the code for the application to run properly I opted-out for running the application on through Visual Studio on a Windows OS machine so I could get the application parallelised. In terms of what I have learned, I usually always utilised Code::Blocks and the mingw 32 and 64 bit compilers when I program in C/C++. This is mainly because the IDE and compiler is free and widely used. However, during this semester, the CAB401 and IGB381 courses showed me how useful Visual Studio can be. The profiler and diagnostic tools allows me to see what functions and code could be further improved. Much easier than slowly debugging your way through the application manually. Another thing I have learnt is how simple OpenMP is to parallelise code with. I've always used POSIX threads when I wanted to parallelise for-loops or create multiple simultaneous executions of work. While there is a difference between the two, low-level vs high-level portable multiprocessing paradigms, it was a good experience to utilise and learn what OpenMP has to offer and how it works.

I believe my attempt at analysing the original code and going beyond trying different techniques to get the application to perform faster was almost a success. The one component that bothers me is the nested for-loop in the CompareAllBacteria function. An issue was encountered here that I could not fix.

5.1 Issues Encountered

I attempted to store the correlated data into a vector, dynamic array by splitting up the objectives. These objective were to calculate the correlation and printing to the console. This code can be seen in Figure 24 below.

```
	std::vector<double> correlation;
	int vectorSize = (number_bacteria * number_bacteria) - number_bacteria;
	correlation.resize(vectorSize);

	#pragma omp parallel for
	for (int i = 0; i < number_bacteria - 1; i++) {
		for (int j = i + 1; j < number_bacteria; j++) {
			correlation[(i * 10) + j] = CompareBacteria(b[i], b[j]);
		}
	}

	for (int i = 0; i < number_bacteria - 1; i++) {
		for (int j = i + 1; j < number_bacteria; j++) {
			printf("%2d %2d -> %.20lf\n", i, j, correlation[(i * 10) +
j]);
		}
	}
```

Figure 24: Restructured Nested For-Loop Attempt

The result of this code sometimes provided the correct correlation values. At other times I found the correct correlation value, being returned by the function CompareBacteria, was

changed when it was stored in the vector. This produced incorrect results. The purpose of this was to allow for the exact run-time to be achieved but with the correlated values printed in order. Splitting these objectives into two components allowed for the CompareBacteria to be parallelised providing a faster run-time. Then a sequential for-loop to print out the results in order.

It annoys me to know that I could have improved the ease of use, printing correlation in order, especially when a colleague of mine in CAB401 did the same thing and it worked for him.

As discussed in section 2.2.2, of this report, it was found that many data dependencies in other functions prevented further changes and parallelism for this application. At times the incorrect correlation between bacteria would occur. Further problems such as infinite loops and application crashes were encountered to further improve the application. However, solutions to these problems provided parallelisation that had no effect on the applications run-time making the parallelisation of multiple sections of code running at the same time on different threads pointless.

For more notes during testing the high-performance version of the Bioinformatics – Genome similarity using Frequency Vectors application can be found commented in the *.cpp file of the Visual Studio project.

6 Appendix

6.1 Original Code

The original code for the Bioinformatics – Genome similarity using Frequency Vectors (C++) application was provided by Dr Wayne Kelly on the CAB401 High Performance and Parallel Computing QUT Blackboard page. A copy of the original code can be seen below. All bacteria files and the Visual Studio 2017 project can be found at the link here https://github.com/Starwolf-001/CAB401/tree/master/Bioinformatics_c_assignment.

```
#include <stdio.h>
#include <string.h>
#include <time.h>
#include <math.h>
#include <iostream>

int number_bacteria;
char** bacteria_name;
long M, M1, M2;
short code[27] = { 0, 2, 1, 2, 3, 4, 5, 6, 7, -1, 8, 9, 10, 11, -1, 12,
13, 14, 15, 16, 1, 17, 18, 5, 19, 3 };
#define encode(ch)        code[ch-'A']
#define LEN               6
#define AA_NUMBER         20
#define EPSILON           1e-010

void Init()
{
      M2 = 1;
      for (int i = 0; i<LEN - 2; i++) // M2 = AA_NUMBER ^ (LEN-2);
            M2 *= AA_NUMBER;
      M1 = M2 * AA_NUMBER;            // M1 = AA_NUMBER ^ (LEN-1);
      M = M1 *AA_NUMBER;              // M  = AA_NUMBER ^ (LEN);
}

class Bacteria
{
private:
      long* vector;
      long* second;
      long one_l[AA_NUMBER];
      long indexs;
      long total;
      long total_l;
      long complement;

      void InitVectors()
      {
            vector = new long[M];
            second = new long[M1];
            memset(vector, 0, M * sizeof(long));
            memset(second, 0, M1 * sizeof(long));
            memset(one_l, 0, AA_NUMBER * sizeof(long));
            total = 0;
            total_l = 0;
            complement = 0;
      }

      void init_buffer(char* buffer)
      {
            complement++;
            indexs = 0;
```

```
53                  for (int i = 0; i<LEN - 1; i++)
54                  {
55                        short enc = encode(buffer[i]);
56                        one_l[enc]++;
57                        total_l++;
58                        indexs = indexs * AA_NUMBER + enc;
59                  }
60                  second[indexs]++;
61            }
62
63            void cont_buffer(char ch)
64            {
65                  short enc = encode(ch);
66                  one_l[enc]++;
67                  total_l++;
68                  long index = indexs * AA_NUMBER + enc;
69                  vector[index]++;
70                  total++;
71                  indexs = (indexs % M2) * AA_NUMBER + enc;
72                  second[indexs]++;
73            }
74
75      public:
76            long count;
77            double* tv;
78            long *ti;
79
80            Bacteria(char* filename)
81            {
82                  FILE * bacteria_file = fopen(filename, "r");
83                  InitVectors();
84
85                  char ch;
86                  while ((ch = fgetc(bacteria_file)) != EOF)
87                  {
88                        if (ch == '>')
89                        {
90                              // skip rest of line
91                              while (fgetc(bacteria_file) != '\n');
92                              char buffer[LEN - 1];
93                              fread(buffer, sizeof(char), LEN - 1,
                                    bacteria_file);
94                              init_buffer(buffer);
95                        }
96                        else if (ch != '\n')
97                              cont_buffer(ch);
98                  }
99
100                 long total_plus_complement = total + complement;
101                 double total_div_2 = total * 0.5;
102                 int i_mod_aa_number = 0;
103                 int i_div_aa_number = 0;
104                 long i_mod_M1 = 0;
105                 long i_div_M1 = 0;
106
107                 double one_l_div_total[AA_NUMBER];
108                 for (int i = 0; i<AA_NUMBER; i++)
109                       one_l_div_total[i] = (double)one_l[i] / total_l;
110
111                 double* second_div_total = new double[M1];
112                 for (int i = 0; i<M1; i++)
113                       second_div_total[i] = (double)second[i] /
                            total_plus_complement;
114                 count = 0;
```

```
115                 double* t = new double[M];
116
117                 for (long i = 0; i<M; i++)
118                 {
119                       double p1 = second_div_total[i_div_aa_number];
120                       double p2 = one_l_div_total[i_mod_aa_number];
121                       double p3 = second_div_total[i_mod_M1];
122                       double p4 = one_l_div_total[i_div_M1];
123                       double stochastic = (p1 * p2 + p3 * p4) *
                          total_div_2;
124
125                       if (i_mod_aa_number == AA_NUMBER - 1)
126                       {
127                             i_mod_aa_number = 0;
128                             i_div_aa_number++;
129                       }
130                       else
131                             i_mod_aa_number++;
132
133                       if (i_mod_M1 == M1 - 1)
134                       {
135                             i_mod_M1 = 0;
136                             i_div_M1++;
137                       }
138                       else
139                             i_mod_M1++;
140
141                       if (stochastic > EPSILON)
142                       {
143                             t[i] = (vector[i] - stochastic) / stochastic;
144                             count++;
145                       }
146                       else
147                             t[i] = 0;
148                 }
149
150                 delete second_div_total;
151                 delete vector;
152                 delete second;
153
154                 tv = new double[count];
155                 ti = new long[count];
156
157                 int pos = 0;
158                 for (long i = 0; i<M; i++)
159                 {
160                       if (t[i] != 0)
161                       {
162                             tv[pos] = t[i];
163                             ti[pos] = i;
164                             pos++;
165                       }
166                 }
167                 delete t;
168
169                 fclose(bacteria_file);
170           }
171     };
172
173     void ReadInputFile(char* input_name)
174     {
175           FILE* input_file = fopen(input_name, "r");
176           fscanf(input_file, "%d", &number_bacteria);
177           bacteria_name = new char*[number_bacteria];
```

```
178
179         for (long i = 0; i<number_bacteria; i++)
180         {
181               bacteria_name[i] = new char[20];
182               fscanf(input_file, "%s", bacteria_name[i]);
183               strcat(bacteria_name[i], ".faa");
184         }
185         fclose(input_file);
186   }
187
188   double CompareBacteria(Bacteria* b1, Bacteria* b2)
189   {
190         double correlation = 0;
191         double vector_len1 = 0;
192         double vector_len2 = 0;
193         long p1 = 0;
194         long p2 = 0;
195         while (p1 < b1->count && p2 < b2->count)
196         {
197               long n1 = b1->ti[p1];
198               long n2 = b2->ti[p2];
199               if (n1 < n2)
200               {
201                     double t1 = b1->tv[p1];
202                     vector_len1 += (t1 * t1);
203                     p1++;
204               }
205               else if (n2 < n1)
206               {
207                     double t2 = b2->tv[p2];
208                     p2++;
209                     vector_len2 += (t2 * t2);
210               }
211               else
212               {
213                     double t1 = b1->tv[p1++];
214                     double t2 = b2->tv[p2++];
215                     vector_len1 += (t1 * t1);
216                     vector_len2 += (t2 * t2);
217                     correlation += t1 * t2;
218               }
219         }
220         while (p1 < b1->count)
221         {
222               long n1 = b1->ti[p1];
223               double t1 = b1->tv[p1++];
224               vector_len1 += (t1 * t1);
225         }
226         while (p2 < b2->count)
227         {
228               long n2 = b2->ti[p2];
229               double t2 = b2->tv[p2++];
230               vector_len2 += (t2 * t2);
231         }
232
233         return correlation / (sqrt(vector_len1) * sqrt(vector_len2));
234   }
235
236   void CompareAllBacteria()
237   {
238         Bacteria** b = new Bacteria*[number_bacteria];
239         for (int i = 0; i<number_bacteria; i++)
240         {
241               printf("load %d of %d\n", i + 1, number_bacteria);
```

```
242                 b[i] = new Bacteria(bacteria_name[i]);
243           }
244
245           for (int i = 0; i<number_bacteria - 1; i++)
246                 for (int j = i + 1; j<number_bacteria; j++)
247                 {
248                       printf("%2d %2d -> ", i, j);
249                       double correlation = CompareBacteria(b[i], b[j]);
250                       printf("%.20lf\n", correlation);
251                 }
252     }
253
254     int main(int argc, char * argv[])
255     {
256           time_t t1 = time(NULL);
257
258           Init();
259           ReadInputFile(argv[1]);
260           CompareAllBacteria();
261
262           time_t t2 = time(NULL);
263           printf("time elapsed: %d seconds\n", t2 - t1);
264
265           system("pause");
266
267           return 0;
277     }
```

6.2 High Performance and Parallel Code

This code for the Bioinformatics – Genome similarity using Frequency Vectors (C++) application was analysed and tested to provide the correct results in a short time as per the requirement for the CAB401 High Performance and Parallel Computing Assignment. This code can be seen below. All bacteria files, notes taken during testing, code and the Visual Studio 2017 project can be found at the link here https://github.com/Starwolf-001/CAB401/tree/master/Bioinformatics_c_assignment_high_performance. There are lines missing in this code. These missing lines of code are commented notes based on the testing, and analysis when parallelising the original Bioinformatics – Genome similarity using Frequency Vectors application.

```
1     #include <stdio.h>
2     #include <string.h>
3     #include <time.h>
4     #include <math.h>
5     #include <iostream>
6     #include <omp.h>
7
8     int number_bacteria;
9     char** bacteria_name;
10    long M, M1, M2;
11    short code[27] = {0, 2, 1, 2, 3, 4, 5, 6, 7, -1, 8, 9, 10, 11, -1, 12,
      13, 14, 15, 16, 1, 17, 18, 5, 19, 3};
12    #define encode(ch)        code[ch-'A']
13    #define LEN               6
14    #define AA_NUMBER         20
15    #define EPSILON           1e-010
16
17    void Init() {
18          M2 = 1;
24          for (int i = 0; i < LEN - 2; i++) {   // M2 = AA_NUMBER ^ (LEN-2);
25                M2 *= AA_NUMBER;
26          }
27          M1 = M2 * AA_NUMBER;            // M1 = AA_NUMBER ^ (LEN-1);
28          M = M1 *AA_NUMBER;              // M  = AA_NUMBER ^ (LEN);
29    }
30
31    class Bacteria {
32    private:
33          long* vector;
34          long* second;
35          long one_l[AA_NUMBER];
36          long indexs;
37          long total;
38          long total_l;
39          long complement;
40
41          void InitVectors() {
42                vector = new long[M];
43                second = new long[M1];
44                memset(vector, 0, M * sizeof(long));
45                memset(second, 0, M1 * sizeof(long));
46                memset(one_l, 0, AA_NUMBER * sizeof(long));
47                total = 0;
48                total_l = 0;
49                complement = 0;
50          }
51
52          void init_buffer(char* buffer) {
```

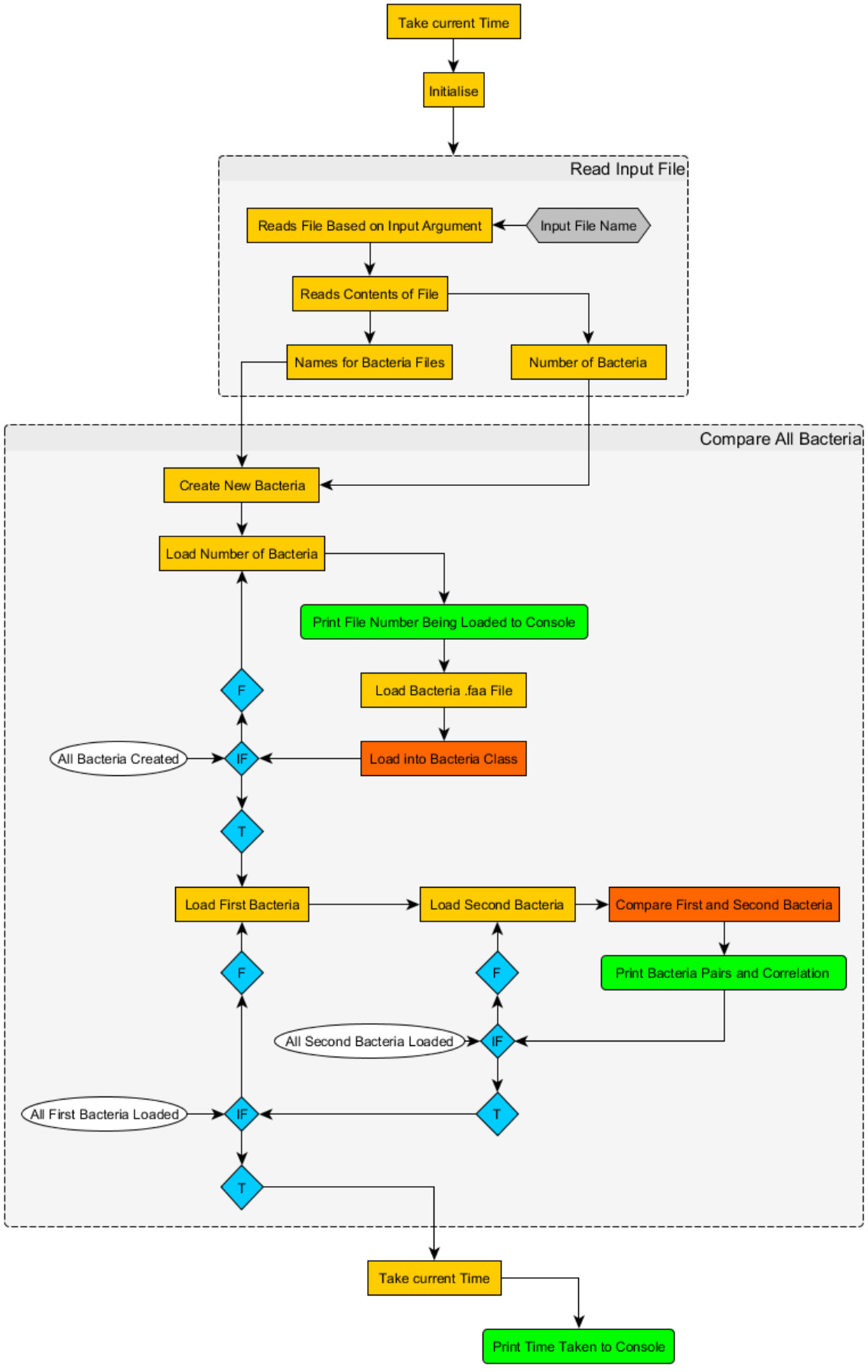
```
53                  complement++;
54                  indexs = 0;
59                  for (int i = 0; i < LEN - 1; i++) {
60                        short enc = encode(buffer[i]);
61                        one_l[enc]++;
62                        total_l++;
63                        indexs = indexs * AA_NUMBER + enc;
64                  }
65                  second[indexs]++;
66            }
67
68            void cont_buffer(char ch) {
69                  short enc = encode(ch);
70                  one_l[enc]++;
71                  total_l++;
72                  long index = indexs * AA_NUMBER + enc;
73                  vector[index]++;
74                  total++;
75                  indexs = (indexs % M2) * AA_NUMBER + enc;
76                  second[indexs]++;
77            }
78
79      public:
80            long count;
81            double* tv;
82            long *ti;
83
84            Bacteria(char* filename) {
92                  FILE * bacteria_file = fopen(filename, "r");
93                  InitVectors();
94
95                  char ch;
96                  while ((ch = fgetc(bacteria_file)) != EOF) {
97                        if (ch == '>') {
98                              while (fgetc(bacteria_file) != '\n'); // skip
                                rest of line
99
100                             char buffer[LEN - 1];
101                             fread(buffer, sizeof(char), LEN - 1,
                                bacteria_file);
102                             init_buffer(buffer);
103                       }
104                       else if (ch != '\n')
105                             cont_buffer(ch);
106                 }
107                 fclose(bacteria_file);
108
109                 long total_plus_complement = total + complement;
110                 double total_div_2 = total * 0.5;
111                 int i_mod_aa_number = 0;
112                 int i_div_aa_number = 0;
113                 long i_mod_M1 = 0;
114                 long i_div_M1 = 0;
115
116                 double one_l_div_total[AA_NUMBER];
117                 double* second_div_total = new double[M1];
130                 for (int i = 0; i < AA_NUMBER; i++) {
131                       one_l_div_total[i] = (double)one_l[i] / total_l;
132                 }
138                 for (int i = 0; i < M1; i++) {
139                       second_div_total[i] = (double)second[i] /
                          total_plus_complement;
140                 }
141
```

```
142                 count = 0;
143                 double* t = new double[M];
144
156                 for (long i = 0; i < M; i++) {
157                       double p1 = second_div_total[i_div_aa_number];
158                       double p2 = one_l_div_total[i_mod_aa_number];
159                       double p3 = second_div_total[i_mod_M1];
160                       double p4 = one_l_div_total[i_div_M1];
161                       double stochastic = (p1 * p2 + p3 * p4) *
                          total_div_2;
162
163                       if (i_mod_aa_number == AA_NUMBER - 1) {
164                             i_mod_aa_number = 0;
165                             i_div_aa_number++;
166                       }
167                       else {
168                             i_mod_aa_number++;
169                       }
170
171                       if (i_mod_M1 == M1 - 1) {
172                             i_mod_M1 = 0;
173                             i_div_M1++;
174                       }
175                       else {
176                             i_mod_M1++;
177                       }
178
179                       if (stochastic > EPSILON) {
180                             t[i] = (vector[i] - stochastic) / stochastic;
181                             count++;
182                       }
183                       else {
184                             t[i] = 0;
185                       }
186                 }
187
188                 delete second_div_total;
189                 delete vector;
190                 delete second;
191
192                 tv = new double[count];
193                 ti = new long[count];
194
195                 int pos = 0;
201                 for (long i = 0; i < M; i++) {
202                       if (t[i] != 0) {
203                             tv[pos] = t[i];
204                             ti[pos] = i;
205                             pos++;
206                       }
207                 }
208                 delete t;
209           }
210     };
211
212     void ReadInputFile(char* input_name) {
213           FILE* input_file = fopen(input_name, "r");
214           fscanf(input_file, "%d", &number_bacteria);
215           bacteria_name = new char*[number_bacteria];
220           for (long i = 0; i < number_bacteria; i++) {
221                 bacteria_name[i] = new char[20];
222                 fscanf(input_file, "%s", bacteria_name[i]);
223                 strcat(bacteria_name[i], ".faa");
224           }
```

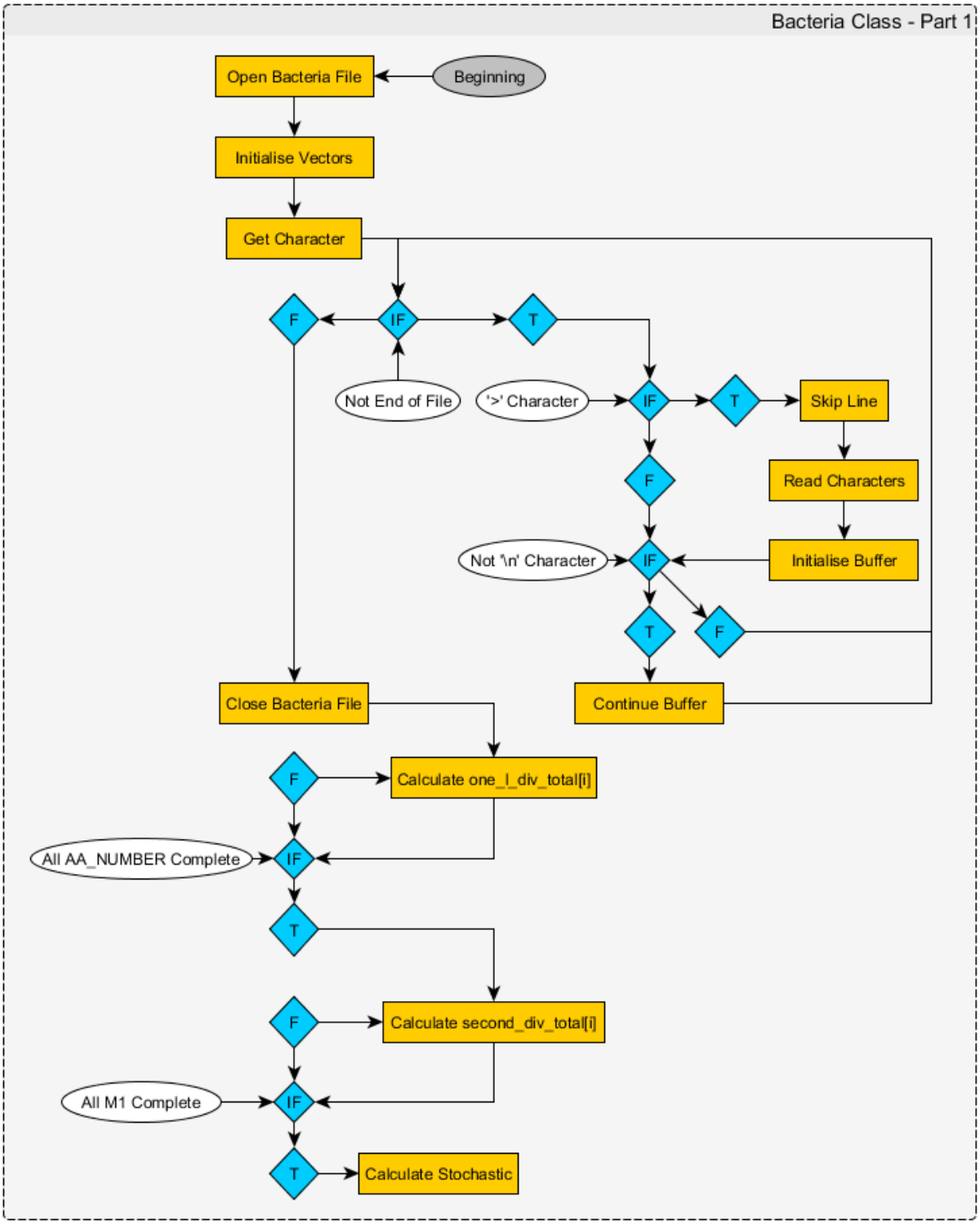
```
225         fclose(input_file);
226     }
227
228     double CompareBacteria(Bacteria* b1, Bacteria* b2) {
229         double correlation = 0;
230         double vector_len1 = 0;
231         double vector_len2 = 0;
232         long p1 = 0;
233         long p2 = 0;
237         while (p1 < b1->count && p2 < b2->count) {
238             long n1 = b1->ti[p1];
239             long n2 = b2->ti[p2];
240             if (n1 < n2) {
241                 double t1 = b1->tv[p1];
242                 vector_len1 += (t1 * t1);
243                 p1++;
244             }
245             else if (n2 < n1) {
246                 double t2 = b2->tv[p2];
247                 p2++;
248                 vector_len2 += (t2 * t2);
249             }
250             else {
251                 double t1 = b1->tv[p1++];
252                 double t2 = b2->tv[p2++];
253                 vector_len1 += (t1 * t1);
254                 vector_len2 += (t2 * t2);
255                 correlation += t1 * t2;
256             }
257         }
264         while (p1 < b1->count) {
265             long n1 = b1->ti[p1];
266             double t1 = b1->tv[p1++];
267             vector_len1 += (t1 * t1);
268         }
274         while (p2 < b2->count) {
275             long n2 = b2->ti[p2];
276             double t2 = b2->tv[p2++];
277             vector_len2 += (t2 * t2);
278         }
279         return correlation / (sqrt(vector_len1) * sqrt(vector_len2));
280     }
281
282     void CompareAllBacteria() {
283         Bacteria** b = new Bacteria*[number_bacteria];
291         #pragma omp parallel for
292         for (int i = 0; i < number_bacteria; i++) {
293             printf("load %d of %d\n", i + 1, number_bacteria);
294             b[i] = new Bacteria(bacteria_name[i]);
295         }
296
342         #pragma omp parallel for
343         for (int i = 0; i < number_bacteria - 1; i++) {
347             for (int j = i + 1; j < number_bacteria; j++) {
348                 double correlation = CompareBacteria(b[i], b[j]);
349                 printf("%2d %2d -> %.20lf\n", i, j, correlation);
350             }
351         }
352     }
353
354     int main(int argc, char * argv[]) {
355         time_t t1 = time(NULL);
364         Init();
365         ReadInputFile(argv[1]);
```

```
366         CompareAllBacteria();
367
368         time_t t2 = time(NULL);
369         printf("time elapsed: %d seconds\n", t2 - t1);
370
371         system("pause");
372
373         return 0;
374     }
```

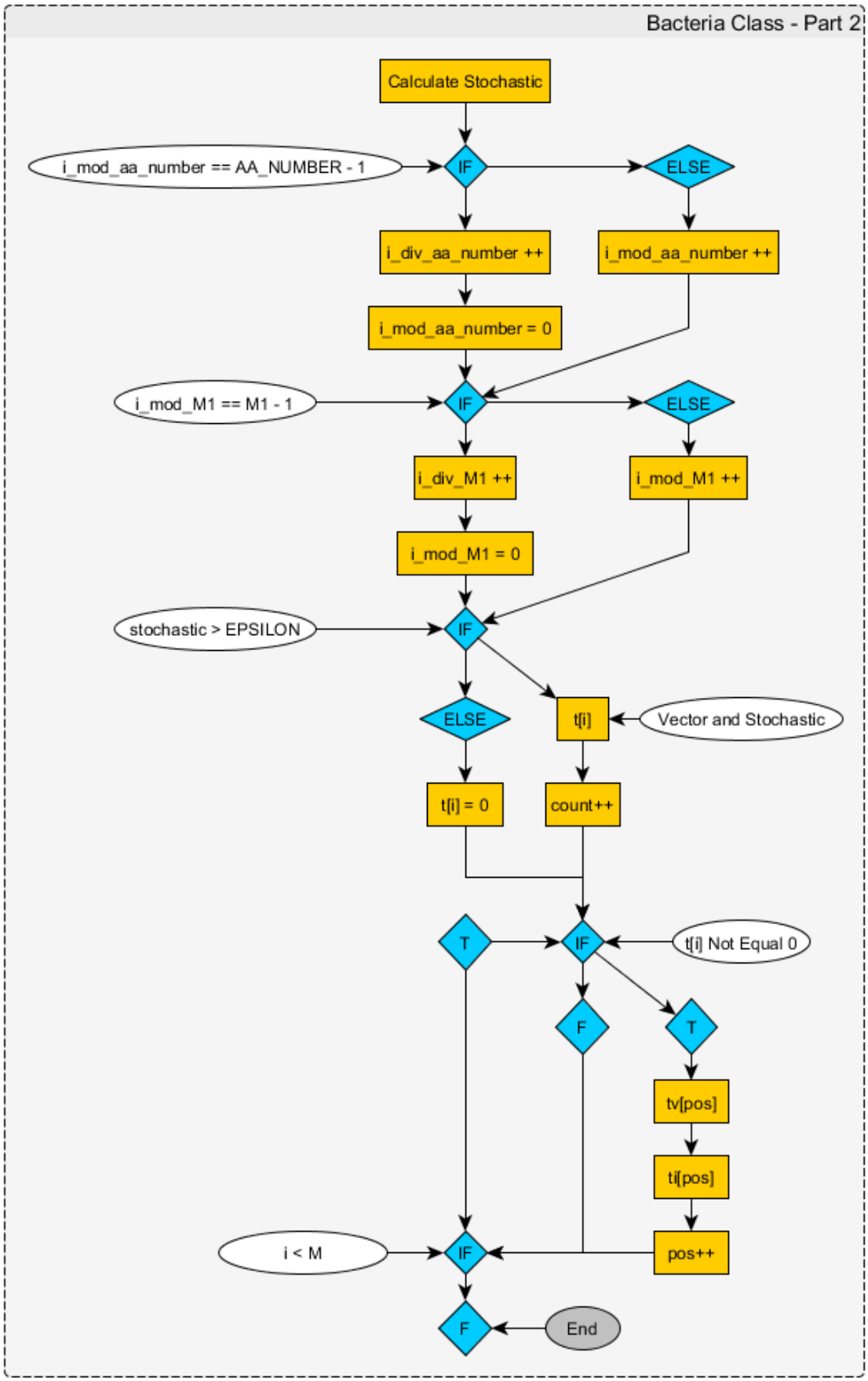
6.3 Detailed Software Architecture



6.4 Bacteria Class – Part 1 Software Architecture



6.5 Bacteria Class – Part 2 Software Architecture



6.6 Compare Bacteria Software Architecture