A C++ IMPLEMENTATION OF A
POLYNOMIAL TIME APPROXIMATION SCHEME
FOR ALIGNING PROTEIN STRUCTURES
BY

CHOR YUN JIA

A REPORT
SUBMITTED TO
Universiti Tunku Abdul Rahman
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for the degree of
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ACKNOWLEDGEMENTS

I would like to express my sincere thanks and appreciation to my supervisor for the opportunity to work on this project on protein structure alignment—my first step towards a career in bioinformatics. Thank you, Dr Ng.

This report is dedicated to my parents and my family for their love, support and continuous encouragement throughout the course.

When I asked for strength, God gave me more burdens to carry.
When I asked for love, God sent me people with problems.
When I asked for wisdom, God gave me more problems to solve.
I see that I did not get the things I asked for but I have been given all the things that I needed. Thank God.
ABSTRACT

This project studies and implements a polynomial time approximation scheme (PTAS) for aligning protein structures proposed by Li and Ng (Li and Ng, 2010). The algorithm addresses the alignment problem called the LCP problem under bottleneck distance. In the problem, each protein structure is modeled as a sequence of 3D points. Given two such sequences, the problem is to find a maximal subset of points from each protein and a bijection between the two subsets, under the restriction that there exists a superposition which brings each pair of points in the bijection to within a specified proximity. Whereas most current algorithms for the problem are heuristic in nature, the algorithm under study provides a solution with theoretical bounds for both runtime and accuracy.

Implementation of the algorithm is complicated by the difficult geometrical manipulations in the algorithm. The basic idea of the algorithm is as follows. Firstly, a rigid transformation is identified to superimpose the two structures. The transformation is searched in a discretized space of resolution $\delta$ – a theorem shows that the discretization will introduce discrepancies of at most $3\delta$. Each pair of points in Q will then be used as a rotation axis upon which P is rotated. During the rotation, the rotation angles where points in P and Q come within the required proximity are noted. At each angle, for each point in P we know a set of points in Q that it can be matched to. This set does not change for each rotation interval where no points come into or out of contact; hence the entire rotation interval can be considered similarly. For each such rotation interval, the problem is to find a bijection which matches the most points in P to Q. To solve this, a bipartite graph is constructed where the vertices are the points in P and Q, and an edge is placed between every two vertices that can be matched; a maximum bipartite matching of the graph gives us the optimal bijection. An exhaustive search of the optimal bijection for all rotation axes and rotation angles gives us the solution to the problem. The algorithm further exploits some geometrical properties as well as overlaps in the intermediate solutions to reduce runtime complexity.

This project gives a full implementation of the algorithm in C++, with very minimal use of external libraries.
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CHAPTER 1 INTRODUCTION

1.1 Motivation and Problem Statement

Proteins are the most important molecules in all living organisms. It functions as enzymes, sensors, antibodies, transporters, among myriads of other roles. To perform their biological function, proteins will fold into one or more specific spatial conformations, driven by some non-covalent interactions. The functions performed are frequently determined by the molecular shape of a protein, and it has been observed that proteins of similar 3D structures are likely to function similarly. This allows us to predict the functions of a protein by comparing its three-dimensional structure to the proteins of known functions.

For this reason, there have been very intense researches on protein structure comparison. Consequently, a large number of approaches, algorithms and software tools have been developed to evaluate the similarity between the 3D proteins structures, under the topic name of Protein Structure Alignment (Li & Ng 2010).

Though there are many protein structure comparison methods, all these methods are heuristic in nature. That is, the principles which the methods are based on common-sense or past experiences, rather than strict mathematical results. For example, they may use readily accessible but loosely applicable information to increase the speed of finding a satisfactory solution. Heuristic methods provide no guarantee on their runtime or the accuracy of their outputs. Since the accuracy of the structure alignment is very important, there is a need to devise methods which guarantees a specified level of accuracy in its output. Such an algorithm to align the protein structures under the bottleneck distance for protein structures is given by Li and Ng (Li & Ng 2010). The algorithm looks for an optimal superposition of the two protein structures in a discretized space to approximate the solution, through the radial pairs (or radial axes) introduced in (Li, Bu, Xu & Li 2008).
1.2 Project Objective and Contribution

The implementation of the algorithm for the LCP problem under the bottleneck distance program will result in a first tool for aligning protein structures with a guarantee in its accuracy. This will help researchers determine such alignments accurately in cases where such accuracy is important – for example, when there is dispute with the results from two different alignment methods.

The technique of radial pair used in the technique has proven to be very useful, and has been successfully used to devise algorithms for so-called model comparison and local continuous segments. To correctly implement the techniques involved in the use of these radial pairs, e.g. the discretization and the rotation axis, is a non-trivial task which requires days, or even weeks, for a programmer. Hence, the implementation of radial pair library is important besides provide standard routines in the manipulation of the radial pairs.

The availability of the radial pair library will be very useful for the implementations of other algorithms which require them. The ease of programming radial pairs using the library will also help in testing new algorithms which makes use of them, spurring faster development of algorithms in structural alignment.
1.3 Background information

The main aim in the study of Protein Structure Alignment is to establish the similarities of two or more polymer structures according to their shapes and three-dimensional conformation. Two important problems studied are:

1. Structure comparison, which is to analyze the similarities and differences between two given structures, while
2. Structure alignment, which is to establish the equivalence between the individual atoms of two given structures.

Specifically, structure alignment requires no prior knowledge on the equivalence of the structures. Thus, structure alignment is very useful for evaluating structures that are predicted purely from protein sequences, that is, through ab initio protein structure prediction methods (Zhang & Skolnick 2005). Structure alignment is also very useful in finding the evolutionary relationship between the proteins which have only a small number of identical sequences, that is, where the evolutionary relationship is difficult to be determined by sequence alignment.

The output expected from a structural alignment typically includes (1) the equivalence between the atoms of the input structures, (2) a minimal root mean square deviation (RMSD) between the structures. The RMSD measures the similarity between the two structures under the best possible superposition of the two structures. The changes in domain relative orientation between two structures can unnaturally increase the RMSD. Hence, structural alignment can be complicated because of the multiple protein domains in one or more input structures.
CHAPTER 2 LITERATURE REVIEW

2.1 Literature Review

Many methods for comparing two protein structures are based on the three following steps. First, detect the common similarities of the two protein structures. Then, align the structures based on such similarities. Lastly, compute a statistical measure on the similarities. Most of these methods do well in recognizing observable similarities between the protein structures. However, it is difficult to align two or more structures. The accuracy may depend on the method used or what the user is about to achieve (Martin, Captriotti, Shindyalow & Bourne 2009). The protein structure alignment methods that are widely used and cited are DALI (Holm and Sander, 1993b), Combinatorial Extension (CE) (Shindyalov and Bourne, 1998), MAMMOTH (Ortiz, Strauss, and Olmea, 2002), RAPIDO (Mosca, Schneider TR.), SALIGN (Sali and Blundell, 1990) and SSAP (Orengo and Taylor, 1996). There are many other new methods that have been published and used. For instance, SABERTOOH, TOPOFIT, SARF2 and ProBis are some known structure alignment methods in the world.

DALI, which is a distance alignment matrix method, represents each structure as a distance matrix. Proteins are transformed into 2D arrays of distance between all Cα atoms (Martin, Captriotti, Shindyalow & Bourne 2009). The method breaks the structures into hexapeptide fragments and generates a comparison distance matrix by evaluating the contact patterns between those successive fragments to align the two structures (Holm & Sander 1996). The matrix diagonal consists of secondary structure features that involve contiguous regions in the sequence’s residues. Other diagonals reflect spatial contacts between the residues that are far from each other in the sequence. The features they represent are parallel if these diagonals are parallel to the main diagonals. On the other hand, their features are anti-parallel whenever they are perpendicular. The features in the square matrix are symmetrical about the main diagonal.

Combinatorial extension (CE) is a method similar to DALI, which breaks structure into fragments before reassembling into a complete alignment. AFPs (aligned fragment pairs) which are a series of pair-wise combinations of fragments are used to identify a similarity matrix through which an optimal path is generated to determine the
final alignment. In order to reduce unnecessary search space and increase the efficiency, only AFPs which satisfy the criteria for local similarity are included in the matrix (Shindyalov & Bourne 1998). Some similarity metrics are possible. CE identifies most alike AFPs between the compared structures by using combinatorial extension algorithm. To increase the performance of the process, the size of each AFP must be within 30 residues distance to the current alignment ends (Martin, Captriotti, Shindyalow & Bourne 2009) and maximum gap size are set to empirically determined value of 8 (Shindyalov & Bourne 1998).

**MAMMOTH** (MAtching Molecular Models Obtained from THegory) transforms coordinates of the protein structure into a set of six unit-vectors which are computed from the Cα trace of the consecutive heptamers. This method decomposes protein structures into short heptapeptides to compare with the heptapeptides of other proteins. It obtains a similarity score between the heptapeptides and store in a similarity matrix by using a unit-vector RMS, which is known as URMS method (Kedem, Chew & Elber 1999). With hybrid dynamic programming, it computes the optimal residue alignment over the similarity matrix. Lastly, identify the largest local structure alignment within a given RMSD threshold by using the non-constant heuristic that is implemented in MaxSub (Martin, Captriotti, Shindyalow & Bourne 2009).

**RAPIDO**, the Rapid Alignment of Proteins In terms of Domains, is actually a web server for crystal structures of different protein molecules in 3D alignment. It identifies fragments that have similar structure in two proteins based on the difference distance matrices. The Matching Fragment Pairs (MFPs) are represented as nodes in a graph. The MFPs are chained together to form an alignment through an algorithm to identify the longest path on a Directed Acyclic Graph (DAG). After finish the alignments of the two structures, the server identify conformational invariant regions by a genetic algorithm (Jogn & Wendy 2004).

**SALIGN** compares structure properties by calculating the 3D coordinates of two or more proteins. This method aligns the coordinates by dynamic programming. SALIGN represents proteins by a set of properties or features which is calculated from protein sequences and structures, or arbitrarily defined by the user. SALIGN can be applied to align three or more protein structures. There are two approaches of SALIGN, which are a
tree-based or a progressive alignment. Progressive alignment has less intensive than the tree-based alignment (Martin, Captriotti, Shindyalow & Bourne 2009).

The SSAP (Sequential Structure Alignment Program) algorithm uses a double dynamic programming optimizer to compare 3D structures based on the atom-to-atom vectors. Instead of using alpha carbons, SSAP uses the $C_\beta$ atoms to generate a set of vectors for all residues except for glycine, a dummy $C_\beta$ is used. A series of inter-residue distance vectors between every residue and its closest non-contiguous neighbours on a protein is constructed. Then, the matrices which consist of the vector differences between $C_\beta$ vectors are constructed. By applying the dynamic programming on each resulting matrix, a set of selected matching position is defined. The final matrix is obtained by comparing vectors between $C_\beta$ atoms at pairs of same protein to the $C_\beta$ atoms from the selected matching position. Then, the final structural alignment is computed over the matrix of scores $S$ by second dynamic programming (Martin, Captriotti, Shindyalow & Bourne 2009).
2.2 Polynomial Time Approximation Scheme to Implement

As stated before, the methods discussed previously are heuristic in nature. Since the accuracy of the structure alignment is very important, there is a need to devise methods which guarantees a specified level of accuracy in its output. Such an algorithm to align the protein structures under the bottleneck distance for protein structures is given by Li and Ng (Li & Ng 2010). The algorithm looks for an optimal superposition of the two protein structures in a discretized space to approximate the solution, through the radial pairs (or radial axes) introduced in (Li, Bu, Xu & Li 2008).

We first describe the alignment problem which the algorithm aims to solve. Given two protein structures, the problem is to find a subset of points from each protein and a bijective matching of the points between the two proteins, with the objective of maximizing the number of pairs of points. The resultant problem is called the largest common point set problem (LCP), which is formally stated in Figure 2.2.1. In the formulation of the problem, each residue in the protein structure is represented as a point in $\mathbb{R}^3$.

<table>
<thead>
<tr>
<th>LCP Problem under Bottleneck Distance</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Input:</strong> Sequences $P = (p_1, ..., p_n)$, $Q = (q_1, ..., q_m)$ and distance threshold $D_c \in \mathbb{R}$. Without loss of generality, assume $m \geq n$.</td>
</tr>
<tr>
<td><strong>Output:</strong> (i) Subsets $P', Q' \subseteq P, Q$, $</td>
</tr>
<tr>
<td>(a) $\max_{p \in P'} |t(p) - f(p)| \leq D_c$</td>
</tr>
</tbody>
</table>

![Figure 2.2.1: LCP Problem under bottleneck distance (Li & Ng 2010)](image-url)

We let $P, Q, f, T, S$ denote an optimal $P'$, $Q'$, $f$, $t$, $S$, respectively. Assume that a pair of points $p_1, p_2 \in P$ is known for the problem. We consider $T$ as consisting of two parts: (1) an initial transformation $T$ which transforms $p_1, p_2$ into their positions under $T$, and (2) a rotation $R$ about an axis through the points $T(p_1)$ and $T(p_2)$, such that $\forall p \in P$, $R(T(p)) = T(p)$. 
Let $P$ and $Q$ be two given structures. A rigid transformation $T$ is to be finding to superimpose the two protein structures.

Assume that two points $p_1, p_2 \in P$, and their corresponding point $q_1, q_2 \in Q$ are known. Let $T$ define an axis where a rotation will complete the transformation $T$. All possible coordinates for $p_1$ and $p_2$ are examined in a discretized space in order to find $T$. $T$, however, may not be within the discretized space. Let $T$ be a transformation within the discretized space which best approximates $T$. We will show that when $p_1$ and $p_2$ fulfills certain properties, the error introduced by $T$ can be bounded by the resolution of the discretization.

**Definition 1 (Radial pair (Li, Bu, Xu & Li 2008)).** Given $p, p' \in P$. We call $p$ and $p'$ a *radial pair* if $p'$ is the furthest point from $p$ among all the points in $P$, which is written as $(p[p'])_p$. Note that $(p[p'])_p$ does not imply $(p[p'])_p$.

**Lemma 2 (Li, Bu, Xu & Li 2008).** Given a set of points $P$, a rigid transformation $T$, $T$ and radial pair $p_1, p_2 \in P$. If $\|T(p_1) - T(p_2)\| \leq \delta$ and $\|T(p_2) - T(p_2)\| \leq \delta$, then there exists a rotation $R$ about an axis through the points $T(p_1)$ and $T(p_2)$, such that $\forall p \in P, \|R(T(p)) - T(p)\| \leq 3\delta$.

Hence an error of $\delta$ introduced by $T$ on $p_1$ and $p_2$ with respect to $T$ will at most introduce an error of $3\delta$ on the rest of the points in $P$, and hence it suffices that we search for the transformation in a discretized space of resolution $\delta$ to obtain a solution of accuracy up to $3\delta$. We now discuss how to perform this search in the discretized space.

Figure 2.2.2: Forming rotation axes with a radial pair within the discretized space
Assume that a radial pair $p_i, p_j$ of $P$ match respectively to $q_k, q_l$ of $Q$. Since we require that $||p_i - p_j|| \leq D_c$ and $||q_k - q_l|| \leq D_c$, it suffices that we examine the coordinates which fulfill these conditions. Then, the sphere of $q_k$ is discretized using cubes of size length $\delta = \epsilon D_c/3$. Every cube corresponds to a grid point in the discretized space. After fixing $p_i$ at a grid point, all possible positions of $p_j$ must be placed on a sphere cap at center $p_i$ and radius $||p_i - p_j||$, as illustrated in Figure 2.2.2. There are $O\left(\frac{1}{\epsilon^3}\right)$ grid points in the sphere and $O\left(\frac{1}{\epsilon^2}\right)$ grid points in the sphere cap, giving us a total of $O\left(\frac{1}{\epsilon^5}\right)$ rotation axes.

That is,

**Lemma 3 (Li, Bu, Xu & Li 2008).** If it is known that $p_i, p_j \in P$ is a radial pair, and that $f(p_i) = q_k$ and $f(p_j) = q_l$ for $q_k, q_l \in Q$, then one only needs to search among $O\left(\frac{1}{\epsilon^5}\right)$ transformations to find a transformation $T$ which will result in at most $\epsilon D_c$ difference to each $p \in P$ transformed by $T$, by way of Lemma 2.

With a rotation axis fixed, we find the angle $\theta \in [0, 2\pi]$ about the axis through $p_i$ and $p_j$ such that the score $S$ is maximized. For a given $p \in P$ and $q \in Q$, we find the rotation angles that move $p$ into and out a distance of $((1 + \epsilon)D_c)$ from $q$, as shown in Figure 3. The angle $\theta_1$ moves $p$ into within a distance of $((1 + \epsilon)D_c)$ from $q$, while the angle $\theta_2$ moves $p$ out from within a distance of $((1 + \epsilon)D_c)$ from $q$. Within the angles $\theta_1$ and $\theta_2$, $p$ may be matched to $q$ while outside of the angles, $p$ cannot be matched to $q$.

![Figure 2.2.3: Rotation angles which move p into and out of contact with q](image)

Given a rotation axis and a rotation angle, we want to find the maximum number of one-one matches between the points in $P$ and $Q$. To do so we construct a graph $G = (V, \mathcal{E})$.
E). Each node in the graph represents a point in either $P$ or $Q$. We place an edge between two nodes if and only if at that angle, the point they represent can be matched. That is, an edge $(u, v) \in E$ iff $u \in P$, $v \in Q$ and $\|u - v\| \leq (1 + \varepsilon) D_c$. It is clear that $G$ is bipartite. To find the maximum one-one matches, it suffices that we find the maximum bipartite matching of $G$ (Schneider 2002). It is clear that for any angle in $\theta \in [0, 2\pi]$ which does not correspond to an angle where a point $p$ comes into, or out of contact with some point $q$, the bipartite graph created will be the same as one where the last change in point contact occurs. Hence, we only need to construct bipartite graphs for the angles where points come into, or out of contact. The angles which define these events divide $[0, 2\pi]$ into $mn$ intervals. We sort the angles that define the rotation intervals in order. The bipartite graph constructed for each subsequent interval differs by at most an edge, and the bipartite matching for one graph can be used as an initial matching for the subsequent graph (Li & Ng 2010), allowing the matching to be performed in $O(1)$ time. The time required for the first bipartite matching, $O(m^{2.5})$, while each of the $O(mn)$ subsequent bipartite matching requires $O(mn)$ time, resulting in a total time complexity of $O(m^{2.5} + m^2n^2)$.

Hence, we are able to determine the maximum number of matches in $O(m^{2.5} + m^2n^2)$ time when a rotation axis is given. Given our discretization scheme, there are at most $O(\frac{1}{\varepsilon^5})$ rotation axes given a radial pair (Lemma 3). However, we do not know which pair is a radial pair of $P$, nor do we know their matching points in $Q$. For this reason we exhaustively search all the possible $m^2n^2$ combinations of pairs of points in $P$ and $Q$. This gives us the following result.

**Theorem 1** (Li, Bu, Xu & Li 2008). There is an algorithm of time complexity $O((n^2m^{4.5} + n^4m^4)/\varepsilon^5)$ for the LCP problem under bottleneck distance.
CHAPTER 3 METHODOLOGY AND TOOLS

3.1 Methodology and Tools

My choice of language to implement the algorithm is C++. The intermediate-level language feature is the reason I chose C++. It comprises the combination of high-level and low-level language features (Herbert 1998).

For the present work, C++ is chosen based on consideration of performance and versatility. My first consideration is speed, since the algorithm has a runtime of a very high polynomial. Due to the intermediate level nature of the C++ language, compiled codes in C++ remain to date faster than those written in most other languages.

Part of the aim of the present work is to realize a library for the manipulation of radial pairs. A major consideration for library codes is the ability to make the codes run under different environments and software development platforms. C++ is perfect for this purpose. A number of interpreters of other programming languages are implemented in C++ language themselves.

To automate the experimentation, I choose to use the UNIX operating system for this project. UNIX also supports many system level programming calls for controlling processes, files, and access rights, such as those to prevent programs from simultaneously accessing the same resource. UNIX is also a natural candidate for program automation, due to its simplicity in the use of plain text and files for inter-process communication (IPC), as well as a wealth of software tools for processing textual data, which can be easily strung together through a command line interpreter using pipes. The use of UNIX shells naturally adds control structures for scripting the software tools. The Bash shell is chosen for this project.
4.1 Program Input and Output

Input of the program:
- Protein Structure 1 file (.pdb)
- Protein Structure 2 file (.pdb)
- Value of $D_c$
- Value of $\epsilon$

Output of the program:
- Maximum number of residue matched.
4.2 Main Procedure of Program

The main procedure of the program is as follows:

1. Get user input.
2. Read .pdb file.
3. Get total length of common residue ID of two input structures (P and Q).
4. Create Structure for the input structures.
5. Identify candidate radial pairs: \( p_1, p_2 \) from \( P \), and corresponding \( q_1, q_2 \) from \( Q \).
6. Transform structure \( Q \) so that \( q_1 \) and \( q_2 \) are along the y-axis.
7. Discretize a sphere of radius \( D_c \) centered at \( q_1 \) as candidate positions for \( p_1 \).
8. Form discretized sphere cap centered at \( q_2 \) as candidate positions for \( p_2 \).
9. For each \( p \) in \( P \) and each \( q \) in \( Q \), find the angles that move \( p \) in and out of contact of \( q \).
10. For each angular interval where there are no changes in the points in \( P \) and \( Q \) that may come into or out of contact, find for each point \( p \) in \( P \) the set of points in \( Q \) that it may be matched to.
11. Construct a bipartite graph out of the contact information obtained for the angular interval in (10).
12. Find the maximum bipartite matching of the bipartite graph in (11).
13. Repeat for each candidate radial pair.
14. Output the maximum number of matching of both structures.

The geometrical manipulations to achieve each of these steps are detailed in the following.
4.2.1 Get user input

```c
Dc = atof(argv[3]);
epsilon = atof(argv[4]);
pdb* nativePdb = new pdb(argv[1]);
pdb* modelPdb = new pdb(argv[2]);
```

Figure 4.2.1.1: Code to Store User Input

Input from the user is specified through command line arguments passed to the program. The first input argument is to be the native structure (structure \(Q\)); the second input argument is to be the model structure (structure \(P\)). The third input argument is to be the value of \(D_c\) while the last input argument is to be the value of \(\epsilon\).

The sample input:

```plaintext
a.pdb b.pdb 0.1 2
```
CHAPTER 4 ALGORITHM IMPLEMENTATION

4.2.2 Read .pdb file

The protein structure file (.pdb) will be read. The total number of residues in the file, residue IDs and also Cα’s x, y and z coordinate will be read.

```cpp
void pdb::readFile()
{
    FILE *fInput=fopen(mPDBFile, "r");
    if(!fInput)
    {
        cerr << "Unsuccessfully open protein file " << mPDBFile << " !" << endl;
        exit(0);
    }

    char temp[80];
    double x,y,z;
    string residueName;
    mNumOfResidue = 0;

    while ( fgets ( temp, sizeof(temp), fInput ) != NULL )
    {
        string line;
        line = temp;
        if(line.substr(0, 6) == "ENDMDL")
            break;
        if(line.substr(0, 6) != "ATOM ")
            continue;
        if(line.substr(12,4) == " CA " || line.substr(12,4) == "CA ")
        {
            x = toDouble(line.substr(30,8));
            y = toDouble(line.substr(38,8));
            z = toDouble(line.substr(46,8));

            mCAAlpha[mNumOfResidue*3] = x;
            mCAAlpha[mNumOfResidue*3+1] = y;
            mCAAlpha[mNumOfResidue*3+2] = z;

            residueName = line.substr(17,3);
            mresidueID[mNumOfResidue] = toInt(line.substr(22,4));

            mNumOfResidue++;
        }unciation;
    }
    fclose(fInput);
}
```

Figure 4.2.2.1: Code of Function readFile

Only Cα atom’s x, y and z coordinates will be needed. Thus the corresponding x, y and z will be stored when the 12th–13th letters of each line is “CA”. The residueID is taken from the 22nd character of each line.

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4.2.3 Get total length of common residue ID of two input structures (P and Q)

```c
int matchPDB(pdb* native, pdb* model)
{
    int natLength = native->mNumOfResidue;
    int modLength = model->mNumOfResidue;

    int* resNative = native->mresidueID;
    int* resModel = model->mresidueID;
    int j = 0, k = 0;
    for(int i = 0; i < natLength; i++)
    {
        for(; j < modLength; j++)
        {
            if(resNative[i] == resModel[j])
            {
                mIndexNative[k] = i;
                mIndexModel[k] = j;
                k++;
                break;
            }
            else if(resNative[i] < resModel[j])
                break;
        }
    }
    if(k == 0)
    {
        cout << "There is no common residues in the input Stuctures" << endl;
        exit(0);
    }
    return k;
}
```

Figure 4.2.3.1: Code of Function matchPDB

In this function, the total number of common residueID of both structures and the index of the common residue will be stored. The coordinates of the common residues will be copied to create two Structure objects as shown in Figure 4.2.4.1.
4.2.4 Create Structure for the input structures

```c
int alignLength = matchPDB(nativePdb, modelPdb);
double* nativeCoord = new double[alignLength*3];
double* modelCoord = new double[alignLength*3];

//copy coordinates of common residues.
for(int i = 0; i < alignLength; i++)
{
    //Native
    nativeCoord[i*3] = nativePdb->mCAlpha[mIndexNative[i]*3]; //x
    nativeCoord[i*3+1] = nativePdb->mCAlpha[mIndexNative[i]*3+1]; //y
    nativeCoord[i*3+2] = nativePdb->mCAlpha[mIndexNative[i]*3+2]; //z

    //Model
    modelCoord[i*3] = modelPdb->mCAlpha[mIndexModel[i]*3]; //x
    modelCoord[i*3+1] = modelPdb->mCAlpha[mIndexModel[i]*3+1]; //y
    modelCoord[i*3+2] = modelPdb->mCAlpha[mIndexModel[i]*3+2]; //z
}
Structure* mNative = new Structure(nativeCoord, alignLength*3);
Structure* mModel = new Structure(modelCoord, alignLength*3);
```

Figure 4.2.4.1: Parts of codes in main function
4.2.5 Identify radial pair candidates from $P$ and $Q$

![Figure 4.2.5.1: Distance of $p$ from $q$ must is at most $D_c$](image)

The condition for a point $p \in P$ to be matched to $q \in Q$ is that the distance between $p$ and $q$ must be within $D_c$ (as shown in Figure 4.2.5.1). Thus, a prerequisite for a pair $p_1$, $p_2 \in P$ to be matched to $q_1$, $q_2 \in Q$ is for $\|\text{distP} - \text{distQ}\| \leq 2D_c$, where $\text{distP} = \|p_1 - p_2\|$ and $\text{distQ} = \|q_1 - q_2\|$. In the program, $\|\text{distP} - \text{distQ}\| \leq 2D_c$ is checked (as shown in Figure 4.2.5.2) before the combination of matching point $p_1$ to $q_1$ and $p_2$ to $q_2$ proceeds to the next step.

![Figure 4.2.5.2: Initial check for matching point $p_1$ to $q_1$ and $p_2$ to $q_2$](image)
void Transformation::matchPoints(int iNative, int jNative, int iModel, int jModel) {
    //Translate p1 and p2 to match q1 and q2.
    //iNative = q1    iModel = p1
    //jNative = q2    jModel = p2
    //------------------Translation to match model to native------------------
    double distP = calDist(mModel->mCoord + iModel, mModel->mCoord + jModel);
    double distQ = calDist(mNative->mCoord + iNative, mNative->mCoord + jNative);
    if(fabs(distP - distQ) <= 2*mDc) {
        //Transform Q structure such that q1 and q2 is along y-axis
        mNative->transformStruct(mNative->mCoord + iNative, mNative->mCoord + jNative);
        //Discretize q1 and try p1 in the grid
        tryP1InGrid(mModel->mCoord + iModel, mNative->mCoord + iNative, mModel->mCoord + jModel, mNative->mCoord + jNative);
    }
}

Figure 4.2.5.3: Code of function matchPoints
4.2.6 Transform structure $Q$ so that it is along the y-axis

The program now proceeds with the assumption that $p_1$ is matched to $q_1$ and $p_2$ is matched to $q_2$. To simplify subsequent geometrical manipulations, I transform the structure $Q$ so that $q_1$ and $q_2$ lies on the y-axis, and $q_1$ is located at the origin (as shown in Figure 4.2.6.1).

Figure 4.2.6.1: Translation of $Q$ so that $q_1$ and $q_2$ are along the y-axis
/*
 * Transform structure such that two points is along y-axis
 */
void Structure::transformStruct(double* q1, double* q2)
{
    double* transStep = new double[3];
    bool q2IsOrigin = false;

    //when one of the point is at origin, no need to do translation, just perform rotation.
    if((q1[0] == 0 && q1[1] == 0 && q1[2] == 0))
    {
        ;
    }
    else if(q2[0] == 0 && q2[1] == 0 && q2[2] == 0)
    {
        q2IsOrigin = true;
    }
    else
    {
        //get the translation step of q1 to origin.
        transStep = q1;

        //translate whole structure so that q1 is at origin.
        translateStruct(transStep);
    }

    if(q2IsOrigin) //ONLY if q2 is origin, we rotate q1.
    {
        rotateStruct(q1);
    }
    else
    {
        //Rotates whole structure so that q2 is on y-axis.
        rotateStruct(q2);
    }
}

Figure 4.2.6.2: Code of function transformStruct
4.2.6.1 Translation

To perform the translation, I first obtain the translation which moves \( q_1 \) to the origin, and apply the translation on the remaining points of the structure. The procedure is skipped when \( q_1 \) or \( q_2 \) is already located at the origin.

```c
/*
 * Translate the whole structure
 */
void Structure::translateStruct(double* transStep)
{
    for(int i = 0; i < mLength; i += 3)
    {
        diff(mCoord + i, transStep, mCoord + i);
    }
}
```

Figure 4.2.6.1.1: Code of function translateStruct

```c
void diff(double* A, double* B, double *ans)
{
    ans[0] = A[0] - B[0];
}
```

Figure 4.2.6.1.2: Code of function diff
4.2.6.2 Rotation

If \( q_2 \) is at origin, \( q_1 \) is rotated so that \( q_1 \) it lies on the \( y \)-axis. Otherwise, \( q_2 \) will be rotated so that it is on the \( y \)-axis as shown in Figure 4.2.6.2.1.

![Figure 4.2.6.2.1: Rotation of \( q_2 \)](image)

To rotate \( q_2 \) to its position along the \( y \)-axis, the rotation axis must first be determined. This rotation axis can be found by using the cross product. The result of cross product is a vector that is perpendicular to both of the vectors that are being multiplied.
4.2.6.3 Cross Product

Figure 4.2.6.3.1: Cross Product

Formula of cross product:

\[
A = \begin{bmatrix}
a_1 \\
a_2 \\
a_3 
\end{bmatrix}
\]

\[
B = \begin{bmatrix}
b_1 \\
b_2 \\
b_3 
\end{bmatrix}
\]

\[
C = A \times B
\]

\[
\begin{bmatrix}
c_1 \\
c_2 \\
c_3 
\end{bmatrix} = \begin{bmatrix}
a_2b_3 - a_3b_2 \\
a_3b_1 - a_1b_3 \\
a_1b_2 - a_2b_1
\end{bmatrix}
\]

void crossProduct(double* A, double* B, double* ans)
{
}

Figure 4.2.6.3.2: Code of function crossProduct
4.2.6.4 Rotation axis

To get the rotation axis, cross product is used. The rotation axis is a vector that is the cross product of $\text{vector1}$ and $\text{vector2}$, where $\text{vector1}$ is the vector of two points ($q_2$ and origin) and $\text{vector2}$ is the vector of two points ($\text{point}$ and origin). Note that $\text{point}$ is a point on y-axis where its value of y is taken from $q_2$. For example, if $q_2 = (3, 5, 2)$, then $\text{point} = (0, 5, 0)$. After obtaining the cross product, $\text{vector3}$, I normalize the vector to make it a unit vector.

The next step is to find the rotation angle on our new rotation axis which will rotate $q_2$ into the y-axis.
/* Rotate structure Q so that q1 and q2 are along y-axis */
void Structure::rotateStruct(double* q2)
{
    double a, b, c;
    double origin[3] = {0, 0, 0};
    double cosC, theta;
    double point[3] = {0, q2[1], 0};
    double vector1[3], vector2[3], vector3[3];

    //get vector1 (a), vector2 (b), vector3 (c), where c = a x b cross product, c = axis of rotation
    diff(q2, origin, vector1);  //a
    diff(point, origin, vector2); //b
    crossProduct(vector1, vector2, vector3); //c: axis of rotation
    normalize(vector3);

    //get angle of rotation using law of cosines
    a = calDist(q2, origin);
    b = calDist(point, origin);
    c = calDist(q2, point);
    
    cosC = (a*a + b*b - c*c) / (2*a*b);

    if(cosC > 1)
        cosC = 1;
    if(cosC < -1)
        cosC = -1;

    theta = acos(cosC);
    rotateStruct(origin, vector3, theta);
}

Figure 4.2.6.4.2: Code of function rotateStruct

void normalize(double* u)
{
    double norm = sqrt(u[0]*u[0] + u[1]*u[1] + u[2]*u[2]);
    u[0] = u[0]/norm;
    u[1] = u[1]/norm;
    u[2] = u[2]/norm;
}

Figure 4.2.6.4.3: Code of function normalize
To find this rotation angle as shown in Figure 4.2.6.4.4, the Law of Cosine (Weisstein, Eric, n.d.) is used. The Law of Cosine is shown in Figure 4.2.6.4.5.

Formula of Law of Cosine:

\[
\cos C = \frac{a^2 + b^2 - c^2}{2ab}
\]
4.2.6.5 Rotation angle

In order to calculate the angle of rotation, I calculate the distance between the origin and \( q_2 \) as \( a \), the distance between origin and point as \( b \) and the distance between point and \( q_2 \) as \( c \). The angle of rotation can then be obtained from:

\[
\cos C = \frac{a^2 + b^2 - c^2}{2ab}
\]

\[
\text{angle of rotation} = \cos^{-1}(\cos C)
\]

Finally, \( Q \) is transformed using the determined rotation axis and rotation angle. The rotation is performed using a rotation matrix. That is, new coordinates for each point in \( Q \) is computed through multiplication with the matrix. The resultant coordinates can be written in the following functional form: For a point \((x, y, z)\) about a line through \((a, b, c)\) with direction unit vector \(<u, v, w>\), where \(u + v + w = 1\), by the angle \(\theta\) (Glenn 2011),

\[
f(x, y, z, a, b, c, u, v, w, \theta) =
\begin{bmatrix}
(a(v^2 + w^2) - u(bv + cw - ux - vy - wz))(1 - \cos \theta) + xc \cos \theta + (-cv + bw - wy + vz)\sin \theta \\
(b(u^2 + w^2) - v(au + cw - ux - vy - wz))(1 - \cos \theta) + yc \cos \theta + (cu - aw + wx - uz)\sin \theta \\
(c(u^2 + v^2) - w(au + bv - ux - vy - wz))(1 - \cos \theta) + zc \cos \theta + (-bu + av - vx + uy)\sin \theta
\end{bmatrix}
\]

Applying the function to the current rotation axis and rotation angle,

\((x, y, z) = \text{points in the structure,}\n
(a, b, c) \text{ would be the origin, so that the point pass through origin.}\n
<u, v, w> would be the vector3, which is the rotation axis, and
\( \theta \) would be the rotation angle.

```c
/* Rotates structure about an axis
   point: a point that the vector(axis) pass through
   axis : vector(axis of rotation)
   theta: rotation angle */
void Structure::rotateStruct(double* point, double* axis, double theta)
{
    for(int i = 0; i < mLength; i+=3)
    {
        rotatesAboutVector(mCoord+i, point, axis, theta, mCoord+i);
    }
}
```

Figure 4.2.6.5.2: Code of function rotateStruct

```c
/*
  //rotatesAboutVector and rotatesAboutArbLine are the same
  //rotatesAboutVector is to convert double* into 3 double
  xyz : point to be rotate
  abc : a point that the rotation axis passes through
  uvw : direction vector (unit vector)
  theta : angle of rotation
  newCoord : the rotated point
*/
void rotatesAboutVector(double* xyz, double* abc, double* uvw, double theta, double* newCoord)
{
    rotatesAboutArbLine(xyz[0], xyz[1], xyz[2], abc[0], abc[1], abc[2], uvw[0], uvw[1], uvw[2], theta, newCoord);
}
```

Figure 4.2.6.5.3: Code of function rotatesAboutVector
Figure 4.2.6.5.4: Code of function rotatesAboutArbLine
4.2.7 Exhaustive search of positions for \( p_1 \) in discretized \( D_c \) sphere around \( q_1 \)

Suppose structure \( Q \) has been transformed so that \( q_1 \) and \( q_2 \) are along the \( y \)-axis. I want to discretize \( q_1 \) and \( q_2 \) with grids of size \( \frac{\varepsilon D_c}{3} \) and exhaustively examine \( p_1 \) and \( p_2 \) at each grid point. Now \( p_1 \) can be at most \((1 + \varepsilon)D_c\) away from \( q_1 \). To find the position for \( p_1 \), I discretize a sphere of radius \((1 + \varepsilon)D_c\) centered at \( q_1 \). However, it is difficult to construct such a discretization with a sphere; to simplify this discretization a cube is used instead. The cube has the same width, length and depth, \( 2(1 + \varepsilon)D_c \), as shown in Figure 4.2.7.1.

![Figure 4.2.7.1: Cube for candidate positions of \( p_1 \)](image)

Then, the cube is discretized with grids of size \( \frac{\varepsilon D_c}{3} \). Positions for \( p_1 \) will be examined on each grid point on the cube and started with the start point and end point as shown in Figure 4.2.7.2. Start point is calculated by using \( x, y \) and \( z \) value of \( q_1 \) subtract \((1 + \varepsilon)D_c\) while end point is calculated by using \( x, y \) and \( z \) value of \( q_1 \) add \((1 + \varepsilon)D_c\), which is as follows:

\[
\text{Start} = (x - (1 + \varepsilon)D_c, y - (1 + \varepsilon)D_c, z - (1 + \varepsilon)D_c) \\
\text{End} = (x + (1 + \varepsilon)D_c, y + (1 + \varepsilon)D_c, z + (1 + \varepsilon)D_c)
\]
Beginning from the start point, I exhaustively examine $p_1$ on the grid. However, since this is a cube, the distance of each grid point to the center ($q_1$) may greater than the radius of a sphere, which is $(1 + \epsilon)D_c$. Hence, I examine the distance from each grid point to the center of the sphere; when the distance is more than $(1 + \epsilon)D_c$, the grid point will not be considered further.
void Transformation::tryP1InGrid(double* p1, double* q1, double* p2, double* q2)
{
    double start[3] = {q1[0] - mThres, q1[1] - mThres, q1[2] - mThres}; //Store each start point of each exist
    double end[3] = {q1[0] + mThres, q1[1] + mThres, q1[2] + mThres}; //Store each end point of each exist
    double coord[3]; // coord = p1 on the grid
    double distQ = calDist(q1, q2); //distance between q1 and q2
    double radius = calDist(p1, p2);
    int count = 1;
    for(double x = start[0]; x <= end[0]; x += mStepSize)
    {
        coord[0] = x;
        for(double y = start[1]; y <= end[1]; y += mStepSize)
        {
            coord[1] = y;
            for(double z = start[2]; z <= end[2]; z += mStepSize)
            {
                coord[2] = z;
                if(isInThres(q1, coord)) //is in sphere of q1
                {
                    //check whether distance(p1,q2) > mThres
                    if(calDist(coord, q2) > mThres)
                    {
                        //check whether p2 is in sphere of q2
                        if(radius >= (distQ - mThres) && radius <= (distQ + mThres))
                        {
                            formSphereCap(p1, coord, p2, q2, radius);
                            cout<<"next"<<endl;
                        }
                    }
                }
            }
        }
    }
}

Figure 4.2.7.4: Code of function tryP1InGrid
4.2.8 Forming a sphere cap for $p_2$

After fixing $p_1$ at a grid point, a sphere cap is to be formed for all possible positions of $p_2$, centered at $p_1$ with radius $\|p_1 - p_2\|$, and the sphere cap must be inside the sphere of $q_2$. The sphere cap is also discretized with grids of size $\frac{\epsilon D_c}{3}$. $p_2$ is then examined on each grid point of the sphere cap.

![Image of sphere cap formation](image)

Figure 4.2.8.1: Forming sphere cap with grid

I check for the condition of whether the distance between the grid point and $q_2$ is greater than $(1 + \epsilon)D_c$. If the grid point is within $(1 + \epsilon)D_c$ from $q_2$, they are approximately matched, and the formation of a sphere cap is not required. In order to form the sphere cap, another condition must be fulfilled. Namely, that the distance $d$ between $p_1$ and $p_2$ must have

- $d \geq \text{distance between } q_1 \text{ and } q_2 - (1 + \epsilon)D_c$, and
- $d \leq \text{distance between } q_1 \text{ and } q_2 + (1 + \epsilon)D_c$, as shown in Figure 4.2.8.2.
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To fulfill the conditions, all the possible positions of $p_2$ form a sphere cap inside the sphere of $q_2$. The sphere cap is generated in the program as follows: starting with a point that forms a straight line with $p_1$ and is parallel to the y-axis (Figure 4.2.8.3). I rotate the point upward, downward, leftward or rightward, until forming a circle, $2\pi$. The step size of the movement is set according to the resolution of the discretization.

Now I want to find the rotation axis and rotation angle to perform the rotations in each of the four directions mentioned. The rotation axis is initialized with a vector that passes through $p_1$ and is parallel to the z-axis as shown in Figure 4.2.8.3.
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The vector (\textit{vector1}) then will be rotated around another vector (\textit{vector2}) that passes through \( p_1 \) and is parallel to the x-axis, to be rotated to the left or right, corresponding to the leftward and rightward movement of the point. Each rotated point will be checked to see if it is still within the sphere of \( q_2 \) by checking whether the distance between the point and \( q_2 \) is within \((1 + \epsilon)D_c\). Otherwise, the rotation continues until \(2\pi\).

To rotate a vector about another vector, the following formula is used:

\[
V = A - [(axis \cdot A)axis \cos \theta] + [(A \times axis)\sin \theta],
\]

where \( A \) is the vector to be rotated, and \( axis \) is the rotation axis (Rotating a vector around an arbitrary axis 2003).

```c
/*
 * A:Vector to be rotate
 * axis:axis
 * V = (A - ((axis.A)*axis)*costheta) + ((A X axis)*sintheta) +
 * (axis.A)*axis)
 */
//must use normalized vector
void rotateVectorAbtVector(double* A, double* axis, double theta, double* ans)
{
    double cross[3], dotAxis[3], dotAxisCosTheta[3], ans1[3], ans2[3],
    ans3[3];
    double dot;
    dot = dotProduct(A,axis);     // (axis.A)
    multiply(dot, axis, dotAxis);  // (axis.A)*axis
    multiply(cos(theta), dotAxis, dotAxisCosTheta);
    ((axis.A)*axis)*costheta
    crossProduct(A,axis,cross);     // (A X axis)
    diff(A, dotAxisCosTheta, ans1); // (A -
    (axis.A)*axis)*costheta)
    multiply(sin(theta), cross, ans2); //((A X axis)*sintheta)
    ans3[0] = dotAxis[0];         // (axis.A)*axis
    ans3[1] = dotAxis[1];
    ans3[2] = dotAxis[2];
    add(ans1, ans2, ans);
    add(ans, ans3, ans);
}
```

Figure 4.2.8.4: Code of function rotateVectorAbtVector

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Figure 4.2.8.5: Method to form the sphere cap. Vector 1 is the rotation axis for $p_2$ to rotate in the up or down direction. Vector 2 is the vector for vector 1 and point $p_2$ to rotate to the left or right. Each rotated point of $p_2$ will be checked to see if it is within the sphere of $q_2$.

The rotation angle is calculated using the formula of arc length, $s = r\theta$. Hence, $\theta = \frac{s}{r}$. For the present purpose, $s = \frac{\varepsilon D_c}{3}$, $r = \text{distance between } p_1 \text{ and } p_2$. Thus $\theta$ is computed as $\frac{\varepsilon D_c}{3\|p_1 - p_2\|}$.

Figure 4.2.8.6: Diagram for formula of arc length
/* Form a sphere cap for p2 on q2 grid, try all coordinates on sphere cap
oriP1: the original p1 before putting on grid
p1 : center of the sphere cap
p2 : point to form sphere cap
q2 : center of sphere where the sphere cap is inside
radius: distance between p1 and p2, radius of forming sphere cap
*/

void Transformation::formSphereCap(double* oriP1, double* p1, double* p2, double* q2, double radius)
{
    double totalangle, totalAOut, PI2;
    // totaltheta must be at most 360 to stop the rotation.
    double coord[3];
    // point on sphere cap (new p2)
    double middleCoord[3];
    // center point of each moving up and down/left and right
    double oriCoord[3];
    // the original point before any rotation
    double vector1[3], vector2[3];
    // axis of rotation
    double angle = mStepSize/radius; // rotation angle
    PI2 = 2*PI;
    bool isWithinQ2 = false;
    // is the coordinate within sphere of q2
    double rotAng;

    // start to form sphere cap with p1 point that form straight line parallel to y-axis
    middleCoord[0] = p1[0];
    middleCoord[2] = p1[2];

    // copy the coordinates to prepare for rotation
    coord[0] = middleCoord[0];
    coord[1] = middleCoord[1];
    coord[2] = middleCoord[2];
    oriCoord[0] = middleCoord[0];
    oriCoord[1] = middleCoord[1];
    oriCoord[2] = middleCoord[2];

    // vector1 to rotate p2 on sphere cap (up and down): firstly parallel to z, will be changed later
    vector1[0] = 0; // parallel to z
    vector1[1] = 0;
    vector1[2] = 1;

    // point that passes through the vector1 and vector2 (axis of rotation) = p1

    // vector2 to rotate p2 on sphere cap (left and right): parallel to x-axis
    vector2[0] = 1;
    vector2[1] = 0;
    vector2[2] = 0;

    totalAOut = 0;
}

Figure 4.2.8.7: Code of function formSphereCap
do
{
  /*prepare to rotates up and down*/
  //going up and down
  totalangle = 0;
  //rotates p2 up and down around vector1
  do
  {
    rotatesAboutVector(coord, p1, vector1, angle, coord);    //going up or down
    totalangle += angle;
    //check whether is in sphere of q2
    isWithinQ2 = isInThres(q2, coord);
    if(isWithinQ2)
    {
      //Move other P respectively
      movePtoPlace(p1, oriP1, coord, p2); //p1: new p1 on grid;
      oriP1: p1 before putting on grid;

      //coord: p2 on sphere cap;  p2: p2 before putting on sphere cap
      //form rotation axis and rotates
      findAngleInOut();
      getMaxMatch(); //get most number of residue matched from
      the maximum bipartite matching for each rotation angle.
    }
  }

  } while(totalangle < PI2);

  //reset coord back to original coord before rotates up&down, to prepare to
  move left/right
  coord[0] = middleCoord[0];
  coord[1] = middleCoord[1];
  coord[2] = middleCoord[2];
  //rotates p2 left and right and rotates vector1 together with same theta
  rotatesAboutVector(coord, p1, vector2, angle, coord);    //going

  left&right
  //rotates also vector1
  rotateVectorAbtVector(vector1, vector2, angle, vector1);
  //normalize vector1
  normalize(vector1);
  totalAOut += angle;

  middleCoord[0] = coord[0];
  middleCoord[1] = coord[1];
  middleCoord[2] = coord[2];

  } while(totalAOut < PI2);
}

Figure 4.2.8.8: Code of function formSphereCap

Having moved $p_1$ and $p_2$ to a grid point around $q_1$ and $q_2$ respectively, all the points in $P$ are to be transformed accordingly. To do so, they are first applied the translation step which moved $p_1$ from its original to its position on the grid point around
Then, they are applied the rotation which moved $p_2$ to its position on the sphere cap around $q_2$. The exact geometrical manipulation follows the same method used earlier to transform $Q$ such that $q_1$ and $q_2$ lie along the $y$-axis. The rotation axis is determined by using cross product and rotation angle is calculated by using the Law of Cosine.

```cpp
/*
 * Move all points in structure P respectively after fixing p1 and p2
 * newP1 : the point on grid(fixed)
 * p1 : the old point before putting on grid
 * newP2 : the point on sphere cap(fixed)
 * p2 : the old point before putting on sphere cap
 */
void Transformation::movePtoPlace(double* newP1, double* p1, double* newP2, double* p2)
{
    //get translation step to translate from old P1 to new P1.
    double transStep[3];
    double vector1[3];
    double vector2[3];
    double vector3[3];
    double theta, a, b, c, cosC;
    diff(p1, newP1, transStep);
    mModel->translateStruct(transStep);

    //get vector1 (a), vector2 (b), vector3 (c), where c = a x b cross product, c = axis of rotation
    diff(newP1, p2, vector1); //a
    diff(newP1, newP2, vector2); //b
    crossProduct(vector1, vector2, vector3); //c:axis of rotation
    normalize(vector3);

    //get angle of rotation using law of cosines
    a = calDist(newP1, p2);
    b = calDist(newP1, newP2);
    c = calDist(p2, newP2);
    cosC = (a*a + b*b - c*c) / (2*a*b);
    if(cosC > 1)
    {
        cosC = 1;
    }
    if(cosC < -1)
    {
        cosC = -1;
    }
    theta = acos(cosC);
    mModel->rotateStruct(newP1, vector3, theta);
}
```

Figure 4.2.8.9: Code of function movePtoPlace
4.2.9 Find angle that moves $P$ in and out of contact of $Q$

![Diagram showing angle that moves $p$ in and out of contact with $q$]

The program proceeds with $p_1$, $p_2$ and $Q$ fixed. The remaining points in $P$ are to be rotated about the axis formed by $p_1$ and $p_2$. In the course of the rotation, points in $P$ might come into contact with some points in $Q$ (that is, within $(1 + \epsilon)D_c$ distance from these points), as well as going out of contact from the points in $Q$ (that is, further than $(1 + \epsilon)D_c$ from these points) which they are originally in contact with.

The program now computes, for each $p$ in $P$ and each $q$ in $Q$, the angle that moves $p$ in and out of contact with $q$ (as shown in Figure 4.2.9.1). Noting that the rotational path of $p$ forms a circle, this can be computed by finding the intersection of a circle and a sphere.

```cpp
/*
 * Get the angle of rotation that moves P into and Out of Contact with Q, 
 * by using intersection between the sphere of Q and unit circle(path of p) 
 */
void Transformation::findAngleInOut()
{
    int indexp, indexq;
    initializeMatch();

    for(int i = 0; i < mNative->mLength; i+=3)
    {
        indexq = i/3;
        for(int j = 0; j < mModel->mLength; j+=3)
        {
            indexp = j/3;
            getIntersectPoint(mModel->mCoord + j, mNative->mCoord + 
            indexp, indexq);
        }
    }
}
```

Figure 4.2.9.2: Code of function findAngleInOut
Initially, the distance between $p$ and $q$ is checked. $p$ is approximately matched to $q$ when the distance between $p$ and $q$ is within $(1 + \epsilon)D_c$. Since the $p$ has been matched to $q$, no rotation is required for the specific $p$ and thus no calculation on intersection of circle and sphere is required. $\theta_1$, the angle that moves $p$ into $q$, is set to 0 since $p$ is already matched to $q$ while $\theta_2$, the angle that moves $p$ out of $q$, is set to $2\pi$.

![Figure 4.2.9.3: Intersection of circle and sphere](image)

To find the intersection of a circle and a sphere, I transform the circle into a plane, then intersect the sphere with the plane. Each circle centered at $(0, B, 0)$ and point $P=(x_1, B, z_1)$. Hence, the plane equation is $Y = B$. The intersection of the plane $Y = B$ and the sphere of $Q$ will be a circle as in Figure 4.2.9.4.
Equation of plane: $Y = B$

Equation of sphere: $(x - x_0)^2 + (y - y_0)^2 + (z - z_0)^2 = ((1 + \epsilon)D_c)^2$

The formula of equation of the intersected circle can be found in (AmBrSoft Quality Softwares, n.d.):

$$(x - x_0)^2 + (y - y_0)^2 + (z - z_0)^2 = r^2,$$

where $r = \sqrt{R^2 - d^2}$,

$R = \text{radius of sphere},$

d = \frac{|Ax_0 + By_0 + Cz_0 + D|}{\sqrt{A^2 + B^2 + C^2}}$

By applying the formula above,

$$d = y_0 - B,$$

$$r = \sqrt{((1 + \epsilon)D_c)^2 - (y_0 - B)^2},$$

which gives the equation:

$$(x - x_0)^2 + (y - y_0)^2 + (z - z_0)^2 = ((1 + \epsilon)D_c)^2 - (y_0 - B)^2,$$
In order to find the intersection of the circle and the sphere, the intersection of the circle (formed by the rotational path of \( p \)) and the intersected circle (intersection of plane and sphere \( Q \)) is calculated as shown in Figure 4.2.9.5.

\[ \theta_1 = \text{Angle that moves } p \text{ into contact with } q \]

\[ \theta_2 = \text{Angle that moves } p \text{ out of contact with } q \]

\( \theta_1 \) and \( \theta_2 \) can be calculated by using the Law of Cosine.

The intersection of two circles can be found analytically. Firstly, since the circles lies on the x-z plane where \( y = B \), there are only two unknowns to solve.

Suppose the radius of the intersected circle is \( \sqrt{((1 + \epsilon)D_c)^2 - (y_0 - B)^2} \) and the radius of the unit circle is \( \sqrt{x_1^2 + z_1^2} \). To simplify the equation, let the radius of intersected circle be \( R \) and the radius of unit circle be \( r \).

The equation of unit circle

\[ x^2 + z^2 = r^2 \quad \text{---------1} \]

The equation of the intersected circle

\[ (x - x_0)^2 + (z - z_0)^2 = R^2 \quad \text{---------2} \]

Expanding (2),

\[ x^2 - 2x_0 x + x_0^2 + z^2 - 2z_0 z + z_0^2 = R^2 \quad \text{---------3} \]
\[ 3 - 1, \]
\[ -2x_0x + x_0^2 - 2z_0z + z_0^2 = R^2 - r^2 \]
\[ x = \frac{r^2 - R^2 + x_0^2 - 2z_0z + z_0^2}{2x_0} \] ———— ④

Substitute ④ into ① and \( \times 4x_0^2 \),
\[ (4x_0^2 + 4z_0^2)z^2 + (-4r^2z_0 + 4R^2z_0 - 4x_0^2z_0 - 4z_0^3)z + (r^4 - 2x_0^2r^2 - 2R^2r^2 + 2z_0^2r^2 + R^4 - 2x_0^2R^2 - 2z_0^2R^2 + x_0^4 + 2x_0^2z_0^2 + z_0^4) = 0 \]

Using quadratic formula,
\[ Z = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}, \]
where \( a = (4x_0^2 + 4z_0^2) \),
\( b = (-4r^2z_0 - 4R^2z_0 - 4x_0^2z_0 - 4z_0^3) \),
\( c = (r^4 - 2x_0^2r^2 - 2R^2r^2 + 2z_0^2r^2 + R^4 - 2x_0^2R^2 - 2z_0^2R^2 + x_0^4 + 2x_0^2z_0^2 + z_0^4) \)

Substitute \( Z \) values into ④,
\[ x = \frac{r^2 - R^2 + x_0^2 - 2z_0z + z_0^2}{2x_0} \]

After getting the intersection points, the angles are calculated using Law of Cosine as shown in Figure 4.2.9.7 and Figure 4.2.9.8.
Figure 4.2.9.7: Angle that moves $p$ into contact with $q$

Figure 4.2.9.8: Angle that moves $p$ out of contact of $q$
void Transformation::getIntersectPoint(double* p, double* q, int indexp, int indexq)
{
    double B = p[1]; //y-coordinate
    double R = sqrt(mThres*mThres - (q[0]-B)*(q[0]-B)); //Radius of Circle1
    double r = sqrt(p[0]*p[0] + p[2]*p[2]); //radius of Circle2
    double R2, r2; //squared of R and squared of r.
    double c2center[3] = {0,B,0}; //center of circle
    R2 = R*R;
    r2 = r*r;

double point1[3],point2[3]; //intersection points between two circles
    double a,b,c,cosC, angle1, angle2;
    double q02, q22; //squared of q[0] and squared of q[2].
    q02 = q[0]*q[0];
    q22 = q[2]*q[2];
    double dist = calDist(p, q); //distance between two centers of circle
    int yes;
    if(dist <= mThres) //p is approximately matched to q
    {
        angle1 = 0;
        angle2 = 2*PI;
    }
    else
    {
        //(-b +/- sqrt(b2-4ac)) / 2a
        double b = -4*r2*q[2] + 4*R2*r2 - 2*R2*2*r2 + 2*2*r2*q22 + R2*R2 - 2*R2*2*q02 - 2*R2*q22 + q02*2*q22 + 2*q02*q22 + q22*q22;
        point1[2] = (-b + sqrt(b*b-4*a*c))/ 2*a; //z1
        point2[2] = (-b - sqrt(b*b-4*a*c))/ 2*a; //z2
        point1[1] = B; //y1
        point2[1] = B; //y2
        point1[0] = (q22 + q02 - 2*q2*point1[2] - R2 + r2) / 2*q[0]; //x1:sub z1
        point2[0] = (q22 + q02 - 2*q2*point2[2] - R2 + r2) / 2*q[0]; //x2:sub z2
    } //end of if
// get angle using law of cosines
// angle that moves P into Q
a = calDist(c2center, p);
b = calDist(c2center, point1);
c = calDist(p, point1);

    cosC = (a*a + b*b - c*c) / (2*a*b);
    angle1 = acos(cosC);

// angle that moves P out of Q using law of cosines
a = calDist(c2center, point2);
c = calDist(point1, point2);

    cosC = (a*a + b*b - c*c) / (2*a*b);
    angle2 = acos(cosC);
}

setRotInterval(angle1, angle2, indexp, indexq);

Figure 4.2.9.10: Code of function getIntersectPoint

All the angles ($\theta_1$ and $\theta_2$) computed thus far are then to be sorted. Suppose this produces the sequence of increasing angles $\phi_1, \phi_2, \phi_3, \ldots$ Then, each interval ($\phi_i, \phi_{i+1}$) represents a region where no two points from $P$ and $Q$ respectively come into or moves out of contact. That is, the ways to match points in $P$ and $Q$ are the same for all the angles in the interval; hence in finding the optimal way to match the points between $P$ and $Q$, only one angle needs to be considered.

To sort the angles, I start with first angle of $\theta_1$. Note that $\theta_1$ and $\theta_2$ come in pair and $\theta_2$ must be next to the $\theta_1$. For each angle, the matching of the respective $p$ and $q$ will be stored. For the first angle, $\theta_1$, there is no respective $p$ and $q$ to be matched, hence -1 is set as its respective index. In $\theta_2$, the respective $p$ and $q$ will be matched; the index combination will be set to 1.
When the next $\theta_1$ is smaller than the first angle in the storage, there will be another angle created after the first angle in the storage as shown in left Figure 4.2.9.12. Then, its pair of $\theta_2$ must be started right after $\theta_1$, as shown in right Figure 4.2.9.12. When the angle is greater than the next cumulative angles, there also will be a new angle created (as in Figure 4.2.9.12).

4.2.10 Find the maximum bipartite matching

After arranging the angles in order and setting the matching for each angle, the maximum bipartite matching for the matching in each angle is to be determined. The Hopcroft-Karp algorithm (Hopcroft & Karp 1973) is used to obtain this matching.

The algorithm takes as input a bipartite graph, and produces as output a maximum cardinality matching, i.e. a set of maximum edges with the property that no two edges share an endpoint. This algorithm runs in $O(|E|\sqrt{V})$ time in the worst case, where $E$ is the number of edges and $V$ is the number of vertices.
the set of edges in the graph and \( V \) is the set of vertices of the graph. The algorithm is able to work with a partial solution, improving on it to produce a maximal set of shortest augmenting paths in order to increase the size of the partial matching. This allows us to use the partial matching for the bipartite graph from an interval \((\phi_{i-1}, \phi_i)\) as initial input to the problem instance for the interval \((\phi_i, \phi_{i+1})\).

The pseudocode of Hopcroft-Karp algorithm is as below:

```c
/*
G = G1 U G2 U \{NIL\}
where G1 and G2 are partition of graph and NIL is a special null vertex
*/

function BFS ()
    for v in G1
        if Pair_G1[v] == NIL
            Dist[v] = 0
            Enqueue(Q,v)
        else
            Dist[v] = \infty
    Dist[NIL] = \infty
    while Empty(Q) == false
        v = Dequeue(Q)
        if Dist[v] < Dist[NIL]
            for each u in Adj[v]
                if Dist[ Pair_G2[u] ] == \infty
                    Enqueue(Q,Pair_G2[u])
            return Dist[NIL] != \infty
```

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function DFS (v)
    if v != NIL
        for each u in Adj[v]
            if Dist[ Pair_G2[u] ] == Dist[v] + 1
                if DFS(Pair_G2[u]) == true
                    Pair_G2[u] = v
                    Pair_G1[v] = u
                    return true
        Dist[v] = ∞
        return false
    return true

function Hopcroft-Karp
    for each v in G
        Pair_G1[v] = NIL
        Pair_G2[v] = NIL
        matching = 0
    while BFS() == true
        for each v in G1
            if Pair_G1[v] == NIL
                if DFS(v) == true
                    matching = matching + 1
    return matching

4.2.11 Output the maximum number of matching of both structures.

```cpp
    if matching > maxMatch
        maxMatch = matching
```

```cpp
    cout << "Maximum number of residue matched: " << maxMatch << endl;
    return 0;
```
4.3 Program Result

Since the program runs for a long time, the program is tested with several .pdb file that has very less number of CA atoms to shorten the time of running. The results have shown the accuracy of the algorithm.

In order to test the accuracy of the program, the same .pdb file has been used for the input of the program. For instance, if protein structure file has two residues of CA atoms, the output of the program should also be two since the two files are the same.

Some test cases of my program testing are as follows:

Test case 1: The program was tested with two same .pdb file, namely a.pdb that has two residues of CA atoms. The result showed that there are two residues matched.

Test case 2: The program was then tested with another .pdb file, that is b.pdb that is also has two residues of CA atoms. The output of the program is two, which is the expected output.
CHAPTER 4 ALGORITHM IMPLEMENTATION

Test case 3: The input protein structure files have four residues of CA atoms. The result of the program is 4.
5.1 Discussion

5.1.1 Achievement

I have successfully implemented the algorithm in 2.2 in C++. Due to the high runtime complexity of the algorithm, the program takes quite a long time to run. The discretization and the forming of sphere cap for pairs of point, which introduces the $O(\frac{1}{\epsilon^8})$ runtime, appears to be the bottleneck. Although this program takes a long time to run, it guarantees the accuracy of the matching of two structures and thus will help researchers to determine the alignments accurately.

The testing of this program has been carried out to ensure the correctness of the program.

However, the analysis of code in order to accelerate the program has not been carried out. The accuracy of its output compared to other methods has also not been examined because of the time taken to run the whole program. The packaging of the codes for handling radial pairs (into an easy to use library) has also not been carried out due to time constraint.

The unfinished work should be continued in the future in order to make the program more useful.

5.1.2 Implementation Issues and Challenges

5.1.2.1 Problem of Installing Cygwin

At the beginning of the project, Microsoft Visual Studio 2010 is used to run my code. However, in the Bioinformatics field, most of the people are using Unix operating system. Thus, I installed Cygwin to run the program. I found that it was difficult to use since it has no GUI. Installing Cygwin also requires some knowledge such as: in order to compile C++ codes, the GCC package has to be installed. The default installation of Cygwin did not include the package, and resulted in some time lost before the problem was identified.
CHAPTER 5 DISCUSSION AND CONCLUSION

After seeking advice from a friend that used Cygwin to run his code, I successfully run my code. He also showed me several commands to compile and run the codes, as well as obtained the packages for me from the internet.

5.1.2.2 Early conceptual mistakes in implementing the algorithm

- **Find radial pair of structure \( P \) for matching structure \( Q \).**

  In finding the radial pair of \( P \), I made a few errors in coding the condition of “\(|p_1 - q_1| \leq D_c \) and \(|p_2 - q_2| \leq D_c \)”. I translated whole structure \( P \) so that \( p_1 \) match \( q_1 \), and then checked the distance between \( p_2 \) and \( q_2 \) to see if it is within \( 2D_c \). This is an error for all the cases because the position of \( p_2 \) and \( q_2 \) might be within \( 2D_c \) after rotation. The checking of the distance between \( p_2 \) and \( q_2 \) after translation is not correct. After discussing with my supervisor, he showed me my mistake and I made the corrections.

![Diagram](image)

**Figure 5.1.2.2.1**: Wrong concept of finding radial pair of \( P \) to match \( Q \)

- **Form sphere cap for \( p_2 \)**

  I had a few conceptual misunderstanding regarding the forming of the sphere caps for \( p_2 \). Initially, I first form grids on the cube of \( q_2 \), and then only form the sphere cap by checking the distance between the grid and the cube center (\( q_2 \)). However, this is wrong as when the sphere cap is not on the grid, the sphere cap could not be formed.
**CHAPTER 5 DISCUSSION AND CONCLUSION**

![Diagram](image.png)

**Figure 5.1.2.2.2: Wrong concept of forming sphere cap**

- **Rotation of $P$ to match $Q$**

  To rotate structure $P$ to match structure $Q$, I have to rotate structure $P$ around an arbitrary axis of $q_1$ and $q_2$. However, I did not know how to do this. I took advice from supervisor to translate structure $Q$ so that $q_1$ and $q_2$ lies along the y-axis. I did not know how to use the rotation matrix to rotate a point about an arbitrary axis. I searched for the formula at Google for days. Finally, I found the formula and also the graphic visualization of the formula. I also did not know how to rotate a vector about an arbitrary axis, which is to change the direction of the rotation axis. I tried to come out with a formula for rotating a point about an arbitrary axis, but failed. I searched for the formula for days and finally found the formula on web. It took me more than a week to complete this step.

- **Total Rotation Angle**

  In my initial tests of the program, the program did not complete even for very small problem instances. At first I suspected that this is a natural consequence of the high time complexity. However, after some debugging, I found that I had written an incorrect condition for enumerating the rotation angles. The enumeration should terminate when the angle is at most $2\pi$, which I wrote $360^\circ$. This, however, caused the program to require $\sim 100$ times the actual time, since the rotation angle should be specified in radian.
5.1.2.4 Lack of knowledge in circle-sphere intersection

Another part of the program which I found difficult to code is the part where I am to find the intersection between a circle and a sphere. I searched for solutions to this problem on many forums on the internet, but was unable to find any information on the problem. There were only methods of finding plane-sphere intersection as well as circle-circle intersection. My supervisor told me to reduce the problem to one of finding circle-circle intersection, by changing the sphere into a circle via a plane-sphere intersection.

Thus, I extended one circle into a plane and cut the sphere with the plane to obtain a circle from the sphere. Then, the problem becomes one of circle-circle intersection.

I also did not know what the equation for a plane is. I discussed this with my supervisor again and finally came out with the complete solution.

5.1.2.4 Implementation of Hopcroft-Karp algorithm

I searched for graphic explanation of Hopcroft Karp algorithm on the internet. However, I could not get any explanation of the algorithm with graphics. I understood the step of finding augmenting path through several powerpoint slides that were available on web. The pseudocode of the Hopcroft-Karp algorithm is available on the internet and I found that someone has already implemented it in C++. The writer posted his code on Blogspot so that the code is able to help some people who need it (as shown below). I tried to run his code but failed to get the expected result since I did not know what the input of the code should be. The program also ran into an infinite loop at a specific line. After trying for days and asking the writer about the input, I managed to get the expected result.

Next, I began to change the input of the function into the form required by my program, namely, matching of the two structures $P$, $Q$ at specific angle. The declaration method of the vector<int> type double array is inappropriate. I tried many declaration methods and resulted in error. An example of a wrong declaration is as follows:

```cpp
vector<int> G[length*length+1];
```

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I followed the method of declaration of original coding to declare a double array of size $length^2 + 1$. But, this did not work as well as it requires a constant whereas length is the parameter that is passed into the function. I found a method to declare this vector<int> with the build-in function “resize”. I make the following declaration and resize in the same function and found that it is also wrong.

```cpp
int hopcroft_karp(int length, int** matching) {
    vector<vector<int>> G;
    G.resize(length+1);
}
```

After trying for few times, I found that the program will work when vector<int> is declared a global variable.

```cpp
vector<vector<int>> G;
int hopcroft_karp(int length, int** matching) {
    G.resize(length+1);
}
```

Nevertheless, I also faced the problem of two uninitialized variables: “dist” and “match”. The original code which I obtained declares them as global variable but I declared them locally. I did not notice this would make a difference. Only after debugging for some times did I realize that there are special meanings to these variable when they are set to zero; dist[] = 0 means that all path is not defined yet and match[] = 0 means that there is no initial matching for the specific combination of points. These details were not documented in the code which I obtained.

Original coding
```
int n, m, match[MAX], dist[MAX];
```

My coding
```
int hopcroft_karp(int length, int** matching) {
    G.resize(length+1);
    int length2 = length*length;
    int *match = new int[length2 + 1];
    int *dist = new int[length2 + 1];
}
```
5.1.3 Runtime Error and Memory Error

There are many memory errors that occurred while testing my program. I have to print out some words for each section to find out which lines caused the memory problem. Typically, these are caused by inappropriate deletion and allocation of memory for the variables. Besides, pointing to a specific memory location that does not exist will also cause the error shown below.

Segmentation fault (core dumped)

5.2 Conclusion

This project started out with the aim to implement an algorithm proposed by Li and Ng in (Li & Ng 2010) to help researchers in structural biology to carry out protein structure comparison. The algorithm solves the LCP problem under bottleneck distance and has a time complexity of $O((n^2m^{4.5} + n^4m^4)/\epsilon^5)$. This aim has been achieved – the algorithm is now a C++ program.

The program turned out to be fairly difficult to code. It involves the use of many mathematical operations and knowledge. It requires a strong foundation of mathematics to complete the program. Any translation, rotation and graph require application of addition, subtraction, vector formulas, rotation matrix, quadratic equation and mathematical logics. Although some other aims of the project, such as comparisons of the algorithm with other heuristic-based algorithms, has not been carried out, the main part of the project has been accomplished.
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APPENDICES

APPENDIX A COMPLETE CODING OF THE WHOLE PROGRAM

A-1 main.cpp

```cpp
#include "pdb.h"
#include "Structure.h"
#include "Transformation.h"
#include <math.h>
#include <iostream>

using namespace std;

int mIndexNative[LONGEST_CHAIN];
int mIndexModel[LONGEST_CHAIN];

// Match both structure to get common residues.
int matchPDB(pdb* native, pdb* model)
{
    int natLength = native->mNumOfResidue;
    int modLength = model->mNumOfResidue;

    int* resNative = native->mresidueID;
    int* resModel = model->mresidueID;
    int j = 0, k = 0;
    for(int i = 0; i < natLength; i++)
    {
        for(; j < modLength; j++)
        {
            if(resNative[i] == resModel[j])
            {
                mIndexNative[k] = i;
                mIndexModel[k] = j;
                k++;
                break;
            }
            else if(resNative[i] < resModel[j])
                break;
        }
        if(k == 0)
        {
            cout << "There is no common residues in the input Structures" << endl;
            exit(0);
        }
    }
    return k;
}
```

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```cpp
int main(int argc, char** argv)
{
    if(argc != 5)
    {
        cout << "Usage: (native pdb) (model pdb) (distance threshold) (epsilon)" << endl;
        exit(0);
    }

double Dc, epsilon;
Dc = atof(argv[3]);
epsilon = atof(argv[4]);

pdb* nativePdb = new pdb(argv[1]);
pdb* modelPdb = new pdb(argv[2]);

int alignLength = matchPDB(nativePdb, modelPdb);
double* nativeCoord = new double[alignLength*3];
double* modelCoord = new double[alignLength*3];

//copy coordinates of common residues.
for(int i = 0; i < alignLength; i++)
{
    //Native
    nativeCoord[i*3] = nativePdb->mCAlpha[mIndexNative[i]*3];
    //x
    nativeCoord[i*3+1] = nativePdb->mCAlpha[mIndexNative[i]*3+1];
    //y
    nativeCoord[i*3+2] = nativePdb->mCAlpha[mIndexNative[i]*3+2];
    //z

    //Model
    modelCoord[i*3] = modelPdb->mCAlpha[mIndexModel[i]*3];
    //x
    modelCoord[i*3+1] = modelPdb->mCAlpha[mIndexModel[i]*3+1];
    //y
    modelCoord[i*3+2] = modelPdb->mCAlpha[mIndexModel[i]*3+2];
    //z
}

Structure* mNative = new Structure(nativeCoord, alignLength*3);
Structure* mModel = new Structure(modelCoord, alignLength*3);

Transformation* transf = new Transformation(mNative, mModel, Dc, epsilon);

int maxMatch = 0;
```
/**Match native to model**
```cpp
for(int iNative = 0; iNative < alignLength*3; iNative+=3) {
    for(int jNative = 0; jNative < alignLength*3; jNative+=3) {
        for(int iModel = 0; iModel < alignLength*3; iModel+=3) {
            for(int jModel = 0; jModel < alignLength*3; jModel+=3) {
                if(iNative != jNative && iModel != jModel) {
                    transf->matchPoints(iNative, jNative, iModel, jModel);
                    maxMatch = transf->mMaxMatch;
                    if(maxMatch < transf->mMaxMatch) {
                        maxMatch = transf->mMaxMatch;
                    }
                }
            }
        }
    }
}
```
```cpp
cout << "Maximum number of residue matched: " << maxMatch << endl;
return 0;
```
A-2 pdb.h

#ifndef _PDB_H_
define _PDB_H_
#include <iostream>
using namespace std;

#define LONGEST_CHAIN 2000

class pdb
{
 public:
  char* mPDBFile;
  int mNumOfResidue;
  float* mCAAlpha;
  int* mresidueID;
  char* mSeq;
  void readFile();
  void write(double** rot, double* shift);

  pdb(char* fileName);
  ~pdb();
};
#endif
A-3 pdb.cpp

```cpp
#include <iostream>
#include <string.h>
#include <string>
#include <stdlib.h>
#include <math.h>
using namespace std;

#include "pdb.h"

double toDouble(string str)
{
    char* tempStr = new char[10];
    int index = 0;
    double ans;

    for(int i=0; i<str.size(); i++){
        if(str[i]!=' ')
            tempStr[index++] = str[i];
    }
    tempStr[index] = '\0';

    ans = atof(tempStr);
    delete [] tempStr;
    return ans;
}

int toInt(string str)
{
    char* tempStr = new char[10];
    int index = 0, ans;

    for(int i=0; i<str.size(); i++){
        if(str[i]!=' ')
            tempStr[index++] = str[i];
    }
    tempStr[index] = '\0';

    ans = atoi(tempStr);
    delete [] tempStr;
    return ans;
}

pdb::pdb(char* fileName){
    mPDBFile = fileName;
    mCAlpha = new float[3*LONGEST_CHAIN];
    mresidueID = new int [LONGEST_CHAIN];
    readFile();
}
```

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pdb::~pdb()
{
    delete [] mCAlpha;
    delete [] mresidueID;
}

void pdb::readFile()
{
    FILE *fInput=fopen(mPDBFile, "r");
    if(!fInput)
    {
        cerr << "Unsuccessfully open protein file " << mPDBFile << " !" << endl;
        exit(0);
    }
    char temp[80];
    double x,y,z;
    string residueName;
    mNumOfResidue = 0;
    while ( fgets ( temp, sizeof(temp), fInput ) != NULL )
    {
        string line;
        line = temp;
        if(line.substr(0, 6) == "ENDMDL")
            break;
        if(line.substr(0, 6) != "ATOM ")
            continue;
        if(line.substr(12,4) == " CA " || line.substr(12,4) == "CA"
          || line.substr(12,4) == " CA"
          || line.substr(12,4) == "CA")
        {
            x = toDouble(line.substr(30,8));
            y = toDouble(line.substr(38,8));
            z = toDouble(line.substr(46,8));

            mCAlpha[mNumOfResidue*3] = x;
            mCAlpha[mNumOfResidue*3+1] = y;
            mCAlpha[mNumOfResidue*3+2] = z;

            residueName = line.substr(17,3);
            mresidueID[mNumOfResidue] = toInt(line.substr(22,4));

            mNumOfResidue++;
        }
    }
    fclose(fInput);
}
A-4 Structure.h

#include <iostream>
using namespace std;

#define LONGEST_CHAIN 2000

class pdb
{
    public:
        char* mPDBFile;
        int mNumOfResidue;
        float* mCAlpha;
        int* mresidueID;
        char* mSeq;
        void readFile();
        void write(double** rot, double* shift);

        pdb(char* fileName);
        ~pdb();
};

#endif
#include "Structure.h"
#include <iostream>

using namespace std;

Structure::Structure(double* coord, int length)
{
    mCoord = coord; //coordinates for translation and rotation
    mLength = length;
}

Structure::~Structure()
{
    delete mCoord;
}

/*
   Translate the whole structure
*/
void Structure::translateStruct(double* transStep)
{
    for(int i = 0; i < mLength; i += 3)
    {
        diff(mCoord + i, transStep, mCoord + i);
    }
}

/*
   Rotates structure about an axis
   point: a point that the vector(axis) pass through
   axis : vector(axis of rotation)
   theta: rotation angle
*/
void Structure::rotateStruct(double* point, double* axis, double theta)
{
    for(int i = 0; i < mLength; i+=3)
    {
        rotatesAboutVector(mCoord+i, point, axis, theta, mCoord+i);
    }
}

/*
   Transform structure such that two points is along y-axis
*/
void Structure::transformStruct(double* q1, double* q2)
{
    double* transStep = new double[3];
    bool q2IsOrigin = false;
// when one of the point is at origin, no need to do translation, just perform rotation.
if((q1[0] == 0 && q1[1] == 0 && q1[2] == 0))
{
    ;
}
else if(q2[0] == 0 && q2[1] == 0 && q2[2] == 0)
{
    q2IsOrigin = true;
}
else
{
    // get the translation step of q1 to origin.
    transStep = q1;
    // translate whole structure so that q1 is at origin.
    translateStruct(transStep);
}
if(q2IsOrigin) // ONLY if q2 is origin, we rotate q1.
{
    rotateStruct(q1);
}
else
{
    // Rotates whole structure so that q2 is on y-axis.
    rotateStruct(q2);
}

/*
Rotate structure Q so that q1 and q2 are along y-axis
*/
void Structure::rotateStruct(double* q2)
{
    double a, b, c;
    double origin[3] = {0, 0, 0};
    double cosC, theta;
    double point[3] = {0, q2[1], 0};
    double vector1[3], vector2[3], vector3[3];

    // get vector1 (a), vector2 (b), vector3 (c), where c = a x b cross product, c = axis of rotation
    diff(q2, origin, vector1); // a
diff(point, origin, vector2); // b
crossProduct(vector1, vector2, vector3); // c: axis of rotation
normalize(vector3);

    // get angle of rotation using law of cosines
    a = calDist(q2, origin);
    b = calDist(point, origin);
    c = calDist(q2, point);
    cosC = (a*a + b*b - c*c) / (2*a*b);
\[
\begin{align*}
\text{if}(\cos C > 1) & \\
\quad & \cos C = 1; \\
\text{if}(\cos C < -1) & \\
\quad & \cos C = -1; \\
\theta & = \arccos(\cos C); \\
\text{rotateStruct}(\text{origin}, \text{vector3}, \theta); \\
\end{align*}
\]
#ifndef _MATHS_OPERATION_H_
#define _MATHS_OPERATION_H_
#include <math.h>
#define PI 3.14159265

double calDist(double* A, double* B);
void add(double* A, double* B, double* ans);
void diff(double* A, double* B, double* ans);
void rotatesAboutVector(double* xyz, double* abc, double*uvw, double theta, double* newCoord);
void rotatesAboutArbLine(double x, double y, double z, double a, double b, double c, double u, double v, double w, double theta, double* newCoord);
void normalize(double* u);
double dotProduct(double* A, double* B);
void crossProduct(double* A, double* B, double* ans);
void multiply(double num, double* A, double* ans);
void rotateVectorAbtVector(double* A, double* axis, double theta, double* ans);

#endif
A-6 MathsOperation.cpp

#include "MathsOperation.h"

double calDist(double* A, double* B)
{
    double sum = 0;
    sum += (A[0] - B[0])* (A[0] - B[0]);
    return sqrt(sum);
}

void add(double* A, double* B, double* ans)
{
    ans[0] = A[0] + B[0];
}

void diff(double* A, double* B, double *ans)
{
    ans[0] = A[0] - B[0];
}

/**<rotatesAboutVector and rotatesAboutArbLine are the same
  //rotatesAboutVector is to convert double* into 3 double
  xyz : point to be rotate
  abc : a point that the rotation axis passes through
  uvw : direction vector (unit vector)
  theta : angle of rotation
  newCoord : the rotated point
*/
void rotatesAboutVector(double* xyz, double* abc, double* uvw, double theta, double* newCoord)
{
    rotatesAboutArbLine(xyz[0], xyz[1], xyz[2], abc[0], abc[1], abc[2], uvw[0], uvw[1], uvw[2], theta, newCoord);
}
void rotatesAboutArbLine(double x, double y, double z, double a, double b, double c, double u, double v, double w, double theta, double* newCoord) {
    double costheta = cos(theta);
    double sintheta = sin(theta);
    double oneMinusCosTheta = 1 - costheta;
    double v2 = v*v;
    double u2 = u*u;
    double w2 = w*w;
    newCoord[0] = (a*(v2 + w2) - u*(b*v + c*w - u*x - v*y - w*z)) * oneMinusCosTheta + x*costheta + (-c*v + b*w - w*y + v*z)*sintheta;
    newCoord[1] = (b*(u2 + w2) - v*(a*u + c*w - u*x - v*y - w*z)) * oneMinusCosTheta + y*costheta + (c*u - a*w + w*x - u*z)*sintheta;
    newCoord[2] = (c*(u2 + v2) - w*(a*u + b*v - u*x - v*y - w*z)) * oneMinusCosTheta + z*costheta + (-b*u + a*v - v*x + u*y)*sintheta;
}

void normalize(double* u) {
    double norm = sqrt(u[0]*u[0] + u[1]*u[1] + u[2]*u[2]);
    u[0] = u[0]/norm;
    u[1] = u[1]/norm;
    u[2] = u[2]/norm;
}

double dotProduct(double* A, double* B) {
}

void crossProduct(double* A, double* B, double* ans) {
}

void multiply(double num, double* A, double* ans) {
    ans[0] = num*A[0];
    ans[1] = num*A[1];
}
/* 
A: Vector to be rotate
axis: axis
V = (A - ((axis.A)*axis)*costheta) + ((A X axis)*sintheta) + 
(axis.A)*axis)
*/
// must use normalized vector
void rotateVectorAbtVector(double* A, double* axis, double theta, double* ans)
{
    double cross[3], dotAxis[3], dotAxisCosTheta[3], ans1[3], ans2[3],
    ans3[3];
    double dot;

dot = dotProduct(A, axis);                // (axis.A)
multiply(dot, axis, dotAxis);            // (axis.A)*axis
multiply(cos(theta), dotAxis, dotAxisCosTheta);  // ((axis.A)*axis)*costheta

crossProduct(A, axis, cross);            // (A X axis)
diff(A, dotAxisCosTheta, ans1);         // (A -
((axis.A)*axis)*costheta)
multiply(sin(theta), cross, ans2);       // (A X axis)*sintheta
ans3[0] = dotAxis[0];                    // (axis.A)*axis)
ans3[1] = dotAxis[1];
ans3[2] = dotAxis[2];

add(ans1, ans2, ans);
add(ans, ans3, ans);
}
A-7 Transformation.h

```c
#ifndef _TRANSFORMATION_H_
#define _TRANSFORMATION_H_
#include "Structure.h"
#include "MathsOperation.h"
#include "Graph.h"

class Transformation
{
    private:
        /*combine all thetas found*/
        int len;
        typedef struct
        {
            double angle;
            int** matching; //adjacency matrix used to store the graph of p and q matching
        } ROTATION;

    public:
        Structure *mNative;
        Structure *mModel;
        double mDc, mEpsilon;
        double mThres, mStepSize;

        ROTATION* mRotInterval; //rotation interval and its matching.
        int mRotItvIndex; //index of rotInterval
        int mMaxMatch; //the maximum number of matched for specific p1,p2 and q1,q2

        Transformation(Structure* native, Structure* model, double Dc, double epsilon);
        ~Transformation();

        void matchPoints(int iNative, int jNative, int iModel, int jModel);

        bool isInThres(double* center, double* points);
        void tryP1InGrid(double* p1, double* center, double* p2, double* q2);

        bool isRadius(double* center, double* coord, double radius);
        void formSphereCap(double* oriP1, double* p1, double* p2, double* q2, double radius);
        void movePtoPlace(double* newP1, double* p1, double* newP2, double* p2);

        void findAngleInOut();
        void getIntersectPoint(double* p, double* q, int j, int i);

        void copyMatching(int** A, int** B);
};
```

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void moveBackwards(int start, int end, double temp2, int **tempArr2);
void insertTheta2(int start, int end, int i, int j, double angle);
void setRotInterval(double theta1, double theta2, int i, int j);
void getMaxMatch();
void initializeMatch();
#include "Transformation.h"
#include <iostream>

using namespace std;

Transformation::Transformation(Structure* native, Structure* model, double Dc, double epsilon)
{
    mNative = native;
    mModel = model;
    mDc = Dc;
    mEpsilon = epsilon;
    mThres = (1 + mEpsilon)* mDc;
    mStepSize = mEpsilon * mDc / 3;
    len = mModel->mLength/3; //total points in mNative or mModel

    mRotInterval = new ROTATION[2*len*len];

    for(int i = 0; i < 2*len*len; i++)
    {
        mRotInterval[i].matching = new int*[len];

        for(int j = 0; j < len; j++)
        {
            mRotInterval[i].matching[j] = new int[len];

            for(int k = 0; k < len; k++)
            {
                mRotInterval[i].matching[j][k] = 0;
            }
        }
    }

    mRotItvIndex = 0;
    mMaxMatch = 0;
}

Transformation::~Transformation()
{
    delete[] mNative;
    delete[] mModel;
    delete[] mRotInterval;
}
void Transformation::matchPoints(int iNative, int jNative, int iModel, int jModel)
{
    //Translate p1 and p2 to match q1 and q2.
    //iNative = q1    iModel = p1
    //jNative = q2    jModel = p2

    double distP = calDist(mModel->mCoord + iModel, mModel->mCoord + jModel);
    double distQ = calDist(mNative->mCoord + iNative, mNative->mCoord + jNative);

    if(fabs(distP - distQ) <= 2*mDc)
    {
        //Transform Q structure such that q1 and q2 is along y-axis
        mNative->transformStruct(mNative->mCoord + iNative, mNative->mCoord + jNative);

        //Discretize q1 and try p1 in the grid
        tryP1InGrid(mModel->mCoord + iModel, mNative->mCoord + iNative, mModel->mCoord + jModel, mNative->mCoord + jNative);
    }
}

/*
Examine p1 in the grid of q1 (all possible positions)
 p1 : coord of p1
 q1 : sphere center
 p2 : another point of structure P.
 q2 : point of structure Q.
*/
void Transformation::tryP1InGrid(double* p1, double* q1, double* p2, double* q2)
{
    double start[3] = {q1[0] - mThres, q1[1] - mThres, q1[2] - mThres}; //Store each start point of each exist
    double end[3] = {q1[0] + mThres, q1[1] + mThres, q1[2] + mThres}; //Store each end point of each exist
    double coord[3]; // coord = p1 on the grid
    double distQ = calDist(q1, q2); //distance between q1 and q2

    double radius = calDist(p1, p2);
    int count = 1;
    for(double x = start[0]; x <= end[0]; x += mStepSize)
    {
        coord[0] = x;
        for(double y = start[1]; y <= end[1]; y += mStepSize)
        {
            coord[1] = y;
            for(double z = start[2]; z <= end[2]; z += mStepSize)
            {
                coord[2] = z;
            }
        }
    }
}
if(isInThres(q1, coord)) //is in sphere of q1
{
    //check whether distance(p1,q2) > mThres
    if(calDist(coord,q2) > mThres)
    {
        //check whether p2 is in sphere of q2
        if(radius >= (distQ - mThres) &&
           radius <= (distQ + mThres))
        {
            formSphereCap(p1, coord, p2, q2, radius);
        }
    }
}

/*
Check whether the points (grid on cube) is within thres (sphere)
center : sphere center
point : point on the grid on cube
*/
bool Transformation::isInThres(double* center, double* point)
{
    if(calDist(center, point) <= mThres)
        return true;
    return false;
}

/*
Form a sphere cap for p2 on q2 grid, try all coordinates on
sphere cap
oriP1: the original p1 before putting on grid
p1 : center of the sphere cap
p2 : point to form sphere cap
q2 : center of sphere where the sphere cap is inside
radius: distance between p1 and p2, radius of forming
sphere cap
*/
void Transformation::formSphereCap(double* oriP1, double* p1, double* p2, double* q2, double radius)
{
    double totalangle,totAOut,PI2; //totaltheta must be at most 360 to stop the rotation.
    double coord[3]; //point on sphere cap (new p2)
    double middleCoord[3]; //center point of each moving up and down/left and right
    double oriCoord[3]; //the original point before any rotation
    double vector1[3], vector2[3]; //axis of rotation
double angle = mStepSize/radius;    //rotation angle
PI2 = 2*PI;
bool isWithinQ2 = false;       //is the coordinate
within sphere of q2

//start to form sphere cap with p1 point that form straight line
parallel to y-axis
middleCoord[0] = p1[0];
middleCoord[2] = p1[2];

//copy the coordinates to prepare for rotation
coord[0] = middleCoord[0];
coord[1] = middleCoord[1];
coord[2] = middleCoord[2];
oriCoord[0] = middleCoord[0];
oriCoord[1] = middleCoord[1];
oriCoord[2] = middleCoord[2];

//vector1 to rotate p2 on sphere cap (up and down): firstly parallel
to z, will be changed later
vector1[0] = 0;   //parallel to z
vector1[1] = 0;
vector1[2] = 1;

//point that passes through the vector1 and vector2(axis of rotation)
= p1

//vector2 to rotate p2 on sphere cap (left and right) : parallel to
x-axis
vector2[0] = 1;
vector2[1] = 0;
vector2[2] = 0;

totalAOut = 0;
do
{
   /*prepare to rotates up and down*/
   //going up and down
   totalangle = 0;
   //rotates p2 up and down around vector1
   do
   {
      rotatesAboutVector(coord, p1, vector1, angle, coord);
      //going up or down
      totalangle += angle;
      //check whether is in sphere of q2
      isWithinQ2 = isInThres(q2, coord);
      if(isWithinQ2)
      {
          //code goes here
      }
   }
   totalangle = 0;
   //rotates p2 up and down around vector1
   do
   {
// Move other P respectively
movePtoPlace(p1, oriP1, coord, p2); // p1: new p1 on grid; oriP1: p1 before putting on grid;
// coord: p2 on sphere cap; p2: p2 before putting on sphere cap
// form rotation axis and rotates
findAngleInOut();
getMaxMatch(); // get most number of residue matched from the maximum bipartite matching for each rotation angle.
}

while (totalangle < PI2);
// reset coord back to original coord before rotates up&down, to prepare to move left/right
coord[0] = middleCoord[0];
coord[1] = middleCoord[1];
coord[2] = middleCoord[2];
// rotates p2 left and right and rotates vector1 together with same theta
rotatesAboutVector(coord, p1, vector2, angle, coord);
// going left&right
// rotates also vector1
rotateVectorAbtVector(vector1, vector2, angle, vector1);
// normalize vector1
normalize(vector1);
totalAOut += angle;
middleCoord[0] = coord[0];
middleCoord[1] = coord[1];
middleCoord[2] = coord[2];
}
while (totalAOut < PI2);

/*
 Move all points in structure P respectively after fixing p1 and p2
 newP1 : the point on grid(fixed)
 p1 : the old point before putting on grid
 newP2 : the point on sphere cap(fixed)
 p2 : the old point before putting on sphere cap
*/
void Transformation::movePtoPlace(double* newP1, double* p1, double* newP2, double* p2)
{
    // get translation step to translate from old p1 to new P1.
double transStep[3];
double vector1[3];
double vector2[3];
double vector3[3];
double theta, a, b, c, cosC;
diff(p1, newP1, transStep);
    mModel->translateStruct(transStep);
    //get vector1 (a), vector2 (b), vector3 (c), where c = a x b
crossProduct(c, vector1, vector2);
    diff(newP1, p2, vector1); //a
diff(newP1, newP2, vector2); //b
crossProduct(vector1, vector2, vector3); //c:axis of rotation
normalize(vector3);

    //get angle of rotation using law of cosines
    a = calDist(newP1, p2);
    b = calDist(newP1, newP2);
    c = calDist(p2, newP2);

    cosC = (a*a + b*b - c*c) / (2*a*b);
    if(cosC > 1)
        cosC = 1;
    if(cosC < -1)
        cosC = -1;
    theta = acos(cosC);

    mModel->rotateStruct(newP1, vector3, theta);
}

void Transformation::initializeMatch()
{
    for(int i = 0; i < 2*len*len; i++)
    {
        for(int j = 0; j < len; j++)
        {
            for(int k = 0; k < len; k++)
            {
                mRotInterval[i].matching[j][k] = 0;
            }
        }
    }
    mRotItvIndex = 0;
}

/*
 * Get the angle of rotation that moves P into and Out of Contact with Q, by using intersection between the sphere of Q and unit circle(path of p)
 */
void Transformation::findAngleInOut()
{
    int indexp, indexq;
    mRotItvIndex = 0;

    for(int i = 0; i < mNative->mLength; i+=3)
APPENDICES

{  
    indexq = i/3;  
    for(int j = 0; j < mModel->mLength; j+=3)  
    {  
        indexp = j/3;  

        getIntersectPoint(mModel->mCoord + j, mNative->mCoord + i, indexp, indexq);  
    }
}

/*
   Get intersection point of circle centered at (0,B,0) and circle centered at (X0, B, Z0) - intersection circle of plane Y=B and sphere of q
   Circle 1: (intersection of plane and sphere) equation: (X-x0)^2 + (Y-B)^2 + (Z-z0)^2 = ((1+eps)Dc)^2 - (y0-B)^2
   Circle 2: (path of p) equation: X^2 + (Y-B)^2 + Z^2 = (x1)^2 + (z1)^2
   p : any point of p (x1,B,z1)
   q : any point of q (x0,y0,z0)
   B : plane to intersect with sphere.
*/
void Transformation::getIntersectPoint(double* p, double* q, int indexp, int indexq)  
{  
    double B = p[1]; //y-coordinate  
    double R = sqrt(mThres*mThres - (q[0]-B)*(q[0]-B)); //Radius of Circle 1  
    double r = sqrt(p[0]*p[0] + p[2]*p[2]); //radius of Circle 2
    double R2, r2; //squared of R and squared of r.
    double c2center[3] = {0,B,0}; //center of circle 2

    R2 = R*R;  
    r2 = r*r;

    double point1[3],point2[3]; //intersection points between two circles
    double a,b,c,cosC, angle1, angle2;

    double q02, q22; //squared of q[0] and squared of q[2].
    q02 = q[0]*q[0];
    q22 = q[2]*q[2];

    double dist = calDist(p, q); //distance between two centers of circle
    int yes;

    if(dist <= mThres) //p is approximately matched to q
    {  
        angle1 = 0;  
        angle2 = 2*PI;
    }
    else  
    {  
        //(-b +- sqrt(b^2-4ac)) / 2a
        a = 4*q02 + 4*q22;
    }
APPENDICES

\[ c = r^2 r^2 - 2q^2 r^2 - 2R^2 r^2 + 2r^2 q^2 + R^2 R^2 - 2R^2 q^2 + q^2 q^2 + 2q^2 q^2 + q^2 q^2 + q^2 q^2 - 2R^2 q^2 + R^2 + r^2 \]

\[ \text{point1[2]} = (-b + sqrt(b*b - 4*a*c)) / 2*a; \]  
\[ \text{point2[2]} = (-b - sqrt(b*b - 4*a*c)) / 2*a; \]

\[ \text{point1[1]} = B; \]  
\[ \text{point2[1]} = B; \]

\[ \text{point1[0]} = (q^2 + q^0 - 2q^0 q^2 + q^2 + R^2 - r^2) / 2q^0; \]
\[ \text{point2[0]} = (q^2 + q^0 - 2q^0 q^2 + q^2 + R^2 - r^2) / 2q^0; \]

//get angle using law of cosines
//angle that moves P into Q
a = calDist(c2center, p);
b = calDist(c2center, point1);
c = calDist(p, point1);

\[ \cos(C) = (a^2 + b^2 - c^2) / (2a*b); \]
\[ \text{angle1} = \cos^{-1}(\cos(C)); \]

//angle that moves P out of Q using law of cosines
a = calDist(c2center, point2);
c = calDist(point1, point2);

\[ \cos(C) = (a^2 + b^2 - c^2) / (2a*b); \]
\[ \text{angle2} = \cos^{-1}(\cos(C)); \]

setRotInterval(angle1, angle2, indexp, indexq);

///////////////////////////////////////////////////////Calculate rotation interval///////////////////////////////////////////////////////

/*
   Copy matching matrix A to matrix B
   A: Matrix to be copied
   B: Copied Matrix
*/
void Transformation::copyMatching(int** A, int** B)
{
for(int i = 0; i < len; i++)
{
   for(int j = 0; j < len; j++)
   {
      B[i][j] = A[i][j];
   }
}
}
APPENDICES

/*
   Move the elements in the array of mRotInterval backwards, based on start and end.
   Start: position to start shift backwards.
   End : mRotInterval array size - mRotItvIndex(usually).
   shift until the end of the array
   temp2 : temporary variable that holds the new value of angle[start].
   tempArr2: temporary array that holds the new value of matching[start].
*/

void Transformation::moveBackwards(int start, int end, double temp2, int** tempArr2)
{
  double temp;
  int** tempArr;

  tempArr = new int*[len];
  for(int i = 0; i < len; i++)
    tempArr[i] = new int[len];

  for(int l = start; l < end; l++)
  {
    temp = mRotInterval[l].angle;
    mRotInterval[l].angle = temp2;
    temp2 = temp;

    copyMatching(mRotInterval[l].matching, tempArr);
    copyMatching(tempArr2, mRotInterval[l].matching);
    copyMatching(tempArr, tempArr2);
  }

  //destroy tempArr in memory address
  for(int i = 0; i < len; i++)
    delete[] tempArr[i];
  delete[] tempArr;
}

/*
   Put in mTheta[i][j]->mTheta2 value in the rotation interval - mRotInterval
   Start: starting position of mRotInterval to trace for theta2. (theta2 must always starts from one element behind theta1)
   End : mRotInterval array size - mRotItvIndex(usually).
   shift until the end of the array
   i : index of p structure
   j : index of q structure
   angle : mTheta[i][j]->mTheta2's value
*/

void Transformation::insertTheta2(int start, int end, int i, int j, double angle)
{
  int** tempArr;

  tempArr = new int*[len];
for(int x = 0; x < len; x++)
    tempArr[x] = new int[len];

double totalTheta = 0;
double temp, temp2;
bool isSet = false;

for(int k = start; k < end; k++)
{
    totalTheta += mRotInterval[k].angle;
    if(angle < totalTheta)
    {
        totalTheta = totalTheta - mRotInterval[k].angle;
        //exclude angle[k]
        temp = mRotInterval[k].angle;
        mRotInterval[k].angle = angle - totalTheta;
        temp2 = mRotInterval[k+1].angle;
        mRotInterval[k+1].angle = temp - angle;
        copyMatching(mRotInterval[k+1].matching, tempArr);
        copyMatching(mRotInterval[k].matching,
                    mRotInterval[k+1].matching);

        //set matching of new matching[k]
        //set also matching for the angle before (for whole totalTheta need to set)
        for(int x = start; x <= k; x++)
        {
            mRotInterval[x].matching[i][j] = 1;
        }
        mRotItvIndex++;

        //move backwards
        moveBackwards(k+2, mRotItvIndex, temp2, tempArr);
        isSet = true;
        break;
    }
    else if(angle == totalTheta)
    {
        for(int l = start; l <= k ; l++)
        {
            mRotInterval[l].matching[i][j] = 1;
        }
        isSet = true;
        break;
    }
}

// angle > totalTheta => add new theta at behind
if(!isSet)
{
    mRotInterval[mRotItvIndex].angle = angle - totalTheta;
    for(int l = start; l <= mRotItvIndex ; l++)
    {
        mRotInterval[l].matching[i][j] = 1;
    }
}
APPENDICES

mRotItvIndex++;
// destroy tempArr in memory address
for(int i = 0; i < len; i++)
    delete[] tempArr[i];
delete[] tempArr;
}

void Transformation::setRotInterval(double theta1, double theta2, int i, int j)
{
    double totalTheta = 0;
    double temp, temp2;
    bool isSet = false;

    int** tempArr;
    /*initialize*/
    tempArr = new int*[len];

    for(int x = 0; x < len; x++)
        tempArr[x] = new int[len];

    totalTheta = 0;
    isSet = false;
    if(mRotItvIndex == 0) // first element, first theta to be insert into array
    {
        if(theta1 > 0)
        {
            mRotInterval[mRotItvIndex].angle = theta1; // angle that moves p to q
            mRotInterval[mRotItvIndex].matching[i][j] = -1;
            mRotItvIndex++;
        }
        mRotInterval[mRotItvIndex].angle = theta2; // angle that moves p out of q
        mRotInterval[mRotItvIndex].matching[i][j] = 1;
        mRotItvIndex++;
    }
    else
    {
        if(theta1 == 0) // insert only theta2 when theta1 = 0
        {
            insertTheta2(0, mRotItvIndex, i, j, theta2);
        }
        else
        {
            for(int k = 0; k < mRotItvIndex; k++)
        }
    }
```{totalTheta += mRotInterval[k].angle;
if (thetal < totalTheta)
{
    totalTheta = totalTheta - mRotInterval[k].angle; //exclude angle[k]
    temp = mRotInterval[k].angle; //copy angle[k] to temp
    mRotInterval[k].angle = thetal - totalTheta; //replace angle[k] with new theta
}
angle[k+1] to temp2
    temp2 = mRotInterval[k+1].angle; //copy angle[k+1] to temp2
    mRotInterval[k+1].angle = temp - thetal; //replace angle[k+1] with new theta
    copyMatching(mRotInterval[k+1].matching, tempArr); //copy matching[k+1] to tempArr
    copyMatching(mRotInterval[k].matching, mRotInterval[k+1].matching); //copy matching[k] to matching[k+1]
    //set matching of new matching[k] //set also matching for the angle before
    (for whole totalTheta also need to set)
    for (int x = 0; x <= k; x++)
    {
        mRotInterval[x].matching[i][j] = -1;
    }
    mRotItvIndex++; //move backwards
    moveBackwards(k+2, mRotItvIndex, temp2, tempArr);
next to the thetal
    insertTheta2(k+1, mRotItvIndex, i, j, theta2); //theta2 - must be the at position that
    isSet = true; break;
}
else if (thetal == totalTheta)
{
    for (int l = 0; l <= k; l++)
    {
        mRotInterval[l].matching[i][j] = -1;
    }
next to the thetal
    insertTheta2(k+1, mRotItvIndex, i, j, theta2); //theta2 - must be the at position that
    isSet = true; break;
}
APPENDICES

// theta1 > totalTheta => add new theta at behind
if(!isSet)
{
    mRotInterval[mRotItvIndex].angle = theta1 - totalTheta;

    for(int l = 0; l <= mRotItvIndex ; l++)
    {
        mRotInterval[l].matching[i][j] = -1;
    }
    mRotItvIndex++;

    //theta2 - must be at the position that next to the theta1
    insertTheta2(mRotItvIndex, mRotItvIndex, i, j, theta2);
}

//destroy tempArr in memory address
for(int x = 0; x < len ; x++)
    delete[] tempArr[x];
delete[] tempArr;


////////////////////////////////////Get maximum bipartite matching////////////////////////////////////
void Transformation::getMaxMatch()
{
    int max = 0;

    for(int i = 0; i < mRotItvIndex; i++)
    {
        max = hopcroft_karp(len, mRotInterval[i].matching);
        if(mMaxMatch < max)
            mMaxMatch = max;
    }
}
#ifndef _GRAPH_H_
define _GRAPH_H_
define NIL 0
define INF (1<<28)
#include <iostream>
#include <queue>
using namespace std;

void insertMatch(int** matching, int length);
bool bfssearch(int n, int* match, int* dist);
bool dfssearch(int v, int* match, int* dist);
int hopcroft_karp(int length, int** matching);

#endif
A-10 Graph.cpp

/*
 * Modified from code on web: 
 http://zobayer.blogspot.com/2010/05/maximum-matching.html
 */
#include "Graph.h"
// nLeft: number of nodes on left side, nodes are numbered 1 to n, G1
// p structure)
// nRight: number of nodes on right side, nodes are numbered n+1 to
// n+m, G2
// q structure)
// G = NIL[0] U\ldots G1[G[1\ldots n]] U\ldots G2[G[n+1\ldots n+m]]

vector<vector<int>> G;
void insertMatch(int** matching, int length)
{
    for(int i = 0; i < length; i++)
    {
        for(int j = 0; j < length; j++)
        {
            if(matching[i][j] == 1)
            {
                j += length; // v += nLeft
                G[i+1].push_back(j+1); // G[u].push_back(v);
            }
        }
    }
}
bool bfs_search(int n, int* match, int* dist)
{
    int u, v, length;
    queue<int> Q;
    //for vertex in G1: from 1 to n
    for(int i = 1; i <= n; i++)
    {
        if(match[i] == NIL) // Pair_G1 = match
        {
            dist[i] = 0;
            Q.push(i);
        }
        else
        {
            dist[i] = INF;
        }
    }
    dist[NIL] = INF;
    while(!Q.empty())
    {
        v = Q.front(); Q.pop(); // vertex = Dequeue(Q), vertex in G1 = u
        if(v != NIL)
        {
            length = G[v].size();
            ...
APPENDICES

//for each u in Adj[v]
for(int i = 0; i < length; i++)
{
    u = G[v][i];
    if (dist[match[u]] == INF)
    {
        dist[match[u]] = dist[v] + 1;
        Q.push(match[u]);
    }
}
}

return (dist[NIL] != INF);

bool dfsearch(int v, int* match, int* dist)
{
    int u, length;
    if (v != NIL)
    {
        length = G[v].size();
        //for each u in Adj[v]
        for(int i = 0; i < length; i++)
        {
            u = G[v][i];
            if (dist[match[u]] == dist[v] + 1)
            {
                if (dfsearch(match[u], match, dist))
                {
                    match[u] = v;
                    match[v] = u;
                    return true;
                }
            }
        }
        dist[v] = INF;
    }
    return false;
}
return true;

int hopcroft_karp(int length, int** matching)
{
    G.resize(length+1);
    int length2 = length*length;
    int *match = new int[length2 + 1];
    int *dist = new int[length2 + 1];

    for(int i = 0; i <= length2; i++)
    {
        match[i] = 0;
        dist[i] = 0;
    }
    insertMatch(matching, length);

int totalMatch = 0;

while(bfsearch(length, match, dist))
{
    for(int i = 1; i <= length; i++)
    {
        if(match[i] == NIL)
        {
            if(dfsearch(i, match, dist))
            {
                totalMatch++;
            }
        }
    }
}

delete match;
delete dist;
return totalMatch;
A-11 Example of .pdb file

ATOM   1  N  MET   1  1.040  0.374 -0.952  1.00  0.00
ATOM   2  CA MET   1  0.000  0.000  0.000  1.00  0.00
ATOM   3  C  MET   1  0.598 -0.376  1.349  1.00  0.00
ATOM   4  O  MET   1  -0.110 -0.827  2.249  1.00  0.00
ATOM   5  CB MET   1  -0.835 -1.146 -0.550  1.00  0.00
ATOM   6  N  SER   2  1.907 -0.187  1.484  1.00  0.00
ATOM   7  CA SER   2  2.623 -0.615  2.679  1.00  0.00
ATOM   8  C  SER   2  2.169  0.169  3.904  1.00  0.00
ATOM   9  O  SER   2  2.381 -0.258  5.039  1.00  0.00
ATOM  10  CB SER   2  4.124 -0.467  2.479  1.00  0.00
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ATOM  13  C  PHE   3  -0.184  1.398  5.417  1.00  0.00
ATOM  14  O  PHE   3  -0.676  1.830  6.460  1.00  0.00
ATOM  15  CB PHE   3  0.534  3.474  4.222  1.00  0.00
ATOM  16  N  ILE   4  -0.620  0.298  4.814  1.00  0.00
ATOM  17  CA ILE   4  -1.688 -0.516  5.381  1.00  0.00
ATOM  18  C  ILE   4  -1.262 -1.139  6.704  1.00  0.00
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