Programming Assignment 5 – 601.455/655 Fall 2024

Score Sheet (hand in with report) Also, PLEASE INDICATE WHETHER YOU ARE IN 601.455 or 601.655 (one in each section is OK)

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Signature (required)	I (we) have followed the rules in completing this assignment			
Grade Factor				
Program (40)				
Design and overall program structure				
Reusability and modularity				
Clarity of documentation and programming				
Results (20)				
Correctness and completeness				
Report (40)				
Description of formulation and algorithmic approach				
Overview of program				
Discussion of validation approach				
Discussion of results				
TOTAL				

NOTE: This is an optional assignment.

If you hand it in, I will use the grade to replace the lowest other programming assignment or written homework assignment with one exception:

You may not drop **both**HW#4 and HW#5. If
these are your two
lowest grades, then I will
drop the lower of those
two under the drop 1
homework scenario and
replace the next lowest
grade (other than the
other of HW#4-5) with
this score

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CIS: Programming Assignment 5

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1 Introduction

The objective of Programming Assignment 5 is to extend the ICP algorithm from PA4 to include deformable registration, allowing transformations of a 3D surface mesh using atlas modes. The deformable registration requires both rigid transformations and atlas-based deformations to correctly align the set of sample points and the 3D surface mesh. This assignment adds iterative processes to both the rigid body transformation and mode weights of the deformable model. The final output includes the computed CT coordinates for the deformed mesh and corresponding mode weights for the atlas.

In the interest of time, we implemented the linear search method to find the closest points on the deformed mesh. We also varied the number of iterations to analyze the impact on accuracy. The same approach can be extended to KDTree and Octree for faster nearest-neighbor searches in larger datasets.

2 Updates from PA4 to PA5

- Extended the ICP algorithm to include deformable registration by incorporating atlas modes.
- Implemented the computation of mode weights (λ_m) using barycentric coordinates and least squares minimization.
- Added iterative refinement for both rigid transformations and mode weights.
- Created readModes.py to parse and load atlas mode data, including the mean shape (Mode 0) and displacement vectors for all modes.
- Developed utility functions:
 - computeBarycentric.py for calculating barycentric coordinates for points relative to triangles.
 - computeQk.py for projecting points onto mean shape or mode displacements.
 - findContainingTriangle.py for determining the triangle containing a given point on the mesh.
- Updated parseMesh.py.
- Varied the number of iterations (1, 3, 9) to study the impact on accuracy and computational cost.

3 Mathematical Approach

3.1 Frame Transformation

To calculate the position of the pointer tip, we used transformations between different coordinate systems. Frame transformations were represented as:

$$F_{ab} = [R_{ab}, p_{ab}]$$

where R_{ab} is the rotation matrix and p_{ab} is a translation vector.

The inverse frame transformation, which is also needed to move between coordinate systems, is computed as:

$$F_{ab}^{-1} = [R_{ab}^{-1}, -R_{ab}^{-1}p_{ab}]$$

3.2 Point Set to Point Set Registration

To compute the optimal rotation matrix and translation vector to align 3D point sets, we first calculated the average value of both point sets. Let source and target be the two point sets. We compute their averages as:

average =
$$\frac{1}{N} \sum_{i=1}^{N} p_i$$

The points were then centered by subtracting the respective average. To solve for the optimal rotation matrix, we implement Arun's method. We compute the covariance matrix H of the centered point sets, given by:

$$H = \sum_{i=1}^{N} (p_{i,\text{source}} - \bar{p}_{\text{source}})(p_{i,\text{target}} - \bar{p}_{\text{target}})^{T}$$

We then apply Singular Value Decomposition (SVD) to the covariance matrix H:

$$H = U\Sigma V^T$$

From the matrices U and V, we find the optimal rotation matrix R using:

$$R = VU^T$$

We ensure that the rotation is correct by checking the determinant of R; if det(R) < 0, we modify V for a valid rotation.

The translation vector p can be computed as:

$$p = \bar{p}_{\text{target}} - R\bar{p}_{\text{source}}$$

We also compute the RMSE between the target and transformed points for algorithm verification:

RMSE =
$$\sqrt{\frac{1}{N} \sum_{i=1}^{N} |p_{i,\text{target}} - Rp_{i,\text{source}} - p|^2}$$

3.3 Finding Pointer A_{Tip} in Body B Coordinates

Given the position of the pointer tip A_{Tip} in local coordinates, for each sample frame k, we calculate its position in Body B coordinates using the given frame transformation:

$$p_{B_{\text{Tip}},k} = F_{B,k}^{-1} F_{A,k} p_{A_{\text{Tip}}}$$

where $F_{A,k}$ and $F_{B,k}$ are the frame transformations from the optical tracker to the local coordinates of pointers A and B, respectively.

3.4 Finding the Closest Point on a Triangle

To determine the closest point on a triangle to a given 3D point \mathbf{a} , where the triangle has vertices $\mathbf{p}, \mathbf{q}, \mathbf{r}$, we used the geometric approach described in the slides. The process consists of two main cases: when the point lies inside the triangle and when it lies outside, which requires projection onto the triangle's edges.

We first calculate the following dot products, which we use to determine the position of ${\bf a}$ relative to the triangle:

$$d_1 = (\mathbf{q} - \mathbf{p}) \cdot (\mathbf{a} - \mathbf{p}),$$

$$d_2 = (\mathbf{r} - \mathbf{p}) \cdot (\mathbf{a} - \mathbf{p}),$$

$$d_3 = (\mathbf{q} - \mathbf{p}) \cdot (\mathbf{q} - \mathbf{p}),$$

$$d_4 = (\mathbf{r} - \mathbf{p}) \cdot (\mathbf{r} - \mathbf{p}),$$

$$d_5 = (\mathbf{q} - \mathbf{p}) \cdot (\mathbf{r} - \mathbf{p}).$$

Using these dot products, we compute the barycentric coordinates u, v, w of point **a** relative to the triangle. The denominator of these coordinates is:

$$denom = d_3 \cdot d_4 - d_5^2.$$

The coordinates v and w are then calculated as:

$$v = \frac{d_4 \cdot d_1 - d_5 \cdot d_2}{\text{denom}},$$

$$w = \frac{d_3 \cdot d_2 - d_5 \cdot d_1}{\text{denom}},$$

$$u = 1 - v - w.$$

If the barycentric coordinates satisfy the conditions $u \ge 0$, $v \ge 0$, and $w \ge 0$, then the point **a** lies inside the triangle. In this case, the closest point on the triangle is the weighted sum of the triangle's vertices:

$$\mathbf{closest_point} = u \cdot \mathbf{p} + v \cdot \mathbf{q} + w \cdot \mathbf{r}.$$

If the point lies outside the triangle, the closest point must be on one of its edges. We compute the closest point on each of the triangle's three edges pq, pr, qr by projecting a onto each segment. The projection of a point a onto a segment with endpoints start and end is:

$$closest_point_segment = start + t \cdot (end - start),$$

where the scalar t is computed as:

$$t = \frac{(\mathbf{a} - \mathbf{start}) \cdot (\mathbf{end} - \mathbf{start})}{(\mathbf{end} - \mathbf{start}) \cdot (\mathbf{end} - \mathbf{start})}.$$

We constrain t to the interval [0,1] to ensure that the projection lies on the segment. The three potential closest points are:

$$closest_pq = closest_point_segment(p, q, a),$$

 $closest_pr = closest_point_segment(p, r, a),$
 $closest_qr = closest_point_segment(q, r, a).$

Finally, we compute the distances from $\bf a$ to each of the potential closest points. The distance between two points $\bf a$ and $\bf b$ is:

$$\operatorname{dist}(\mathbf{a}, \mathbf{b}) = \|\mathbf{a} - \mathbf{b}\|.$$

The closest point is the one that minimizes the distance:

$$\mathbf{closest_point} = \begin{cases} \mathbf{closest_pq} & \mathrm{if\ dist}(\mathbf{a}, \mathbf{closest_pq}) < \mathrm{dist}(\mathbf{a}, \mathbf{closest_pr}) \ \mathrm{and\ dist}(\mathbf{a}, \mathbf{closest_pq}) < \mathrm{dist}(\mathbf{a}, \mathbf{closest_pr}) \\ \mathbf{closest_pr} & \mathrm{if\ dist}(\mathbf{a}, \mathbf{closest_pr}) < \mathrm{dist}(\mathbf{a}, \mathbf{closest_qr}), \\ \mathbf{closest_qr} & \mathrm{otherwise}. \end{cases}$$

3.5 Linear Search through Triangles

For the linear search through triangles, the process involves passing a point and the current triangle into the closest point on triangle method. After computing the closest point on the triangle, the distance between the query point and the closest point is calculated using the following:

$$distance = \|\mathbf{pt} - \mathbf{closest_point}\|_2$$
.

The triangle with the closest point is selected by comparing these distances across all triangles (Brute Force).

3.6 K-D Tree Nearest-Neighbor Search

We can optimize the search for the closest triangle using a K-D Tree. The K-D Tree is built from the centroids of the triangles, and the nearest neighbor search is performed to find the closest triangle to the query point. The implementation is described in 3.6.

The centroid C of a triangle with vertices $\mathbf{v}_1(x_1, y_1, z_1), \mathbf{v}_2(x_2, y_2, z_2), \mathbf{v}_3(x_3, y_3, z_3)$ is computed as:

$$\mathbf{C}_{i} = \frac{1}{3} \left((x_{1}, y_{1}, z_{1}) + (x_{2}, y_{2}, z_{2}) + (x_{3}, y_{3}, z_{3}) \right).$$

Using the K-D Tree, we can find the nearest centroid to the current point, and the corresponding triangle can be retrieved.

3.7 Octree Search

An Octree can also be used to further optimize the search by partitioning the space into cubes. Each cube contains the triangles whose centroids fall within it. The implementation is described in 3.8.

3.8 Iterative Refinement of Transformation (F_{reg})

The Iterative Closest Point algorithm builds on the initial transformation F_{reg} by iteratively refining it to minimize the distance between points (s_k) and the closest points on the mesh (c_k) . This process ensures convergence to an optimal alignment.

First, apply the current transformation F_{reg} to the d_k points (pointer tip positions in Body B coordinates) to generate s_k :

$$s_k = F_{reg} \cdot d_k$$

Next, for each transformed point s_k , determine the closest point c_k on the surface mesh using one of the previous search methods. Then, register the d_k points to the c_k points by recalculating the transformation F_{reg} with point set registration:

$$F_{reg} = \begin{bmatrix} R & p \\ 0 & 1 \end{bmatrix}$$

where R and p are updated. Finally, evaluate the Frobenius norm of the difference between successive transformations:

$$\Delta F = \|F_{reg}^{(i+1)} - F_{reg}^{(i)}\|_F$$

If $\Delta F < \text{tol (e.g., } 1e^{-5})$ or the maximum number of iterations is reached, stop. Now, update F_{reg} and repeat steps 1-4 until convergence.

3.9 Convergence Parameters and Tolerance

Convergence is monitored using:

$$\Delta F = \|F_{reg}^{(i+1)} - F_{reg}^{(i)}\|_F$$

where $\|\cdot\|_F$ is the Frobenius norm. This ensures that eventually, updated transformations differ by a negligible amount. The maximum number of iterations is capped (in our case, 10), and the tolerance for convergence is set to $1e^{-5}$ to optimize computational cost.

3.10 Deformable Registration

Deformable registration extends the ICP algorithm by incorporating a statistical shape model. The deformed vertex positions are computed as:

$$\mathbf{v}_k = \mathbf{v}_k^{(0)} + \sum_{m=1}^{N_{\mathrm{modes}}} \lambda_m \mathbf{d}_{k,m},$$

where:

- $\mathbf{v}_k^{(0)}$: Average position of vertex k (Mode 0).
- $\mathbf{d}_{k,m}$: Displacement vector for vertex k in mode m.

• λ_m : Weight for mode m.

The barycentric coordinates $[\zeta, \xi, \psi]$ for a point **c** in a triangle defined by vertices $\mathbf{v}_0, \mathbf{v}_1, \mathbf{v}_2$ are computed as:

$$\xi = \frac{d_{11}d_{20} - d_{01}d_{21}}{\text{denom}},$$

$$\psi = \frac{d_{00}d_{21} - d_{01}d_{20}}{\text{denom}},$$

$$\zeta = 1 - \xi - \psi,$$

where d_{ij} represents dot products of vectors formed by the vertices and \mathbf{c} , and denom = $d_{00}d_{11} - d_{01}^2$. The projection of \mathbf{c} onto a specific mode m is given by:

$$\mathbf{q}_{k}^{(m)} = \zeta \mathbf{v}_{0}^{(m)} + \xi \mathbf{v}_{1}^{(m)} + \psi \mathbf{v}_{2}^{(m)}.$$

4 Algorithm Overview

4.1 Frame Transformations

Our implementation uses 3D points and transformation matrices to handle rotations and translations in homogeneous coordinates. The transformation matrix has the form:

$$T = \begin{bmatrix} R & p \\ 0 & 1 \end{bmatrix}$$

where R is a 3×3 rotation matrix, and p is a 3×1 translation vector.

Inverse transformations are computed as:

$$T^{-1} = \begin{bmatrix} R^{-1} & -R^{-1}p \\ 0 & 1 \end{bmatrix}$$

This allows us to transform points between coordinate systems efficiently.

4.2 Point Set to Point Set Registration

The registration algorithm computes the optimal transformation (rotation and translation) to align two sets of corresponding 3D points.

- 1. Compute the average positions of both the source and target point sets.
- 2. Center each point set by subtracting averages.
- 3. Compute covariance matrix of centered point sets.
- 4. Perform Singular Value Decomposition on the covariance matrix.
- 5. Compute the rotation matrix R from the SVD results. If det(R) < 0, adjust for a valid rotation.
- 6. Handle cases where singular values are zero or near-zero.
- 7. Compute translation vector p using the computed rotation.
- 8. Return final transformation matrix combining R and p.

Update: We included a check for zero or near-zero singular values to maintain stability during SVD.

4.3 Finding the Pointer Tip in Body B Coordinates

To compute the pointer tip position in Body B coordinates:

1. Use the transformation matrices (F_A) and (F_B) to compute the pointer tip position.

$$d_k = F_B^{-1} \cdot F_A \cdot A_{\rm tip}$$

2. Extract position of the pointer tip from transformed coordinates.

4.4 Finding the Closest Point on a Triangle

The closest point to a given 3D point on a triangle is computed as follows:

- 1. Calculate barycentric coordinates to determine if the point lies inside the triangle.
- 2. If the point is inside the triangle, return it.
- 3. If the point lies outside the triangle, compute projections onto each triangle edge and find closest edge point.
- 4. Return closest point found.

4.5 Linear Search for Closest Point on a Mesh

Brute force:

- 1. For each triangle in the mesh:
 - (a) Compute closest point on the triangle to the point.
 - (b) Calculate distance between query point and closest point.
- 2. Keep track of smallest distance and corresponding point.
- 3. Return closest point found.

4.6 Optimizing with K-D Trees

To improve efficiency, we use a K-D Tree.

- 1. Build K-D Tree from the centroids of all triangles in the mesh.
- 2. For a given point,
 - (a) Find nearest centroid using the K-D Tree.
 - (b) Retrieve corresponding triangle and compute closest point on it.
- 3. Return closest point found.

4.7 Octree-Based Search

For also tested using Octrees:

- 1. Build Octree by recursively dividing the 3D space into octants.
- 2. For a given point,
 - (a) Traverse Octree, starting from the root node.
 - (b) Check triangles in leaf nodes for closest point.
- 3. Return closest point found.

4.8 Iterative Closest Point (ICP) Algorithm

Our most recent update for PA4 was including the iterative component of the ICP algorithm:

- 1. Start with initial transformation matrix (the identity matrix).
- 2. Transform ource points using current transformation.
- 3. Find closest points on mesh for each transformed source point (using a previous method).
- 4. Compute new transformation by registering source points to their corresponding closest points.
- 5. Check for convergence using the Frobenius norm:

$$\Delta F = ||F_{\text{new}} - F_{\text{old}}||_F$$

6. Stop if change is below a threshold or the maximum number of iterations is reached.

Update: Convergence is monitored with a tolerance of 10^{-5} and a maximum of 10 iterations.

4.9 Deformable Registration

- 1. Initialization:
 - Parse Mode 0 (mean shape) and mode displacement data using readModes.py.
 - Parse vertices and triangles using parseMesh.py.
 - Initialize \mathbf{F}_{reg} as the identity matrix and mode weights $\lambda_m = 0$.
 - 2. Transform sampled points \mathbf{d}_k into CT coordinates using the current rigid transformation:

$$\mathbf{s}_k^{(t)} = \mathbf{F}_{\text{reg}}^{(t)} \cdot \mathbf{d}_k.$$

- 3. Compute closest points \mathbf{c}_k on the deformed mesh:
- Use linear search with a specified number of iterations (This can be extended to KD trees or Octrees upon successful implementation).
- Use findContainingTriangle.py to determine the triangle containing \mathbf{c}_k .
- Compute barycentric coordinates with computeBarycentric.py.
- 4. Solve for λ_m using least squares:

$$\mathbf{A} = \text{reshape}(\mathbf{q}_k^{(m)}, N_s, N_m \cdot 3), \quad \mathbf{b} = \mathbf{s}_k - \mathbf{q}_k^{(0)}.$$

5. Update vertex positions using the new mode weights:

$$\mathbf{v}_k = \mathbf{v}_k^{(0)} + \sum_{m=1}^{N_{ ext{modes}}} \lambda_m \mathbf{d}_{k,m}.$$

- 6. Recalculate \mathbf{F}_{reg} using $\mathbf{pointSetRegistration.py}$.
- 7. Compute the Frobenius norm of successive transformations:

$$\Delta F = \|\mathbf{F}_{\text{reg}}^{(t+1)} - \mathbf{F}_{\text{reg}}^{(t)}\|_F.$$

Stop if ΔF is below the tolerance.

8. Write transformed points, closest points, mode weights, and residual errors to an output file.

5 Program Structure

5.1 Overview

Input Data Handling (readData):

- parseMesh.py: Parses mesh files containing vertices and triangles.
- parseData.py: Reads body marker coordinates and sample readings.
- readModes.py: Reads mode displacement data for Mode 0 and additional modes.

Utility Files (util):

- geometry.py: Contains Vertex and Triangle classes.
- calculateTransformation.py: Computes frame transformations between Body A and Body B using point set registration.
- pointSetRegistration.py: Implements Arun's method for registering point sets.
- iterativeRegistration.py: Implements the iterative closest point (ICP) algorithm for refining transformations.
- computeBarycentric.py: Computes barycentric coordinates for a point relative to a triangle.

- computeQ_k.py: Computes the projection of a point onto the mode displacements.
- findContainingTriangle.py: Determines the triangle containing a point on the mesh.

Data Structure Building (build):

- buildKDTree.py: Builds a KD-tree structure.
- buildOctree.py: Builds an octree structure.

Main, Search Optimization, and Generating Output:

- main.py: Reads input files, calculates transformations, finds the closest points on a mesh, and generates the output.
- findClosestPoint.py: Computes the closest point on a triangle.
- findPointOnMesh.py: Linear Search to finds closest point.
- findPointOnMeshKDTree.py: KD-tree Search.
- findPointOnMeshOctree.py: Octree Search.
- **generateOutput.py:** Writes transformed tip positions and closest points on the mesh to an output file.
- generateOutputPA4.py: Performs similar output generation tasks as generateOutput.py, adapted for PA4 to include ICP.
- **generateOutputPA5.py**: Manages the iterative process, updating transformations and mode weights.

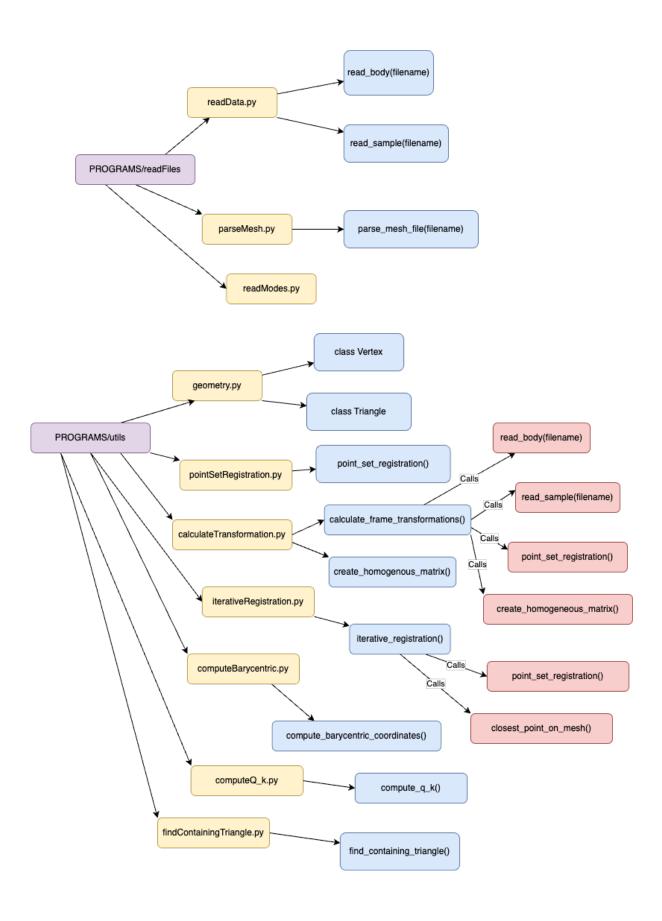
Error and Performance Metrics (errorCalculation):

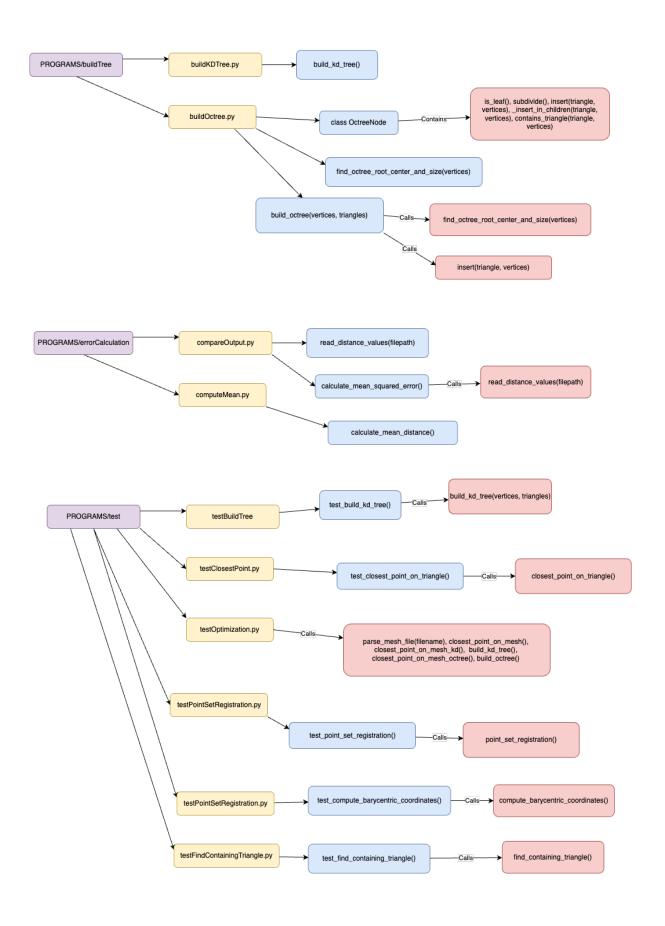
- computeMean.py: Computes the mean distance from the last column of output files.
- compareOutput.py: Computes the Mean Squared Error between the results and expected outputs.

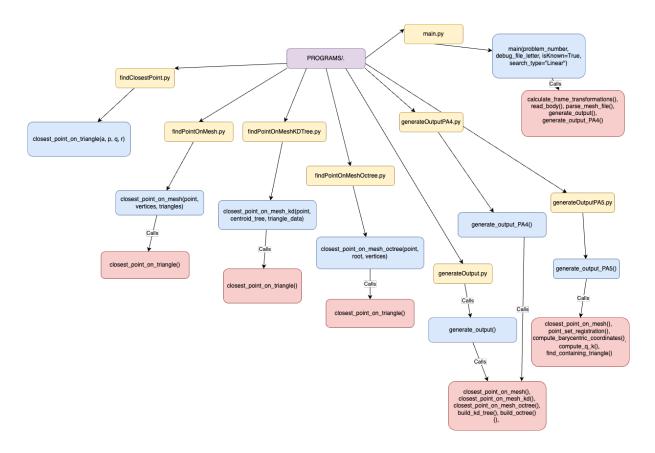
Please look at the README for the file tree expressed as relative paths from the root.

5.2 Visual Representation

We extend the file structure from PA3 and PA4 by incorporating the additional files required for PA5.







5.3 File Descriptions

readData.py

The readData.py file handles data input operations to read body marker and sample data files.

- \bullet ${\bf read_body(filename):}$ Reads marker LED coordinates and tip data.
 - Input:
 - * filename (str): Prefix of calibration body file ("Problem3-BodyA").
 - Output:
 - * N_markers (int): Number of marker LEDs in calibration body.
 - * marker_coords (list of list of float): List of coordinates for each marker.
 - * tip_coords (list of float): Coordinates of the pointer tip.
- read_sample(filename): Reads sample readings, including marker coordinates for body A, body B, and dummy markers across multiple frames.
 - Input:
 - * filename (str): Prefix of the sample readings file ("PA3-A-Debug-SampleReadingsTest").
 - Output:
 - * NA (int): Number of A LED markers.
 - * **NB** (int): Number of B LED markers.
 - * ND (int): Number of dummy LED markers.
 - * Nsamps (int): Number of sample frames.
 - * readings (list of dict): List of sample frame data:
 - · 'A' (np.ndarray): Coordinates of A body markers.
 - · 'B' (np.ndarray): Coordinates of B body markers.
 - · 'D' (np.ndarray): Coordinates of dummy markers.

parseMesh.py

The parseMesh.py file reads and processes the mesh data, including vertices and triangles.

- parse_mesh_file(filename): Reads vertex and triangle data.
 - Input:
 - * filename (str): Path to mesh file ("PROGRAMS/data/Problem3MeshFile.sur").
 - Output:
 - * vertices (list of Vertex): A list of Vertex objects representing the coordinates (x, y, z) of each vertex in mesh.
 - * triangles (list of Triangle): A list of Triangle objects representing the vertices and neighbor information for each triangle in the mesh. Each triangle includes:
 - · v1, v2, v3 (int): Indices of the vertices forming the triangle.
 - · n1, n2, n3 (int): Indices of the neighboring triangles.

readModes.py

The **readModes.py** file reads and parses mode displacement data, including the mean shape (Mode 0) and additional atlas modes.

- read_modes(filename): Reads mode data from specified file.
 - Input:
 - * filename (str): Path to the mode file.
 - Output:
 - * mode_data (list of np.ndarray): List containing mode displacement arrays, including the mean shape as Mode 0.

geometry.py

The ${f geometry.py}$ file defines classes for vertices and triangles.

- Vertex Class:
 - **Description:** 3D point with x, y, and z coordinates.
 - Attributes:
 - * x (float): x-coordinate
 - * y (float): y-coordinate
 - * z (float): z-coordinate
 - Initialization:
 - * Constructor $_$ init $_$ (x, y, z) initializes the vertex with the given x, y, and z coordinates.
- Triangle Class:
 - Description: Represents a triangle in a 3D mesh, defined by vertex indices and neighboring triangle indices.
 - Attributes:
 - * vertices (tuple of int): A tuple containing the indices of three vertices that form the triangle.
 - * neighbors (tuple of int): A tuple containing indices of three neighboring triangles.
 - Initialization:
 - * Constructor __init__(v1, v2, v3, n1, n2, n3) initializes the triangle with the given vertex indices (v1, v2, v3) and neighbor indices (n1, n2, n3).

pointSetRegistration.py

The **pointSetRegistration.py** file from PA1/2. This file implements Arun's method for aligning two sets of 3D points. It also includes a check for degenerate cases where singular values are zero.

- point_set_registration():
 - Inputs:
 - * source (numpy.ndarray): An (N,3) array representing source point set.
 - * target (numpy.ndarray): An (N,3) array representing target point set.
 - Outputs:
 - * R (numpy.ndarray): A (3,3) array representing the optimal rotation matrix.
 - * p (numpy.ndarray): A (3,) array representing the optimal translation vector.

calculateTransformation.py

The **calculateTransformation.py** file computes the frame transformations between the Body A and Body B coordinate systems for each frame in the sample data. It utilizes point set registration.

- calculate_frame_transformations():
 - Inputs:
 - * body_filename_a (str): Filename prefix for Body A marker LED data, "Problem3-BodyA".
 - * body_filename_b (str): Filename prefix for Body B marker LED data, "Problem3-BodyB".
 - * sample_filename (str): Filename prefix for the sample readings file, "PA3-A-Debug-SampleReadingsTest".
 - Outputs:
 - * transformations (list): A list of tuples $(F_{A,k}, F_{B,k})$, where $F_{A,k}$ and $F_{B,k}$ are 4x4 homogeneous transformation matrices for each frame.
- create_homogeneous_matrix():
 - Inputs:
 - * R (numpy.ndarray): A 3×3 rotation matrix.
 - * p (numpy.ndarray): A 3×1 translation vector.
 - Outputs:
 - * homogeneous_matrix (numpy.ndarray): A 4 × 4 transformation matrix in homogeneous coordinates.

iterativeRegistration.py

The **iterativeRegistration.py** file performs iterative point cloud registration to align a set of 3D points to a target mesh using an ICP algorithm.

- iterative_registration():
 - Inputs:
 - * **d_points** (numpy.ndarray): A $N \times 3$ array of points to be registered.
 - * vertices (list of Vertex): A list of Vertex objects representing the vertices of the mesh.
 - * triangles (list of Triangle): A list of Triangle objects representing the mesh's triangles.
 - * max_iterations (int, optional): Maximum number of iterations (default: 100).
 - * tol (float, optional): Convergence tolerance (default: 1×10^{-5}).
 - Outputs:
 - * **F_reg** (numpy.ndarray): A 4×4 homogeneous transformation matrix representing the registration transformation.

computeBarycentric.py

The **computeBarycentric.py** file computes barycentric coordinates for a point with respect to a triangle.

• compute_barycentric_coordinates(c, triangle, vertices): Computes barycentric coordinates for a point relative to a triangle.

```
Input:
* c (np.ndarray): Closest point (3,).
* triangle (np.ndarray): Indices of the triangle vertices (3,).
* vertices (np.ndarray): Vertex coordinates (Nvertices, 3).
Output:
* bary_coords (np.ndarray): Barycentric coordinates [ζ, ξ, ψ].
```

computeQ_k.py

The **computeQ_k.py** file computes the projection of a point onto either the mean shape or mode displacements.

• compute_q_k(bary_coords, triangle, mode_data, mode_index): Computes the projection of a point.

```
Input:
* bary_coords (np.ndarray): Barycentric coordinates [ζ, ξ, ψ].
* triangle (np.ndarray): Indices of the triangle vertices (3,).
* mode_data (list of np.ndarray): List of modes (mean shape + displacements).
* mode_index (int): Index of the mode.
Output:
* q_k (np.ndarray): Projection onto the specified mode (3,).
```

findContainingTriangle.py

The findContainingTriangle.py file determines the triangle containing a specified point on the mesh.

• find_containing_triangle(c, triangles, vertices): Finds the triangle that contains the given point.

```
Input:
c (np.ndarray): Closest point (3,).
triangles (np.ndarray): Array of triangles.
vertices (np.ndarray): Vertex coordinates.
Output:
triangle (np.ndarray): Indices of the vertices of the containing triangle.
```

buildKDTree.py

The **buildKDTree.py** file is responsible for building a KD-tree structure for 3D mesh data using **build_kd_tree()**.

```
build_kd_tree():Inputs:
```

- * vertices (list of Vertex): A list of Vertex objects.
- * triangles (list of Triangle): A list of Triangle objects.

- Outputs:

- * **KDTree:** A KD-tree built from the centroids of the triangles. Each centroid represents the average position of a triangle's vertices.
- * triangle_data (list of tuple): A list where each entry is a tuple containing three Vertex objects, corresponding to the vertices of each triangle.

buildOctree.py

The buildOctree.py file is responsible for constructing an octree structure from 3D mesh data.

- OctreeNode Class: Represents a node in the octree, which divides 3D space into 8 components.
 - Attributes:
 - * center (np.array): Center point of the cube.
 - * size (float): Length of the side of the cube.
 - * children (list): A list of child OctreeNode objects representing subdivided regions.
 - * triangles (list): A list of Triangle objects contained within this node.

- Methods:

- * is_leaf(): Returns True if the node has no children.
- * **subdivide():** Divides the node into 8 smaller sub-nodes, each representing an octant of the original cube.
- * insert(triangle, vertices): Inserts a triangle into the node. If the node exceeds a threshold of 5 triangles, it subdivides and redistributes the triangles among its children.
- * _insert_in_children(triangle, vertices): Attempts to insert a triangle into one of the child nodes.
- * contains_triangle(triangle, vertices): Checks if a triangle is fully contained within a node.
- find_octree_root_center_and_size(vertices):
 - Inputs:
 - * vertices (list of Vertex): A list of Vertex objects representing the mesh's vertices in 3D space.
 - Outputs:
 - * center (np.array): The computed center point of the octree root node.
 - * size (float): The length of the side of the root node's cube.
- build_octree(vertices, triangles):
 - Inputs:
 - * vertices (list of Vertex): A list of 3D vertices.
 - * triangles (list of Triangle): A list of triangles.
 - Outputs:
 - * OctreeNode: The root node of the constructed octree.

main.py

The **main.py** file orchestrates overall program execution by coordinating input parsing, transformation calculations, mesh processing, and output generation.

- Parses Input Files:
 - Reads body marker data for Body A and Body B using read_body() from readData.py.
 - Reads sample readings using read_sample() from readData.py.
 - Parses mesh data using parse_mesh_file() from parseMesh.py.
- Calculates Transformations:
 - Calls calculate_frame_transformations() from calculateTransformation.py to compute the frame transformations $F_{A,k}$ and $F_{B,k}$ for each frame.
- Generates Output:

- Computes the closest points on the mesh using different search algorithms (Linear, KDTree, or Octree).
- Writes the transformed tip positions and closest points to an output file.
- For Problem 3: Calls generate_output() from generateOutput.py.
- For Problem 4: Calls generate_output_PA4() from generateOutputPA4.py.

• Outputs Results:

 Outputs are written to the specified directory (./OUTPUT) with filenames indicating the problem number, dataset type, and search method.

• Inputs:

- problem_number (int): Specifies the problem number (3 or 4).
- debug_file_letter (str): Specifies the test case ('A', 'B', etc.).
- isKnown (bool): Indicates whether the dataset is known or unknown.
- search_type (str): Specifies the search algorithm (Linear, KDTree, or Octree).

• Outputs:

Output File: Writes results to a file named PA{problem_number}-{debug_file_letter}-OurOutput-{search in the ./OUTPUT directory.

findClosestPoint.py

The findClosestPoint.py file computes the closest point on a triangle to a given point via the closest_point_on_triangle() method:

• Inputs:

- a (tuple): Coordinates of the query point (x, y, z).
- p, q, r (tuple): Coordinates of the triangle vertices (x, y, z).

• Outputs:

 Closest Point (numpy.ndarray): The closest point on the triangle or its edges to the query point.

findPointOnMesh.py

The **findPointOnMesh.py** file finds the closest point on a mesh via linear search in the **closest_point_on_mesh()** function.

- Loops through all triangles: Iterates through each triangle in the mesh.
- Computes closest point on each triangle: For each triangle, calculates the closest point to the given point by calling closest_point_on_triangle() with the triangle's vertex coordinates.
- Tracks the closest point: Compares distances from the point to the closest points on all triangles and updates.

Inputs:

- point (array-like): The point as (x, y, z).
- vertices (list of Vertex): A list of vertices in the mesh.
- triangles (list of Triangle): A list of triangles.

Outputs:

• Closest Point (numpy.ndarray): The 3D coordinates of the closest point on the mesh to the given point.

findPointOnMeshKDTree.py

The findPointOnMeshKDTree.py file uses the KD-tree for faster nearest-point searches via closest_point_on_mesh_kd():

- Finds nearest centroids: Utilizes the KD-tree to quickly find the closest triangle centroids to the given point.
- Computes closest points: For each triangle corresponding to the nearest centroids, calculates the closest point on the triangle using closest_point_on_triangle().
- Selects the closest point: Compares the distances from the point to all candidate points and selects the closest one.

Inputs:

- point (array-like): The point as (x, y, z).
- centroid_tree (KDTree): A KD-tree built from the centroids of the triangles in the mesh.
- triangle_data (list of tuple): A list where each entry contains three vertices corresponding to the vertices of a triangle.

Outputs:

• Closest Point (numpy.ndarray): The 3D coordinates of the closest point.

findPointOnMeshOctree.py

The findPointOnMeshOctree.py file uses an octree structure for faster spatial searches.

- Traverses the octree: Begins at the root of the octree and iteratively checks all relevant nodes.
- Handles leaf nodes: For each triangle in a leaf node, calculates the closest point on the triangle using closest_point_on_triangle().
- Tracks the closest point: Maintains the minimum distance and updates the closest point if a better candidate is found.
- Processes child nodes: If the node is not a leaf, recursively checks its children to continue the search.

Inputs:

- point (tuple): The point as (x, y, z).
- root (OctreeNode): The root of the octree containing the mesh triangles.
- vertices (list of Vertex): A list of vertices, where each vertex provides its 3D coordinates.

Outputs:

• Closest Point (tuple): The 3D coordinates of the closest point on the mesh.

generateOutput.py

The **generateOutput.py** file writes the computed results to an output file.

- Handles search structures: Builds the KDTree or Octree search structure if the corresponding search type is specified.
- Calculates transformed tip position: For each frame, computes the transformed tip position d.
- Finds closest points: Determines the closest point c on the mesh to d using closest_point_on_mesh() for Linear search, closest_point_on_mesh_kd() for KDTree, or closest_point_on_mesh_octree() for Octree.

- Writes output: Records d, c, and the magnitude of their difference $|d_k c_k|$ to the output file.
- Computes timing metrics: Measures and prints the average build and search times for the specified search method.

Inputs:

- output_dir (str): Directory path where the output file will be saved.
- filename (str): Name of the output file.
- \bullet search_type (str): Search method to use ("Linear", "KDTree", or "Octree").
- frames (list): List of transformation matrices $F_{A,k}$ and $F_{B,k}$ for each frame.
- Atip (numpy.ndarray): Initial tip position in local coordinates.
- vertices (list of Vertex): List of vertices representing the mesh.
- triangles (list of Triangle): List of triangles in the mesh.

Outputs:

- Output File: Contains d (transformed tip position), c (closest point on the mesh), and $|d_k c_k|$ (magnitude of their difference) for each frame.
- Timing Metrics: Average build and search times for the specified search method.

generateOutputPA4.py

The **generateOutputPA4.py** file writes the computed results to an output file. It iteratively refines a transformation F_{reg} using the ICP algorithm and calculates the transformed tip position s_k and its closest point c_k on a mesh:

- Initial tip positions: Computes initial d_k positions for each frame using the frame transformation matrices and the initial tip position A_{tip} .
- Builds search structures: Constructs KDTree or Octree structures for faster nearest-point searches if the corresponding search type is specified.
- Iterative refinement: Applies ICP to refine F_{reg} , transforming d_k into s_k and computing their closest points c_k on the mesh.
- Output results: Writes s_k , c_k , and $|s_k c_k|$ to the output file, along with timing metrics.

Inputs:

- output_dir (str): Directory path where the output file will be saved.
- filename (str): Name of the output file.
- search_type (str): Search method to use ("Linear", "KDTree", or "Octree").
- frames (list): List of transformation matrices $F_{A,k}$ and $F_{B,k}$ for each frame.
- Atip (numpy.ndarray): Initial tip position in local coordinates.
- vertices (list of Vertex): List of vertices representing the mesh.
- triangles (list of Triangle): List of triangles in the mesh.
- max_iterations (int, optional): Maximum number of ICP iterations. Defaults to 10.
- tol (float, optional): Convergence tolerance for the Frobenius norm of F_{reg} updates. Defaults to 1×10^{-5} .

Outputs:

- Output File: Contains s_k (transformed tip position), c_k (closest point on the mesh), and $|s_k c_k|$ (magnitude of their difference) for each frame.
- Timing Metrics: Average build and search times for the specified search method.

generateOutputPA5.py

The **generateOutputPA5.py** file performs deformable registration with iterative updates to rigid transformations and mode weights.

• generate_output_PA5(output_dir, filename, search_type, frames, Atip, vertices, triangles, modes, max_iterations, tol): Executes deformable registration and writes results to an output file.

- Input:

- * output_dir (str): Directory to save the output file.
- * filename (str): Output file name.
- * search_type (str): Search method (Linear or KDTree).
- * frames (list): Rigid transformations for sampled points.
- * Atip (np.ndarray): Pointer tip coordinates (3,).
- * vertices (np.ndarray): Mean shape vertices (Mode 0).
- * triangles (np.ndarray): Array of triangles.
- * modes (list of np.ndarray): Array of mode displacements.
- * max_iterations (int): Maximum number of iterations.
- * tol (float): Convergence tolerance.

- Output:

* None.

computeMean.py

The **computeMean.py** file calculates the mean of the last column from the output files via the **calculate_mean_distance**(assignment_number, file_letter, search_type) function.

- Reads data from the output file: Opens the specified file and extracts the last column values, which represent the magnitude of the difference $|s_k c_k|$.
- Calculates the mean: Computes the mean of the last column values if the file contains valid data.
- Handles missing or empty files: Returns None if the file is missing or contains no data, along with an appropriate message.

Inputs:

- assignment_number (int): The assignment number (3,4).
- file_letter (str): The letter identifier for the file ('A', 'B').
- search_type (str): The search type ('Linear', 'KDTree', or 'Octree').

Outputs:

- Mean Value (float or None): The mean of the last column values if successful, or None if the file is missing.
- Console Message: Prints the mean value or an error message if the file is missing.

compareOutput.pv

The **compareOutput.py** file computes the Mean Squared Error between the results from an output file and a corresponding debug output file.

• read_distance_values(filepath): Reads the last column values from the specified file. If the file does not exist, it returns None and prints an error message.

• calculate_mean_squared_error(assignment_number, file_letter, search_type): Calculates the MSE between the last column values of the specified result file and the corresponding debug file. It ensures both files exist and have the same number of rows before computation.

Inputs:

- assignment_number (int): The assignment number (3, 4).
- file_letter (str): The letter identifier for the file ('A', 'B').
- search_type (str): The search type ('Linear', 'KDTree', or 'Octree').

Outputs:

- Mean Squared Error (float or None): MSE value if successful, or None if there is an issue.
- Console Message: Prints the MSE value.

6 Debugging Methods

In our testing approach, we utilized unit tests to verify the correctness of various functions. We generated synthetic data for testing by manually defining vertices and triangles in controlled configurations, including right, equilateral, and axis-aligned triangles. Test points were selected with known closest projections on these triangles, enabling us to calculate expected results manually. Using these baseline expectations, we performed unit tests for individual functions and integration tests across components to ensure accuracy and consistency in finding closest points.

6.1 KD-Tree Construction (testBuildTree.py)

Test Data:

- Vertices: A set of points (e.g., [0, 0, 0], [1, 0, 0], etc.) was used to create a mock scenario for testing.
- **Triangles:** Mock triangles were formed using the indices of these vertices, ensuring a variety of points and edges were included to test the tree's response to different configurations.

How we verified it: We checked that the returned KDTree object was an instance of KDTree and that the number of elements in the triangle_data list matched the number of input triangles. For further verification, the centroid data of the KD-tree was printed, and the triangles were manually inspected to ensure they corresponded to the correct vertices.

6.2 Closest Point on Triangle (testClosestPoint.py)

Test Data:

- **Point inside the triangle:** We picked an interior point (e.g., (0.5, 0.5, 0)) and tested if the function returned this point as the closest point.
- Points outside the triangle: We then tested points outside the triangle, which were closest to specific edges or vertices of the triangle. Each test case involved setting up the point and the expected closest point on the triangle using manual calculations for reference.

How we verified it: For each case, we used the expected closest point (calculated manually) and compared it with the output of the closest_point_on_triangle function using np.allclose to ensure numerical precision. If the computed result deviated from the expected outcome, an error message would indicate the mismatch.

6.3 Optimization Comparison (testOptimization.py)

Test Data:

- **Test point:** A point in 3D space ((1.5, 9.5, 0.5)) was selected to test how the different algorithms handle the query.
- Meshes: A mesh of vertices and triangles was parsed from an input file (Problem3MeshFile.sur) to simulate data.

How we verified it: For each algorithm, we calculated the closest point using the respective method and measured the time taken for each search. The output was verified manually by checking whether the point found by each method was reasonable given the configuration of the mesh. We also ensured that the KD-tree and octree algorithms were significantly faster than the linear search.

6.4 Point Set Registration (testPointSetRegistration.py)

Test Data:

- **Pure translation:** We translated a simple set of points $(\{(0, 0, 0), (0, 0, 1), (0, 1, 0), (1, 0, 0)\})$ by a fixed vector (1, 2, 3).
- Rotation by 45 degrees: We manually calculated the expected rotation matrix and used this to verify that the registration correctly identified the rotation matrix when applied to the point set.
- Combined rotation and translation: A 90-degree rotation around the Z-axis and a translation vector (1, 1, 1).

How we verified it: For the translation test, we manually checked that the translation vector was correctly identified. For rotation, we verified the orthogonality of the rotation matrix and checked that its determinant was close to 1. For the combined rotation and translation test, we manually calculated the expected result and confirmed that both the rotation and translation were correct.

6.5 Barycentric Coordinate Computation (testComputeBarycentric.py)

Test Data:

- Point inside the triangle: A point inside a triangle, [0.25, 0.25, 0.0], was tested to ensure the barycentric coordinates were correctly computed.
- Point on a vertex: A point exactly on a vertex, [0.0, 0.0], was tested to verify that the barycentric coordinates reflected full weight on the vertex.
- Point on an edge: A point on the edge of a triangle, [0.5, 0.5, 0.0], was tested to confirm the barycentric coordinates showed contributions from the edge's vertices only.
- Point outside the triangle: A point outside the triangle, [-0.5, -0.5, 0.0], was tested to ensure at least one barycentric coordinate was negative.

How we verified it: For each test case, the expected barycentric coordinates were computed manually and compared with the function's output using np.allclose to ensure numerical precision. For points outside the triangle, we verified that at least one barycentric coordinate was negative, indicating the point's exclusion from the triangle.

6.6 Triangle Containment (testFindContainingTriangle.py)

Test Data:

- Point inside triangle 0: A point inside the first triangle, [0.25, 0.25, 0.0], was tested to verify that the correct triangle was identified.
- Point inside triangle 1: A point inside the second triangle, [0.75, 0.75, 0.0], was tested to ensure proper triangle identification.

- Point on a shared edge: A point on the shared edge between two triangles, [0.5, 0.5, 0.0], was tested to confirm the return of one of the triangles containing the edge.
- Point outside all triangles: A point outside the mesh, [1.5, 1.5, 0.0], was tested to verify that the function raised an appropriate exception.

How we verified it: For points inside triangles, the function's output was checked against the manually identified containing triangle. For edge points, the function was verified to return one of the two triangles sharing the edge. For points outside the mesh, we confirmed that the function raised a ValueError.

7 Results

Program File	1 Iteration (Mean Error)	3 Iterations (Mean Error)	9 Iterations (Mean Error)
PA5-A	2.1857	0.7494	0.2069
PA5-B	2.6963	1.3445	0.2522
PA5-C	1.4033	0.6992	0.1172
PA5-D	3.0018	1.3861	0.3083
PA5-E	3.2020	1.5858	0.4991
PA5-F	2.7997	1.2083	0.2422
PA5-G	3.0808	1.2254	0.2690
PA5-H	2.5943	1.0220	0.2025
PA5-J	2.0695	1.0801	0.2530

Table 1: Mean Error $(|s_k - c_k|)$ for 1, 3, and 9 Iterations Using Linear Search

Program File	1 Iteration (Sec)	3 Iterations (Sec)	9 Iterations (Sec)
PA5-A	15.681631	47.620175	146.030969
PA5-B	15.452038	47.775990	144.270322
PA5-C	15.529976	47.156470	145.189145
PA5-D	15.900215	46.718556	142.923090
PA5-E	41.151457	125.557943	378.545361
PA5-F	42.945079	125.157587	386.399761
PA5-G	16.168253	47.780417	152.823812
PA5-H	41.247603	126.595372	426.836293
PA5-J	42.020385	128.140480	385.877159

Table 2: Total Time for 1, 3, and 9 Iterations Using Linear Search

Program File	1 Iteration (MSE)	3 Iterations (MSE)	9 Iterations (MSE)
PA5-A	6.445199	0.851422	0.080164
PA5-B	10.231764	2.563318	0.130745
PA5-C	3.267470	0.821596	0.021223
PA5-D	14.379790	3.347131	0.164347
PA5-E	18.607876	4.063636	0.370883
PA5-F	10.859920	2.124181	0.078749

Table 3: Mean Squared Error (MSE) Between Output Files and Debug Files for 1, 3, and 9 Iterations

8 Discussion

8.1 Impact of Iteration Count

The results for 1, 3, and 9 iterations of deformable registration using the linear search method revealed the impact of increasing the number of iterations on accuracy and computational cost, as summarized in Tables 1 and 2.

8.1.1 Known Data (A-F)

The results for known data files (PA5-A to PA5-F) show that the accuracy improves significantly with an increased number of iterations:

- 1 Iteration: Initial results for 1 iteration show relatively large mean errors, ranging from 1.4033 (PA5-C) to 3.2020 (PA5-E). The Mean Squared Error (MSE) against debug outputs ranges from 3.267470 (PA5-C) to 18.607876 (PA5-E), indicating that the algorithm is far from convergence.
- 3 Iterations: Increasing the iterations to 3 significantly improves alignment. The mean errors decrease to a range of 0.6992 (PA5-C) to 1.5858 (PA5-E), with corresponding MSE values between 0.821596 (PA5-C) and 4.063636 (PA5-E). Thus, iteration optimizes the algorithm.
- 9 Iterations: At 9 iterations, the algorithm achieves high accuracy. Mean errors range from 0.1172 (PA5-C) to 0.4991 (PA5-E), and the MSE values drop to as low as 0.021223 (PA5-C).

8.1.2 Unknown Data (G-J)

For unknown data files (PA5-G to PA5-J), the patterns observed for the known data files are consistent:

- 1 Iteration: Mean errors range from 2.0695 (PA5-J) to 3.0808 (PA5-G), reflecting suboptimal alignment due to insufficient iterations.
- 3 Iterations: The errors improve significantly, ranging from 1.0220 (PA5-H) to 1.2254 (PA5-G).
- 9 Iterations: At 9 iterations, mean errors drop to a range of 0.2025 (PA5-H) to 0.2690 (PA5-G).

8.2 Computational Cost

The computational cost increases proportionally with the number of iterations, as shown in Table 2:

- For known data files, the total time for 1 iteration ranges from 15.452 seconds (PA5-B) to 42.945 seconds (PA5-F). At 3 iterations, this increases to 47.156 seconds (PA5-C) to 125.557 seconds (PA5-E). For 9 iterations, the total time ranges from 142.923 seconds (PA5-D) to 386.399 seconds (PA5-F).
- For unknown data files, the total time follows a similar trend, with 1 iteration taking 16.168 seconds (PA5-G) to 42.020 seconds (PA5-J), and 9 iterations taking 152.823 seconds (PA5-G) to 385.877 seconds (PA5-J).

There is a significant trade-off between accuracy and computational efficiency, particularly for larger datasets at high iteration counts.

8.3 Optimizing Linear Search with Bounding Boxes or Spatial Trees

The linear search method used in this implementation is computationally expensive, especially for large datasets. The performance can be significantly improved by leveraging spatial partitioning structures:

- **Bounding Boxes:** Subdividing the mesh into bounding boxes reduces the number of triangles to search for nearest neighbors.
- **KD Trees:** Constructing a KD Tree for the vertices and triangles can optimize the nearest-neighbor search, as previously shown in PA3 and PA4. The hierarchical structure allows logarithmic search complexity.
- Octrees: An Octree divides 3D space into smaller, recursively refined octants. Although this method has not been sufficiently optimized in previous PAs, it may be appropriate in this setting.

9 Who Did What?

9.1 Program

- Ben wrote the following files:
 - readData.py
 - pointSetRegistration.py
 - testPointSetRegistration.py
- Aryavrat did everything else related to the program, including:
 - Implementing the core algorithms
 - Unit testing and optimizing
 - Handling integration of different data structures

9.2 Report

- Aryavrat was responsible for:
 - Debugging the code
 - Generating the results
 - Program Structure Visualization
- Ben did everything else for the report, including:
 - Writing the Mathematical and Algorithmic Approach
 - Writing the Program Structure
 - Writing the Discussion