UNIVERSITÀ DEGLI STUDI FIRENZE

Parallel KMeans

Parallel Programming for Machine Learning

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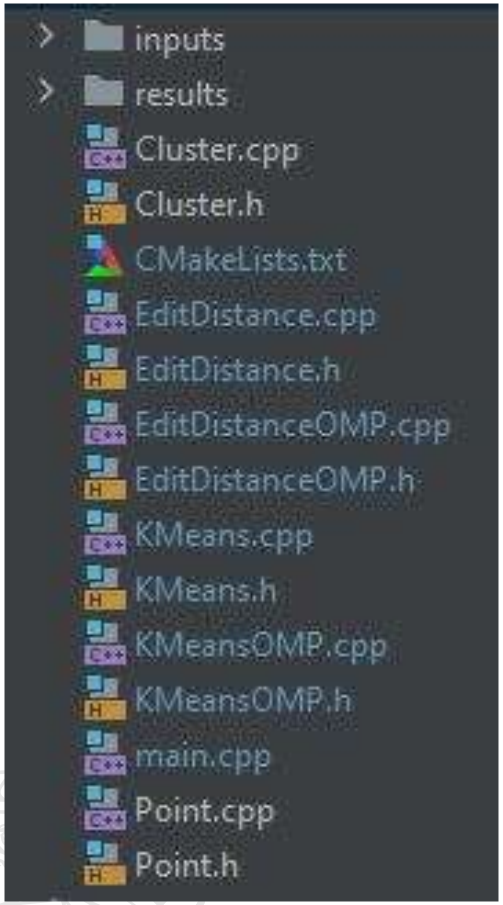
Introduction

The program written for this project implements **K-means**, an unsupervised learning clustering algorithm. Given a dataset of points and a number **K** of clusters, K-means assigns each point to one of the K clusters, minimizing the mean squared error.
The **convergence** of the algorithm is set by a maximum number of iterations, 35, and by the percentage of points that change clusters after each iteration. If this percentage falls below 0.1%, the algorithm terminates.

There are two implementations of K-means: one **sequential** and one **parallel**. The purpose of this work is to observe the speedup obtained with the parallel version compared to the sequential one.

The programming language used is C++ (MinGW compiler, CLion IDE), and parallelization was done with **OpenMP**.
All experiments were conducted on the ssh server "papavero.dinfo.unifi.it".

Code organization



inputs
results
Cluster.cpp
Cluster.h
CMakeLists.txt
EditDistance.cpp
EditDistance.h
EditDistanceOMP.cpp
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KMeans.cpp
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Point.cpp
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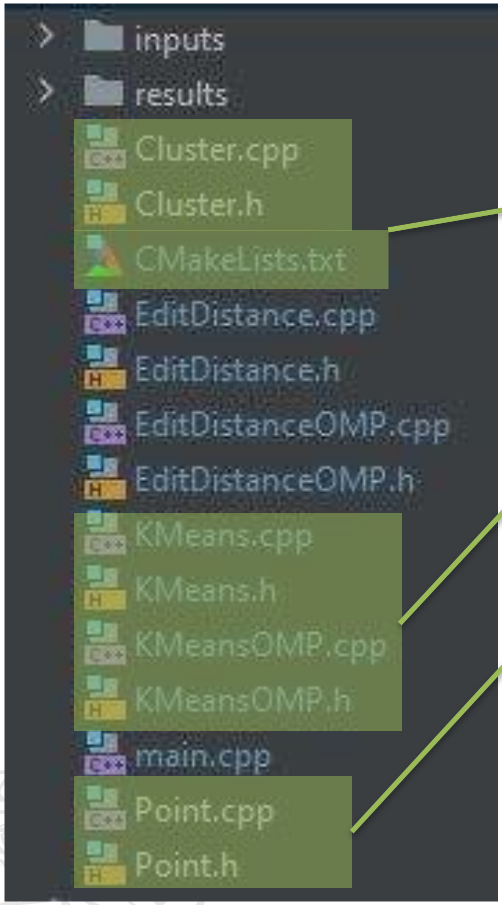
Code organization



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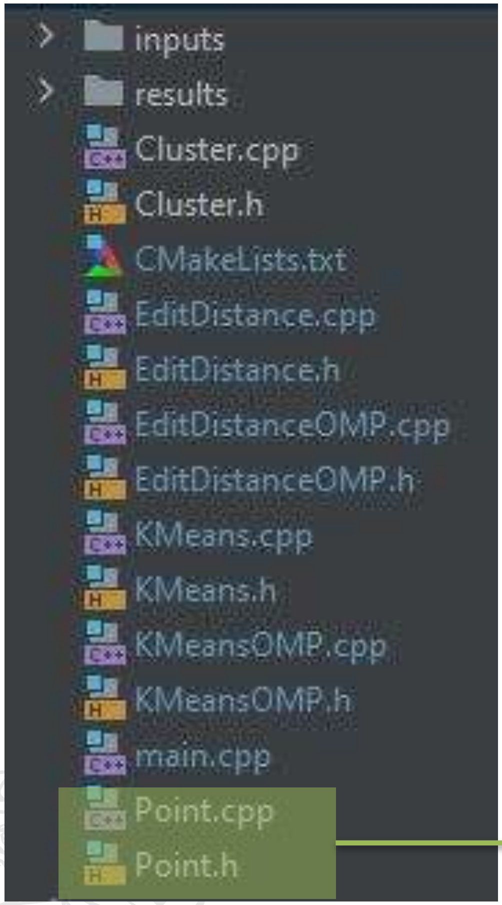
Files included in this project. The remaining ones are related to another project with a common directory.

Code organization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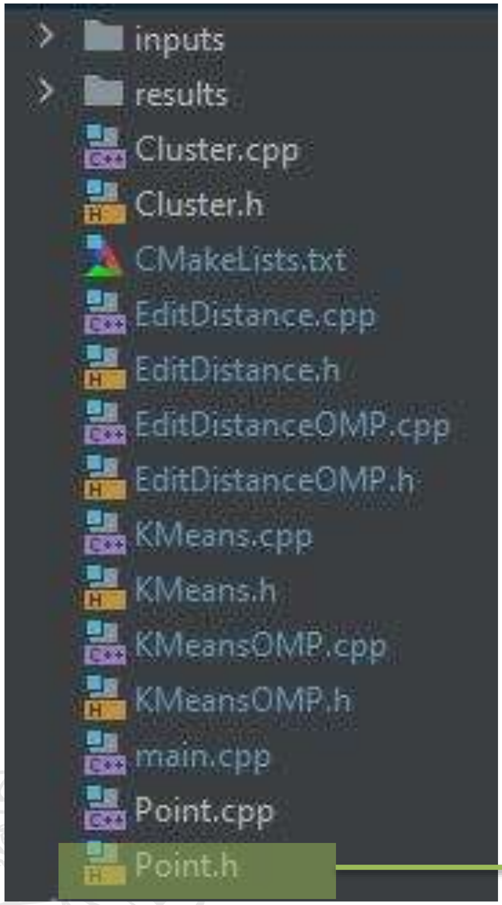
Files related to the definition and declaration of the Point class, which represents the points on which K-means will be executed.

Code organization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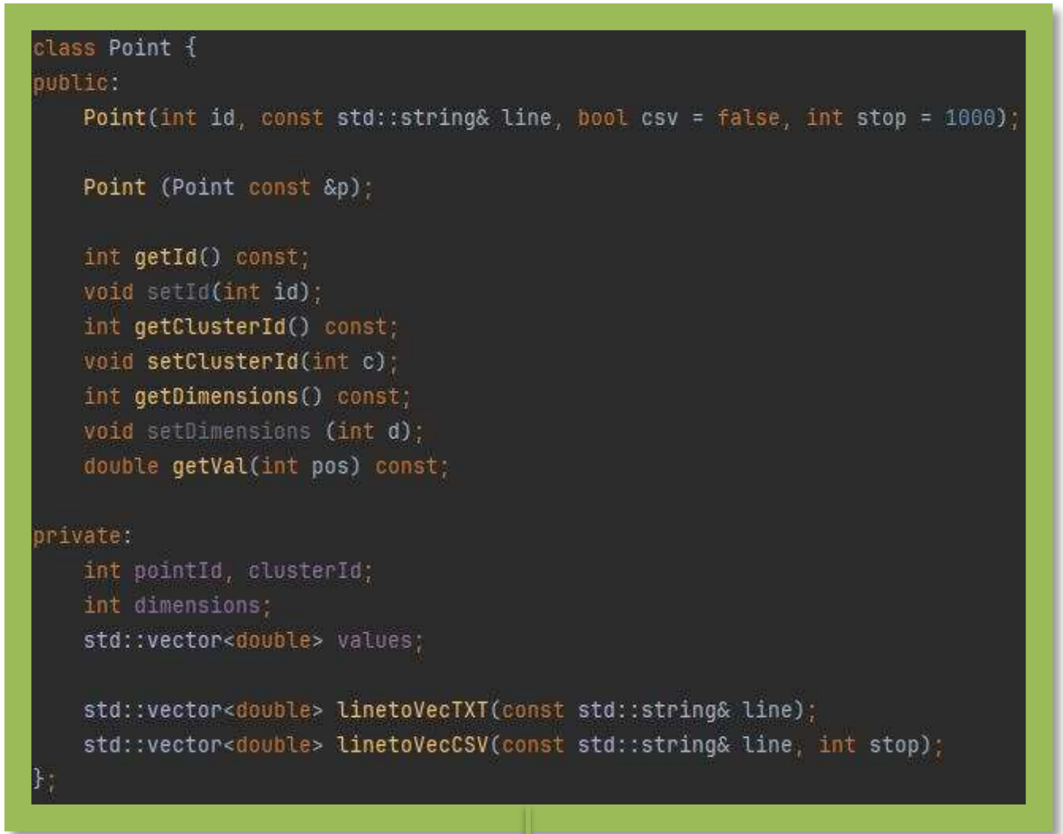
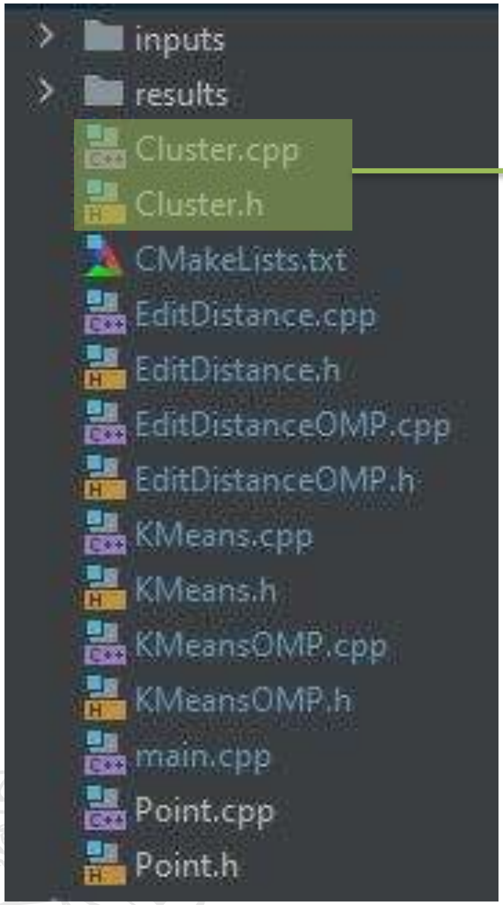

```
class Point {
public:
    Point(int id, const std::string& line, bool csv = false, int stop = 1000);

    Point (Point const &p);

    int getId() const;
    void setId(int id);
    int getClusterId() const;
    void setClusterId(int c);
    int getDimensions() const;
    void setDimensions (int d);
    double getVal(int pos) const;

private:
    int pointId, clusterId;
    int dimensions;
    std::vector<double> values;

    std::vector<double> linetoVecTXT(const std::string& line);
    std::vector<double> linetoVecCSV(const std::string& line, int stop);
};
```

Code organization



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KMeansOMP.h
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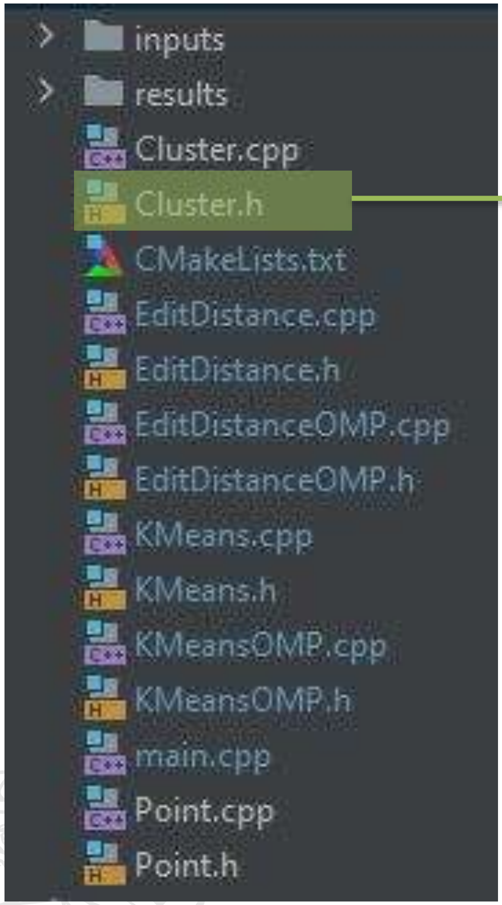
Point.h
```

Files related to the definition and declaration of the Cluster class, which represents the clusters that the points will be grouped into.

Code organization



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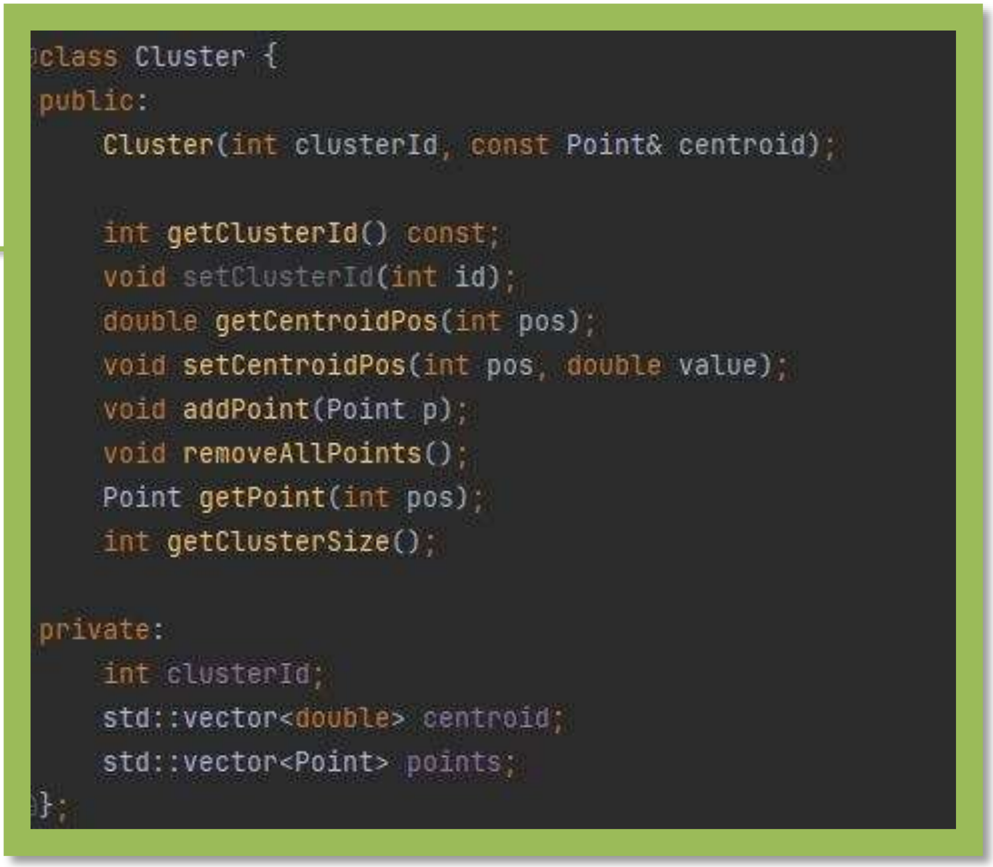
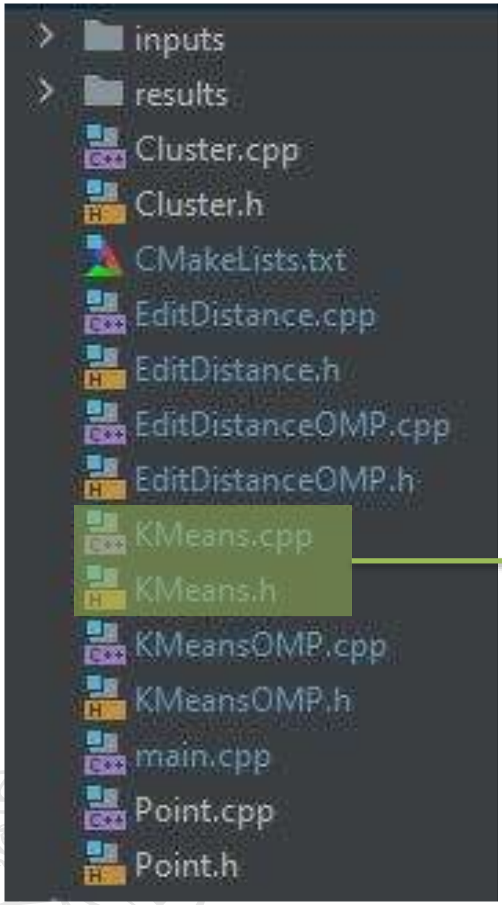


```
class Cluster {
public:
    Cluster(int clusterId, const Point& centroid);

    int getClusterId() const;
    void setClusterId(int id);
    double getCentroidPos(int pos);
    void setCentroidPos(int pos, double value);
    void addPoint(Point p);
    void removeAllPoints();
    Point getPoint(int pos);
    int getClusterSize();

private:
    int clusterId;
    std::vector<double> centroid;
    std::vector<Point> points;
};
```

Code organization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```
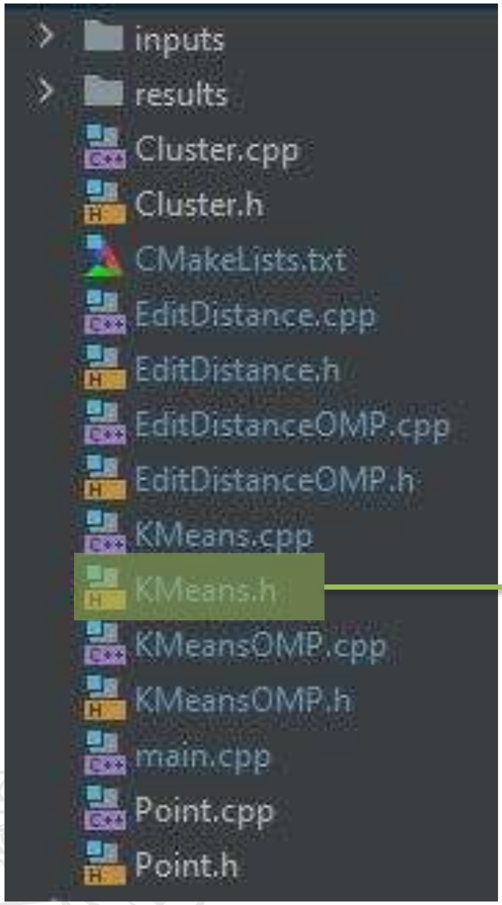

Files related to the definition and declaration of the KMeans class, which encapsulates the parameters and the method to execute the algorithm.

Code organization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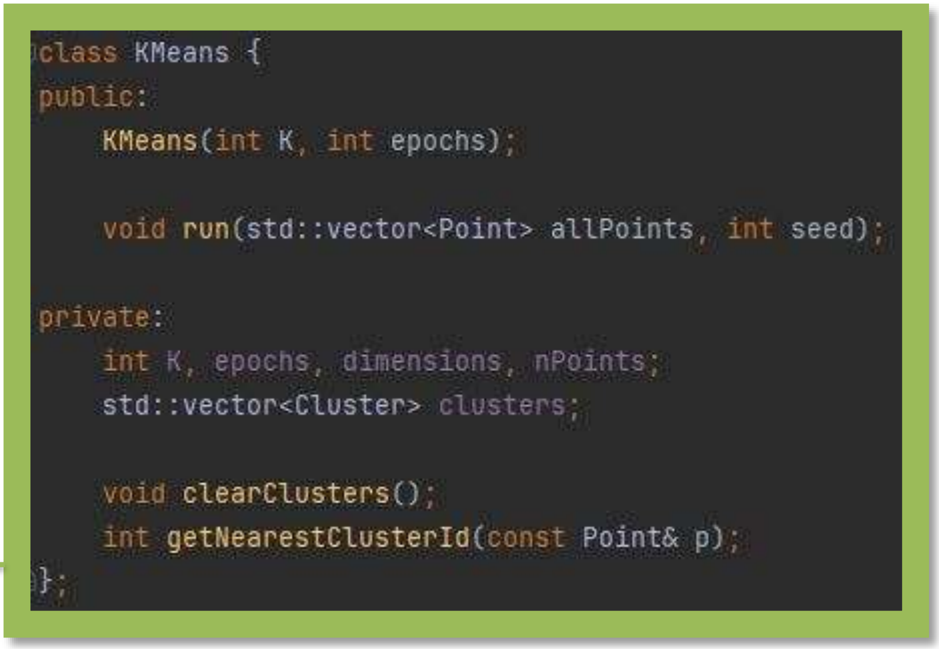
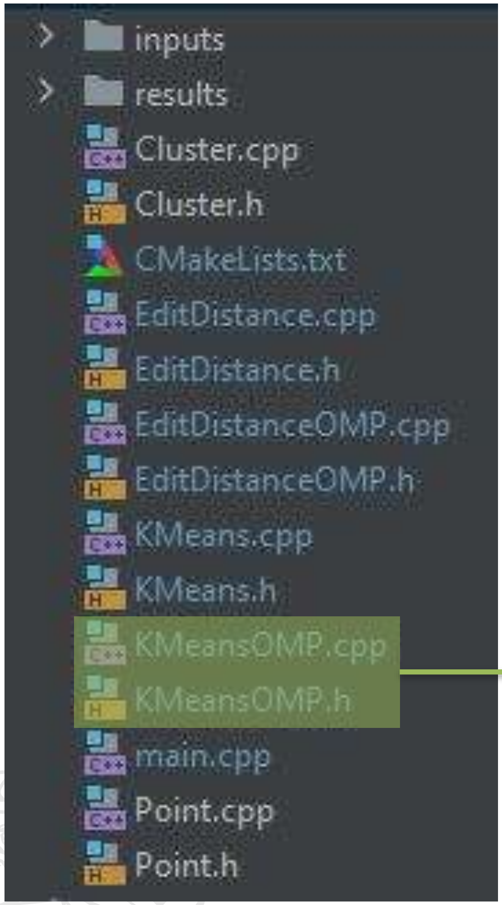

```
class KMeans {
public:
    KMeans(int K, int epochs);

    void run(std::vector<Point> allPoints, int seed);

private:
    int K, epochs, dimensions, nPoints;
    std::vector<Cluster> clusters;

    void clearClusters();
    int getNearestClusterId(const Point& p);
};
```

Code organization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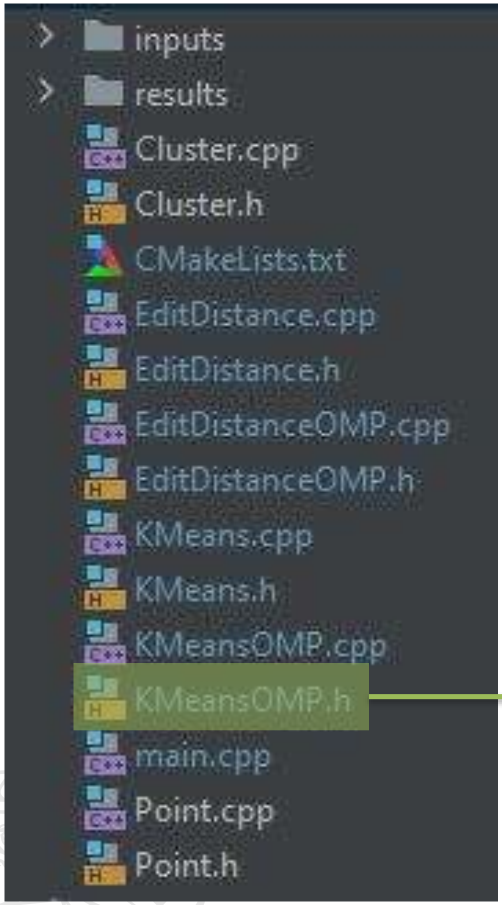
Files related to the definition and declaration of the KMeansOMP class, which encapsulates the parameters and the parallelized method to execute the algorithm.

Code organization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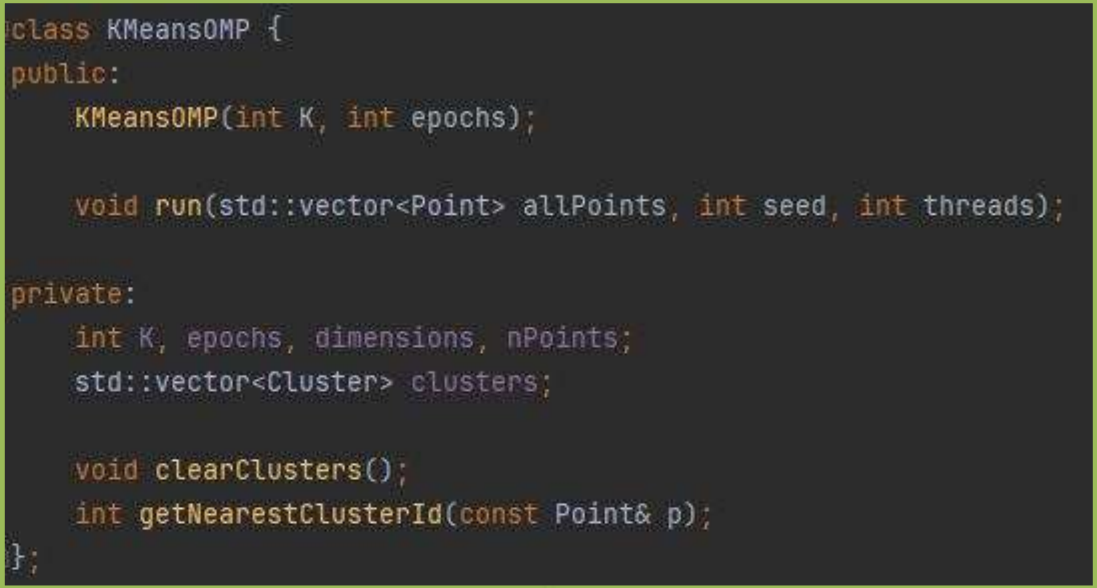
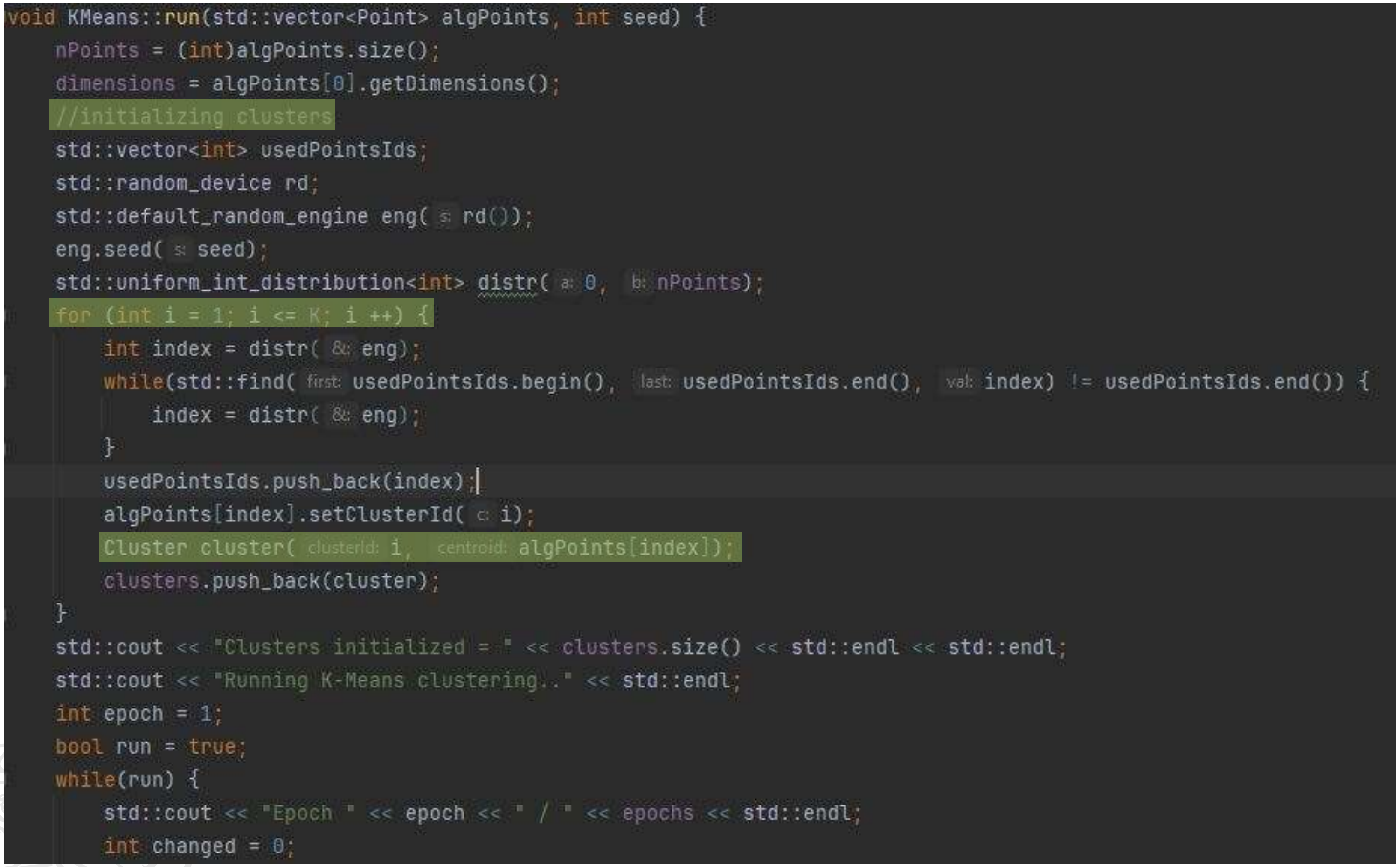
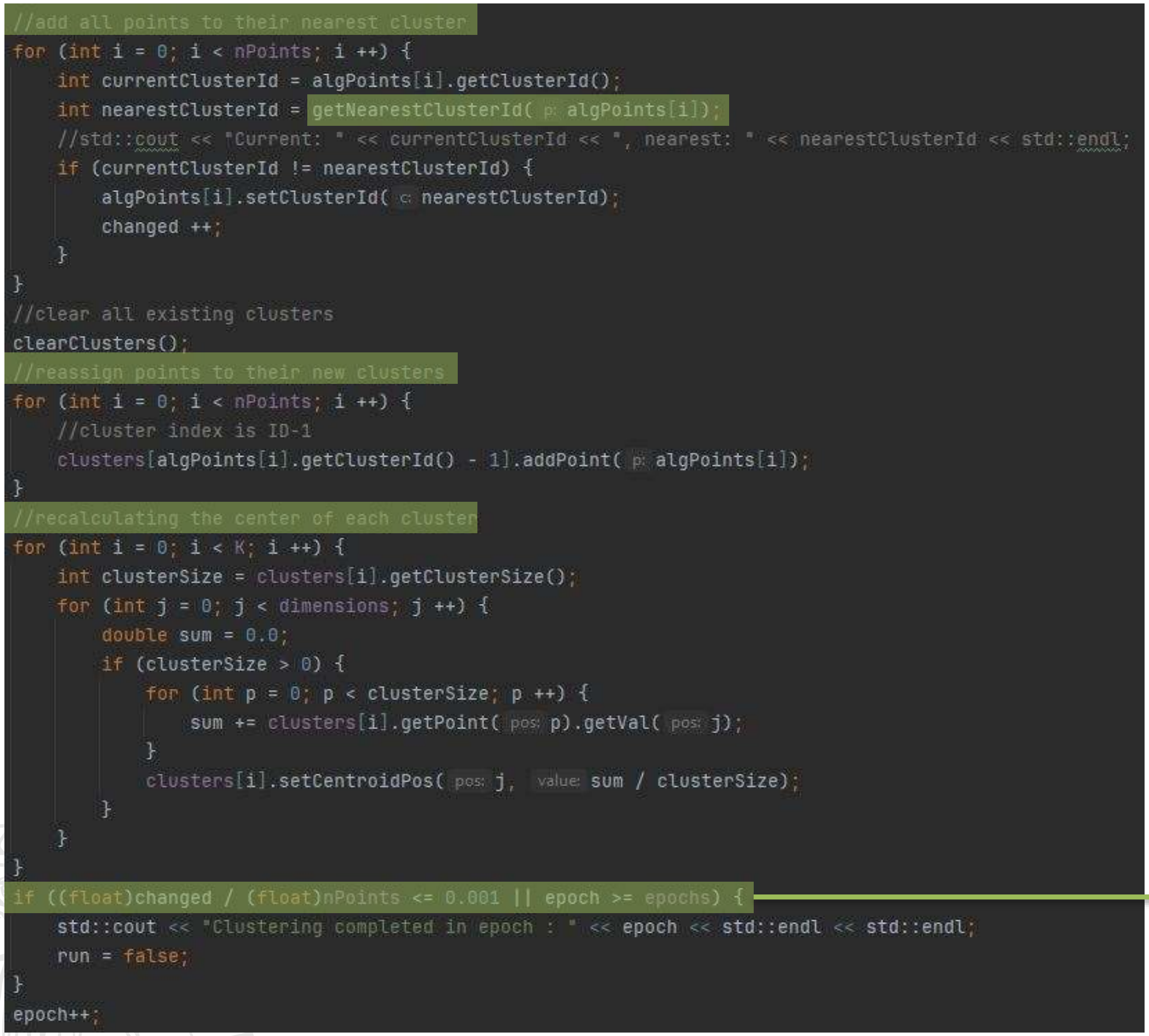

```
class KMeansOMP {
public:
    KMeansOMP(int K, int epochs);

    void run(std::vector<Point> allPoints, int seed, int threads);

private:
    int K, epochs, dimensions, nPoints;
    std::vector<Cluster> clusters;

    void clearClusters();
    int getNearestClusterId(const Point& p);
};
```

Sequential Algorithm



```
void KMeans::run(std::vector<Point> algPoints, int seed) {
    nPoints = (int)algPoints.size();
    dimensions = algPoints[0].getDimensions();
    //initializing clusters
    std::vector<int> usedPointsIds;
    std::random_device rd;
    std::default_random_engine eng( s: rd());
    eng.seed( s: seed);
    std::uniform_int_distribution<int> distr( a: 0,  b: nPoints);
    for (int i = 1; i <= K; i ++) {
        int index = distr( &: eng);
        while(std::find( first: usedPointsIds.begin(),  last: usedPointsIds.end(),  val: index) != usedPointsIds.end()) {
            index = distr( &: eng);
        }
        usedPointsIds.push_back(index);
        algPoints[index].setClusterId( c: i);
        Cluster cluster( clusterId: i,  centroid: algPoints[index]);
        clusters.push_back(cluster);
    }
    std::cout << "Clusters initialized = " << clusters.size() << std::endl << std::endl;
    std::cout << "Running K-Means clustering.." << std::endl;
    int epoch = 1;
    bool run = true;
    while(run) {
        std::cout << "Epoch " << epoch << " / " << epochs << std::endl;
        int changed = 0;
```

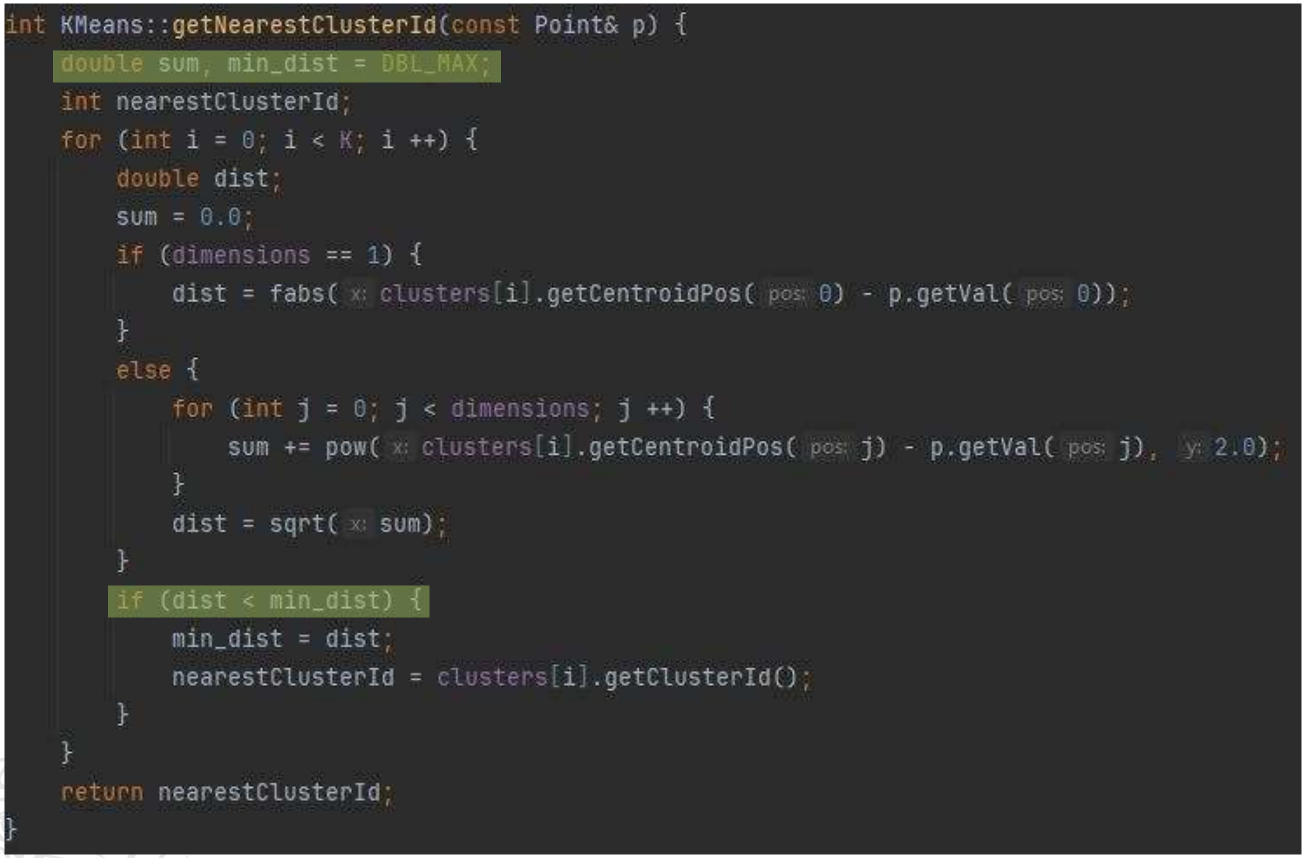
Sequential Algorithm



```
//add all points to their nearest cluster
for (int i = 0; i < nPoints; i ++) {
    int currentClusterId = algPoints[i].getClusterId();
    int nearestClusterId = getNearestClusterId( p: algPoints[i]);
    //std::cout << "Current: " << currentClusterId << ", nearest: " << nearestClusterId << std::endl;
    if (currentClusterId != nearestClusterId) {
        algPoints[i].setClusterId( c: nearestClusterId);
        changed ++;
    }
}
//clear all existing clusters
clearClusters();
//reassign points to their new clusters
for (int i = 0; i < nPoints; i ++) {
    //cluster index is ID-1
    clusters[algPoints[i].getClusterId() - 1].addPoint( p: algPoints[i]);
}
//recalculating the center of each cluster
for (int i = 0; i < K; i ++) {
    int clusterSize = clusters[i].getClusterSize();
    for (int j = 0; j < dimensions; j ++) {
        double sum = 0.0;
        if (clusterSize > 0) {
            for (int p = 0; p < clusterSize; p ++) {
                sum += clusters[i].getPoint( pos: p).getVal( pos: j);
            }
            clusters[i].setCentroidPos( pos: j,  value: sum / clusterSize);
        }
    }
}
if ((float)changed / (float)nPoints <= 0.001 || epoch >= epochs) {
    std::cout << "Clustering completed in epoch : " << epoch << std::endl << std::endl;
    run = false;
}
epoch++;
```

Termination of the algorithm

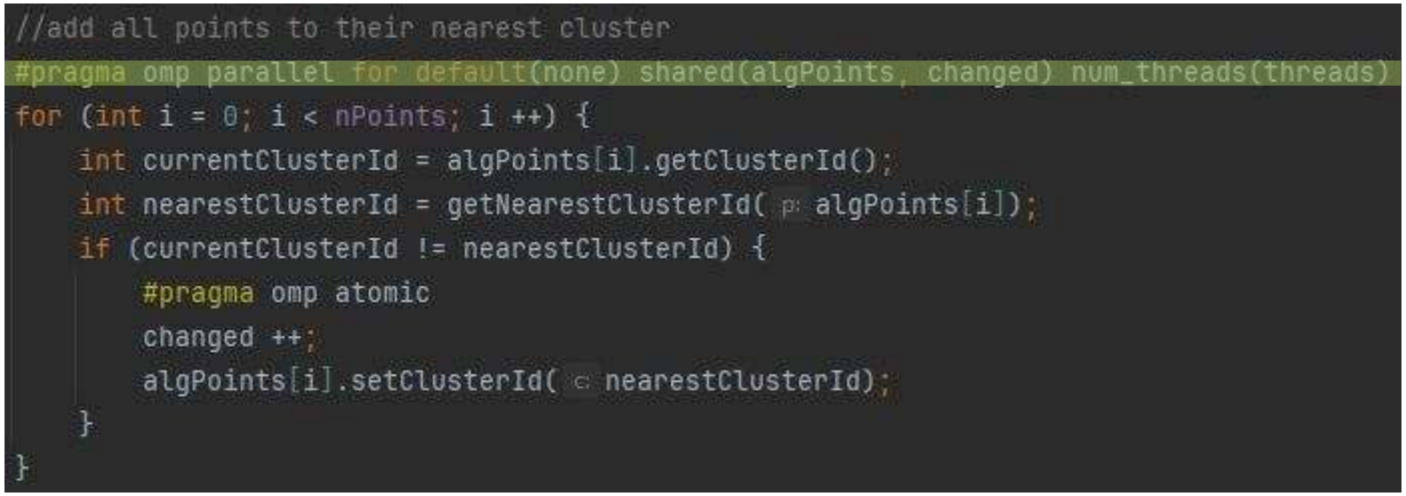
Function getNearestClusterId()



```cpp
int KMeans::getNearestClusterId(const Point& p) {
    double sum, min_dist = DBL_MAX;
    int nearestClusterId;
    for (int i = 0; i < K; i ++) {
        double dist;
        sum = 0.0;
        if (dimensions == 1) {
            dist = fabs( x: clusters[i].getCentroidPos( pos: 0) - p.getVal( pos: 0));
        }
        else {
            for (int j = 0; j < dimensions; j ++) {
                sum += pow( x: clusters[i].getCentroidPos( pos: j) - p.getVal( pos: j),  y: 2.0);
            }
            dist = sqrt( x: sum);
        }
        if (dist < min_dist) {
            min_dist = dist;
            nearestClusterId = clusters[i].getClusterId();
        }
    }
    return nearestClusterId;
}
```

Parallel Algorithm

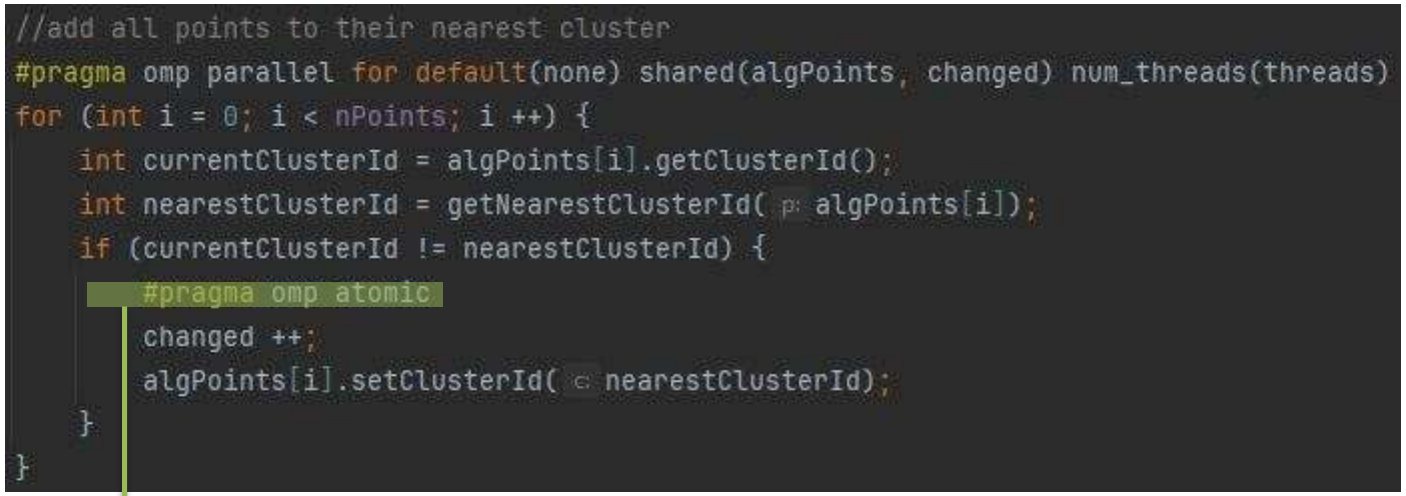
Parallelization of assigning points to the nearest clusters



```
//add all points to their nearest cluster
#pragma omp parallel for default(none) shared(algPoints, changed) num_threads(threads)
for (int i = 0; i < nPoints; i ++) {
    int currentClusterId = algPoints[i].getClusterId();
    int nearestClusterId = getNearestClusterId( p: algPoints[i]);
    if (currentClusterId != nearestClusterId) {
        #pragma omp atomic
        changed ++;
        algPoints[i].setClusterId( c: nearestClusterId);
    }
}
```

Parallel Algorithm

Parallelization of assigning points to the nearest clusters

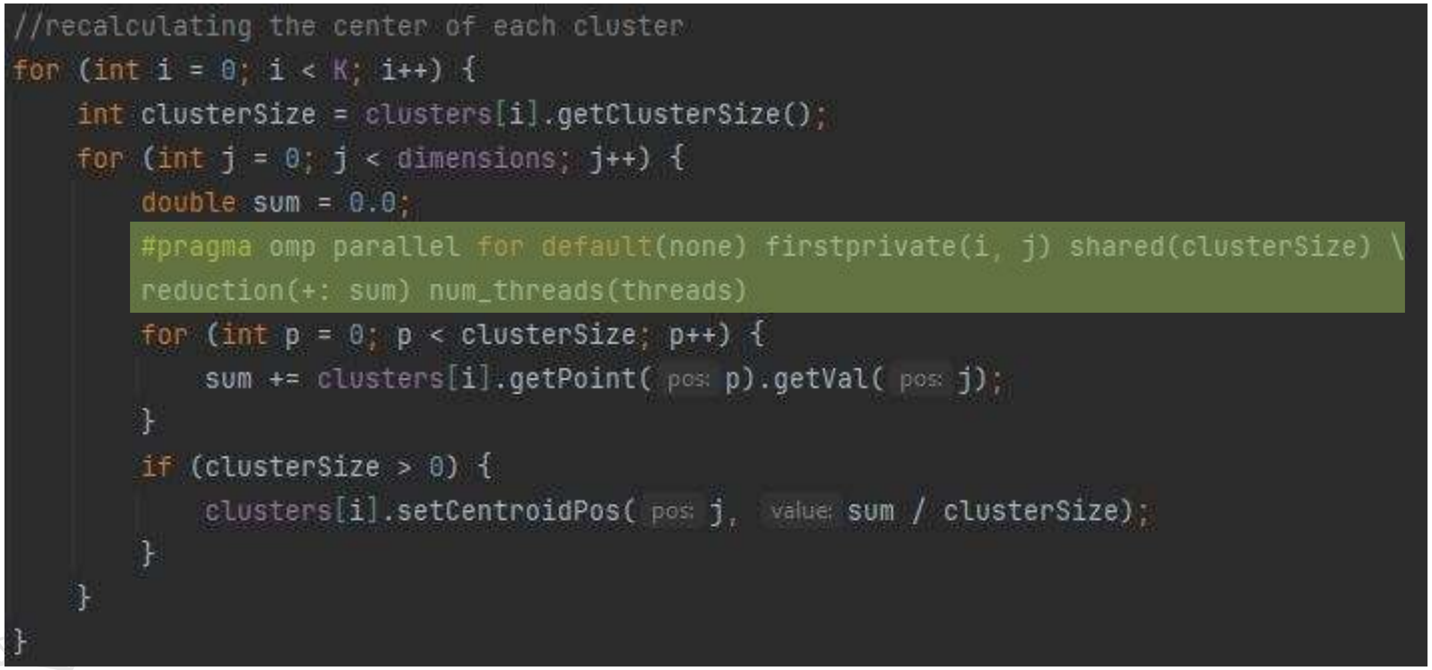


```
//add all points to their nearest cluster
#pragma omp parallel for default(none) shared(algPoints, changed) num_threads(threads)
for (int i = 0; i < nPoints; i ++) {
    int currentClusterId = algPoints[i].getClusterId();
    int nearestClusterId = getNearestClusterId( p: algPoints[i]);
    if (currentClusterId != nearestClusterId) {
        #pragma omp atomic
        changed ++;
        algPoints[i].setClusterId( c: nearestClusterId);
    }
}
```

Increment management of the shared variable changed.

Parallel Algorithm

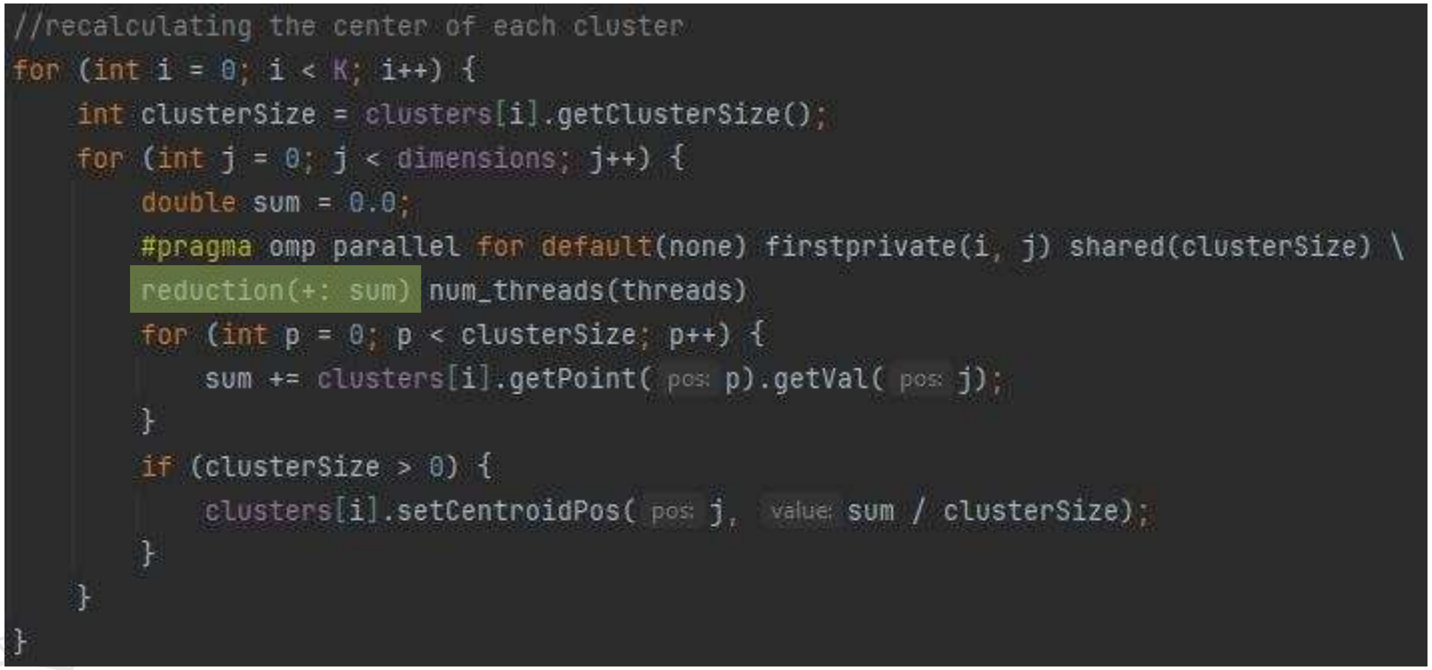
Parallelized computation of the coordinates of the new centroids



```
//recalculating the center of each cluster
for (int i = 0; i < K; i++) {
    int clusterSize = clusters[i].getClusterSize();
    for (int j = 0; j < dimensions; j++) {
        double sum = 0.0;
        #pragma omp parallel for default(none) firstprivate(i, j) shared(clusterSize) \
        reduction(+: sum) num_threads(threads)
        for (int p = 0; p < clusterSize; p++) {
            sum += clusters[i].getPoint( pos: p).getVal( pos: j);
        }
        if (clusterSize > 0) {
            clusters[i].setCentroidPos( pos: j,  value: sum / clusterSize);
        }
    }
}
```

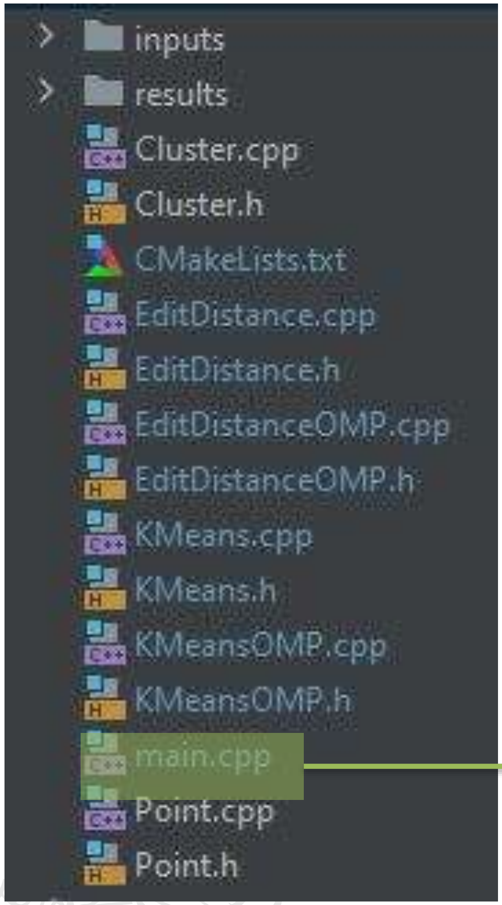
Parallel Algorithm

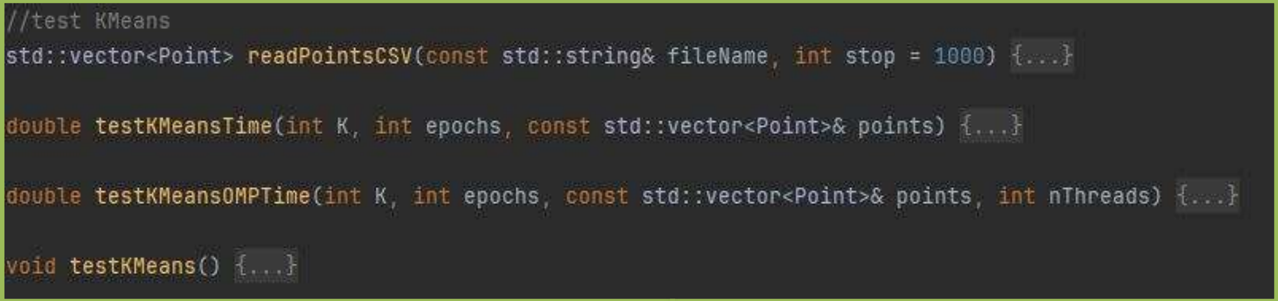
Parallelized computation of the coordinates of the new centroids



```
//recalculating the center of each cluster
for (int i = 0; i < K; i++) {
    int clusterSize = clusters[i].getClusterSize();
    for (int j = 0; j < dimensions; j++) {
        double sum = 0.0;
        #pragma omp parallel for default(none) firstprivate(i, j) shared(clusterSize) \
        reduction(+: sum) num_threads(threads)
        for (int p = 0; p < clusterSize; p++) {
            sum += clusters[i].getPoint( pos: p).getVal( pos: j);
        }
        if (clusterSize > 0) {
            clusters[i].setCentroidPos( pos: j,  value: sum / clusterSize);
        }
    }
}
```

Test





```
//test KMeans
std::vector<Point> readPointsCSV(const std::string& fileName, int stop = 1000) {...}

double testKMeansTime(int K, int epochs, const std::vector<Point>& points) {...}

double testKMeansOMPTime(int K, int epochs, const std::vector<Point>& points, int nThreads) {...}

void testKMeans() {...}
```

Tests are located in the file main.cpp.

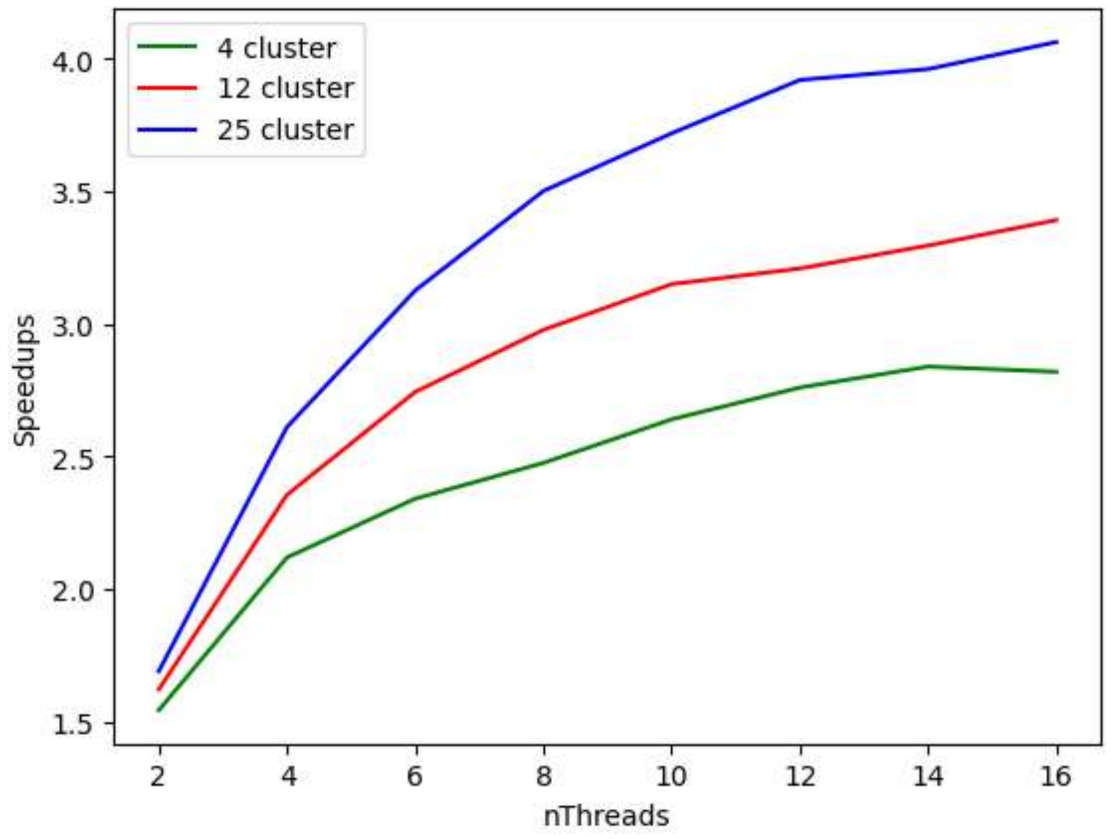
Test 1

Minimum number of points to prefer parallel execution.

	3000 points 2D	19000 points 8D
4 threads, K = 3-5	0.946291	2.23869
8 threads, K = 3-5	0.948598	3.27011
4 threads, K = 6-8	0.989534	2.64693
8 threads, K = 6-8	0.964235	3.29542

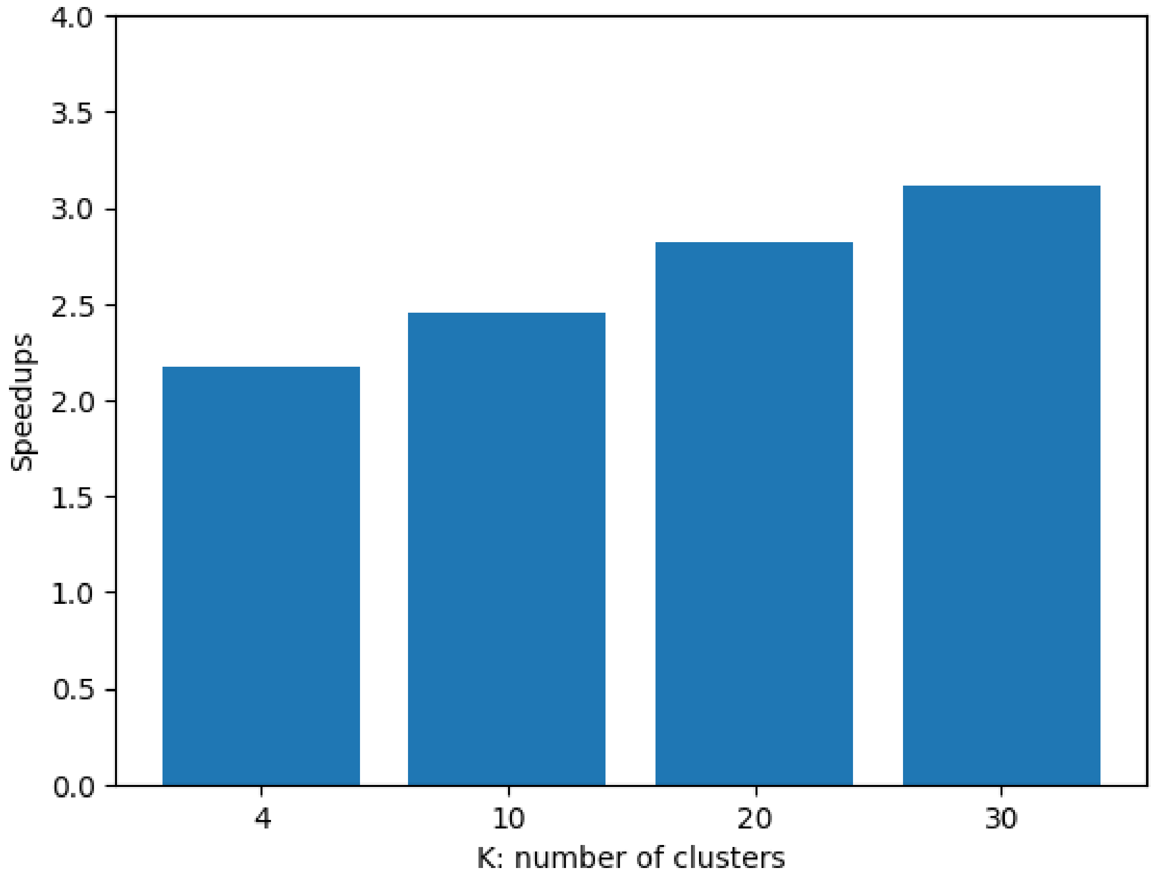
Test 2

Varying the number of threads and the value of K, with 500,000 points in 5D



Test 3

Varying the value of K, on 4 million points in 3D and with 8 threads



Test 4

Considerations about the number of points to run KMeans on

	Speedup con 8 threads
3000 punti 2D, K = 3	0.948598
19000 punti 8D, K = 5	3.27011
500000 punti 5D, K = 4	2.47619
4mln di punti 3D, K = 4	2.17211