Parallel and Multicore Computing Project 2

Shuang Li 1044137

Introduction

This report outlines and analyses an implementation of a message passing parallel algorithm for k-means++ clustering and the n-body simulation.

The algorithm is implemented with Open MPI where a number of nodes collaborate and passes messages to each other to carry out the task required.

The task is described as follows (n denotes the total number of points and m denotes the total number of nodes):

1. n points are sampled by all m nodes from a Gaussian mixture model (GMM).

2. All nodes collaborate to cluster the points into m clusters using k-means++.

3. Each cluster is moved into one single node so that a single node contains all points of a cluster.

4. The nodes collaborate with each other to perform n-body simulation where each point represents a body with a mass of 1 and bodies are attracted to each other via gravity.

The implementation for sampling all n points and clustering them with k-means++ are all rather naive and straightforward. The interesting part is the n-body gravity simulation.

To reduce the simulation time, the Barnes-Hut simulation approximation algorithm is used so that points over a certain distance away are simplified into a single center of mass when calculating the force they exert on another point. To reduce the communication overhead, each node constructs a Barnes-Hut tree and then prune the tree for each other nodes so that the tree only contains the nodes that are actually needed for the calculation of points in each other node. This pruned tree will from now on be referred to as the partial tree.

For node A to construct a partial tree to be sent to node B, we would like to make sure that any node of the tree where $s/d < \theta$ is kept, where s is the width of the region the node of the tree represent, d is the distance between the center of mass of the node and the closest point in cluster B to the center of mass to the node, and θ is a predefined constant. However, we do not want to calculate the closest points in cluster B to every node in the Barnes-Hut tree for cluster A and that would be slow in both computation time and communication overhead. Hence, we instead take the closest point in cluster B with respect to the center of mass of all points in cluster A, and calculate a hyperplane that is perpendicular to the line through the center of mass and the closest point, that goes through the closest point. Assuming that all points in each cluster are closer to their center of mass than any points in other clusters, the distance from any point within cluster A to this hyperplane should be shorter than the distance from point within cluster A to any point within cluster B.

The pseudocode describing the algorithm is shown in Algorithm 1, with the function that it calls shown in Algorithm 2 to 7. Note that the pseudocode is written in the perspective on one computing node.

While in theory, this algorithm should be faster than naively parallelizing Barnes-Hut algorithm by transferring all points to a root cluster and calculating one single Barnes-Hut tree to be sent to all clusters. In practice, it turns out the algorithm has a number of other overheads.

These overheads include calculating m partial trees (again here m is the total number of computing nodes), encoding them into an array of bytes to be sent over to each node and decoding the bytes into a partial tree, plus the extra computing time of creating m^2 partial trees. Furthermore, because each simulation step relies on the assumption of points of each all points in each cluster are closer to their center of mass than any points in other clusters being true, the clusters have to be recomputed and points that changed clusters sent over the corresponding nodes. This adds additional overheads that,

Algorithm 1

1: $\theta \leftarrow 0.1$
2: $DeltaTime \leftarrow 0.01$
3: $m \leftarrow$ number of compute nodes.
4: $NodeIndex \leftarrow$ the index for the compute node.   ▷ This is equivalent to MPI_Comm_rank but 1 indexed.
5: $N \leftarrow$ number of points
6: $D \leftarrow$ number of dimensions
7: $c \leftarrow$ number of GMM components
8: **for** $i \leftarrow 1$ **to** c **do**
9:     $prob[i] \leftarrow$ the probability of the ith GMM component
10:     $gmmc[i] \leftarrow$ the ith GMM component
11: **end for**
12: **for** $i \leftarrow 1$ **to** N/m **do**
13:     $points[i] \leftarrow$ SAMPLE($gmmc[$SAMPLEWEIGHTEDDISCRETEDISTRIBUTION($prob$)])
14:     ▷ SAMPLEWEIGHTEDDISCRETEDISTRIBUTION($weights$) generate a random number between 1 and the length of $weights$ with the number i having a probability of $weights[i]/$SUM($weights$)
15: **end for**
16: $centroids[1] \leftarrow$ CHOOSERANDOMONE($points$)   ▷ choose centroid for k-means++
17: **for** $i \leftarrow 2$ **to** m **do**   ▷ choose m centroids for m clusters
18:     **for** $j \leftarrow 1$ **to** LEN($points$) **do**
19:         $distances[i] \leftarrow$ distance of $points[i]$ to the closest centroid
20:     **end for**
21:     $DistSum \leftarrow$ sum of distances
22:     **if** $NodeIndex = 1$ **then**
23:         **for** $i \leftarrow 1$ **to** m **do**
24:             $AllSum[i] \leftarrow DistSum$ from node i
25:         **end for**
26:         $NextCentroidNode \leftarrow$ SAMPLEWEIGHTEDDISCRETEDISTRIBUTION($AllSum$)
27:     **end if**
28:     $NextCentroidNode \leftarrow NextCentroidNode$ from node 1
29:     **if** $NodeIndex = NextCentroidNode$ **then**
30:         $NextCentroid \leftarrow points[$SAMPLEWEIGHTEDDISCRETEDISTRIBUTION($distances$)$]$
31:     **end if**
32:     $centroids[i] \leftarrow NextCentroid$ from node $NextCentroidNode$
33: **end for**
34: $ClusterIndices \leftarrow$ KMEANS($centroids, points$)
35: $points \leftarrow$ points in $NodeIndex^{th}$ cluster as indicated by $ClusterIndices$ in all nodes   ▷ Significant implementation detail of message passing between nodes omitted.
36: **for** $i \leftarrow 1$ **to** LEN($points$) **do**
37:     $velocities[i] \leftarrow 0$
38: **end for**
39: $InitVariance \leftarrow$ GETVARIANCE($points$)
40: **while** $True$ **do**
41:     SIMULATE($points, velocities$)
42:     $CurrentVariance \leftarrow$ GETVARIANCE($points$)
43:     **if** $Currentvariance < InitVariance/2$ **then**
44:         **break while loop**
45:     **end if**
46:     $ClusterIndices \leftarrow$ KMEANS($centroids, points$)   ▷ one iteration only, implemented separately in real code but reusing pseudocode here.
47:     $points \leftarrow$ points in $NodeIndex^{th}$ cluster as indicated by $ClusterIndices$ in all nodes
48: **end while**

Algorithm 2

1: **function** KMEANS(centroids, points)
2:     **while** centroids changed since last iteration **do**
3:         **for** $i \leftarrow 1$ **to** LEN($points$) **do**
4:             $ClusterIndices[i] \leftarrow$ index of centroid closest to $points$
5:         **end for**
6:         **for** $i \leftarrow 1$ **to** LEN($points$) **do**
7:             $sums[ClusterIndices[i]] \leftarrow sums[ClusterIndices[i]] + points[i]$
8:             $counts[ClusterIndices[i]] \leftarrow counts[ClusterIndices[i]] + 1$
9:         **end for**
10:        **if** NodeIndex == 1 **then**
11:            **for** $i \leftarrow 1$ **to** LEN($centroids$) **do**
12:                $allSums \leftarrow$ sum of $sums[i]$ from all nodes
13:                $allCounts \leftarrow$ sum of $counts[i]$ from all nodes
14:                $centroids[i] \leftarrow allSums/allCounts$ ▷ Here it is actually each dimension of $allSums$ divided by $allCounts$.
15:            **end for**
16:        **end if**
17:        $centroids \leftarrow centroids$ from node 1
18:     **end while**
19:     **return** $ClusterIndices$
20: **end function**

Algorithm 3

1: **function** GETVARIANCE(points) ▷ should really be named: get sum of distance to overall center of mass
2:     $mean \leftarrow$ average of all points
3:     **if** $NodeIndex = 1$ **then**
4:         $sum \leftarrow 0$
5:         $allSize \leftarrow 0$
6:         **for** $i \leftarrow 1$ **to** m **do**
7:             $means[i] \leftarrow mean$ from node i
8:             $sizes[i] \leftarrow$ LEN($points$) from node i
9:             $sum \leftarrow sum + means[i] * sizes[i]$
10:            $allSize \leftarrow allSize + sizes[i]$
11:         **end for**
12:         $allMean \leftarrow sum/allSize$
13:     **end if**
14:     $mean \leftarrow allMean$ from node 1
15:     $variance \leftarrow 0$
16:     **for** $i \leftarrow 1$ **to** LEN($points$) **do**
17:         $variance \leftarrow variance +$ DISTANCE($points[i], mean$)
18:     **end for**
19:     $allVariance \leftarrow$ sum of all $variance$ from all nodes
20:     **return** $allVariance$
21: **end function**

Algorithm 4

1: **function** SIMULATE(points, velocities)
2:     $b1 \leftarrow points[1]$
3:     $b2 \leftarrow points[1]$
4:     **for** $i \leftarrow 2$ **to** LEN($points$) **do**
5:         **for** each dimension **do**
6:             $b1[dimension] \leftarrow$ MIN($b1[dimension], points[i][dimension]$)
7:             $b2[dimension] \leftarrow$ MAX($b2[dimension], points[i][dimension]$)
8:         **end for**
9:     **end for**
10:     $MaxDiff \leftarrow 0$
11:     **for** each dimension **do** $MaxDiff \leftarrow$ MAX($MaxDiff, b2[dimension] - b1[dimension]$)
12:     **end for**
13:     **for** each dimension **do**
14:         $CurDiff \leftarrow b2[dimension] - b1[dimension]$
15:         $Expand \leftarrow (MaxDiff - CurDiff)/2$
16:         $b2[dimension] \leftarrow b2[dimension] + Expand$
17:         $b1[dimension] \leftarrow b1[dimension] - Expand$
18:     **end for**   ▷ Now $b1$ and $b2$ encapsulate a hypercube where all *points* are in it.
19:     $BHTree \leftarrow$ BARNESHUTTREE($points, b1, b2$)
20:     **for** $i \leftarrow 1$ **to** m **do**
21:         $means[i] \leftarrow centerOfMass$ from $BarnesHutTree$ of node i
22:         $ClosestPoints[i] \leftarrow$ points with the shortest distance to $means[i]$
23:     **end for**
24:     **for** $i \leftarrow 1$ **to** m **do**
25:         $hyperplanes[i] \leftarrow$ hyperplane that go through $ClosestPoints[i]$ which is perpendicular to the line through $ClosestPoints[i]$ and $centerOfMass$ of local cluster
26:     **end for**
27:     **for** $i \leftarrow 1$ **to** m **do**
28:         $PartialTrees[i] \leftarrow$ GETPARTIALTREE($hyperplane[i], BHTree$)
29:     **end for**
30:     **for** $i \leftarrow 1$ **to** m **do**
31:         **if** $i \neq NodeIndex$ **then**
32:             $BHTrees[i]$ $PartialTrees[NodeIndex]$ from node i
33:         **end if**
34:     **end for**
35:     $BHTrees[NodeIndex] \leftarrow BHTree$
36:     **for** $i \leftarrow 1$ **to** LEN($points$) **do**
37:         $acceleration \leftarrow 0$
38:         **for** $j \leftarrow 1$ **to** LEN($BHTrees$) **do**
39:             $acceleration \leftarrow acceleration +$ GETACCELERATION($points[i], BHTrees[j]$)
40:         **end for**
41:         $velocities[i] \leftarrow velocities[i] + acceleration * DeltaTime$
42:         $points[i] \leftarrow points[i] + velocities[i] * DeltaTime$
43:     **end for**
44: **end function**

Algorithm 5

1: **function** BARNESHUTTREE(points, b1, b2)
2:   **if** All *points* are identical **then**
3:     NUMCHILDREN($BHTreeNode$) $\leftarrow$ 0
4:     MASS($BHTreeNode$) $\leftarrow$ LEN($points$)
5:     CENTEROFMASS($BHTreeNode$) $\leftarrow$ $points[1]$
6:   **else**
7:     CHILDREN($BHTreeNode$) $\leftarrow$ empty array
8:     **for** $nb1$, $nb2 \leftarrow$ every hyperoctant of the hypercube $b1$, $b2$ represent **do**
9:       $npoints \leftarrow$ empty array
10:       **for** $point \leftarrow points$ **do**
11:         **if** $point$ in hypercube represented by $nb1$, $nb2$ **then** PUSHBACK($npoints, point$)
12:         **end if**
13:       **end for**
14:       **if** LEN($npoints$) > 0 **then**
15:         PUSHBACK(CHILDREN($BHTreeNode$), BARNESHUTTREE($npoints, nb1, nb2$))
16:       **end if**
17:       NUMCHILDREN($BHTreeNode$) $\leftarrow$ LEN(CHILDREN($BHTreeNode$))
18:       CENTEROFMASS($BHTreeNode$) $\leftarrow$ 0
19:       MASS($BHTreeNode$) $\leftarrow$ 0
20:       **for** $child \leftarrow$ each CHILDREN($BHTreeNode$) **do**
21:         $ChildMass \leftarrow$ CENTEROFMASS($child$) * MASS($child$)
22:         CENTEROFMASS($BHTreeNode$) $\leftarrow$ CENTEROFMASS($BHTreeNode$) $+ ChildMass$
23:         MASS($BHTreeNode$) $\leftarrow$ MASS($BHTreeNode$) + MASS($child$)
24:       **end for**
25:       CENTEROFMASS($BHTreeNode$) $\leftarrow \frac{\text{CENTEROFMASS}(BHTreeNode)}{\text{MASS}(BHTreeNode)}$
26:     **end for**
27:   **end if**
28:   B1($BHTreeNode$) $\leftarrow b1$
29:   B2($BHTreeNode$) $\leftarrow b2$
30:   **return** $BHTreeNode$
31: **end function**

Algorithm 6

1: **function** GETPARTIALTREE(hyperplane, BHTreeNode)
2:   CENTEROFMASS($PartialNode$) $\leftarrow$ CENTEROFMASS($BHTreeNode$)
3:   MASS($PartialNode$) $\leftarrow$ MASS($BHTreeNode$)
4:   B1($PartialNode$) $\leftarrow$ B1($BHTreeNode$)
5:   B2($PartialNode$) $\leftarrow$ B2($BHTreeNode$)
6:   **if** $\frac{\text{B1}(BHTreeNode) - \text{B2}(BHTreeNode)}{\text{DISTANCE}(hyperplane, \text{CENTEROFMASS}(BHTreeNode))} < \theta$ **then**
7:     NUMCHILDREN($PartialNode$) $\leftarrow$ 0
8:   **else**
9:     NUMCHILDREN($PartialNode$) $\leftarrow$ NUMCHILDREN($BHTreeNode$)
10:     CHILDREN($PartialNode$) $\leftarrow$ empty array
11:     **for** $child \leftarrow$ each CHILDREN($BHTreeNode$) **do**
12:       PUSHBACK(CHILDREN($PartialNode$), GETPARTIALTREE($hyperplane, child$))
13:     **end for**
14:   **end if**
15:   **return** $PartialNode$
16: **end function**

Algorithm 7

1: **function** GETACCELERATION(point, BHTreeNode)
2:     $acceleration \leftarrow 0$
3:     **if** $\frac{\text{B1}(BHTreeNode) - \text{B2}(BHTreeNode)}{\text{DISTANCE}(point, \text{CENTEROFMASS}(BHTreeNode))} < \theta \vee \text{NUMCHILDREN}(BHTreeNode) = 0$ **then**
4:         $com \leftarrow \text{CENTEROFMASS}(BHTreeNode)$
5:         $acceleration \leftarrow \text{ACCELERATIONFROMCOM}(point, com, \text{MASS}(BHTreeNode))$
6:     **else**
7:         **for** $child \leftarrow$ every CHILDREN($BHTreeNode$) **do**
8:             $acceleration \leftarrow acceleration + \text{GETACCELERATION}(point, child)$
9:         **end for**
10:     **end if**
11:     **return** $acceleration$
12: **end function**

when combined with all the other overheads mentioned above, might outweigh the benefit of not having to send all points to all nodes.

In the future, it would be interesting to compare the performance of the current implementation against the naively parallelized Barnes-Hut algorithm described above.

Due to time constraint, the implementation is also not parallelized within a node. As a result, this does not take advantage of the multicore nature of each node. In the future, it'll be interesting to see how much extra performance can be extracted via parallelization within each node.

Methodology

To measure the performance of the implementation and whether parallelization sped up the simulation or not and by how much, the program was run on spartan with 1, 2, 4, 8, 16, 32 and 64 nodes. Because the implementation doesn't utilize OpenMP for inner process / inner node parallelization, each node only have one core allocated to run the simulation. Furthermore, to investigate how the communication overhead between the different nodes effect the overall runtime, the program is also run on a single spartan compute node with 1, 2, 4, 8, 16, 32 and 64 threads. This should significantly reduce the communication overhead between the Open MPI processes and give us more insight to how the extra communication overhead between different spartan compute nodes effect the performance of the program.

To allow more fine-grained observation of the program's performance, the runtime measurement is done on each process for the following stages of the program:

- Generating the points (by sampling from the GMM components).
- Choosing centers as needed by the k-means++ algorithm.
- Collaborating to cluster points using k-means algorithm after the centers are chosen.
- Sending points across the nodes so that all points of each cluster are on a single node.
- The N-Body simulation.

Originally, the N-Body simulation would stop when the sum of square of the distance between every point and the overall center of mass fall below 1/4 of the initial value. However, during the experiments, it is observed that sometimes the sum of square distance never goes below 1/4 of the initial value. It is believed that there are several reasons of this happening.

First, when two points get too close together, they experience strong gravitation attraction towards each other and hence receive large value of acceleration that increases their velocities to a very high value. Because the simulation's time is discrete, by the next time step, the points have already flew past each other and the gravitational attraction between them are no longer strong enough to slow them down. These points fly off away from all the other points in high velocity and the square of their distance to the overall center of mass dominate the sum of square distance. This problem has been fixed in two ways. First, by not having the point exert any gravitational forces upon each other when they're less than 0.05 distance away. This is a physically justifiable approximation because during the very short time period

when two points fly through each other in proximity, the total acceleration through that short period of time add up to be zero, as they act in opposite direction for equal amount of time. Second, by using sum of distance and the threshold being 1/2 of the initial value instead of sum of square distance. This reduces the influence of points very far away from the overall center of mass have on the sum.

Second, if the points are too close to each other at the start, they quickly fly past each other and the sum of distances increase after a short decrease. This is because our model has no mechanism for energy lost. As a result, after the points get close enough to each other, a significant portion of the points will gain enough energy from other points and get ejected from the center and fly away forever. This is solved by having the points further away from each other at the start so that the sum of distance will dip below 1/2 of the initial value before any points get ejected.

Experiments

Analysis & Discussion