Parallel Searches

Team Parallel Professional

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Outline

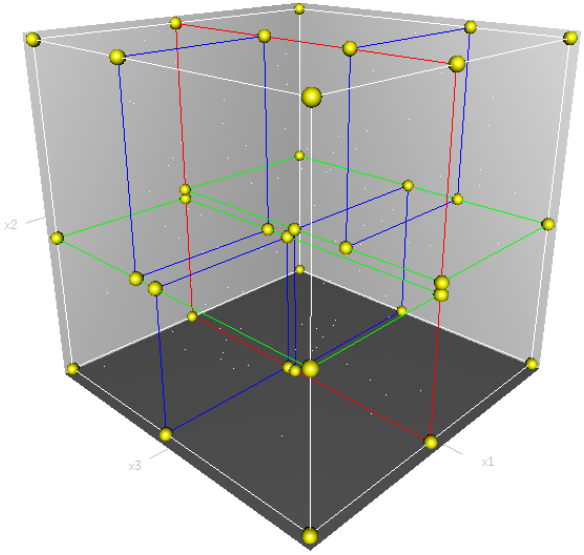
- Logic
- Code
- Results
- Challenges

Introduction

- k-d tree is a data structure used for organizing some number of points in a space with k dimensions.
- Parallel k-d tree construction requires sorting

data across ranks using MPI

- Goals:
  1. Build k-d tree with 10 billion points
  2. Search k-d tree for 20 million targets
  3. Search using 3 radii



Source:Wiki

Functions Outline

1. Create_array_datatype
2. readFromFileAllRead(datapoints, array)
3. buildTreeGlobal(array, num, &headNode, -1)
   - (A) getMaxMinGlobal(array, num, colIndex, anode→max, anode→min)
   - (B) getLargestDimensionGlobal(anode→max, anode→min, &colIndex);
   - (C) globalSort(array, &num, colIndex, &globalNum)
     - (i) do_sort(array, *num, colIndex);
     - (ii) getallCount(*num, colIndex, array, allCounts)
       - (a) qsort(LDiv, (num_ranks)*num_ranks, sizeof(float), compare_longfloat)
       - (b) getCounts(num, colIndex, array, L, totalCount, allCounts)
       - (c) checkBalance(&balanced, totalCount)
       - (d) adjustL(num, colIndex, array, L, allCounts, totalCount, &balanced)
     - (iii) struct data_struct *recv_array = AllToAllSend(array, &total_recv_counts, allCounts)
     - (iv) do_sort(recv_array, *num, colIndex)
   - (D) splitRanks()
   - (E) getMaxMin(array, num, -1, anode→max, anode→min)
4. globalTreeMaster(&Gtree, localHead)
5. readFromFile(fname, targetSize, targetArray)
6. buildTree(array, num, localHead, -1)
7. getSendArray(&Gtree,0.1, targetArray, targetSize,sendArray, sendSize[i],i)
8. localSearch(localHead, sendArray[sendi], childArray, &radiCounts[radi])

Data Structures

```
struct data_struct{
   long int num;
   float xyz[3];
};
struct node{
   float max[3], min[3], maxRadius;
   struct node *left, *right;
   int num_below;
   struct data_struct *center;
};
struct Gnode{
   float max[3], min[3], maxRadius;
   struct Gnode *left, *right, *parent;
   int this_rank, num_below, assigned;
   struct data_struct *center;
};
```

New MPI data type

```
void create_array_datatype(){

  MPI_Datatype data_type[2];
  int data_length[2];
  MPI_Aint displ[2], lower_bound, extent;

  MPI_Type_create_resized(MPI_LONG_INT, 0, sizeof(long int), &li_type);
  MPI_Type_commit(&li_type);

  MPI_Type_create_resized(MPI_FLOAT, 0, sizeof(float), &ld_type);
  MPI_Type_commit(&ld_type);

  displ[0] = 0;
  data_type[0] = li_type;
  data_length[0] = 1;

  MPI_Type_get_extent(li_type, &lower_bound, &extent);
  displ[1] = data_length[0] * extent;
  data_type[1] = ld_type;
  data_length[1] = 3;

  MPI_Type_create_struct(2, data_length, displ, data_type, &array_type);
  MPI_Type_commit(&array_type);
}
```

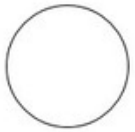
Create Comms

```
1: MPI_Comm_size(MPI_COMM_WORLD, &num_ranks);
2: MPI_Comm_rank(MPI_COMM_WORLD, &my_rank);
3: j = MPI_Comm_dup(MPI_COMM_WORLD, &dup_comm_world);
4: MPI_Comm_group( dup_comm_world, &world_group );
5: MPI_Comm_create( dup_comm_world, world_group, &MPI_LOCAL_COMM );
6: if num_ranks >1 then
7:    MPI_Barrier(MPI_LOCAL_COMM)
8:    if my_rank <num_ranks/2 then
9:       cflag = 0
10:   else
11:      cflag = 1
12:   end if
13: end if
14: MPI_Comm_split(MPI_LOCAL_COMM , cflag, my_rank, &MPI_TEMP_COMM );
15: MPI_Comm_free(&MPI_LOCAL_COMM);
16: MPI_Comm_dup(MPI_TEMP_COMM, &MPI_LOCAL_COMM);
17: MPI_Comm_free(&MPI_TEMP_COMM);
18: MPI_Comm_size(MPI_LOCAL_COMM, &num_ranks);
19: MPI_Comm_rank(MPI_LOCAL_COMM, &my_rank);
```

Tree Traversal: 4 Methods

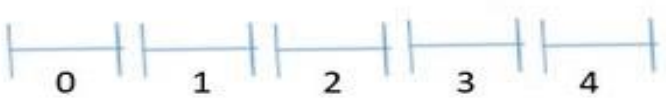
A. Recursive
   - Relic
   - Most Memory Usage
B. Sequential Flags
   - Used for Global Tree Build Rank 0
   - Traverses Tree from Leaf to Head
   - Requires a flag variable in struct
   - Extra Memory Usage
C. Sequential Array: Adjust Index
   - Used for targetSize and targetArray
   - Elements are moved around child array
   - Slower than Round Robin by 10^2
D. Sequential Array: Round Robin
   - Used for local search
   - Element indexes managed in child array

Sequential Flag Method

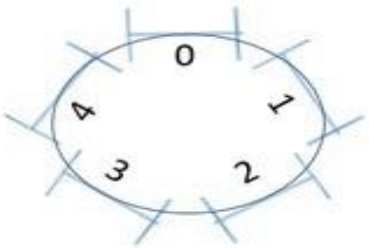


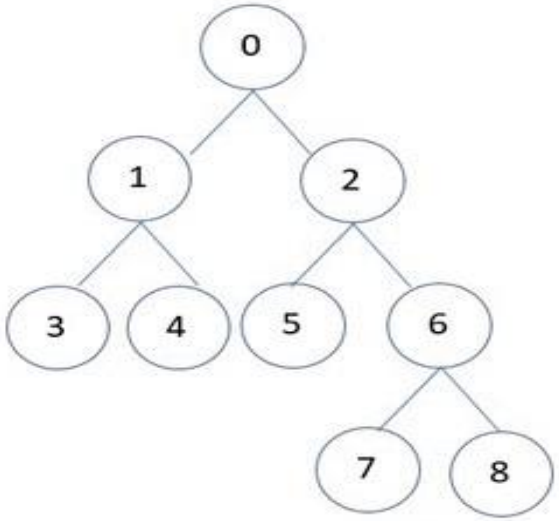
Sequential Array Methods

Adjust Position

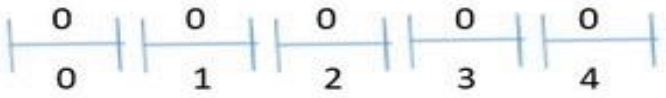


Round Robin

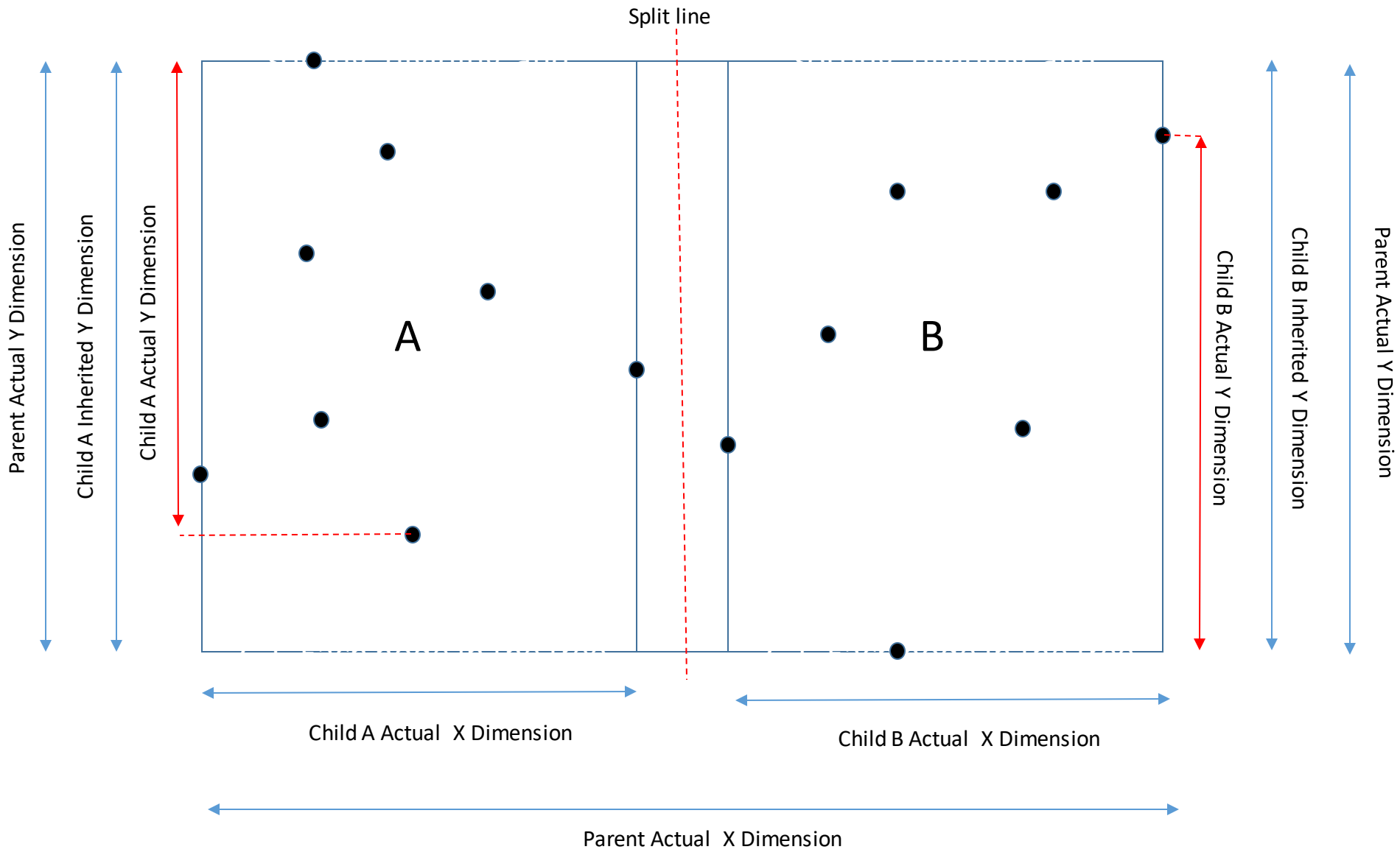




Leaf count

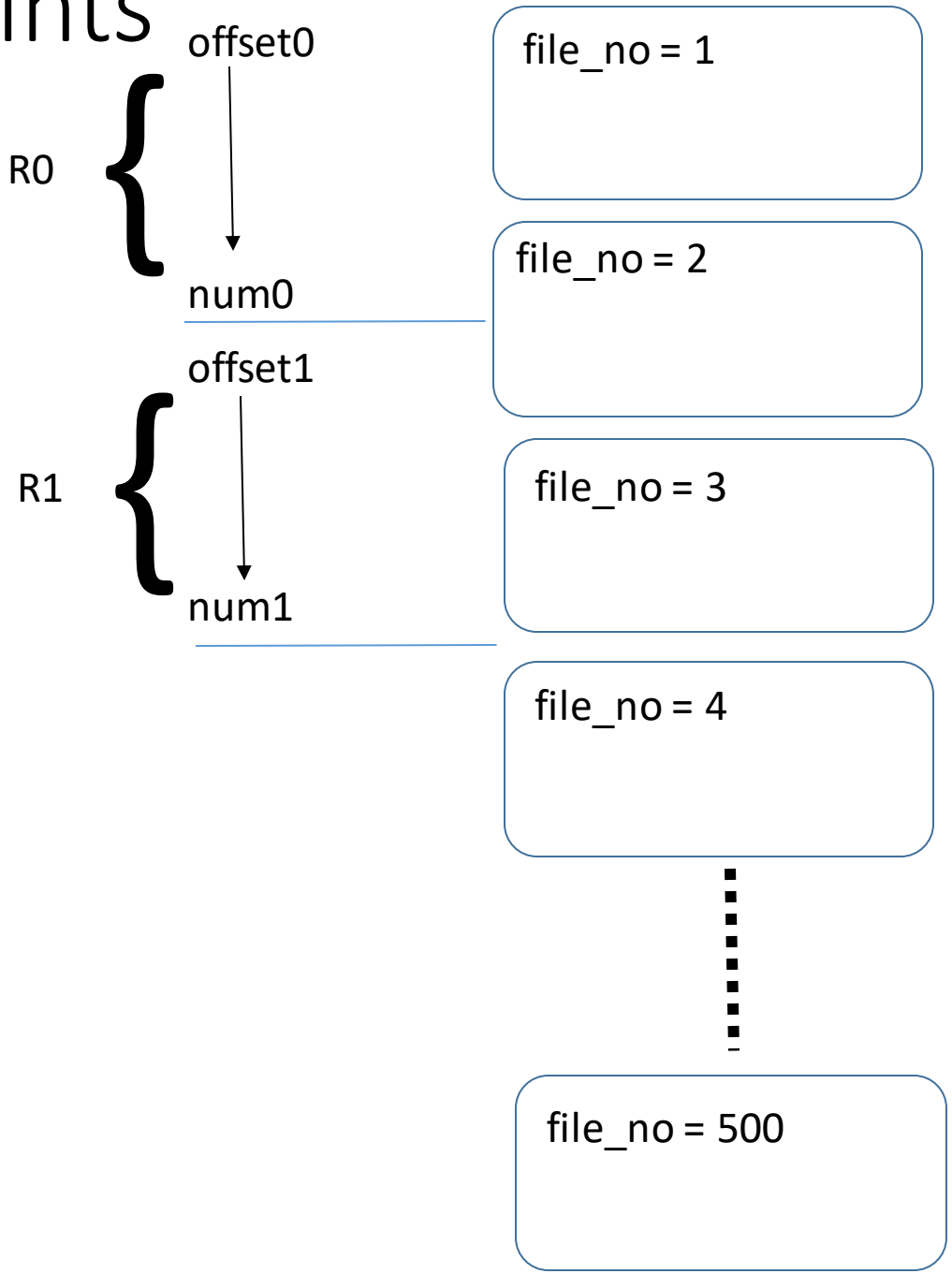


Node Split Logic

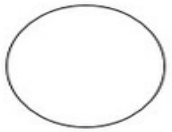


Read data points

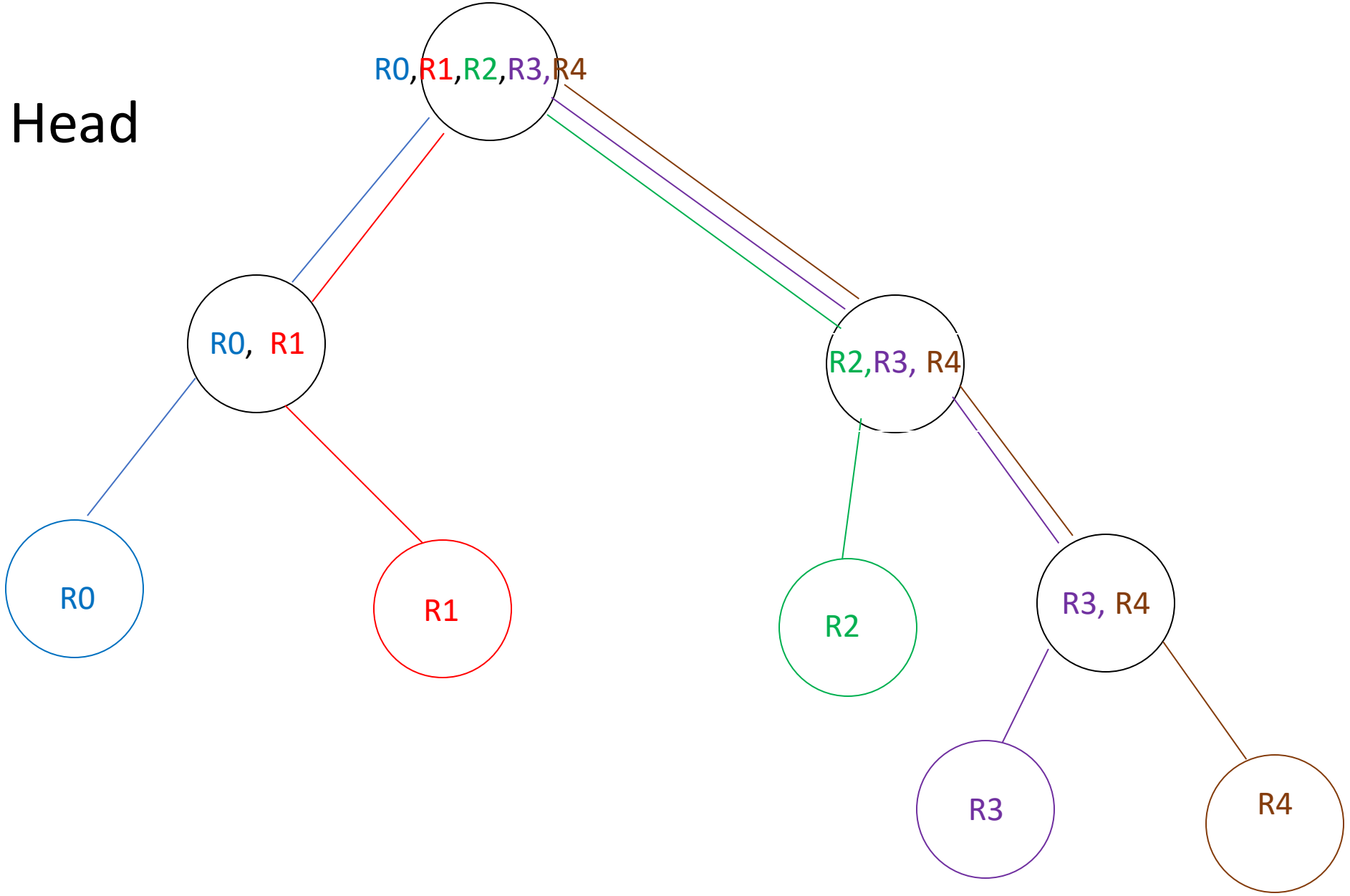
```
int datapoints = atoi(argv[1]);
int num;
if (my_rank == num_ranks-1){
    num = (int)datapoints/num_ranks + datapoints%num_ranks;
  }else{

    num = (int)datapoints/num_ranks;
  }

long int file_no, startline=0, tsize, size;
size_t offset = 0;
size_t dataSize = sizeof(long long int) +  3*sizeof(long double);
char fname[80];

if (my_rank < num_ranks-1){
  size = sizeOnAll/num_ranks;
  file_no = (long int)(size*my_rank/20000000 + 1);
  if (my_rank != 0){
    startline = (long int)(my_rank*size%20000000) + 1;
    offset = (startline-1)*dataSize;
  }
}else{
  tsize = sizeOnAll/num_ranks;
  size = tsize + sizeOnAll%num_ranks;
  file_no = (long int)(tsize*my_rank/20000000 + 1);
  startline = (long int)(my_rank*tsize%20000000) + 1;
  offset = (startline-1)*dataSize;
}
```



Get Local Head



Get Local Head



Get Local Head

Algorithm 1 Get Local Head

```
1: struct node *anode;
2: int datapoints = atoi(argv[1]);
3: struct data_struct* array = (struct data_struct *) malloc(num * sizeof(struct
   data_struct));
4: readFromFileAllRead(datapoints, array );
5: if my_rank == global_num_ranks-1 then
6:    num = (int)datapoints/num_ranks + datapoints%num_ranks;
7: else
8:    num = (int)datapoints/num_ranks;
9: end if
10: while num_ranks > 0 do
11:    getMaxMinGlobal(array, num, colIndex, anode→max, anode→min);
12:    getLargestDimensionGlobal(anode→max, anode→min, &colIndex);
13:    array = globalSort(array, &num, colIndex, &globalNum);
14:    splitRanks();
15: end while
```

GetMaxMinGlobal

```
void getMaxMinGlobal(void* varray, int size,  int colIndex, float *arrayMax, float *arrayMin){
  struct data_struct* array = (struct data_struct *)varray;
  float *allMax = (float *) malloc(3 * num_ranks * sizeof(float));
  float *allMin = (float *) malloc(3 * num_ranks * sizeof(float));

  int i,j,k;
  if (colIndex < 0){
    for (i=0;i<3;i++){
      arrayMax[i] = array[0].xyz[i];
      arrayMin[i] = array[0].xyz[i];
    }

    for (i=1;i<size;i++){
      for (j=0;j<3;j++){
        if (arrayMax[j] < array[i].xyz[j])
          arrayMax[j] = array[i].xyz[j];
        else if (arrayMin[j] > array[i].xyz[j])
          arrayMin[j] = array[i].xyz[j];
      }
    }
  }else{
    arrayMax[colIndex] = array[0].xyz[colIndex];
    arrayMin[colIndex] = array[0].xyz[colIndex];


    for (i=1;i<size;i++){

      if (arrayMax[colIndex] < array[i].xyz[colIndex])
        arrayMax[colIndex] = array[i].xyz[colIndex];
      else if (arrayMin[colIndex] > array[i].xyz[colIndex])
        arrayMin[colIndex] = array[i].xyz[colIndex];

    }
  }

  MPI_Allgather(arrayMax, 3, ld_type, allMax, 3,ld_type, MPI_LOCAL_COMM);
  MPI_Allgather(arrayMin, 3, ld_type, allMin, 3,ld_type, MPI_LOCAL_COMM);
```

Get Largest Dimension

```
void getLargestDimensionGlobal(float *arrayMax, float *arrayMin, int *colIndex){
  float range = arrayMax[0] - arrayMin[0];
  *colIndex = 0;
  if (range < (arrayMax[1] - arrayMin[1])){
    *colIndex = 1;
    range = arrayMax[1] - arrayMin[1];
  }
  if (range < (arrayMax[2] - arrayMin[2])){
    *colIndex = 2;
    range = arrayMax[2] - arrayMin[2];
  }

}
```

Global Sort

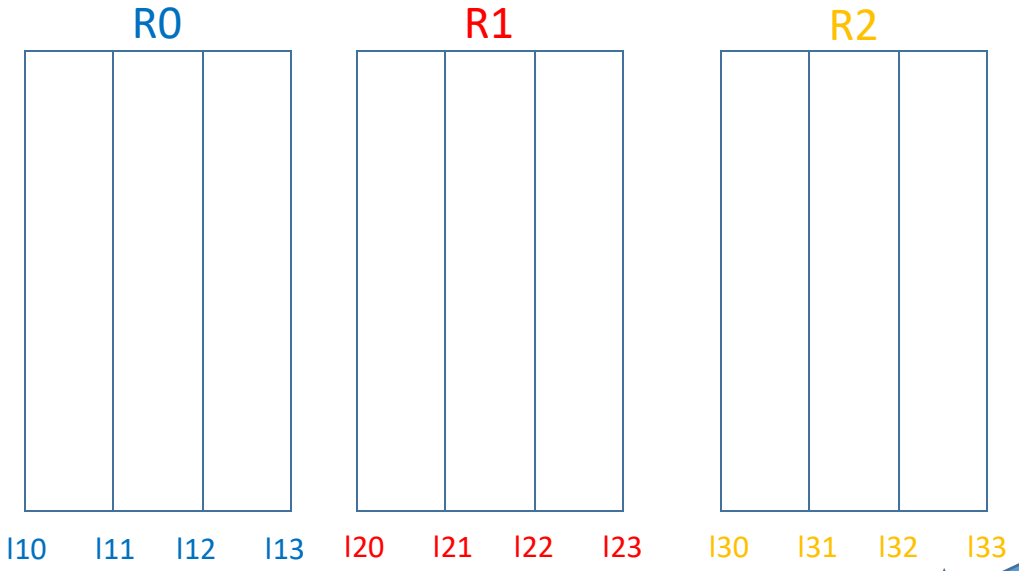
- localsort
- getBuckets
- adjustBuckets
- SendItems
- localsort

localsort

```
int compare_datastruct(const void* s1, const void* s2, int index){
  struct data_struct  *p1 = (struct data_struct *) s1;
  struct data_struct  *p2 = (struct data_struct *) s2;
  return p1->xyz[index] > p2->xyz[index];
}

int compare_x(const void* s1, const void* s2){
  return compare_datastruct(s1, s2, 0);
}

int compare_y(const void* s1, const void* s2){
  return compare_datastruct(s1, s2, 1);
}

int compare_z(const void* s1, const void* s2){
  return compare_datastruct(s1, s2, 2);
}

void do_sort(struct data_struct *array, int num, int colIndex){

  if (colIndex == 0)
    qsort(array, num, sizeof(struct data_struct), compare_x);
  else if (colIndex == 1)
    qsort(array, num, sizeof(struct data_struct), compare_y);
  else if (colIndex == 2)
    qsort(array, num, sizeof(struct data_struct), compare_z);
  else{
    printf("colIndex is between 0 and 2\n");
    exit(0);
  }
}
```

GetBuckets

lij = jth local lower limit for ith rank



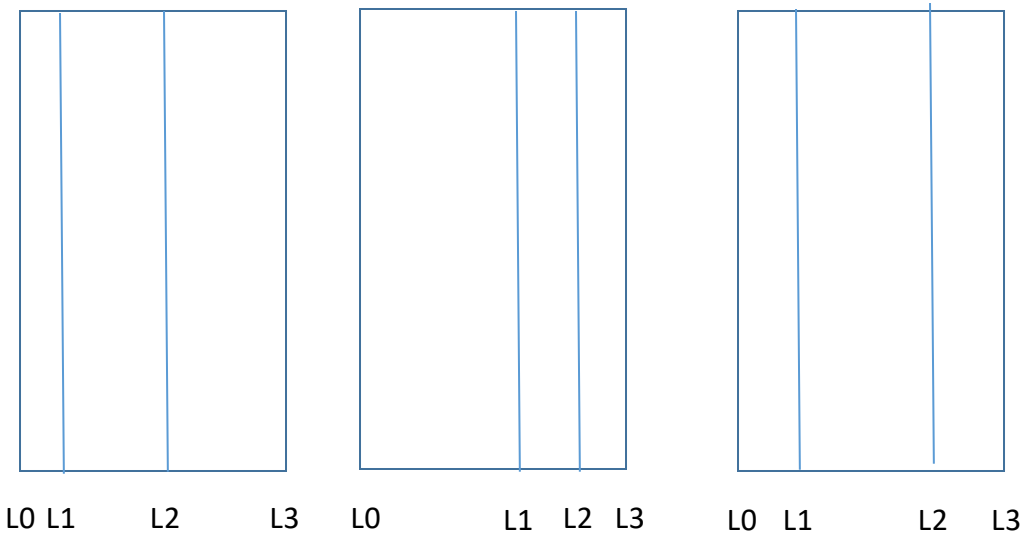
Min	li1	li2	Max
l10	l11	l12	l13
l20	l21	l22	l23
l30	l31	l32	l33

SORT

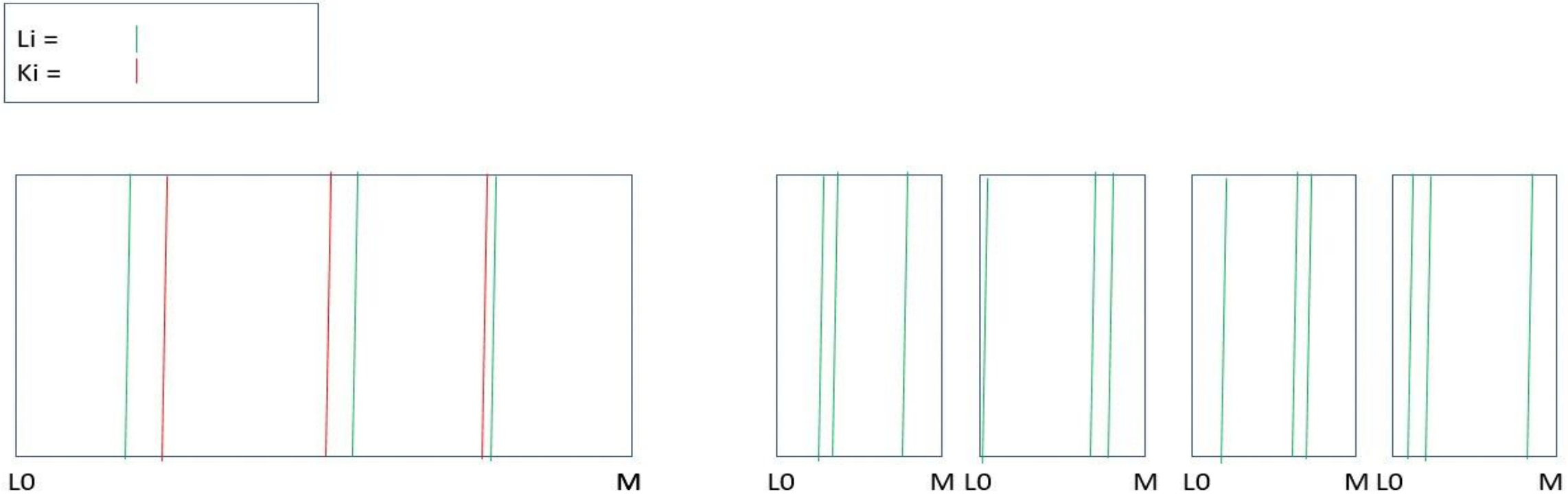
Lj = jth global lower limit

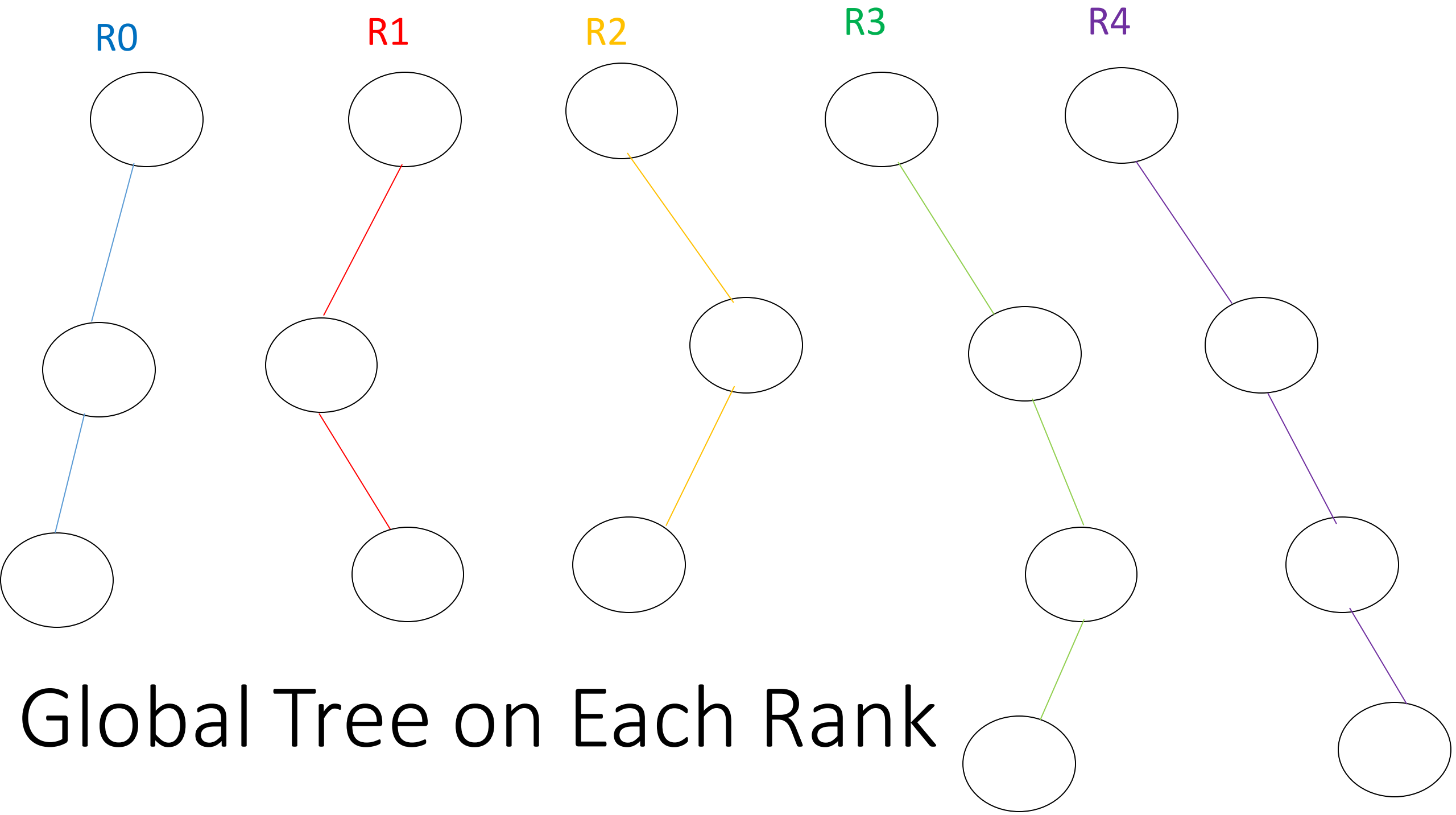
L0-2	N/A	N/A	L3
l30	l20	l10	l31
l11	l21	l12	l32
l22	l33	l23	l13

L0=l30, L1=l11, L2=l22, L3=l13



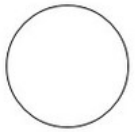
AdjustBuckets



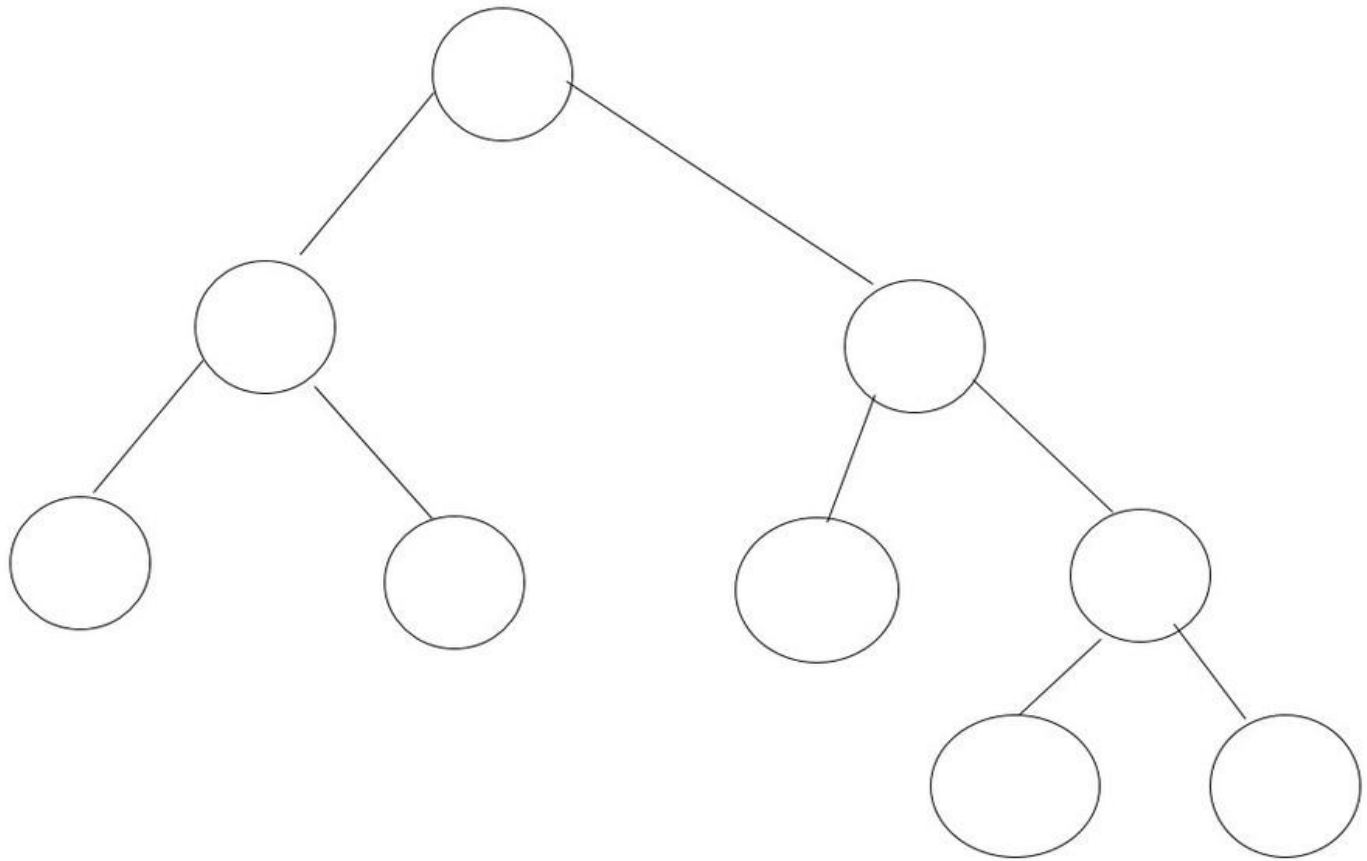


Global Tree on Each Rank

Build Global Tree Rank 0 Down



Build Global Tree up



Build Global Tree (Sequential Flag)

Algorithm 3 Build Global Tree

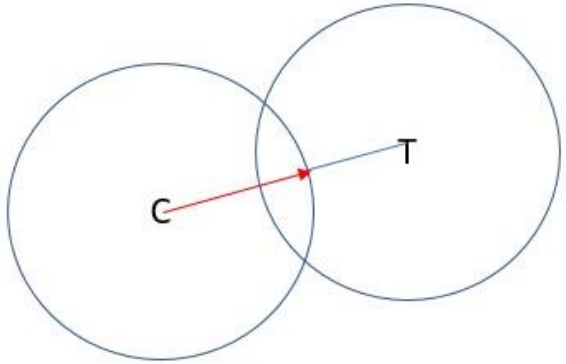
```
1:  struct Gnode *Gtree;
2:  currNode = buildEmptyGtree(Gtree, ranks_below, 0)
3:  j = num_ranks - 1
4:  while j > 0 do
5:     if currNode→assigned == -1 then
6:        if currNode→num_below <= 1 then
7:           Receive max and min of the leaf from rank j;
8:           currNode→this_rank = j;
9:           currNode = currNode→parent;
10:          j −;
11:       else
12:          if currNode→right→assigned == -1 then
13:             currNode = currNode→right;
14:          else if currNode→left→assigned == -1 then
15:             currNode = currNode→left;
16:          else
17:             Build the node up
18:             currNode = currNode→parent;
19:          end if
20:       end if
21:    end if
22: end while
```

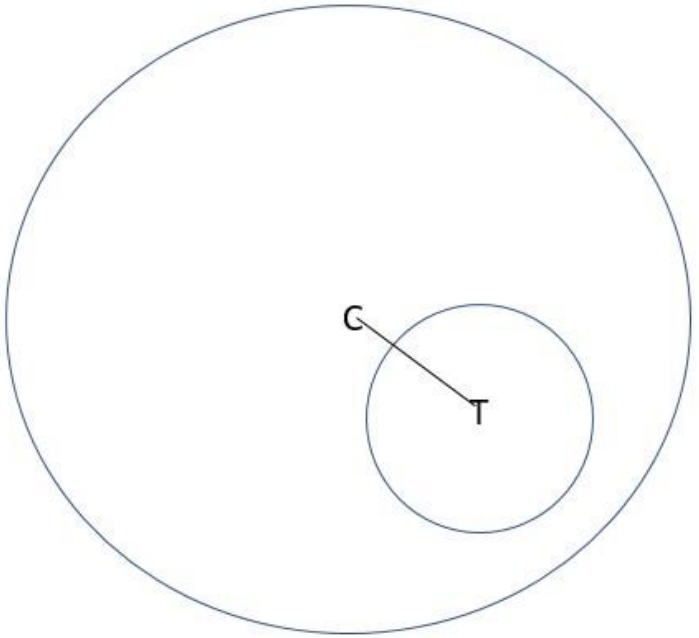
Read Target

- Only the master rank reads the target file named file501
- Number of targets read is specified as a command line argument.
- The file is converted to binary and stored as long doubles as discussed in the ”Read datapoints” section

Search Comparison Logic

```
for (i=0;i<3;i++){
  temp = (anode->max[i] + anode->min[i])/2;
  targetDir[i] = (target.xyz[i]-temp);
  targetMagnitude += targetDir[i]*targetDir[i];
}
targetMagnitude = sqrt(targetMagnitude);
for (i=0;i<3;i++){
  temp = (anode->max[i] + anode->min[i])/2;
  targetDir[i] = targetDir[i]/targetMagnitude;
  targetDir[i] *= anode->maxRadius;
  targetPoint[i] = temp + targetDir[i];
  testRadius += pow(target.xyz[i] - targetPoint[i],2);
}
testRadius = sqrt(testRadius);
if (targetMagnitude < anode->maxRadius || testRadius < radius){
  caSize = 2;
  start = 0;
  end = 1;
  childArray[0] = anode->left;
  childArray[1] = anode->right;
}
```





Get Targets (Round Robin)

- For Master rank

```
sendArray = (struct data_struct *) malloc(maxSendSize * sizeof(struct data_struct));
for (i = 1; i<global_num_ranks; i++){
    getSendArray(&Gtree, 0.1, targetArray, targetSize, sendArray, &sendSize[i], i);
    MPI_Send(sendArray, sendSize[i], array_type, i, 0, MPI_COMM_WORLD);
}
```

- For other ranks

```
MPI_Probe(0, 0, MPI_COMM_WORLD, &stat);
MPI_Get_count(&stat,array_type,&mySendSize);
sendArray = (struct data_struct *) malloc(mySendSize * sizeof(struct data_struct));
MPI_Recv(sendArray, mySendSize, array_type, 0, 0, MPI_COMM_WORLD, &mystat);
```

Build Local Tree (Adjust Index)

```
while ( caSize > 0){
  anode = childArray[0];
  start = starts[0];
  num = ends[0];
  if (num > 1){
    getMaxMin(&array[start], num, colIndex, anode->max, anode->min);
    getLargestDimension(anode->max, anode->min, &colIndex);
    do_sort(&array[start], num, colIndex);
    getNode(num, anode);
    anode->left = (struct node *)malloc(sizeof(struct node));
    anode->right = (struct node *)malloc(sizeof(struct node));
    for (i=0;i<3;i++){
      anode->left->max[i] = anode->max[i];
      anode->left->min[i] = anode->min[i];
      anode->right->max[i] = anode->max[i];
      anode->right->min[i] = anode->min[i];
    }
    for (i=0;i<caSize;i++){
      childArray[i] = childArray[i+1];
      starts[i] = starts[i+1];
      ends[i] = ends[i+1];
    }
    caSize += 1;
    childArray[caSize-2] = anode->left;
    starts[caSize-2] = start;
    ends[caSize-2] = (int)num/2;
    childArray[caSize-1] = anode->right;
    starts[caSize-1] = start + (int)num/2;
    if (num%2 == 0){
      ends[caSize-1] = (int)num/2;
    }else{
      ends[caSize-1] = (int)num/2 + 1;
    }
```

Local Count (Round Robin)

- Get number of datapoints within radius of target
- Same Logic as getSendArray
- Send total counts to master rank

```
while (caSize > 0){
  anode = childArray[start];
  targetMagnitude = testRadius = 0;
  if (anode->num_below > 1){
    for (i=0;i<3;i++){
      temp = (anode->max[i] + anode->min[i])/2;
      targetDir[i] = (target.xyz[i]-temp);
      targetMagnitude += targetDir[i]*targetDir[i];
    }
    targetMagnitude = sqrt(targetMagnitude);
    if (targetMagnitude < anode->maxRadius){
      caSize += 1;
      start = (start + 1)%numOfLeaves;
      end = (end + 1)%numOfLeaves;
      childArray[end] = anode->left;
      end = (end + 1)%numOfLeaves;
      childArray[end] = anode->right;
    }else{
      for (i=0;i<3;i++){
        temp = (anode->max[i] + anode->min[i])/2;
        targetDir[i] = targetDir[i]/targetMagnitude;
        targetDir[i] *= anode->maxRadius;
        targetPoint[i] = temp + targetDir[i];
        testRadius += pow(target.xyz[i] - targetPoint[i],2);
      }
      testRadius = sqrt(testRadius);
      if (testRadius < radius){
        caSize += 1;
        start = (start + 1)%numOfLeaves;
        end = (end + 1)%numOfLeaves;
        childArray[end] = anode->left;
        end = (end + 1)%numOfLeaves;
        childArray[end] = anode->right;
      }else{
        start = (start + 1)%numOfLeaves;
        caSize -= 1;
      } // BOUNDARY TO TARGET ( TEST RADIUS)
    } // CENTER TO TARGET ( TARGET MAGNITUDE)
```

Global Count

- Master rank receives counts from other ranks
- Sum up all counts for a given target with a radius
- Displays final outputs

```
if {my_global_num_ranks == 0}{
    i = 0;
    while (i<nonZeroRanks){
          MPI_Probe(MPI_ANY_SOURCE, 123, MPI_COMM_WORLD, &stat);
          d = stat.MPI_SOURCE;
          radiCounts = (long int *)malloc(tsendSize[d]*sizeof(long int));
          MPI_Recv(radiCounts,tsendSize[d] , li_type, d, 123, MPI_COMM_WORLD, &mystat);
          i++;
          for (radi=0;radi<tsendSize[d];radi+=4){
              k = (int)(radiCounts[radi]-targetArray[0].num)*3;
              for (j=1; j<=3;j++)
                   allRadiCounts[k+j-1] += radiCounts[radi+j];
          }
          free(radiCounts);
    }
 }else{
   mySendSize *=4;
   if (mySendSize > 0)
        MPI_Send(radiCounts, mySendSize, li_type, 0, 123, MPI_COMM_WORLD);
}
```

0 <= assignedi < number of targets assigned to rank
radiCounts[assignedi] = [id1,x1,y2,z2,id2,x2,y2,z2, …. idn,xn,yn,zn]

0 <= k < number of targets (k represents target id)
allRadiCounts[k] = [x1,y1,z1,x2,y2,z2, … xn,yn,zn]

Validation

- Used file001 to validate our code
- Used a function named 'targetTest.c' to verify if a point is within the radius of the target.
- Compared the result of targetTest.c with the result of our program for file001 and file501
- Matched the global tree leaves with the local tree heads.

Validation File 001

INDIVIDUAL COMPARES

TargetID	0.01	0.05	0.1
1	1	10	49
2	1	40	320
3	1	17	121
4	1	31	244
5	1	22	152
6	1	20	185
7	1	15	89
8	1	7	58
9	15	2085	3853
10	2	15	152
11	3	220	1276
12	1	9	74
13	1	9	67
14	8	1462	3558
15	6	2060	3561
16	48	2985	4640
17	1	76	593
18	2	300	1467
19	1	152	879
20	21	2129	4578
21	1	37	373
22	1	13	69
23	1	14	107
24	1	3	40
25	2	14	129
26	20	1558	3725
27	107	3242	3557
28	1	16	151
29	32	2313	3858
30	1	42	274
31	1	4	68
32	1	23	175
33	147	3345	3560
34	1	114	825
35	41	2558	4624
36	1	22	115
37	2	115	779
38	1	29	237
39	1	11	59
40	3	100	671
41	1	17	147

TREE SEARCH

TargetID	0.01	0.05	0.1
1	1	10	49
2	1	40	320
3	1	17	121
4	1	31	244
5	1	22	152
6	1	20	185
7	1	15	89
8	1	7	58
9	15	2085	3853
10	2	15	152
11	3	220	1276
12	1	9	74
13	1	9	67
14	8	1462	3558
15	6	2060	3561
16	48	2985	4640
17	1	76	593
18	2	300	1467
19	1	152	879
20	21	2129	4578
21	1	37	373
22	1	13	69
23	1	14	107
24	1	3	40
25	2	14	129
26	20	1558	3725
27	107	3242	3557
28	1	16	151
29	32	2313	3858
30	1	42	274
31	1	4	68
32	1	23	175
33	147	3345	3560
34	1	114	825
35	41	2558	4624
36	1	22	115
37	2	115	779
38	1	29	237
39	1	11	59
40	3	100	671
41	1	17	147

Validation file 501

INDIVIDUAL COMPARES			
TargetID	0.01	0.05	0.1
10000000001	38	2715	4646
10000000002	1	94	633
10000000003	0	28	194
10000000004	4	186	1131
10000000005	0	32	184
10000000006	36	2625	3865
10000000007	0	12	82
10000000008	0	6	74
10000000009	33	2695	4617
10000000010	0	14	104
10000000011	4	84	645
10000000012	10	856	3312
10000000013	0	9	68
10000000014	0	79	557
10000000015	93	3250	3566
10000000016	0	37	325
10000000017	0	11	120
10000000018	0	16	109
10000000019	0	96	563
10000000020	0	12	131
10000000021	0	132	1028
10000000022	0	15	108
10000000023	199	3453	3564
10000000024	0	22	153
10000000025	0	34	227
10000000026	0	22	168
10000000027	0	11	91
10000000028	0	16	106
10000000029	4	618	2893
10000000030	0	32	232
10000000031	1	39	264
10000000032	0	12	75
10000000033	0	31	226
10000000034	0	5	65
10000000035	1	134	908
10000000036	0	85	583
10000000037	0	79	683
10000000038	1	177	1122
10000000039	0	23	189
10000000040	0	11	89

TREE SEARCH			
TargetID	0.01	0.05	0.1
10000000001	38	2715	4646
10000000002	1	94	633
10000000003	0	28	194
10000000004	4	186	1131
10000000005	0	32	184
10000000006	36	2625	3865
10000000007	0	12	82
10000000008	0	6	74
10000000009	33	2695	4617
10000000010	0	14	104
10000000011	4	84	645
10000000012	10	856	3312
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10000000019	0	96	563
10000000020	0	12	131
10000000021	0	132	1028
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10000000023	199	3453	3564
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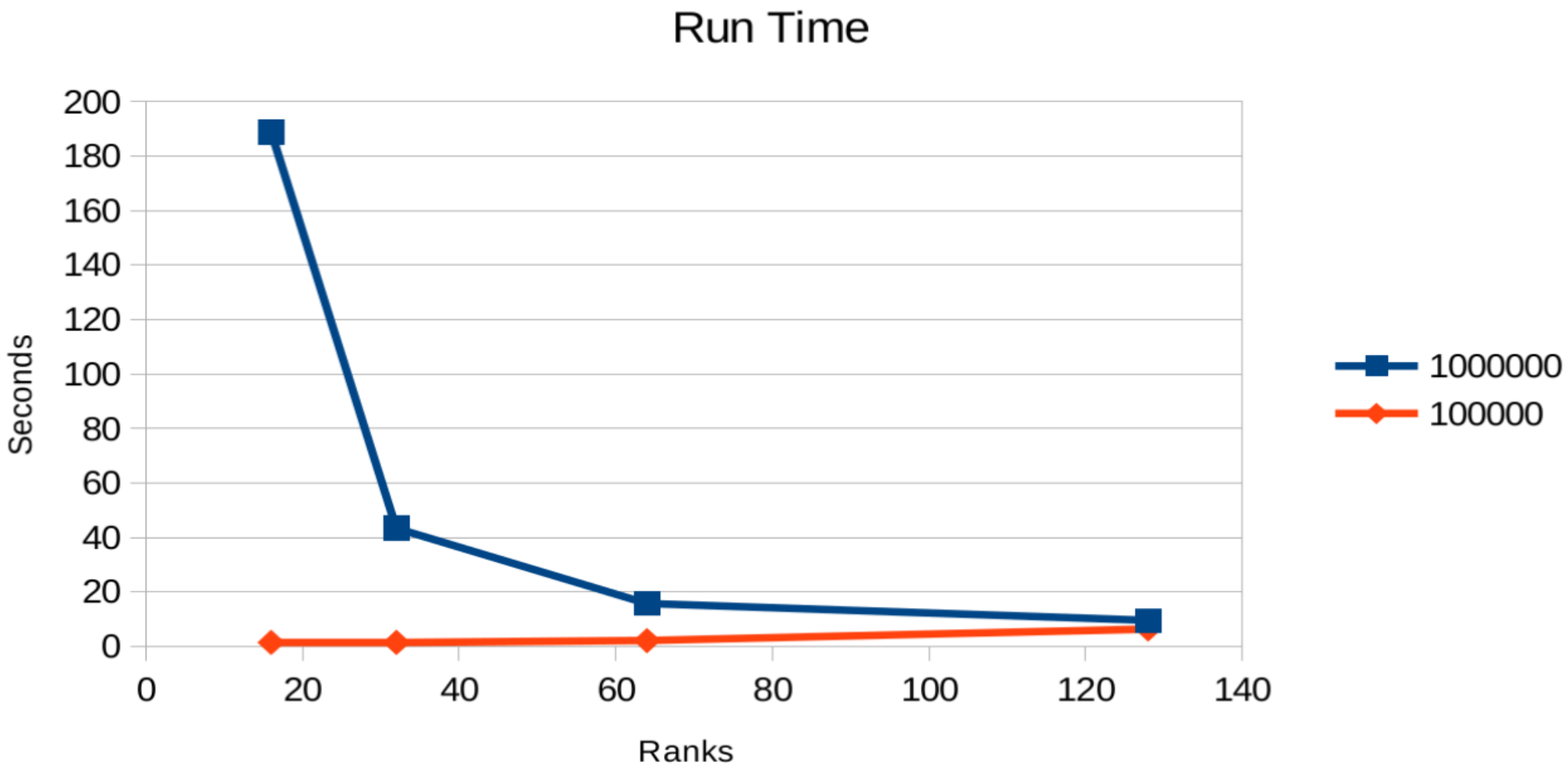
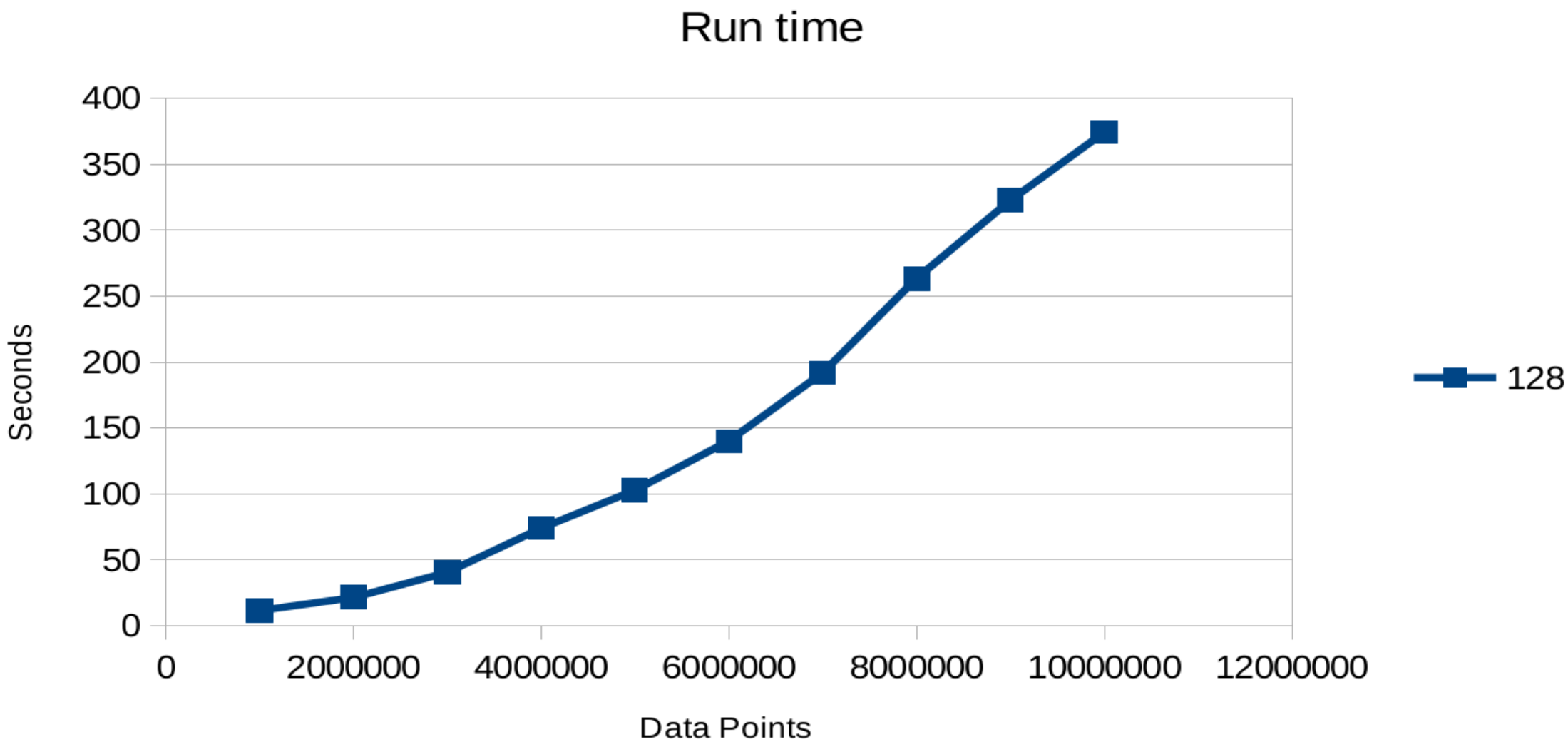
10000000025	0	34	227
10000000026	0	22	168
10000000027	0	11	91
10000000028	0	16	106
10000000029	4	618	2893
10000000030	0	32	232
10000000031	1	39	264
10000000032	0	12	75
10000000033	0	31	226
10000000034	0	5	65
10000000035	1	134	908
10000000036	0	85	583
10000000037	0	79	683
10000000038	1	177	1122
10000000039	0	23	189
10000000040	0	11	89

Timing Data


Run Time
Seconds
200
180
160
140
120
100
80
60
40
20
0
0
20
40
60
80
100
120
140
Ranks
1000000
100000

Timing Data


Run time
Seconds
400
350
300
250
200
150
100
50
0
0
2000000
4000000
6000000
8000000
10000000
12000000
Data Points
128

Search Results

Table 1: Time required for 1000000 with different nodes.

Data	Nodes	read	LocalH	GloTr	Targ	LocTr	asignTarg	localC	gloC	TotT
1000000	16	0.65	0.43	0	0.02	18.37	0.01	0	0.02	188.82
1000000	32	0.9	0.43	0	0.02	5.66	0.01	0	0.04	43.32
1000000	64	0.5	0.61	0	0.01	1.42	0.01	0	0.03	15.64
1000000	128	0.48	1.24	0	0.01	0.01	0.01	0	0.02	9.44

Bottleneck

- Build Local Tree (when points is large)
- Reading data files (when points is large)
- Get Local Head (when ranks is large)
- Assigning the target (when targets is large)
- Local search (when targets is large)

Program Execution

- Python script "runTests.py" to run the different test by varying number of ranks, datapoints and target size.
- This python script creates qsub file for each run with particular target size, rank and datapoint.
- Qlogin for quick test
- Git version control.
- Each state timing data stored in .txt file
- Python code "killprocess.py" that kill the running process for all the used node for qsub job ID.

Challenges

- Splitting / Grouping MPI COMM WORLD. (Spent weeks on this)
- Print statements
- Cluster usage overload.
- Memory issue for large data sets and rank.
- Recursive call.
- Malloc/ Calloc.
- Global tree leaves match with local head on each rank.
- Get size of target matching, size of target array.

Challenges

- Split ranks
  - Without groups(no barriers)
  - With groups (with barrier)

- Comm Collections
  - With COMM(ranks<128)
  - Withouts COMS
    - Custom Collectives(unstable)
    - Split ranks(datapoints<1 milions)

Challenges

- Print Formats
- Reallocate the array

Work Distribution

- Gabriel Toban: Adjust Buckets, Round Robin, Integration
- Khem Poudel: MPI Comms, Data Read
- Toheeb Biala: MPI Functions, Local Sort

Conclusion

- Successful implementation of an orthogonal recursive bisection (ORB) of the dataset along N-dimensions with serial and parallel sort.
- Implemented for a parallel spatial binary tree that searches millions/ billion points.
- Find how many points are within 3 search radii of 20 million targets .

Thank you !!!