kd-tree construction and analysis with OpenMP and OpenMPI

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1 Introdution

A K Dimensional tree (or k-d tree) is a tree data structure that is used to represent points with more than one property in a k-dimensional space. It is a convenient way to organize points by several criteria at once and it provides eg. a convenient way to search, cluster points by their overall similarity.

In this work a way to build and parallelize such a tree is presented.

2 Algorithm

The construction of the tree is done by:

- Finding median/pivot by median of medians of the input array. Each section of constant length is sorted by insertion sort.
- Recursively proceed on left and right portions on the left and right of the found median. Each median is a node.
- Terminate when length of a portion is 0.
- Return root node.

The time complexity of the divide and conquer algorithm is O(nlogn) since the pivot is chosen in O(nlogn) time. If the partitioning would be done in a non optimal way (choosing as pivot the lowest, largest element of the array), the complexity would be $O(n^2)$.

```
Algorithm 1 Build kD-tree
    Input arrayOfNodes
   Output treeRootNode
1: function BuildKDTree(startNode, length, axis, dim)
       if length = 0 then
2:
                                                               ▶ base case
3:
          return 0
       end if
4:
5:
       myaxis \leftarrow round robin approach between 0 and 1
6:
       medianNode \leftarrow MedianOfMedianS(startNode, startNode + length)
   -1, myaxis, len)
       medianNode.left \leftarrow BuildKDTree(startNode, medianNode -
7:
   startNode, myaxis, dim)
       medianNode.right \leftarrow BuildKDTree(startNode, startNode +
8:
   length - (medianNode + 1), myaxis, dim)
       return treeNode
9:
10: end function
11: function MedianOfMedians(startNode, endNode, myaxis, length)
       if length < 10 then
                                                               ▷ base case
12:
          InsertionSort(startNode, length, myaxis)
13:
14:
          median \leftarrow middleElement
       else
15:
          subarrays \leftarrow ceiling(n/5)
16:
          allocate array medians of length subarrays
17:
          for i \leftarrow 1, subarrays do
18:
              InsertionSort(startNode, length, myaxis)
19:
              medians[i] \leftarrow middleElement
20:
          end for
21:
          if numSubarrays = high then
22:
23:
              median \leftarrow \text{MedianOfMedians}(medians, end, myaxis, length)
          end if
24:
       end if
25:
       return median
27: end function
28: procedure InsertionSort(startNode, length, axis)
       similar to the sorting of playing cards in hands
30: end procedure
```

3 Implementation

Herein the strategy used for OpenMP, OpenMP and their hybrid solution.

3.1 OpenMP

OpenMP is one of the application programming interfaces that facilitates the employment of a shared memory paradigm for parallelization within a node. Below the simplified, decorated Algorithm1 with the instruction read by OpenMP during compilation.

```
Algorithm 2 Build kD-tree w/ OpenMP
    Input arrayOfNodes
    Output treeRootNode
1: function MAIN
       #pragma omp parallel
2:
3:
       #pragma omp single nowait
       initialize random arrayOfNodes
4:
       root \leftarrow BuildKDTree(arrayOfNodes, length, 0, 2)
5:
6:
       #pragma omp barrier
7:
       printroot
8: end function
9: function BuildKDTree(startNode, length, axis, dim)
10:
       if length = 0) then
                                                                ▶ base case
          return 0
11:
       end if
12:
13:
       myaxis \leftarrow round robin approach between 0 and 1
       medianNode \leftarrow MedianOfMedianS(startNode, startNode + length)
14:
   -1, myaxis, len)
15:
       #pragma omp task
       medianNode.left \leftarrow BuildKDTree(leftPoints, length, myaxis, dim)
16:
17:
       #pragma omp task
18:
       medianNode.right \leftarrow BuildKDTree(rightPoints, length, myaxis,
   dim)
19:
       return treeNode
20: end function
21: function MEDIANOFMEDIANS(startNode, endNode, myaxis, length)
       if length < 10 then
                                                                ▷ base case
22:
          InsertionSort(startNode, length, myaxis)
23:
          median \leftarrow middleElement
24:
       else
25:
          for i \leftarrow 1, subarrays do
26:
27:
              #pragma omp parallel for
              InsertionSort(startNode, length, myaxis)
28:
              medians[i] \leftarrow middleElement
29:
          end for
30:
                                     5
          median \leftarrow medians[middleElement]
31:
32:
       end if
       return median
33:
34: end function
```

- 35: **procedure** InsertionSort(startNode, length, axis)
- 36: similar to the sorting of playing cards in hands
- 37: end procedure

3.2 Hybrid solution

The hybrid solution, other than leveraging parallelization within a node, leverages also the different nodes that reside in a cluster, scaling up the solution. To achieve this, point-to-point messaging needs to be designed along the NUMA node on disposal, since each node has its own memory space. Once a task receives it's message, each one computes the assignment on its portion of data using OpenMP threads, as under subsection OpenMP.

In order for each task to get it's portion of data, rank0, the master rank, get's to find the tree nodes up until the level of the kdtree from where it is possible to assign the unique, fairly balanced, and only portions of data for each task (the left-most chunk being processed by rank 0). This approach was decided upon, to ensure load balancing and to easily reconstruct the tree, by sending the subtrees back to rank0.

MPI calls are made inside parallel regions, but there is no restriction when a certain thread receives the message from the master rank, hence the $MPI_THREAD_MULTIPLE$ paradigm is flagged.

Below the function that employs tasks, and the main function.

```
Algorithm 3 Build kD-tree w/ Hybrid
   Input arrayOfNodes, numProcs, rank
   Output treeRootNode
 1: function MAIN
      MPI\_Init\_thread(..., MPI\_THREAD\_MULTIPLE,...)
2:
      #pragma omp parallel
3:
       #pragma omp single nowait
4:
5:
      initialize random arrayOfNodes
      if rank = 0 then
6:
          root \leftarrow
                      FINDFIRSTNODES(arrayOfNodes, length, 0,
7:
   depth=0,rank = -1)
                                                      8:
      else
9:
          MPI\_Recv(length, 1, MPI\_INT, 0, 2, MPI\_COMM\_WORLD, ...)
          MPI\_Recv(portion, length, MPI\_BYTE, 0, 0, MPI\_COMM\_WORLD, ...)
10:
          toSend \leftarrow BuildKDTree(portion, length, myaxis, 2)
11:
   ideally the head of the subtree would be sent back to rank 0, for full tree
   construct
      end if
12:
      MPI\_Finalize()
13:
14: end function
15: function FINDFIRSTNODES(startNode, length, axis, dim)
16:
      myaxis \leftarrow round robin approach between 0 and 1
17:
      if depth == log2(numProcs) then
                                                             ▶ base case
          return 0
18:
      end if
19:
      medianNode \leftarrow MedianOfMedianS(startNode, startNode + length)
20:
   -1, myaxis, len)
21:
       #pragma omp task
      if depth == log2(numProcs) - 1 then
22:
          rank \leftarrow rank + 1
                                                ▷ no round robin needed
23:
         if rank = 0 then
24:
             toSend \leftarrow BuildKDTree(leftPoints, leftLength, myaxis, 2)
25:
26:
          else
             MPI\_Send(leftLength, 1, MPI\_INT, rank, 2, MPI\_COMM\_WORLD)
27:
             MPI\_Send(leftPoints, leftLength, MPI\_BYTE, rank, 0, MPI\_COMM\_WORLD)
28:
                                   7
          end if
29:
          rank \leftarrow rank + 1
                                               ▷ no round robin needed
30:
          MPI\_Send(rightLength, 1, MPI\_INT, rank, 2, MPI\_COMM\_WORLD)
31:
          MPI\_Send(rightPoints, rightLength, MPI\_BYTE, rank, 0, MPI\_COMM\_WORLD)
32:
```

end if

33:

Continuing ...

```
34: depth ← depth + 1
35: medianNode.left ← FINDFIRSTNODES(leftPoints, length, myaxis, dim, depth, rank)
36: #pragma omp task
37: depth ← depth + 1
38: medianNode.right ← FINDFIRSTNODES(rightPoints, length, myaxis, dim, depth, rank)
39: return treeNode
40: end function
```

4 Performance model and scaling

Measurements for speedup and efficiency graphs are used to acquire an indication of how well the implementation is performing in regard to some reference implementation. As reference, the corresponding serial execution of the code is used, on the same hardware.

4.1 Hardware

• Device: Tesla V100-PCIE-32GB

• Multiprocessors: 48

• CUDA Cores/MP: 64

• Maximum number of threads per MP: 2048, per block 1028

4.2 Parallel speed-up

In order to compute the parallel speed-up of the implementation, the following formula is used:

$$S(P) = T(1)/T(P) \tag{1}$$

, where T(1) is the serial execution time, and T(P) is the parallel execution time of the same problem size, with P tasks.

4.3 Strong scaling

Parallel efficiency, also referred to as strong scaling, is calculated by:

$$E(P) = S(P)/P \tag{2}$$

When S(P) = P it is considered a perfect speed-up. This in "real-life" is not a goal, since the code usually has parts that need to execute in a serial fashion. Ahmdal hence defined a way to model these more common, realistic implementations:

$$Sahm(P) = 1/(s + (p/N)) \tag{3}$$

In case of the above described implementation, the purely serial part (s) is the initialization of the array of nodes. Furthermore, a show-stopper to a full parallelization is the part where rank 0 computes the nodes up until a certain level of the tree.

4.4 Weak scaling

Gustafson pointed out, that in practice the sizes of problems scale with the amount of available resources. This is called weak scaling, where the scaled speedup is calculated based on the amount of work done for a scaled problem size (in contrast to Amdahls law which focuses on fixed problem size).

$$Sgus(P) = s + pN \tag{4}$$

4.5 Thread equilibrium for Hybrid solution

To understand better the optimal number of threads to be used for the hybrid approach, further analysis is needed. Using for the purpose the OpenMP function omp_get_wtime .

5 Conclusion

OpenMPI strategy could have been used to find the pivot element. In that case, rank 0 would have scattered the sections to the ranks, the ranks would have computed the insertion sort, to then send back their medians to rank 0, rank 0 gathering them.