CS601: Software Development for Scientific Computing

Autumn 2021

Week12:

N-Body problems and Hierarchical Methods

Course Progress..

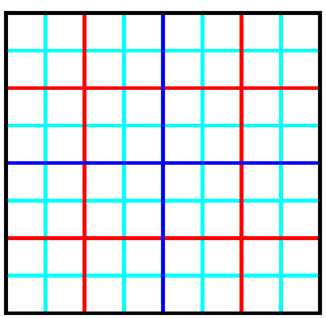
- Particle (Simulation) Methods / N-Body Problems
  - PP, PM, P3M.
  - Hierarchical Methods
    - Tree-based codes

      - Preliminaries – Metric Trees

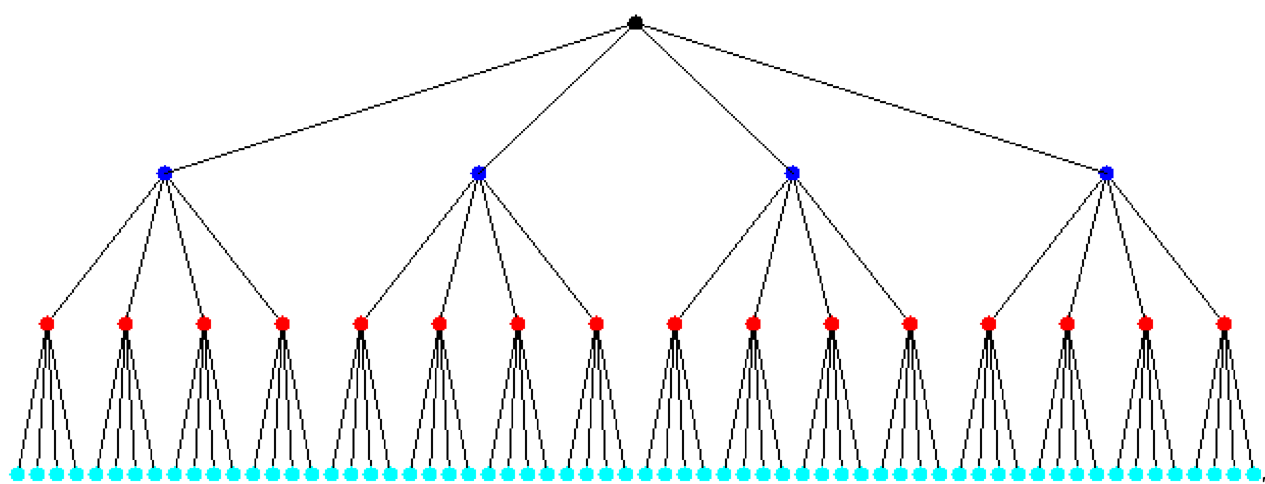
      - Quad Trees
- Applications:
  - Fluid Dynamics, Electromagnetics, Molecular Dynamics, Statistics, Astrophysics etc.

Quad Tree

- Data structure to subdivide the plane
  - Nodes can contain coordinates of center of box, side length.
  - Eventually also coordinates of CM, total mass, etc.
- In a complete quad tree, each non-leaf node has 4 children



A Complete Quadtree with 4 Levels



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Using Quad Tree and Octree

1. Begin by constructing a tree to hold all the particles
   – Interesting cases have nonuniformly distributed particles
   – In a complete tree most nodes would be empty, a waste of space and time
   – Adaptive Quad (Oct) Tree only subdivides space where particles are located
2. For each particle, traverse the tree to compute force on it

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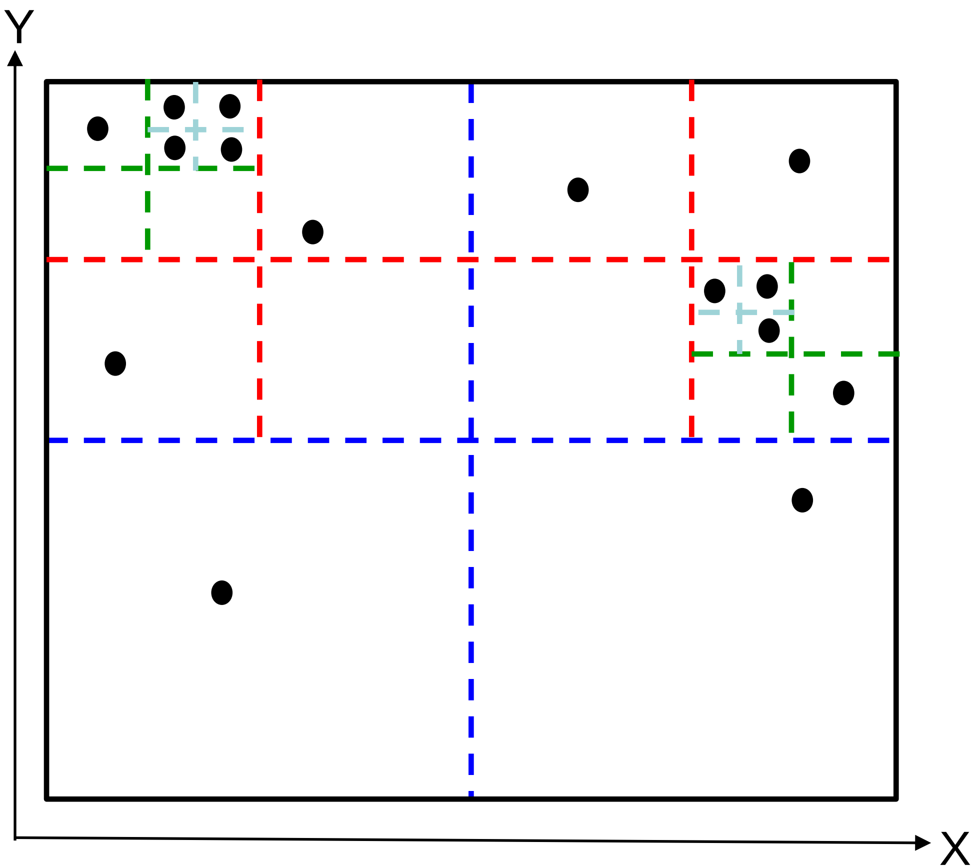
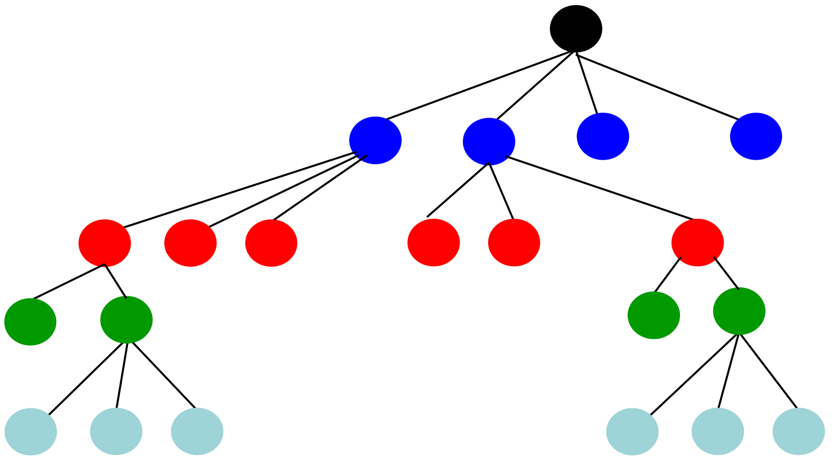
Adaptive Quad Tree





- In practice, #particles/square > 1. tuning parameter
- Child nodes numbered as per *Z-order numbering*

Adaptive Quad Tree Construction

```
Procedure Quad_Tree_Build
   Quad_Tree = {emtpy}
   for j = 1 to N                              … loop over all N particles
      Quad_Tree_Insert(j, root)                  … insert particle j in QuadTree
   endfor
   …   At this point, each leaf of Quad_Tree will have 0 or 1 particles
   …   There will be 0 particles when some sibling has 1
   Traverse the Quad_Tree eliminating empty leaves  … via, say Breadth First Search

Procedure Quad_Tree_Insert(j, n)  … Try to insert particle j at node n in Quad_Tree
   if n an internal node                  … n has 4 children
      - determine which child c of node n contains particle j
      - Quad_Tree_Insert(j, c)
   else if n contains 1 particle   …  n is a leaf
      - add n's 4 children to the Quad_Tree
      - move the particle already in n into the child containing it
      - let c be the child of n containing j
      - Quad_Tree_Insert(j, c)
   else                                   …  n empty
      - store particle j in node n
   end
```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Adaptive Quad Tree Construction – Cost?

```
Procedure Quad_Tree_Build
   Quad_Tree = {emtpy}                        ≤ N *max cost of Quad_Tree_Insert
   for j = 1 to N                          … loop over all N particles
       Quad_Tree_Insert(j, root)           … insert particle j in QuadTree
   endfor
   …  At this point, each leaf of Quad_Tree will have 0 or 1 particles
   …  There will be 0 particles when some sibling has 1
   Traverse the Quad_Tree eliminating empty leaves  … via, say Breadth First Search
```

```
Procedure Quad_Tree_Insert(j, n) … Try to insert particle j at node n in Quad_Tree
   if n an internal node            … n has 4 children
      - determine which child c of node n contains particle j
      - Quad_Tree_Insert(j, c)
   else if n contains 1 particle    … n is a leaf
      - add n's 4 children to the Quad_Tree
      - move the particle already in n into the child containing it
      - let c be the child of n containing j
      - Quad_Tree_Insert(j, c)                    ≤ max depth of Quad Tree
   else                             … n empty
      - store particle j in node n
   end
```


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Adaptive Quad Tree Construction – Cost?

- Max Depth of Tree:
  - For uniformly distributed points?
  - For arbitrarily distributed points?

- Total Cost = ?

Adaptive Quad Tree Construction – Cost?

- Max Depth of Tree:
  - For uniformly distributed points? = O(log N)
  - For arbitrarily distributed points? = O(bN)
    - b is number bits used to represent the coordinates

- Total Cost = $O(\,b\,N)$ or $O(N * \log N)$

Barnes-Hut

- Simplest hierarchical method for N-Body simulation
  - "A Hierarchical O(n log n) force calculation algorithm" by J. Barnes and P. Hut, Nature, v. 324, December 1986
- Widely used in astrophysics
- Accuracy $\geq$ 1% (good when low accuracy is desired/acceptable. Often the case in astrophysics simulations.)

Barnes-Hut: Algorithm

(2D for simplicity)

1) Build the QuadTree using QuadTreeBuild
   … already described, cost = O(N log N) or O(b N)

2) For each node/subsquare in the QuadTree, compute the
   Center of Mass (CM) and total mass (TM) of all the particles it contains.

3) For each particle, traverse the QuadTree to compute the force on it,

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Barnes-Hut: Algorithm (step 2)

Goal: Compute the Center of Mass (CM) and Total Mass (TM) of all the particles in each node of the QuadTree. (TM, CM) = Compute_Mass(root)

```
(TM, CM)  = Compute_Mass( n )    //compute the CM and TM of node n
   if n contains 1 particle
        //TM and CM are identical to the particle's mass and location
        store (TM, CM) at n
        return (TM, CM)
  else
     for each child c(j) of n  //j = 1,2,3,4
           ( TM(j), CM(j) ) = Compute_Mass( c(j) )
     endfor
     TM = TM(1) + TM(2) + TM(3) + TM(4)
     //the total mass is the sum of the children's masses
     CM = ( TM(1)*CM(1) + TM(2)*CM(2) + TM(3)*CM(3) + TM(4)*CM(4) ) / TM
     //the CM is the mass-weighted sum of the children's centers of mass
     store ( TM, CM ) at n
     return ( TM, CM )
  end if
```


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Barnes-Hut: Algorithm (step 2 cost)

(2D for simplicity)

1) Build the QuadTree using QuadTreeBuild
   … already described, cost = O(N log N) or O(b N)

2) For each node/subsquare in the QuadTree, compute the
   Center of Mass (CM) and total mass (TM) of all the particles it contains.
   … cost = O(number of nodes in the tree) = O(N log N) or O(b N)

3) For each particle, traverse the QuadTree to compute the force on it,

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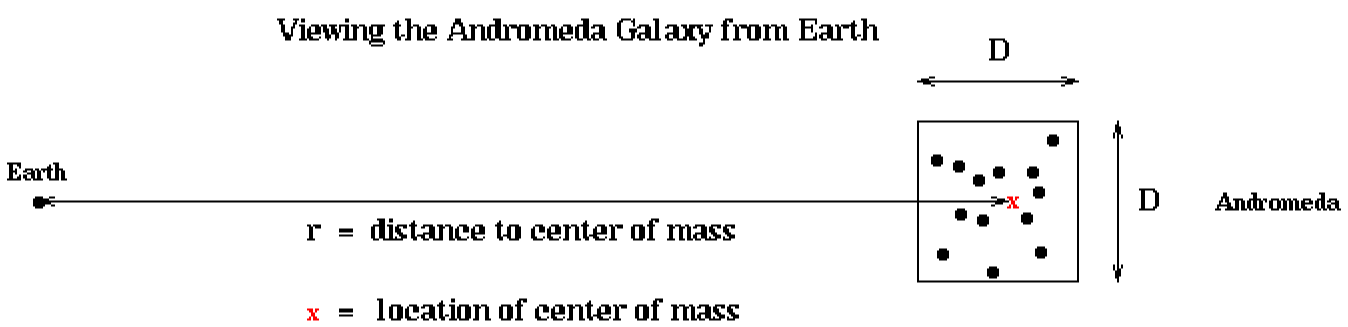
Barnes-Hut: Algorithm (step 3)

Goal: Compute the force on each particle by traversing the tree. For each particle, use as few nodes as possible to compute force, subject to accuracy constraint.

- For each node = square, can approximate force on particles outside the node due to particles inside node by using the node's CM and TM
- This will be accurate enough if the node if "far away enough" from the particle
- Need criterion to decide if a node is far enough from a particle
  - **D = side length of node**
  - **r = distance from particle to CM of node**
  - **θ = user supplied error tolerance < 1**
  - **Use CM and TM to approximate force of node on box if D/r < θ**



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Barnes-Hut: Algorithm (step 3)

```
//for each particle, traverse the QuadTree to compute the force on it
for k = 1 to N
    f(k) = TreeForce( k, root )
    //compute force on particle k due to all particles inside root (except k)
endfor
function f = TreeForce( k, n )
    //compute force on particle k due to all particles inside node n (except k)
    f = 0
    if n contains one particle (not k)  //evaluate directly
        return f = force computed using direct formula
    else
        r = distance from particle k to CM of particles in n
        D = size of n
        if  D/r  < q    //ok to approximate by CM and TM
             return f = computed approximately using CM and TM
        else                 //need to look inside node
             for each child c(j) of n //j=1,2,3,4
                   f = f + TreeForce ( k, c(j) )
             end for
             return f
        end if
    end if
```


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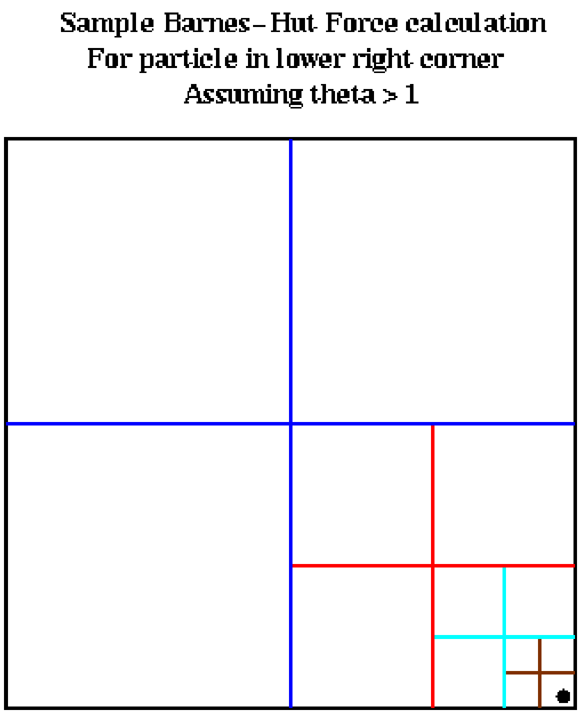
Barnes-Hut: Algorithm (step 3 cost)

- Correctness follows from recursive accumulation of force from each subtree
  - Each particle is accounted for exactly once, whether it is in a leaf or other node
- Complexity analysis
  - Cost of TreeForce(k, root) = O(depth in QuadTree of leaf containing k)
  - Proof by Example (for $\theta>1$):
  - For each undivided node = square, (except one containing k), $D/r < 1 < \theta$
  - There are at most 3 undivided nodes at each level of the QuadTree.
    - –There is O(1) work per node
    - –Cost = O(level of k)

Total cost = $O(\Sigma_k$ level of k) = O(N log N)

Strongly depends on θ



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Barnes-Hut: Algorithm (step 3 cost)

(2D for simplicity)

1) Build the QuadTree using QuadTreeBuild
   … already described, cost = O(N log N) or O(b N)

2) For each node/subsquare in the QuadTree, compute the
   Center of Mass (CM) and total mass (TM) of all the particles it contains.
   … cost = O(number of nodes in the tree) = O(N log N) or O(b N)

3) For each particle, traverse the QuadTree to compute the force on it,
   … cost depends on accuracy desired (θ) but still O(N log N) or O(bN)

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