A fast algorithm for identifying Friends-of-Friends halos

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Abstract

We describe a simple and fast algorithm for identifying friends-of-friends clusters and prove its correctness. The algorithm avoids unnecessary expensive neighbor queries, uses minimal memory overhead, and rejects slowdown in high over-density regions. We define our algorithm formally based on pair enumeration, a problem that has been heavily studied in fast 2-point correlation codes and our reference implementation employs a dual KD-tree correlation function code. We construct halos in a hierarchical merger tree, and use a splay operation to reduce the average cost of identifying the root of a cluster from $O[\log L]$ to $O[1]$ ($L$ is the size of a cluster) without additional memory costs. This reduces the overall time complexity of merging trees form $O[L \log L]$ to $O[L]$, reducing the number of operations per by orders of magnitude. We next introduce a pruning operation that skips pair enumeration between two fully self-connected KD-tree nodes. This improves the robustness of the algorithm, reducing cost of exploring to high density peaks from $O[\delta^2]$ to $O[\delta]$. We show that for cosmological data set the algorithm eliminates more than half of enumerations for typically used linking lengths $b \sim 0.2$, and empirically scales as $O[\log b]$ at large $b$ (linking length) limit. Furthermore, our algorithm is extremely simple and easy to implement on top of an existing pair enumeration code, reusing the optimization effort that has been invested in fast correlation function codes.

Keywords: cosmology, halo, cluster, simulation, algorithm, feature identification

1. Introduction

Friends-of-Friends clustering (FOF) is a common problem in cosmology for identifying features in density fields. Three common uses are 1) to find halos from N-body computer simulations in the 3-dimensional configuration space\cite{Davis,1985}; 2) to find sub structures inside halos from N-body computer simulations in the 6-dimensional phase space\cite{White,2010, Behroozi,2013}; and galaxy clusters from observational catalogs\cite{Murphy,2012} in the red-shifted configuration space.

Simply put, the problem is identifying the clusters of points that are (spatially) separated by a distance that is less than a threshold (linking length $b$) and assigning them a common label. A typical algorithm that solves this involves a breadth-first-search (henceforth BFS). During each visit of BFS, a neighbor query returns all of the particles within the linking length of a given particle. The cluster label of these neighbors are examined and updated, and the neighbors whose labels are modified are appended to the search queue for a revisit. The first description of the friends-of-friends algorithm with breadth-first-search in the context of astrophysics following this paradigm is by\cite{Geller,1983}. A popular implementation is by \textit{Nbody-Shop}\cite{Bryan,2014}, and more recently by\cite{Koda,2016}.

Another widely used algorithm creates the friends-of-friends clusters by hierarchical merging\cite{Springel,2005}. This was originally used for parallelization on large distributed computer architectures, as it allows a very large concurrency with a simple decomposition of the problem onto spatially disjoint domains. Hence it is implemented in the popular simulation software GADGET-2 and variants, including AMR codes such ENZO\cite{Bryan,2014}, but probably existed long before. To improve upon spatial queries, GADGET incrementally increase the linking length with multiple iterations. During each iteration, the algorithm performs a neighbor query on a selected set of points, and merges the proto-clusters hosting these points by updating the labels of all constituent points of these two proto-clusters. The iterations are repeated till no additional merging is possible.

In the GADGET implementation, the proto-clusters are maintained as a series of linked lists. During a merge operation, the shorter linked list is traversed and the tail pointer are updated to the tail pointer of the longer tree. Two additional storage spaces of $O[N]$ are required to keep track of the size of proto-clusters and the threading linked list. The traverse (important to maintain the invariant properties of tail pointers) increases the cost to merge a cluster of length $L$ to $O[L \log L]$, which can be a factor of a few more than optimal in terms of wall clock time. This
short-coming of a linked list representation is discussed in detail in [Cormen et al., 2009].

Due to these multiple traversals of the data, each making many expensive spatial queries (that slows down significantly as over-density grows) required in the existing algorithms, FOF has been generally considered a slow algorithm. As a result, algorithms that leads to exact solution are rarely discussed in any detail in the literature of cosmology and astrophysics, while numerous approximated FOFs have been proposed as better alternatives to trade the speed with accuracy, some with more desirable physical characters (e.g. avoid bridging). The general idea of these approximated methods is that accurately tracking the outskirts of halos (clusters) is not important as it is already dominated by shot-noise in the numerical scheme of solvers. A few examples are improving the speed by using density information [Eisenstein and Hut 1998], stochastic sub-sampling [Liu et al., 2008], and a relaxed linking length [Nbody-Shop a].

Conceptually the FOF problem of cosmology is the same as a well known problem of computer science— that of identifying the maximum connected components (MCC) from a graph, where the graph is induced from the data set with an adjacent matrix

$$A(i, j) = \begin{cases} 0, & \text{Dist}(i, j) > b \\ 1, & \text{Dist}(i, j) \leq b, \end{cases}$$

where $b$ is the linking length. Put differently, if there is a path between two points, then they belong to the same cluster, which are represented by a disjoint set. This problem is well studied and has a wide range of applications beyond the field of astrophysics. Numerous example implementations are freely available on the internet. (e.g. Shun and Blelloch [2013].

In this paper we apply well known data structures and algorithms from computer science to derive a fast exact friends-of-friends algorithm that avoids expensive neighbor queries, uses minimal memory overhead, and rejects over-density slow down.

Our main inspiration is from the dual-tree algorithm introduced by [Moore et al., 2001]. The dual-tree algorithm efficiently calculates correlation functions by walking two spatial index trees simultaneously and avoids expensive and unnecessary neighbor queries. We use KD-Tree in the example implementation, though this can be replaced with a ball-tree for higher dimensional data and a chaining mesh for low dimensional data to achieve better performance. (for latter, see [Sinha 2016].) Most importantly, dual-tree algorithm calculates the correlation function with a single traversal of the data, and we make use of this cost-reduction by expressing FOF algorithm in terms of pair enumeration.

While it is difficult to rewrite the breadth-first-search algorithm with pair enumerations, we realize that the hierarchical merging algorithm is not affected by the ordering of occurrence of pairs. The main issue in the hierarchical merging algorithm, as pointed above, is the costly merging of clusters. We address this by representing the clusters with a tree/forest data structure, and apply a splay operation in the merge procedure, which moves recently accessed nodes closer to the root, accelerating root finding operations in the average case [Cormen et al., 2009]. This reduces the average case complexity to construct a final cluster of length $L$ to $O(L)$ (as compared to $O(L \log L)$ with a linked list, as implemented in GADGET). It also eliminates the need to use additional $O[N]$ storage space for threading and balancing, resulting an extremely simple implementation. For completeness, we give an intuitive proof of finding correct solution with a single pass of pair enumeration with the splay tree data structure.

To further speed up our algorithm, especially in case of heavily over dense region where spatial queries become increasingly expensive (scaling as $O((1 + \delta)b^2)$ where $b$ is the linking length and $\delta$ is the over density), we implement another important optimization. We show that if two KD-Tree nodes (proto-clusters) are known to be fully-connected, the nodes need not be further opened and their respective hosting proto-clusters can be directly merged. This optimization basically eliminates the pair enumeration in dense region and is particularly relevant in high resolution simulations that resolves Kpc scale structures and over-density peaks of $\delta \gg 10^3$ (if we push high resolution simulations such as Hopkins et al., 2014 to a cosmological volume), though even for current generation of simulations it already gives a near 50% reduction in the number of pairs enumerated. We will prove the correctness of this optimization.

The algorithm can be directly applied as the local part of a parallel friend of friend halo finding routine. Our implementation of the algorithm is available at [https://github.com/rainwoodman/kdcount/blob/master/kdcount/kd_fof.c]. We note that our reference dual tree pair enumeration code is not particularly optimized for performance, and hence we rather focus on the theoretical aspects of the algorithm and optimizations in this work. One can easily port these optimizations to existing highly optimized fast correlation function codes to further improve the performance of FOF halo identification on actually problems.

The paper is organized as the following: in Section 2, we define the plain dual-tree friends-for-friends algorithm and prove its correctness; in Section 3, we will discuss the optimization; in Section 4, we perform scaling tests of the algorithm on two realistic cosmological simulation data sets.

2. Dual tree Friends-of-Friends algorithm

In this section, we describe our main algorithm, which is based on walking simultaneously two KD-trees that spatially indexes the data set being analyzed.
Definition 1. We define a KD-Tree with $M$ nodes as a tuple of \((L[0 : M], R[0 : M], P[0 : M])\), where \(L[m]\) is the left child of \(m\), \(R[m]\) is the right child of \(m\), and \(P[m]\) is the list of points contained by \(m\). Several operations are also defined, such as \(\text{Dist}(i,j)\) \(\equiv\) distance between \(i\)-th and \(j\)-th point in the dataset, \(\text{MinDist}(m,n)/\text{MaxDist}(m,n)\) \(\equiv\) minimal / maximal distance between \(m\)-th and \(n\)-th node. We also follow the convention that \(0\)-th node is the root node.

The FOF algorithm is based on pair enumeration and therefore we first briefly review the relevant pieces of the pair enumeration algorithm for clarity and completeness.

2.1. Pair enumeration with KD-Tree

Although the dual tree pair enumeration algorithm formally starts from two trees, we follow the auto-correlation scenario described in [Moore et al., 2001] and set both starting location to the root node of the KD-Tree. Here, we simply give an outline of the algorithm and refer the readers to the original reference [Moore et al., 2001] for proofs and detailed discussions.

The pseudo code in Algorithm 1 describes the operation \(\text{enum}(m, n, b)\) that returns a list of all pairs of data points that are maximally separated by distance \(b\) and contained in \(m\)-th and \(n\)-th nodes.

Algorithm 1 \(\text{enum}\): enumerate the edges that connect a pair of particles with distance less than \(b\) with the dual tree method on tree \((L, R, P)\). We have written it as a generative function that yields the pairs to emphasize that the full list does not need to be saved in memory.

\[
\text{procedure } \text{ENUM}(L, R, P, m, n, b) \!
\begin{align*}
&\text{if } m \text{ is a leaf then} \\
&\quad \text{Swap } m \text{ and } n \\
&\text{end if} \\
&\text{if } \text{MaxDist}(m,n) < b \text{ or } m \text{ is a leaf then} \\
&\quad \text{for all } i \in P[m], j \in P[n] \text{ do} \\
&\quad\quad \text{if } \text{Dist}(i,j) < b \text{ then} \\
&\quad\quad\quad \text{yield } i, j \\
&\quad\text{end if} \\
&\quad\text{end for} \\
&\text{else} \\
&\quad \text{if } \text{MinDist}(m,n) < b \text{ then } \text{\triangledown Ignore the nodes that are too far apart}. \\
&\quad \quad \text{yield all } \text{enum}(L, R, P, L[m], n, b) \\
&\quad \quad \text{yield all } \text{enum}(L, R, P, R[m], n, b) \\
&\quad \text{end if} \\
&\text{end if} \\
\end{align*}
\]

2.2. Friends-of-friends with pair enumeration

Next we describe the dual tree friends-of-friends algorithm. In addition to the data structures spatially indexing the data points, this algorithm requires us to maintain (both as an output and as a scratch space) an associated array storing the labels of the (proto-) clusters the given point belongs to.

Definition 2. We define an array \(H[0 : N]\) to represent friends-of-friends clusters, where \(N\) is the number of points in the data set. If \(p\) is the parent of \(i\), we set \(H[i] = p\). The root of a (proto-)cluster satisfies \(H[r] = r\) and thus acts as the label of the (proto-)cluster.

\(H\) thus defines a forest and we can find the root \(r_i = \text{root}(i)\) of the proto cluster hosting \(i\) by back-tracking in \(H\). Since the root acts as the label of the proto-cluster, merging two proto-clusters with root \(r_i, r_j\) is done by setting \(H[r_i] = r_j\).

Given the definition of \(H\) and the pair enumeration algorithm, we are ready to describe our friends-of-friends algorithm. The algorithm consists of three steps:

1. At the beginning of the algorithm, we initialize \(H[i] = i\), such that each point forms a proto-cluster of size 1 containing the point itself.
2. For each pair \((i, j)\) yielded by the pair enumeration algorithm (and hence is closer than the linking length \(b\) \(\Rightarrow\) belong to the same proto-cluster), we find the roots for \(i\) and \(j\), \(r_i, r_j\) by backtracking in \(H\) and merge the two proto-clusters.
3. At the end of the algorithm, set \(H[i] = r_i\).

However, this naive way of merging proto-clusters leads to very deep sub-trees with increasingly expensive root-query by back-tracking in \(H\). For instance, to merge a proto-cluster of length \(l\), the root-query takes \(O(l)\) time and thus doing this for all the \(L\) particles to generate a length \(L\) cluster, in worst case, can take up to \(O(L^2)\) time.

To motivate our splay optimization further, we re-iterate here that linked list implementation of FOF algorithms (as done in GADGET) overcomes this by keeping track of size of proto-cluster and during merge operation, it traverses the shorter tree and merges all its leaves directly to the root of longer tree \((H[k] \Leftarrow r_j\) such that root \((k) = \text{root}(i))\). This makes the root-query of \(O(1)\). However, since the shorter array needs to be traversed to update labels, the overall time complexity to merge a size \(L\) tree reduces only to \(O(L \log L)\). This can be seen by considering that at every stage, the size of the shorter tree (whose labels \(H[i]\) are changed) is at least doubled. Thus, for any point \(i\) in the cluster of size \(L\), the maximum number of times its labels change is \(\log L\) and thus for all \(L\) points, time taken is \(O(L \log L)\). (Also discussed in Cormen et al. [2009])

2.3. Optimization with splay

We augment the merge procedure of root(i) with a splay operation that reattaches i itself as a direct child of the root \(r_i\) by setting \(H[i] = r_i\). This decreases the depth of \(i\), while maintaining root(i) invariant. After a splay, complexity of sequential queries to root(i) is reduced to \(O[1]\). Put in simpler terms, we do not ensure that every
leaf of the smaller proto-cluster becomes a direct leaf of the root of the bigger cluster (like GADGET linked list implementation above), but we maintain that the last accessed point becomes a direct leaf of the root. What we are exploiting here is that a pair enumeration visits the same point many times, and hence this reduction implies that the average depth of the merger tree is $O[1]$. However, we realize that for a malicious data set, this optimization can instead lead to significantly worse results.

The hierarchical merging tree $H$ is unbalanced, and can reduce to a linked list. For example, consider the final step where we need to update $H[i]$ to root$(i)$ for all points in the data set. If the tree is reduced to a linked list, and the iteration starts from the deepest point, the complexity becomes $O[N^2]$.

Therefore, we also advocate a safe guard operation during splay, by reattaching every parent accessed while back-tracing $H[i]$ as an immediate child of the root. This does not change the scaling of the root tracing and splay operation, but improves the reduction in the depth of the merger tree. The complexity of previous malicious example drops from $O(N^2)$ to $O[N]$. In fact, it can be show that the average time complexity to form a cluster of length $L$ in any data set for this algorithm is $O[Lo(L)]$ where $\alpha$ is a slowly increasing function, upper bounded by $4$. (Couch et al. 2009). The splay operation thus achieves $O[L]$ complexity without adding additional book-keeping cost in space and time. We find that for cosmological data set, enabling the guard indeed bounds the average depth of the tree closer to $O[1]$, though disabling the safe guard gives slightly (5%) better performance. We refer the reader to Figure 1 in Section 4 for more discussion on the issue.

The pseudo-code for our FOF algorithm along with the splay optimization is listed in Algorithm 2. For completeness, we include a proof in the appendix that the pair enumeration algorithm indeed gives correct solution.

### 3. Optimization for fully-connected KD-tree nodes

The pair enumeration algorithm produces a large number of pairs in highly over-dense regions such as the cores of halos. We can write down the total number of pairs in a cell of size $b$ (linking length) per side with an over-density of $\delta$,

$$N_{op} = [b^3/(1 + \delta)]^2.$$  \hspace{1cm} (1)

$N_{op}$ can be huge. For example, a typical halo profile predicts an over-density of $\delta \sim 10^6$ at 1 Kpc (e.g. Martizzi et al. 2012). In a high resolution simulation that resolves sub Kpc structures, a typical length of $b = 0.2$ leads to $N_{op} \sim 10^{12}$ operations inside the cell. Often, this becomes the most expensive part of the computation. However here, we argue that it is possible to eliminate almost all of the edge enumeration in very dense regions. For this, we begin with the definition of self-connectedness and neighbors.

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**Algorithm 2** Dual tree Friends-of-Friends with splay.

**Ensure:** $H[i] = H[j]$ if $i$ and $j$ belongs to the same FOF halo.

**procedure** splay($H, i$)  
find the subtree root $r$ of a particle $i$, and reattach the particle as an immediate leaf of the root.

while $H[r] \neq r$ do

$r \leftarrow H[r]$  
end while  

return $H[i] \leftarrow r$

**end procedure**

**procedure** merge($H, i, j$)  
merge the two subtrees containing $i$ and $j$ respectively

$r \leftarrow \text{splay}(H, i)$

$s \leftarrow \text{splay}(H, j)$

$H[r] \leftarrow s$

**end procedure**

**procedure** fof($H, L, R, P, b$)

$H[0 : N] \leftarrow 0 \ldots N - 1$

for all $i, j \in \text{enum}(L, R, P, 0, 0, b)$ do

merge($H$, $i, j$)

end for

for $i \in 0 \ldots N - 1$ do

splay($H, i$)

end for

**end procedure**
**Definition 3.** A KD-Tree node is **self-connected** when the node $m$ is smaller than the linking length $b$, $\maxDist(m,m) < b$.

**Definition 4.** Two nodes $m$ and $n$ are neighboring if and only if

$$\minDist(m,n) = \min_{i \in P[m], j \in P[n]} \Dist(i,j) < b.$$ 

If a node $m$ is self-connected, then any pair of points $(i,j) \in P[m]$ is separated by at most the linking length $b$. The set of points in $P[m]$, or alternatively node $m$, forms a proto-cluster. This proto-cluster can be quickly created by enumerating the points, at a cost of $O(b^3(1+\delta))$. This motivates our optimization in **Theorem 1**.

**Theorem 1.** Visiting and merging an arbitrary single pair from two neighboring self-connected nodes is equivalent to visiting and merging all pairs. We can therefore visit only the first pair.

**Proof.** Consider the case when two self-connected nodes $m$, $n$ are neighboring. By definition, there exists a pair $(i,j)$ such that $\Dist(i,j) < b$ and $i \in P[m]$, $j \in P[n]$. Because the nodes $m$ and $n$ are fully connected, $r_u = r_i$ for any $u \in P[m]$, and $r_v = r_j$ for any $v \in P[n]$. Hence, regardless the pair $u,v$ that is visited, $r_i$ and $r_j$ are the only proto-clusters that are merged. Therefore, regardless of merging an arbitrary single pair $u,v$, or all pairs of the two proto-halos, $r_i$ and $r_j$ (and only) are merged. 

Thus, in our optimized algorithm, we first initialize proto-clusters of all self-connected nodes before the pair enumeration. We then perform a modified pair enumeration, where most pairs of two neighboring are skipped. We describe the optimized algorithm in Algorithm 3 and 4. Due to **Theorem 1** the optimization does not alter the result of the original algorithm.

### 4. Benchmarks

In this section we show the performance of our algorithm on two cosmological simulation data sets, each with a total of 16 million points.

Low A FastPM Simulation in a box of 100 Mpc/h per side with $256^3$ particles. FastPM is a Particle Mesh cosmological simulation code. ([Feng et al., 2016](#))

High An NyX Simulation in a box of 10 Mpc/h per side with $256^3$ particles. NyX is an AMR cosmological simulation code. ([Almgren et al., 2013](#))

The tests are performed with a single computing core on a computing node of the Cray XC-30 super-computer Edison at National Energy Research Scientific Computing Center. For each simulation, we perform two sets of runs: one with and one without the safe-guard operation. We

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**Algorithm 3** Pair enumeration aware of self-connected nodes.

```javascript
procedure CONNECT(H, P, F, m, b, f)
if f == 0 then
    if \text{dist}(m) < b then
        for all $i \in P[m]$ do
            $H[i] \leftarrow P[m][0]$
        end for
        $F[m] \leftarrow 1$
    end if
    else \triangleright m must be self-connected because the parent
    $F[m] \leftarrow 1$
end if
CONNECT(H, P, F, m=L[m], b, f=F[m])
CONNECT(H, P, F, m=R[m], b, f=F[m])
end procedure
```

**Algorithm 4** Friends-of-friends algorithm avoiding self-connected nodes.

**Ensure:** $H[i] = H[j]$ if $i$ and $j$ belongs to the same FOF halo.

```javascript
procedure FOFP2(H, F, T, b)
$H[0 : N] \leftarrow 0 \ldots N - 1$
$F[0 : \text{LEN}(T)] \leftarrow 0$
CONNECT($H, P, F, m = 0, b, f = 0$)
for all $i, j \in \text{ENUM2}(H, L, R, P, F, m = 0, n = 0, b)$
do
    MERGE($H, i, j$)
end for
for $i \in 0 \ldots N - 1$ do
    SPLAY($H, i$)
end for
end procedure
```
use 10 different linking lengths, spanning from 0.01 to 1.0 in units of the mean particle separation.

The main results are shown in Figure 1. Our algorithm shows robust performance: when the resolution (inverse of mean particle separation) increases by a factor of 10, the wall clock time increases only by a factor of 30 percent. The scaling of wall clock time against linking length appears to be asymptotically logarithmic.

We empirically confirm that the safe guard operation reduces the average depth of the hierarchical merger tree. Without the safe guard operation, both data set gives depths of $3 \sim 4$ at the limit of large linking length (which results larger clusters). With the safe guard, the average depth is bound to slightly more than 2.0. However, the safe guarded version performs slightly slower for most cases because it doubles the cost of a splay operation.

In Figure 2, we investigate the performance due to the choice of representation of the proto-cluster data structure. We compare our algorithm with a splay tree against the linked list data structure (which is used in GADGET-2). For short linking length $b < 0.1$ where most resulted clusters are small, the algorithms showed little difference, since the time spent in maintaining the hierarchy is negligible. However, as the size of the clusters increase with $b$, the number of visits to the linked list per merge operation increases rapidly to the order of hundreds, while the number of visits to the splay tree remains almost a constant up to a few (also seen in the right panel of Figure 1). As a result, the linked list representation performs considerably worse than the splay tree as the clusters grow. For the low resolution test data set we used, when $b > 0.4$, the size of the largest halo increases to more than 5 million points, and the computation of the linked list code could not finish in 20 minutes; while the splay tree representation finished in less than 50 seconds. We expect the difference to be more drastic in data sets with even larger halos.

In Figure 3, we show that as the linking length increases, the self-connected optimization reduces the number of pair enumerations by a large fraction. At linking length of 0.2, the reduction rate is a factor of $\sim 0.5$ on both data sets. For extremely large data set, the reduction rate approaches 1, which could be the reason for the logarithmic asymptotic behavior at large linking length we observe in the left panel of Figure 1.

Finally, our base implementation of the KD-Tree pair enumeration emphasizes on clarity rather than performance, even though this implementation is already quite fast: for linking length of 0.2, the algorithm takes close to 30 seconds to process 16 million points. These numbers are comparable to the amount of time spent in reading in the data and preparing the initial KD-Tree (6 seconds). There is a huge space for fine tuning, as our KD-Tree implementation is slightly slower than cKDTree in scipy, comparable to halotools (Hearin et al., 2016), twice slower than TreeCorr (Jarvis et al., 2004) and 20 times slower than CorrFunc, an amazingly fast chaining-mesh code (Sinha, 2016). We expect a large margin of improvement in speed by adapting a fine-tuned implementation for the base pair enumeration code.

5. Conclusion

We describe a fast algorithm for identifying friends-of-friends halos in cosmological data sets. The algorithm is defined on pair enumeration which visits all edges of the connected graph induced by the linking length and is constructed on a dual KD-tree correlation function code. We present two optimizations that significantly speed up the FOF algorithm - use of a splay tree and pruning the enumeration of self-connected KD-tree nodes - both of which can be very easily ported to any of the existing pair-enumeration codes.

We began by pointing out that the although the friends-and-friends problem is identical to the maximum connected component problem in graph theory, with spatial data such as a cosmological simulation, the elements of adjacent matrix are implied via expensive neighbor queries. Therefore, the dual-tree pair enumeration algorithm that we use is advantageous because it systematically eliminates expensive neighbor queries by tracking two tree nodes simultaneously.

We implement two important optimizations to improve the scaling and robustness of the algorithm for merging proto-clusters against input data. The first optimization is to append a splay operation to the root query in the hierarchical merger tree of proto-clusters. The splay operation significantly reduces the average number of traverses,
Figure 1: Benchmarks. We show the wall clock time and average depth of the merger tree as a function of linking length. Two data sets are used: the Low resolution FastPM simulation data set (black) and the high resolution NyX simulation data set (red). We show the benchmarks with and without the safe guard operation (dashed / solid) defined in Section 3. Left: wall clock time. Right: average depth of the merger tree.

Figure 2: Comparing splay tree and linked list implementation. Left: wall clock time. Right: average number of visits (operations) per merging with linked list / splay. Red crosses: linked list. (Runs with $b > 0.4$ did not finish in 20 minutes and are not presented). Black diamonds: splay tree (this work). Note that splay algorithm is already 30% faster than linked list at $b = 0.2$, where the number of visits is reduced by almost two orders of magnitude.
making root-query a $O[1]$ process, without requiring significant additional storage space. The second optimization is to skip pair enumerations while merging neighboring self-connected KD-Tree nodes. Reducing the number of pair enumerations significantly speeds up the algorithm in high-over-density regions and with large linking lengths. We also proved the correctness of this optimization. After these two optimizations we find that our algorithm reduces the number of operations for constructing friends of friends halos by almost two orders of magnitude comparing to a naive implementation with linked list for generally used linking lengths of $b = 0.2$.

We note that in our application, the time spent in local friends-of-friends finding becomes sub-dominant compared to the time in global merging of the catalog. We plan to investigate an optimal distributed algorithm by combining our algorithm with the fast distributed memory parallel algorithm by (e.g. Fu et al. 2010).

Finally, as an advantage due to insisting on constructing the algorithm with an abstract hierarchical pair enumeration operation, we expect further improvement of speed from our naive implementation by porting the algorithm to a highly optimized correlation function code beyond KD-Tree (e.g. Sinha 2016).

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References

References

Almgren, A.S., Bell, J.B., Lijewski, M.J., Lukić, Z., Van Andel, E., 2013. Nyx: A Massively Parallel AMR Code for Computational Cosmology. ApJ 765, 39. doi:10.1088/0004-637x/765/1/39

Behroozi, P.S., Wechsler, R.H., Wu, H.Y., 2013. The ROCKSTAR Phase-space Temporal Halo Finder and the Velocity Offsets of Cluster Cores. ApJ 762, 109. doi:10.1088/0004-637x/762/2/109

Bryan, G.L., Norman, M.L., O’Shea, B.W., Abel, T., Wise, J.H., Turk, M.J., Reynolds, D.R., Collins, D.C., Wang, P., Skillman, S.W., Smith, B., Harkness, R.P., Bordner, J., Kim, J.H., Kuhlen, M., Xu, H., Goldbaum, N., Hummels, C., Kritsuk, A.G., Tinker, E., Skory, S., Simpson, C.M., Hahn, O., Oishi, J.S., So, G.C., Zhao, F., Cen, R., Li, Y., Enzo Collaboration, 2014. ENZO: An Adaptive Mesh Refinement Code for Astrophysics. ApJS 211, 19. doi:10.1088/0067-0049/211/2/19

Cormen, T.H., Leiserson, C.E., Rivest, R.L., Stein, C., 2009. Introduction to Algorithms, Third Edition. 3rd ed., The MIT Press.

Davis, M., Efstathiou, G., Frenk, C.S., White, S.D.M., 1985. The evolution of large-scale structure in a universe dominated by cold dark matter. ApJ 292, 371–394. doi:10.1086/163168

Eisenstein, D.J., Hut, P., 1998. HOP: A New Group-Finding Algorithm for N-Body Simulations. ApJ 498, 137–142. doi:10.1086/305535

Feng, Y., Chu, M.Y., Seljak, U., 2016. FastPM: a new scheme for fast simulations of dark matter and halos. ArXiv e-prints

Fu, B., Ren, K., López, J., Fink, E., Gilson, G., 2010. Discﬁnder: A data-intensive scalable cluster finder for astrophysics, in: Proceedings of the 19th ACM International Symposium on High Performance Distributed Computing, ACM, New York, NY, USA, pp. 348–351. URL: http://doi.acm.org/10.1145/1851476.1851527

Geller, M.J., Huchra, J.P., 1983. Groups of galaxies. III - The CFA survey. ApJS 52, 61–87. doi:10.1086/190859

Hearin, A., Campbell, D., Tollerud, E., Behroozi, P., Diemer, B., Goldbaum, N.J., Jennings, E., Leauthaud, A., Mao, Y.Y., More, S., Parejko, J., Sinha, M., Sipocz, B., Zentner, A., 2016. High-Precision Forward Modeling of Large-Scale Structure: An open-source approach with Halotools. ArXiv e-prints

Hopkins, P.F., Kereš, D., Oñorbe, J., Faucher-Giguère, C.A., Quataert, E., Murray, N., Bullock, J.S., 2014. Galaxies on FIRE (Feedback In Realistic Environments): stellar feedback explains cosmologically inefficient star formation. MNRAS 445, 581–603. doi:10.1093/mnras/stu1738

Jarvis, M., Bernstein, G., Jain, B., 2004. The skewness of the aperture mass statistic. MNRAS 352, 335–352. doi:10.1111/j.1365-2966.2004.07926.x

Koda, J., Blake, C., Beutler, F., Kazin, E., Marin, F., 2016. Fast and accurate mock catalogue generation for low-mass galaxies. MNRAS 459, 2118–2129. doi:10.1093/mnras/stw763

Liu, H.B., Hsieh, B.C., Ho, P.T.P., Lin, L., Yan, R., 2008. A New Galaxy Group Finding Algorithm: Probability Friends-of-Friends. ApJ 681, 1046–1057. doi:10.1086/588183

Martizzi, D., Teyssier, R., Moore, B., Wentz, T., 2012. The effects of baryon physics, black holes and active galactic nucleus feedback on the mass distribution in clusters of galaxies. MNRAS 422, 3081–3091. doi:10.1111/j.1365-2966.2012.20879.x

Moore, A.W., Connolly, A.J., Genovese, C., Gray, A., Grone, L., Randic, I., Ran, C., Nichol, R.C., Schneider, J., Szalay, A.S., Szapudi, I., Wasserman, L., 2001. Fast Algorithms and Efﬁcient Statistics: N-Point Correlation Functions, in: Banday, A.J., Zaroubi, S., Bartelmann, M., (Eds.), Mining the Sky, p. 71. doi:10.1007/10849171_5

Murphy, D.N.A., Geach, J.E., Bower, R.G., 2012. ORCA: The Overdense Red-sequence Cluster Algorithm. MNRAS 420, 1861–1881. doi:10.1111/j.1365-2966.2011.19782.x

Noody-Shop, a. Approximated Friends-of-Friends. URL: http://www-hpcc.astro.washington.edu/tools/fof.html

Shun, J., Blelloch, G.E., 2013. Ligra: A lightweight graph processing framework for shared memory. SIGPLAN Not. 48, 135–146. URL: http://doi.acm.org/10.1145/2517327.2442530

Sinha, M., 2016. Corrfunc: Corrfunc-1.0.0. URL: http://dx.doi.org/10.5281/zenodo.55161

Springel, V., 2005. The cosmological simulation code GADGET-2. MNRAS 364, 1105–1134. doi:10.1111/j.1365-2966.2005.09655.x

White, M., Cohn, J.D., Smith, R., 2010. Cluster galaxy dynamics and the effects of large-scale environment. MNRAS 408, 1818–1834. doi:10.1111/j.1365-2966.2010.17248.x
Appendix A. Proof of the algorithm

Theorem 2 guarantees the algorithm finds a solution to the maximum connected component problem.

Theorem 2. The clusters in $H$ after the algorithm are fully connected and maximum: $H[i] = H[j]$ if and only if $i, j$ is connected by a path (belongs to the same cluster)

Proof. We first prove that if $\text{root}(i) = \text{root}(j)$, then $i$ and $j$ are connected. We can show this by induction. At the beginning of the algorithm, this is clearly true, since there is no $i \neq j$ such that $\text{root}(i) = \text{root}(j)$. Without losing generality we consider the case where a visit to $i, j$ sets $H[r_j] = r_i$, and the claim is true before the visit. Denote the points in the two old subtrees $A(r_i)$ and $A(r_j)$, then by the assumption, $A(r_i)$ is connected and $A(r_j)$ is connected. Because $i \in A(r_i), j \in A(r_j)$ and $i, j$ are connected, $A(r_i) \cup A(r_j)$ is also connected. Since $A(r_j)$ are the only points that has changed root, the algorithm maintains the invariant at each iteration. Note that the last step of the algorithm ensures $H[i] = \text{root}(i)$.

Next we prove that if $i$ and $j$ are connected, then $H[i] = H[j]$. We show this by contradiction. Assume there exists point $i$ and $k$, where $H[k] \neq H[i]$, and $\text{Dist}(i, k) < b$. Because any $(i, j)$ such that $\text{Dist}(i, j) < b$ has been visited, the pair $i, k$ must have been visited during the pair enumeration. A merge operation ensures $j = \text{root}(k) = \text{root}(i)$. Any later merge operations will only change the root of $j$. Thus $\text{root}(k) = \text{root}(j)$ from this point on till the end of enumeration, resulting $H[k] = H[i]$. The contradiction shows that there is no such pair $i, k$. Therefore every cluster we have identified is maximized.

Because every cluster is fully connected and maximized, the algorithm has identified all friends-of-friends clusters from the data set. ∎