A Highly Scalable Graph Clustering Library based on Parallel Union-Find

Karthik Senthil

Parallel Programming Laboratory
University of Illinois at Urbana-Champaign

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Problem Statement

Graph clustering or connectivity is the process of detecting connected components in a given graph

- **Connected component** : Maximal-size subgraph where a path exists between every pair of vertices in the subgraph

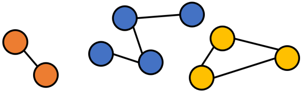

Figure 1: Connected components in a graph

Two schools of algorithms :

- Graph traversal algorithm
- Union-Find based algorithm

Outline

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1. Related Work
2. Parallel Union-Find in Charm++
3. Path Compression
4. Implementation
5. Performance Evaluation
6. What's In Store

Related Work

Connectivity in a graph is a well-studied problem

- Shiloach, Yossi, and Uzi Vishkin. “An O (logn) parallel connectivity algorithm.” Journal of Algorithms 3.1 (1982): 57-67.
- Nassimi, David, and Sartaj Sahni. “Finding connected components and connected ones on a mesh-connected parallel computer.” SIAM Journal on computing 9.4 (1980): 744-757.
- Krishnamurthy, A., Lumetta, S., Culler, D. E., & Yelick, K. (1997). “Connected components on distributed memory machines”. Third DIMACS Implementation Challenge, 30, 1-21.
- Manne, Fredrik, and Md Patwary. “A scalable parallel union-find algorithm for distributed memory computers.” Parallel Processing and Applied Mathematics (2010): 186-195.

Our motivation : A scalable parallel implementation using union-find data structures in a distributed asynchronous environment

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Algorithm

- Given a graph $G = (V, E)$, with $n = |V|$ and $m = |E|$
- An edge $e = (v_1, v_2)$ represents a union operation

Our algorithm:

1. Message v_1 for the operation $find(v_1)$
2. v_1 messages parents till $boss_1 = find(v_1)$
3. $boss_1$ messages v_2 for operation $find(v_2)$ and carries info of $boss_1$
4. When $boss_2 = find(v_2)$, align parent pointers of bosses

- Effectively we are constructing a forest of inverted trees; each tree is a unique connected component
- Root of a tree (boss) = Representative of the component

Algorithm

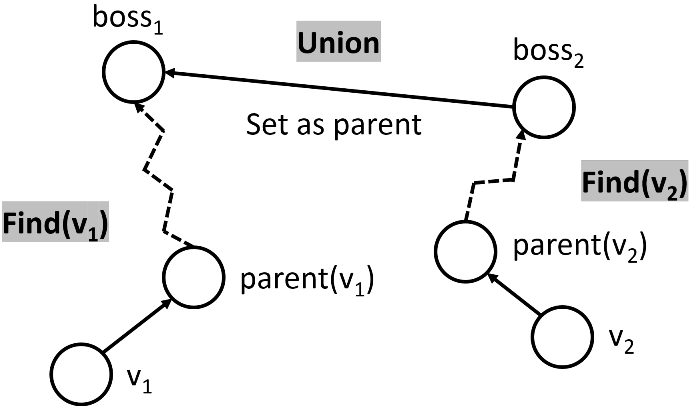
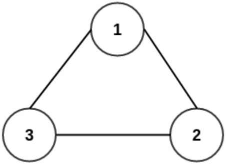


Figure 2: Asynchronous union-find algorithm

Solving Race Conditions



Consider 3 PEs, one chare on each PE

union(1, 2) on chare 0
union(2, 3) on chare 1
union(3, 1) on chare 2

An example scenario

- Enforce a strict ordering in the union operation based on vertex ID
- Brings in an additional min-heap like property to the inverted trees
  - ID of a parent node is always lesser than IDs of its children
  - A possible cycle edge can be detected if a node with lower ID is asked to point to node with higher ID

High Level Pseudo-Code

```
union_request($v_1$, $v_2$) {
    if ($v_1.ID$ > $v_2.ID$)
        union_request($v_2$, $v_1$)
    else
        find_boss1($v_1$, $v_2$)
}
```

Listing 1: union_request

```
find_boss1($v_1$, $v_2$) {
    if ($v_1.parent$ == -1)
        find_boss2($v_2$, $boss_1$)
    else
        find_boss1($v_1.parent$, $v_2$)
}
```

Listing 2: find_boss1

```
find_boss2($v_2$, $boss_1$) {
    if ($v_2.parent$ == -1) {
        if ($boss_1.ID$ > $v_2.ID$)
           union_request($v_2$, $boss_1$)
        else
           $v_2.parent$ = $boss_1$
    }
    else
        find_boss2($v_2.parent$, $boss_1$)
}
```

Listing 3: find_boss2

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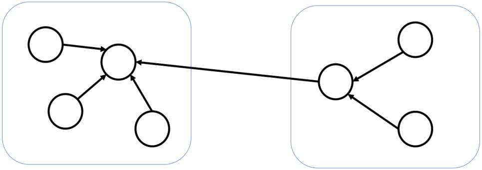
Local Path Compression

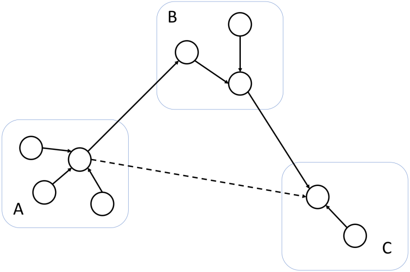
- Make the local subtree constructed in every chare completely shallow i.e. rooted star
- During **Find**, if next parent on current path is on a different chare then sequentially update parent pointer for all nodes on path



- Increases amount of sequential work per chare but greatly boosts speed of future Find operations

Global Path Compression

- Pointer jumping operation to grandparent
- Short circuits paths that are spanning across multiple chares



- Increases communication due to more messages, but overhead is reduced by aggregating messages using TRAM

Outline

Library Design

- Library designed using bound-array concept
- Connected components detection
  - **Phase 1** : Build the forest of inverted trees using our asynchronous union-find algorithm
  - **Phase 2** : Identify the bosses of each component and label all vertices in that component
  - **Phase 3** : Prune out insignificant components
- Used TRAM to aggregate all messages in Phase 1 and Phase 2
- Tested and verified with protein structures from RCSB PDB
- Large scale testing with synthetic and real-world graphs

Phase 3 - Discussion

- Perform a global reduction to gather membership statistics for each component from all the chares
- Initially implemented using a custom reducer with each chare contributing an `std::map`
- Reduced final map is broadcast and rebuilt on each PE (using a group)

Figure 3: Overheads in map-based reducers for Phase 3

Library Design - Updated

- **Phase 1** : Build the forest of inverted trees using our asynchronous union-find algorithm
- **Phase 2** :
  (a) Parallel prefix scan to get total boss count and relabel all bosses with sequential identifiers
  (b) Identify the bosses of each component and label all vertices in that component
- **Phase 3** : Prune out insignificant components
  - Use fixed size array based reduction for the counts
  - Arrays can be sparse, but this implementation is very scalable and has minimal overhead

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Experiments

Experiments performed:

1. Phase runtime evaluation
    - Mesh configurations : 1024^2 (1M), 2048^2 (4M), 4096^2 (16M), 8192^2 (64M)
    - Probabilities : 2D40, 2D60, 2D80
    - Problem size per chare fixed at : 128x128 mesh piece
2. Strong scaling performance
    - Mesh configuration : 8192^2 (64M), 16384^2 (256M), 2D60
    - Number of cores : 64, 256, 1024, 4096
3. Real world graphs
    - `com-Orkut` : 3M vertices, 117M edges
    - `com-Amazon` : 330K vertices, 925K edges

All experiments were performed on the Blue Waters (Cray XE) supercomputer maintained by NCSA.

Results - Phase Runtime

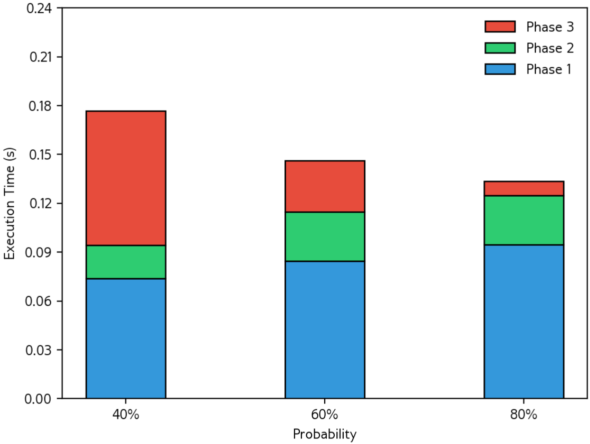


Figure 4: Mesh size 1024x1024 on 64 cores

Results - Phase Runtime

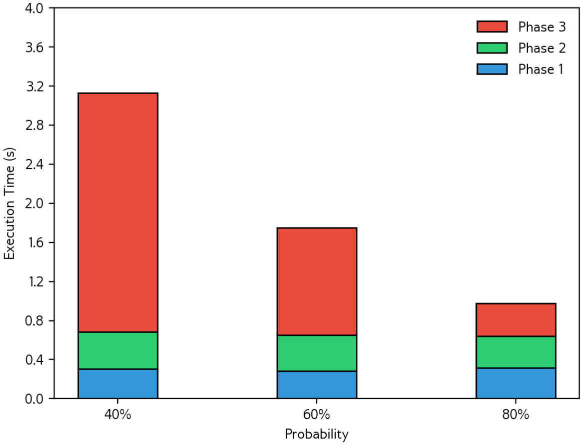
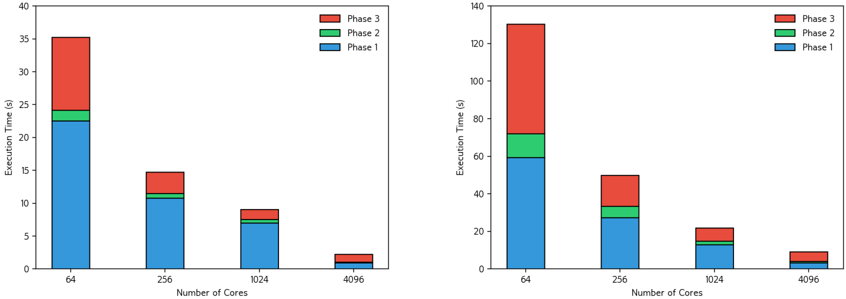


Figure 5: Mesh size 8192x8192 on 4096 cores

Results - Strong Scaling



Mesh 8192x8192

Mesh 16384x16384

Figure 6: Strong scaling runs

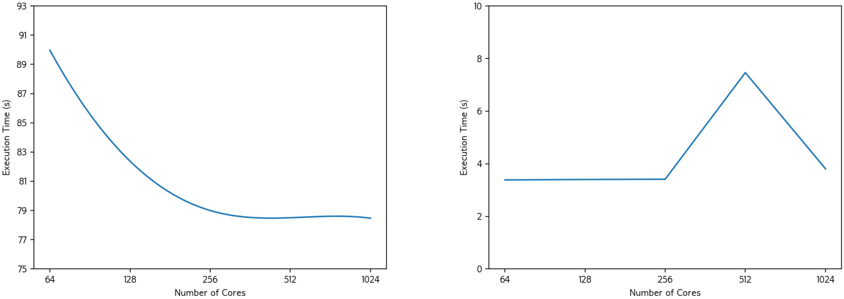
Comparison

Mesh Size	**Last Workshop**	**Current Workshop**
4096^2	113.730437 s	0.815045 s
8192^2	195.767054 s	1.749127 s
16384^2	NA	9.178887 s

Table 1: Improvements in performance

Kudos to path compression optimizations and TRAM!

Results - Real World Graphs



`com-Orkut` `com-Amazon`

Figure 7: Experiments with real world graphs

Current Issues

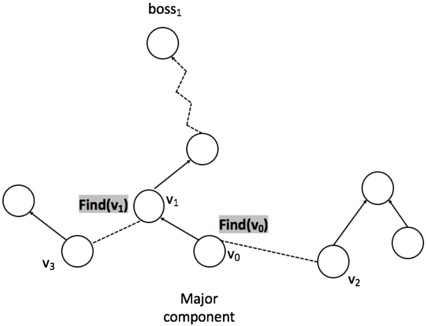


Figure 8: Bottleneck will be observed at $boss_1$ when edges (v_1, v_3) and (v_0, v_2) are processed during later stages of Phase 1

- Potential bottlenecks at the root of the biggest inverted tree for dense graphs with very few number of components
- Cases where component roots are unevenly distributed among the chares leading to load imbalance in Phase 2

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Future Work

On the to-do list:

- Optimizing Phase 1 to remove bottleneck and improve weak scalability
- Performance evaluation using large ChaNGa datasets
- Implement a Python interface for library using Charmpy

Code and examples on Gerrit: users/karthik/unionFind

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Thank You