Scalable Graph Algorithms for Cluster Finding

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ChaNGa (CHArm++ N-body GrAvity solver) is built as a Charm++ application that employs a tree algorithm to represent the simulation space.

Edges are discovered during tree traversals.

Cluster finding.

Component Pruning: Tinier components need to be deleted.
Connected components detection

Vertices:
{0, 1, 2, 3, 5, 6, 7, 8}

Edges:
(1, 3)
(2, 3)
(0, 3)

Connected components: 5

- Detect connected components.
- Label these components.
- Prune components (1).
Anchor Algorithm

- Each vertex has a parent.
- Union Operation: Edge (a, b) -> union (a, b)
- Challenge: To prevent race condition
- Anchor (hook-up):
  - a -> b ; if a > b
  - b -> a ; if b <= a
- Union operations are executed in parallel.
- Edges can be generated on any PE.
Parallel Union-Find (Cluster finding)

**Vertices:**

- 1
- 2
- 3
- 0
- 5
- 6
- 7
- 8

**Edges:**

- (1, 3)
  - Send a message to 3 to anchor itself to 1.
- (2, 3)
  - Send a message to 3 to anchor itself to 2.
  - But, 3 has a parent, so it sends a message to its parent (1) to anchor to 2 (tree climbing).
  - 1 sees that 2 is > than itself, so it in-turn sends a message to 2 to anchor itself to 1.
  - 2 obliges. (If 2 had a parent, the tree climbing would have happened here)
- (0, 3)
Parallel Union-Find (Cluster finding)

Components:

Phases:

Tree construction
Component Labeling
Pruning (ChaNGa specific)
Parallel Union-Find (Cluster finding)

Vertices:

Path compression

Local path compression: within PE

Global path compression
Parallel Union-Find (Cluster finding)

Problem: Too many messages clog the system.

Batch processing of edges in the union-find tree construction.
(Phase 1: batch 1) -> (Phase 1: batch 2) -> (Phase 1: batch N) -> Phase 2 -> Phase 3

Not known:
• How many total edges will be processed when the run starts.
• On which PE a single find traversal will terminate.
  • All union-find operations might terminate on a single PE!
• Who will inform the application to start a new batch?
  • None of the PEs know what the other PEs are doing.
• When to start a new batch?
10 PEs, 100 edges batch size.

Can there be a deadlock?
Example scenario: 10 PEs with a batch size of 100 edges.

**Algorithm:**

- Each PE informs PE[0] as soon as it sees 6 union-find terminations.
- PE[0] informs the application to start a new batch as soon as it receives 50 union-find terminations.

- In general \((\text{avg} + 1)\) as the trigger point to send a message to PE-0 will work, where \(\text{avg} = \text{batch size}/\# \text{ PEs}\). The trigger point should be changed if the trigger point for PE-0 to inform the application to start a new batch changes (but can similarly be derived).
15 PEs, 1000 edges batch size
Varying thresholds. (1/4)

**Can there be a deadlock?**
15 PEs, 1000 edges batch size

Scenario 1: $499 + 124 \times 2 + 30 \times 4 + 6 \times 8 = 915$

85 edges remaining to be processed.
**Stampede2**
- 68 cores per node
- 4 hardware threads
- 272 threads per node

per node: 7 mpi_tasks/logical nodes
+ppn 8
+pemap 1-8,10-17,19-26,28-35,37-44,46-53,55-62
+commap 0,9,18,27,36,45,54
ofi layer

**Parallel Union-Find (Cluster finding)**

4 Billion Particles

Execution time in seconds

Nodes

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16
Component Labeling

Iterate over the vertices in the node, and only those vertices that have their parent in a different node send messages to their parent requesting for a component ID. (The number of messages sent is recorded)

Root replies back the component ID. Only after all the messages are received, iterate over the vertices, and label them. Quiescence Detection (QD) -> Inform the application.
## Parallel Union-Find (Cluster finding)

### Orkut data set:

<table>
<thead>
<tr>
<th></th>
<th>tree construction time (s)</th>
<th>component detection (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 PE</td>
<td>84.3</td>
<td>0.8</td>
</tr>
<tr>
<td>64 PEs</td>
<td>80.3</td>
<td>7.4</td>
</tr>
<tr>
<td>256 PEs</td>
<td>85.3</td>
<td>3.4</td>
</tr>
<tr>
<td>512 PEs (8 nodes)</td>
<td><strong>51.4</strong></td>
<td><strong>1.7</strong></td>
</tr>
<tr>
<td>768 PEs</td>
<td>131.3</td>
<td>1.2</td>
</tr>
<tr>
<td>1024 PEs</td>
<td>154.5</td>
<td>1</td>
</tr>
</tbody>
</table>
Orkut: Strided (8PEs)

Distribution of vertices.

Timeline
Parallel Union-Find (Cluster finding)

Other optimizations (Results from Orkut):

• Do component labeling (global path compression) at regular intervals.
  Phase 1 -> Phase 2 -> Phase 1 -> ...
  Phase 1 -> global path compression -> Phase 2 -> ...

• Drop an edge if both its vertices belong to the same component.

• Shared parent data structure across PEs.
  • Phase 1 still sends messages so as to avoid race conditions during tree construction.
  • More edges can be dropped (component label information is treated as read-only).

<table>
<thead>
<tr>
<th># batches</th>
<th>total_time</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>56.9</td>
</tr>
<tr>
<td>2</td>
<td>94.4</td>
</tr>
<tr>
<td>3</td>
<td>153.2</td>
</tr>
<tr>
<td>5</td>
<td>225.4</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th># batches</th>
<th>total_time</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>81.7</td>
</tr>
<tr>
<td>3</td>
<td>85.1</td>
</tr>
<tr>
<td>5</td>
<td>141.9</td>
</tr>
</tbody>
</table>
Other optimizations:

- Overlap Phase 1 and Phase 2.
- Mini batches of edge injection.
- Child pointers at vertices.
Related work:

• **ParConnect:** A parallel connectivity algorithm for de Bruijn graphs in metagenomic applications by Patrick Flick, Chirag Jain, Tony Pan and Srinivas Aluru (SC 2016).
  
  on de Bruijn graphs: 1.8B vertices; 135B vertices + edges; 22 minutes on 1280 cores.

• **LACC:** A Linear-Algebraic Algorithm for Finding Connected Components in Distributed Memory by Ariful Azad and Aydin Buluc (IPDPS 2019). (~5.1x faster than ParConnect)

• **ChaNGa:** Edges are generated dynamically.
Backup Slides
Component Pruning

**Up-Pass:**
A node sends component count to its respective parent.

Parent knows how many counts it will receive for that component. (Because in the labelling phase the count of the buffered requests was stored).

Adds them up and sends the sum to its parent.

Root finally has the total count.

**Down-Pass:**
The root sends back the total count. The total count is trickled down. Component pruning.
Charm++ is a generalized approach to writing parallel programs.

Three design principles: Overdecomposition, Migratability, and Asynchrony.

Smallest Unit: Chare
Overview

Processor 0

Scheduler

Message Queue

Processor 1

Scheduler

Message Queue

A.foo(…)

Source: Charm Workshop '18
Chare is the smallest unit.

Application execution is distributed across Processing Elements (PEs), which are OS threads or processes. On each PE, there is a scheduler operating with its own private pool of messages.

Group chares when created exist on every PE.
Anchor Algorithm

We leverage a parallel data-structure, the union forest, $T = (V, E_T)$. The union forest leverages a global ordering $<$ of the vertices in $V$, in particular, it ensures that if $v$ is a parent of $w$, so $(v, w) \in E_T$, then $v < w$. Our analysis assumes this ordering is random. The data structure support ANCHOR queries. Each vertex in $T$ knows only its parent,

$$
\pi(v) = \begin{cases} 
    u : (u, v) \in E_T \\
    v : \exists u \in V \text{s.t.} (u, v) \in E_T 
\end{cases}
$$

**Algorithm 2** $[u] = \text{ANCHOR}(w)(T, v)$

**Require:** $T = (V, E_T)$ is a forest, if $(s, t) \in E_T$, $\pi(t) = s$, if $t$ is a root $\pi(t) = t$, $v, w \in V$. The anchor function is invoked on the vertex $w$ (only $\pi(w)$ is known).

**Ensure:** If $v$ and $w$ are not in the same tree, an edge is added to $E_T$ to connect the smaller of the two roots ($r$) of the trees containing $v$ and $w$, to the first ancestor of the other vertex ($p$) satisfying $p < r$, in particular $\pi(r) = p$.

1: if $w < v$ then
2: \hspace{1em} $\text{ANCHOR}(\pi(v))(T, w)$
3: else if $\pi(w) = w$ then
4: \hspace{1em} $\pi(w) = v$
5: else
6: \hspace{1em} $\text{ANCHOR}(\pi(w))(T, v)$
7: end if
Example scenario: 10 PEs with a batch size of 100 edges.

- **Scenario-1**: 9 PEs witnessed 5 terminations, so PE-x will observe 55 terminations, hence would have informed PE-0 9 times that it has seen 6 terminations. PE-0 would have informed the application to start a new batch.

- **Scenario-2**: 4 PEs: 5; 4 PEs: 11. The remaining PEs should see 34 among them. This still does not lead to a deadlock.