Software and Algorithms for Graph Queries on Massively Multithreaded Architectures

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Outline

- **Graph-based informatics**
- **Massively-multithreaded architectures**
- **Sandia's prototype Multithreaded Graph Library (MTGL)**
- **Algorithmic case studies on the Cray MTA-2**
- **Current and future directions, opportunities for collaboration**

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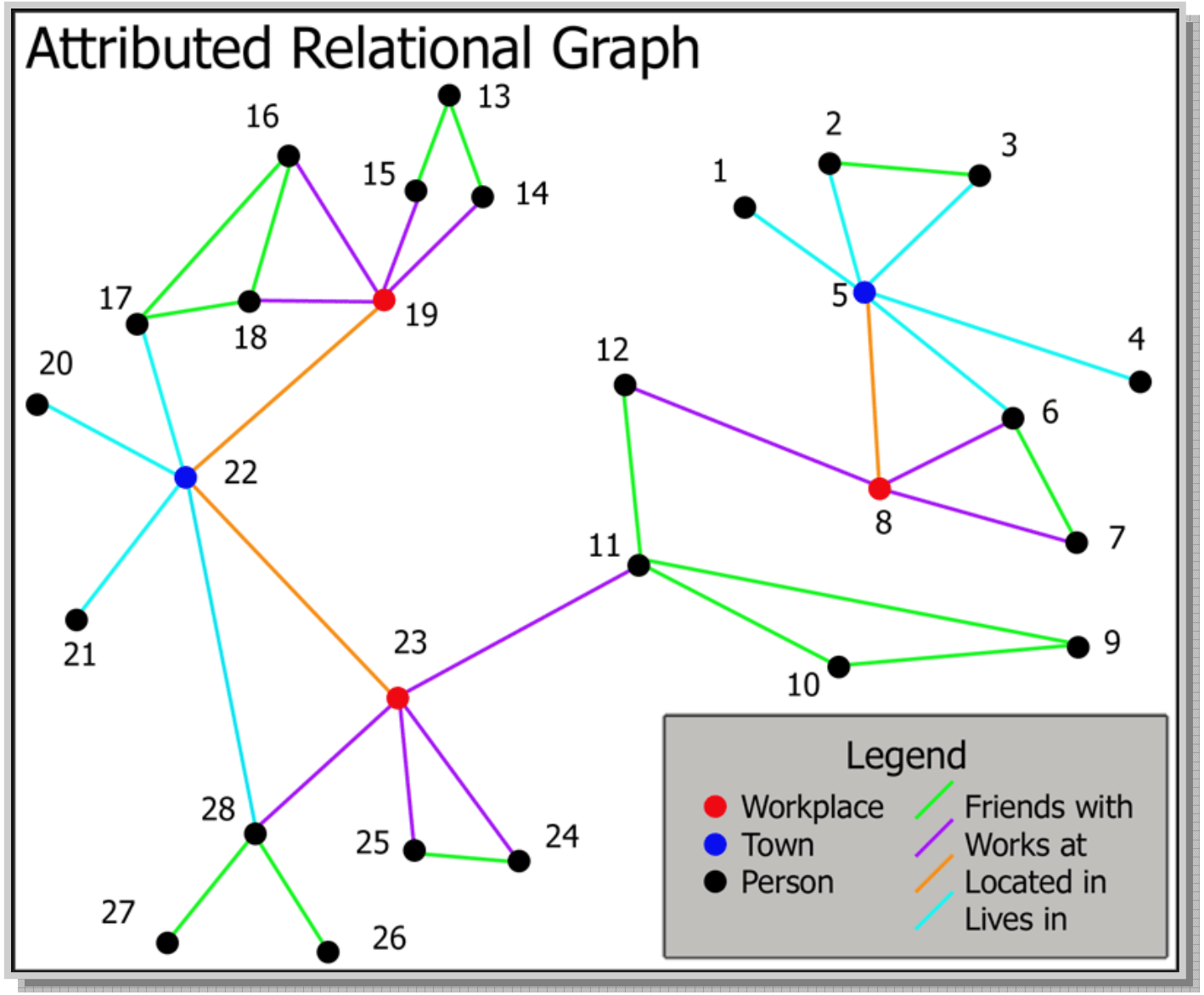
Graph-Based Informatics



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Massive Multithreading: e.g., The Cray MTA-2

- **Slow clock rate (220Mhz)**
- **128 “streams” per processor**
- **Global address space**
- **Fine-grain synchronization**
- **Simple, serial-like programming model**
- **Advanced parallelizing compilers**

No Data Cache

Latency Tolerant:

important for Graph Algorithms

Hashed Memory

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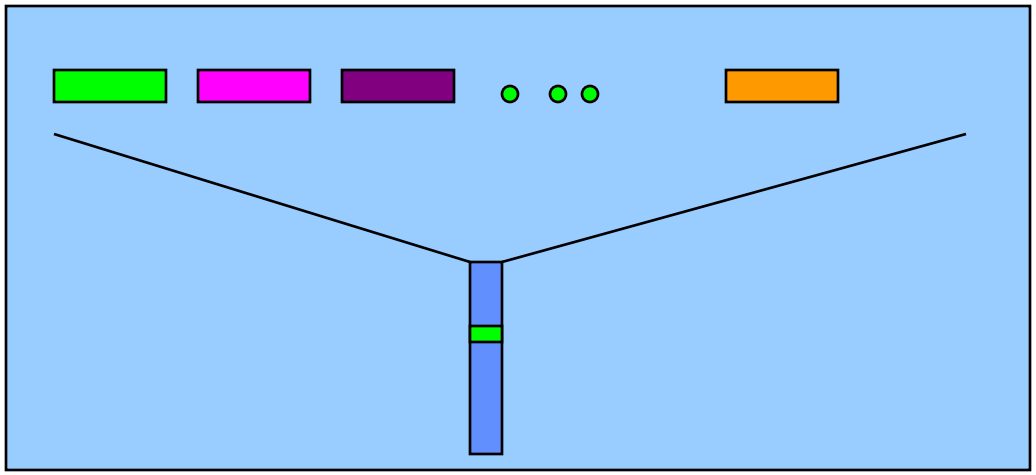
Cray MTA Processor



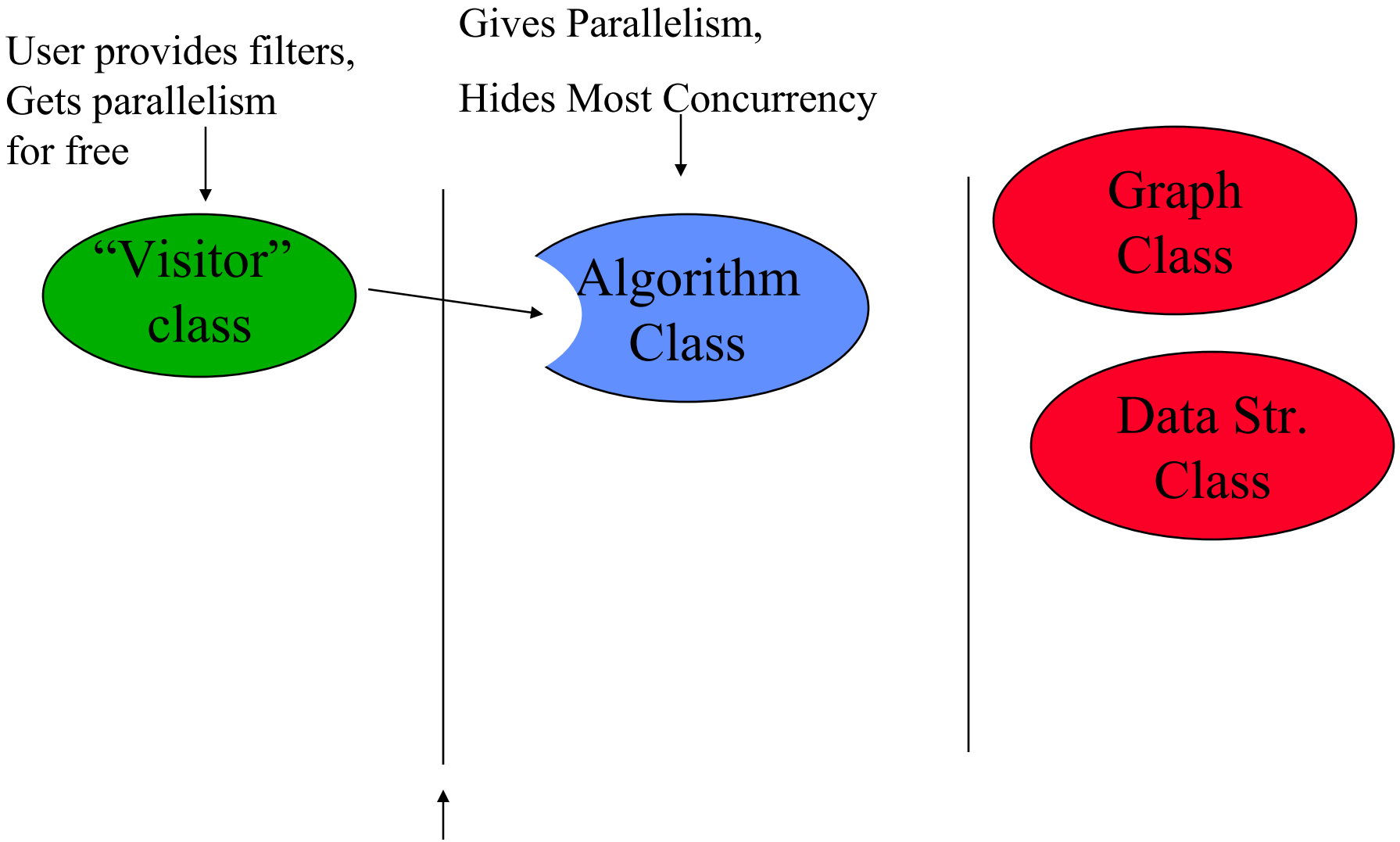
- Each thread can have up to 8 memory refs in flight
- Round trip to memory ~150 cycles

The MultiThreaded Graph Library (MTGL)

- **Recent work**
  - Design & implement the Multithreaded Graph Library (MTGL)
    - Boost GL-like, but not Boost-based
    - In the process of open-sourcing
    - Develop, run, debug codes on workstations and/or MTA/XMT
  - Design multithreaded algorithms
    - Simon Kahan's connected components algorithm
    - "Bully" connected components algorithm
    - Subgraph isomorphism for semantic graphs

- **Current work**
  - Adapt the MTGL to run on SMP's
  - Flesh out the MTGL with community finding, etc.
  - Integrate the MTGL with visualization frameworks

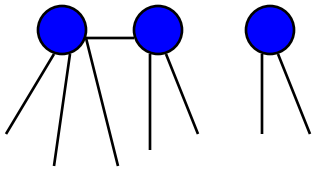
MTGL: C++ Design Levels



Four Modes of MTGL Graph Exploration

for v in V: visit_adj

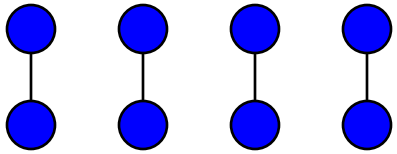
visit v's neighbors



~10 memref/edge

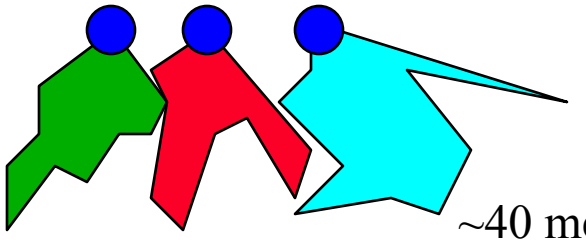
for e in E: visit_edges

visit e's endpoints



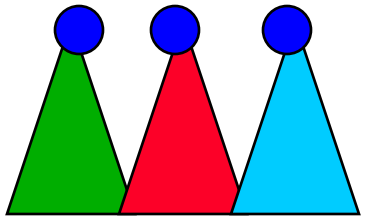
~10 memref/edge

recursive parallel search psearch



~40 memref/edge

breadth-first search bfs



~20-40 memref/edge

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Current MTGL Algorithms

- Connected components (psearch, visit_edges, visit_adj)
- Strongly-connected components (psearch)
- Maximal independent set (visit_edges)
- Typed subgraph isomorphism (psearch, visit_edges)
- S-t connectivity (bfs)
- Single-source shortest paths (psearch)
- Betweenness centrality (bfs-like)
- Connection subgraphs (bfs, sparse matrix, mt-quicksort)
- Find triangles (psearch)
- Find assortativity (psearch)
- Find modularity (psearch)

Under development:

- Optimize modularity via simulated annealing (visit_adj, visit_edges)
- Count edges in 1, 2 neighborhoods (various)
- more

MTGL PSearch Primitive: visitors

```
DefaultVisitor {
   sr(v) {}       # search root
   d(v) {}        # discover
   vt(v) {}       # visit test
   te(v,w) {}  # tree edge
   oe(v,w) {} # "other" edge
   …
}
```

The search primitives give the programmer these opportunities to react to search events

Pseudocode for this talk uses these shortened method names

Abuse of notation: multiple edges *are* allowed

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MTGL Search Primitives (e.g)

```
PSearch<OR,vis>(v)
{
   vis.d(v)
   for (v,w) in E(v):
        if (v,w) unvisited OR vis.vt(v,v')
             vis.te(v,w)
             PSearch<OR,vis>(w)
        else
             vis.oe(vw)
}
```

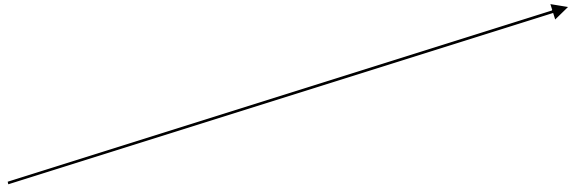
```
PSearch<AND,vis>(v)
{
   vis.d(v)
   for (v,w) in E(v):
      if vis.vt(v,v')
        if (v,w) unvisited
             vis.te(v,w)
             PSearch<AND,vis>(w)
        else
             vis.oe(vw)
}
```

More general, but details omitted here…

MTGL Synchronization Primitives

MTA Primitive	Meaning	Pseudocode	MTGL
b = int_fetch_add(a,i)	Atomic read, increment of *a*	$b \xleftarrow{\text{ifa}} a, i$	mt_incr(a,i)
b = readfe(&a)	Wait for *a* to be "full," read *a,* leave empty	$b \xleftarrow{\text{fe}} a$	mt_readfe(a)
b = readff(&a)	Wait for *a* to be "full," Read *a,* leave full	$b \xleftarrow{\text{ff}} a$	mt_readff(a)
writeef(&a, v)	Wait for *a* to be "empty," Write *a,* leave full	$b \xleftarrow{\text{ef}} a$	mt_write(a,v)

Overloaded for different platforms



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Case Studies: Algorithm Kernels

- **Connected Components**
- **Subgraph Isomorphism**
- **S-T Connectivity (i.e., use of BFS)**

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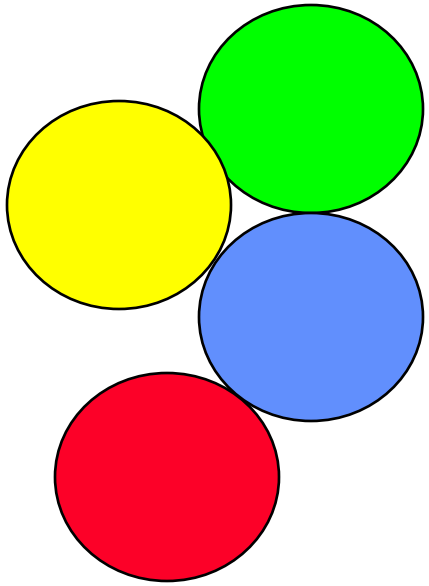
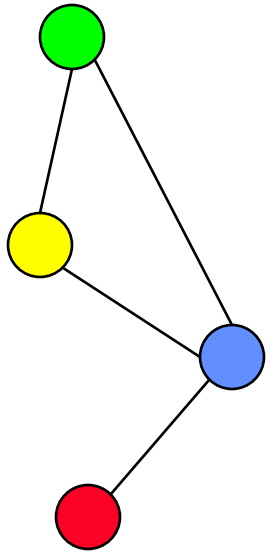
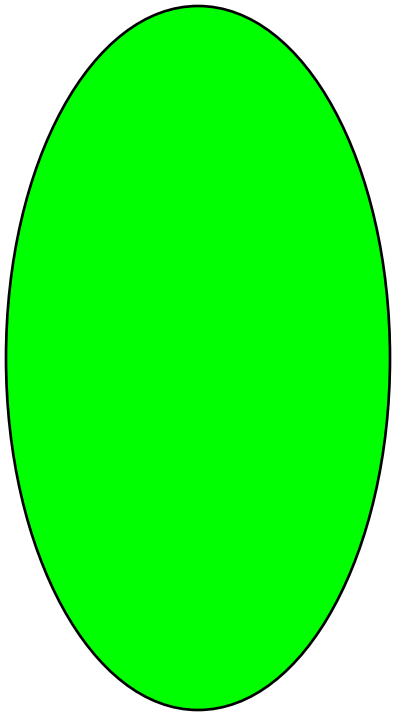
Kahan's Algorithm for Connected Components



Phase 1:
concurrent
searches

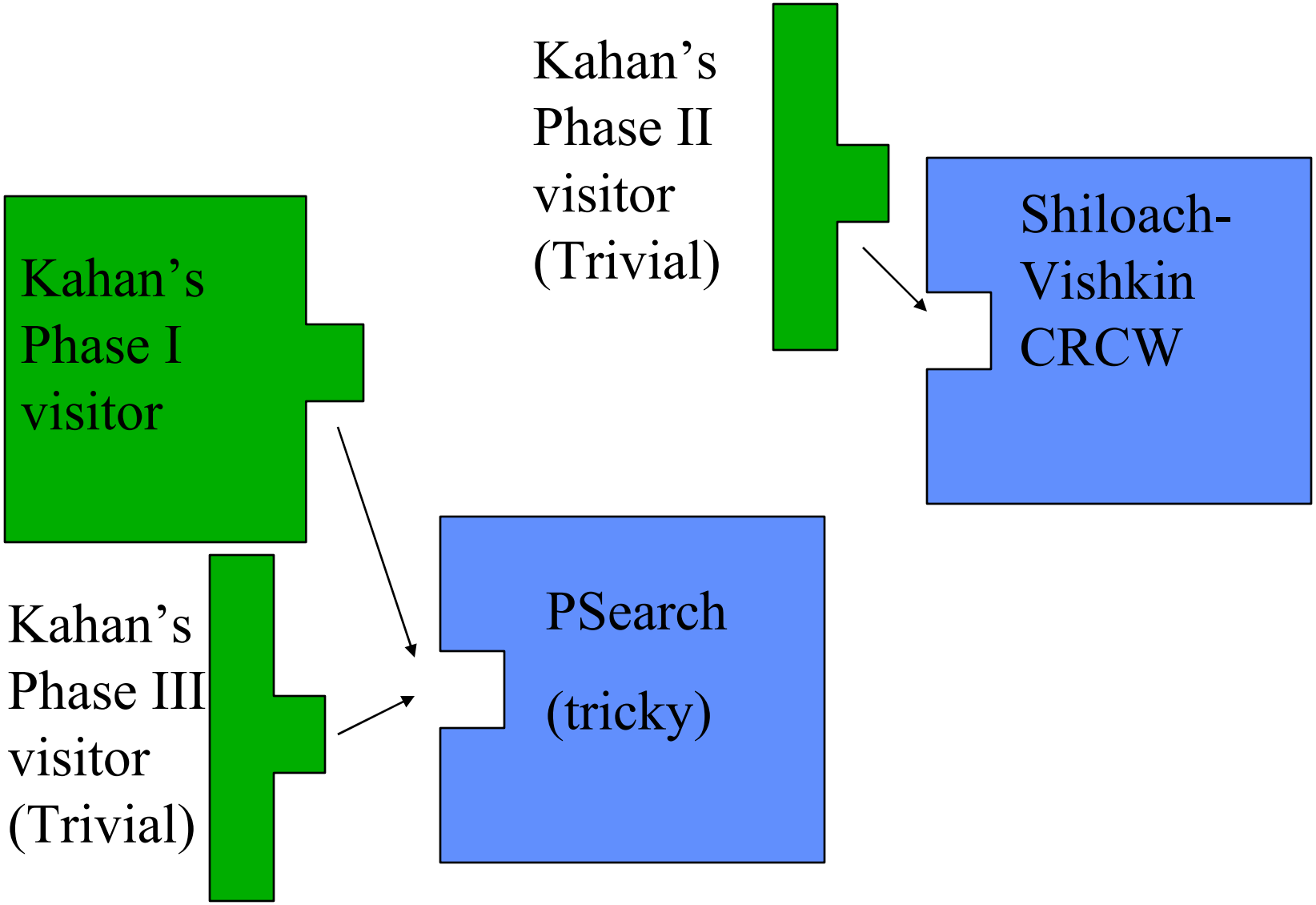


Phase 2: CRCW
(Shiloach-Vishkin)



Phase 3:
relabel

MTGL Implementation of Kahan's Algorithm



MTGL Implementation of Kahan's Algorithm

Phase I visitor:

$V_1 = \{$

$C \leftarrow$ user array of $|V(G)|$ ints

$T \leftarrow$ hash table of (int, int) pairs

sr(v) $\{ C[v] \xleftarrow{ef} v \}$

te(v, w) $\{ C[w] \xleftarrow{ef} C[v] \}$

oe(v, w) $\{ cv \xleftarrow{ff} C[v];$

$cw \xleftarrow{ff} C[w];$

$T \xleftarrow{ts} T \cup \{(cv, cw)\}$

$\}$

$\}$

"component" values were defined by user to start "empty"

Wait until both full

Thread-safe Add to hash table

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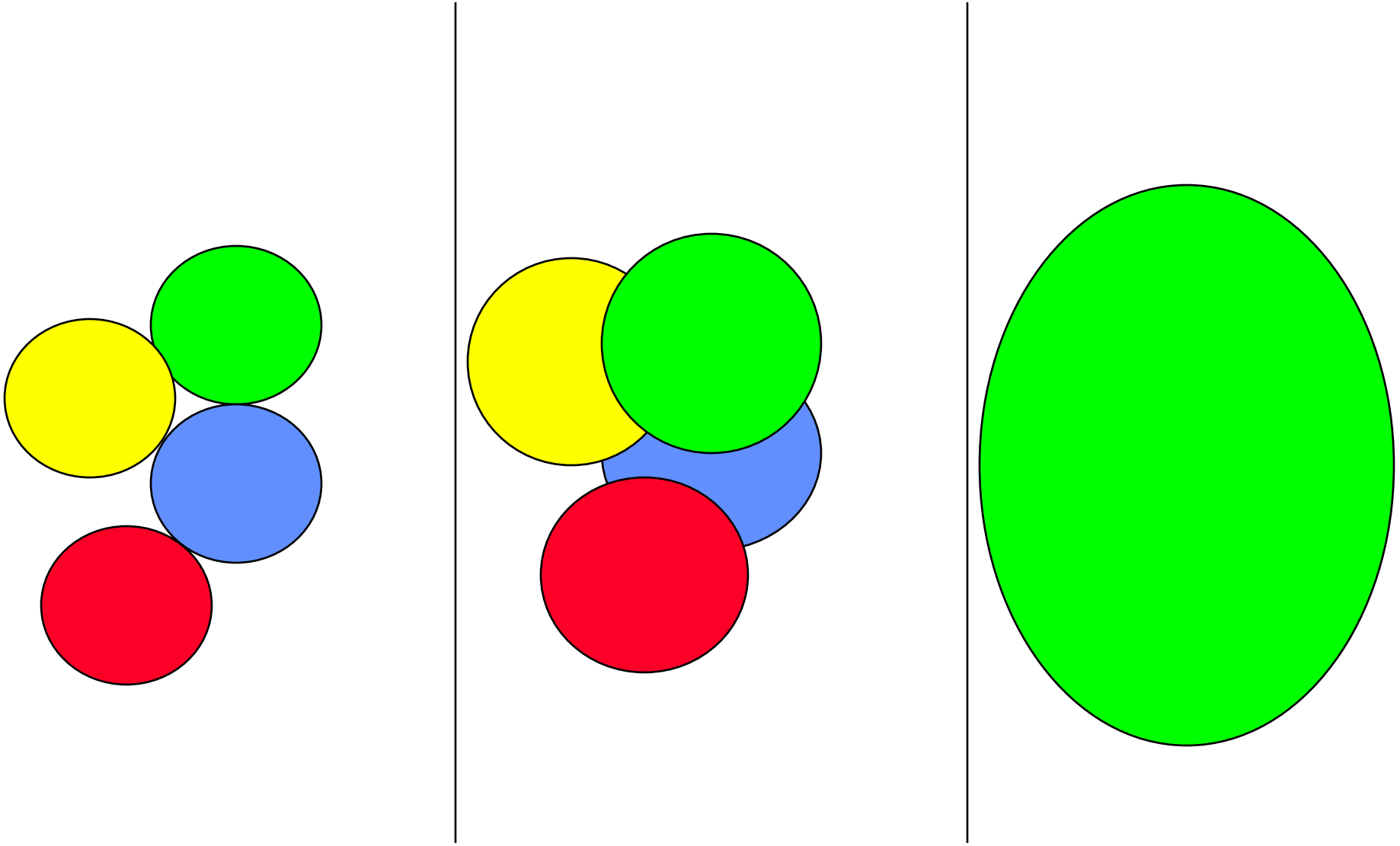
More General Filtering: The “Bully” Algorithm



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MTGL Implementation of the Bully Algorithm

$V_b = \{$

.....

vt(v, w) $\{cv \xleftarrow{ff} C[v];\quad cw \xleftarrow{ff} C[w];$

return $(cv < cw)$;

$\}$

te(v, w) $\{cv \xleftarrow{ff} C[v];\quad cw \xleftarrow{fe} C[w];$

if w unvisited OR $(cv < cw)$

$C[w] \xleftarrow{ef} C[v]$

else

$C[w] \xleftarrow{ef} cw$

$\}$

$\}$

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Parallelized Shiloach-Vishkin (Bader, Feo, Cong'06)

```
edge   **edges    = g->edges.getStore();
   while (graft) {
        numiter++;
        graft = 0;
        #pragma mta assert parallel
        for (int i=0; i<m; i++) {
            int u = edges[i]->vert1->id;
            int v = edges[i]->vert2->id;
            if (D[u] < D[v] && D[v] == D[D[v]]) {
                D[D[v]] = D[u];
                graft = 1;
            }
            if (D[v] < D[u] && D[u] == D[D[u]]) {
                D[D[u]] = D[v];
                graft = 1;
            }
        }
        #pragma mta assert parallel
        for (int i=0; i<n; i++) {
            while (D[i] != D[D[i]]) D[i] = D[D[i]];
        }
   }
```

"Graft"

"Hook"

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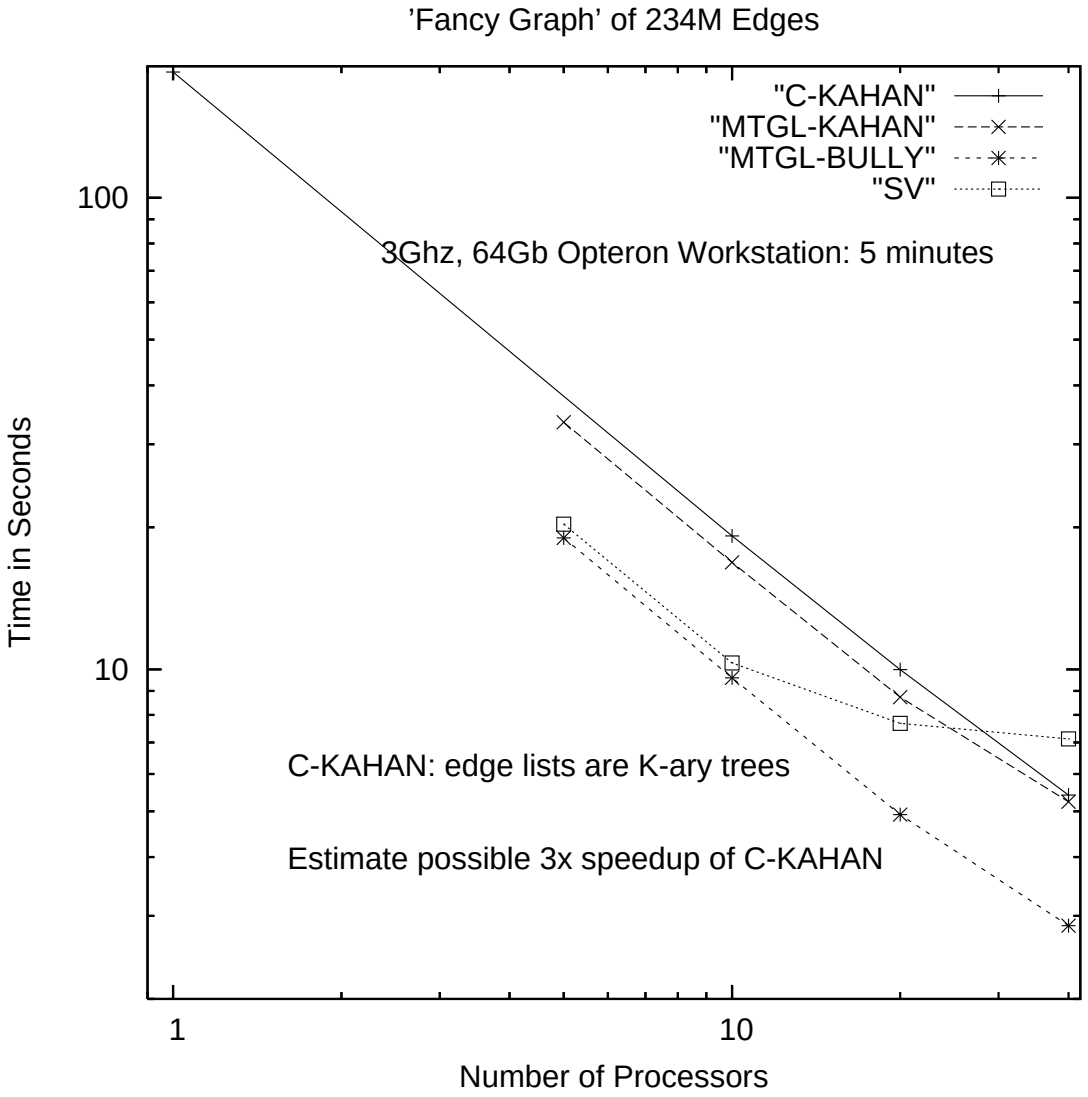
Connected Components Performance (1)



~2.9s

~40 memref/edge

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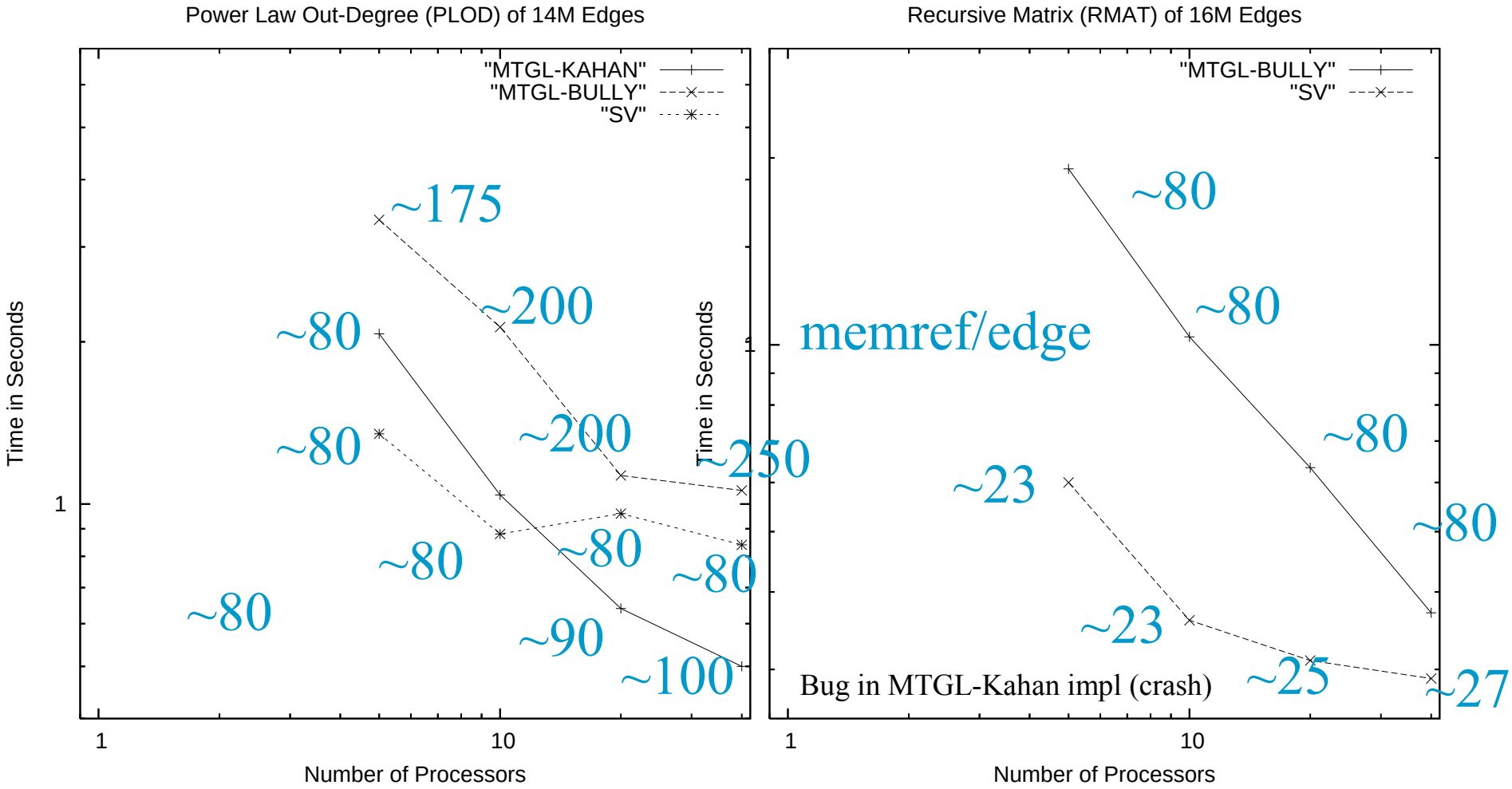
Connected Components Performance (2)



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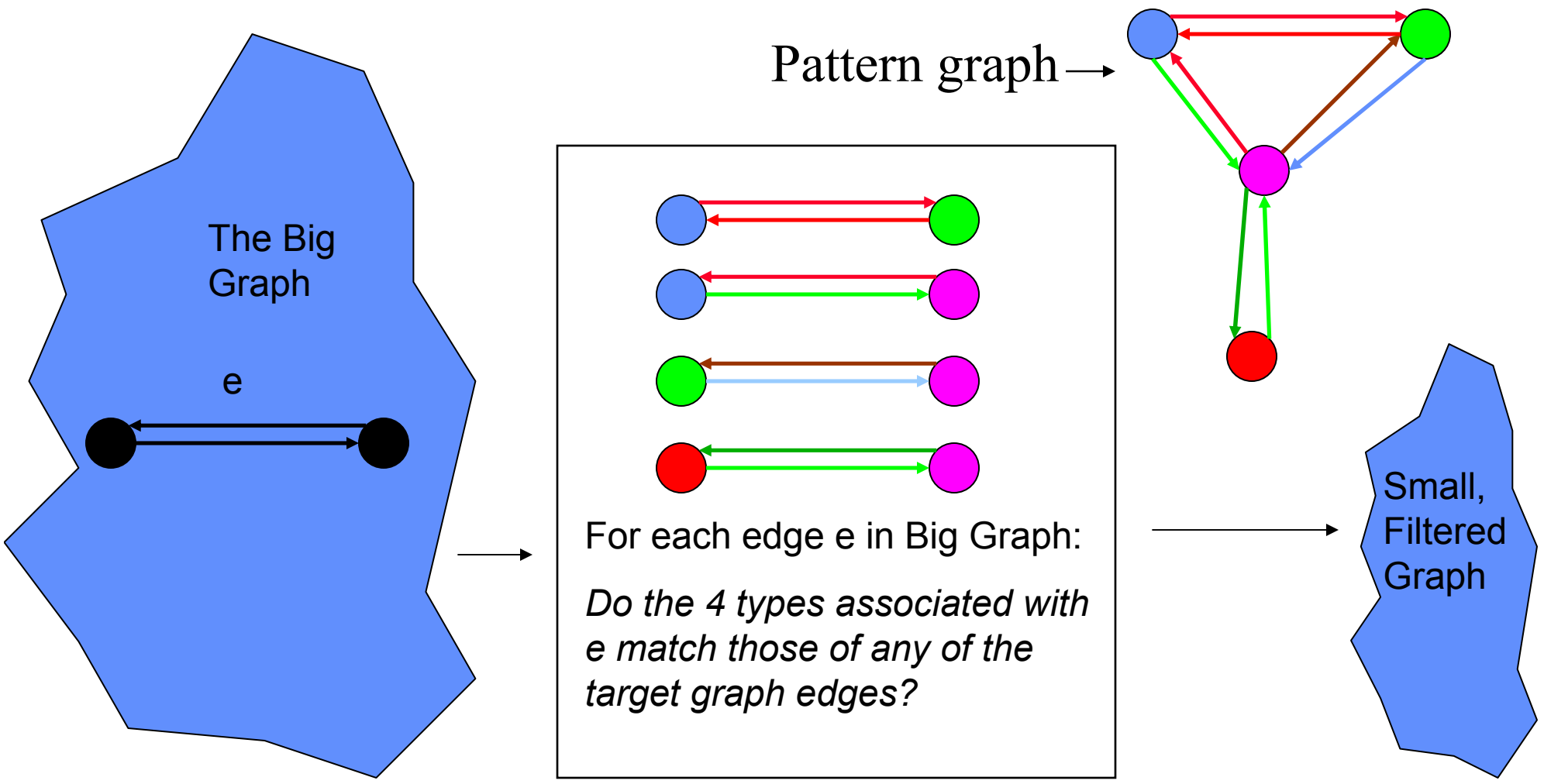
Case Study: Subgraph Isomorphism Kernel

- **Objective: find exact or inexact matches of a small pattern graph within a large semantic graph**

Instance-Specific Type Filtering for Subgraph Iso.



Subgraph Isomorphism: Input

The Target Graph:

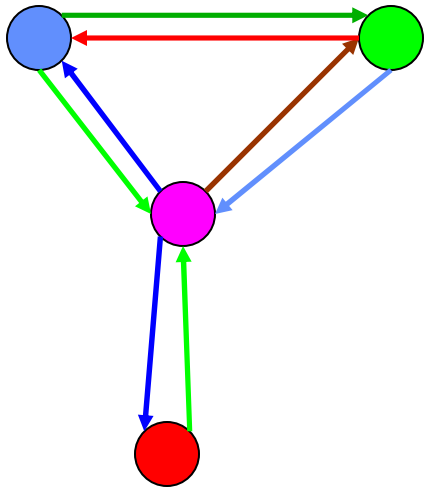


Table of Type and Auxiliary Information:

T																	
V	**2**		**2**		**3**		**2**		**3**		**1**		**3**		**2**		**2**

Ideal: Euler Tour

Our Experiments: Random Walk

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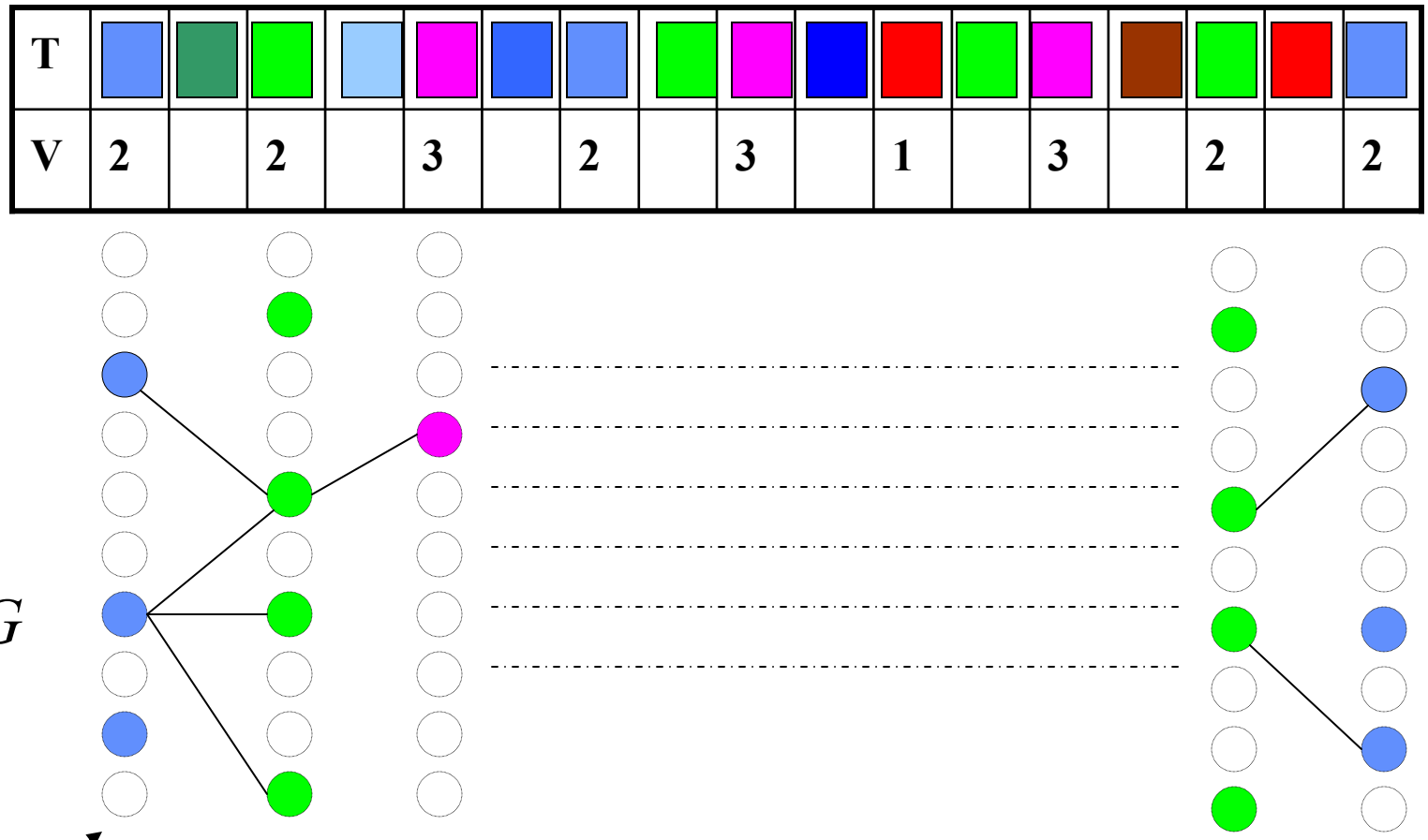
Subgraph Isomorphism: Creating a Bipartite Graph

Small, Filtered Graph (SFG)

k times:
visit each edge of SFG

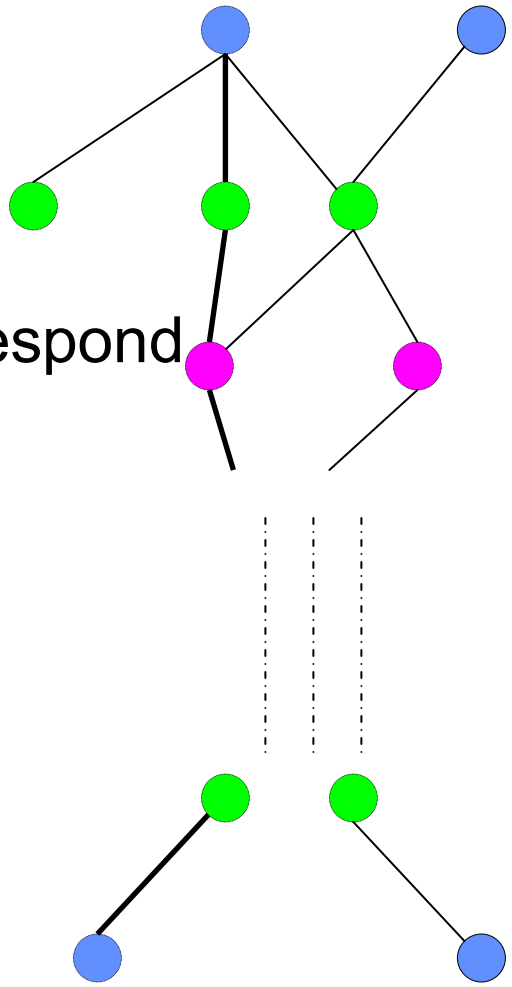


Logical placeholders for vertices in the SFG.

Subgraph Isomorphism: Creating a Bipartite Graph

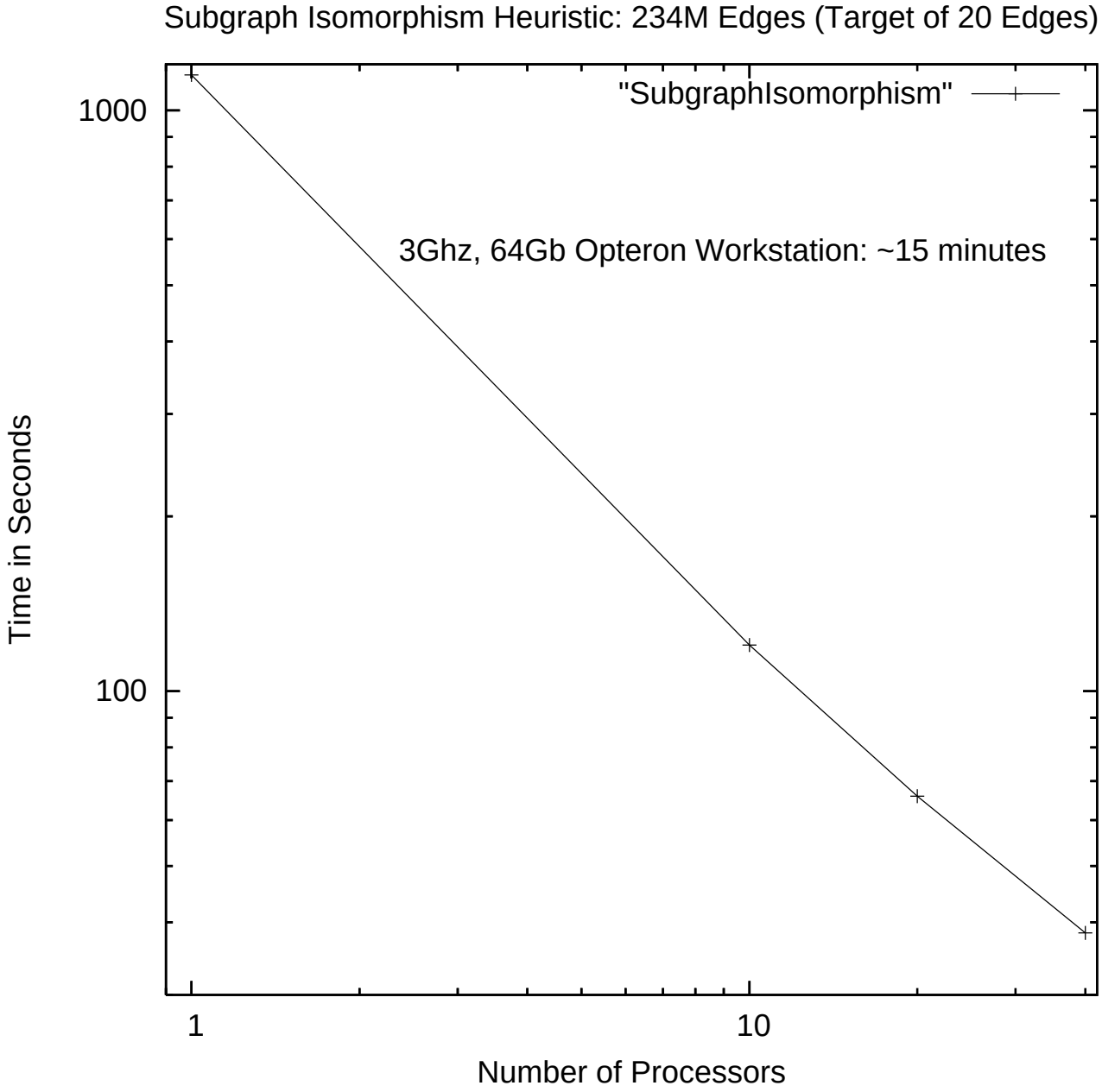
S-T shortest paths (top to bottom) correspond to candidate matches.

Branch and bound to Find better matches.



Visitor object tailors Search so that it never goes up (similar to "Bully" algorithm).

Computational Results: Subgraph Isomorphism



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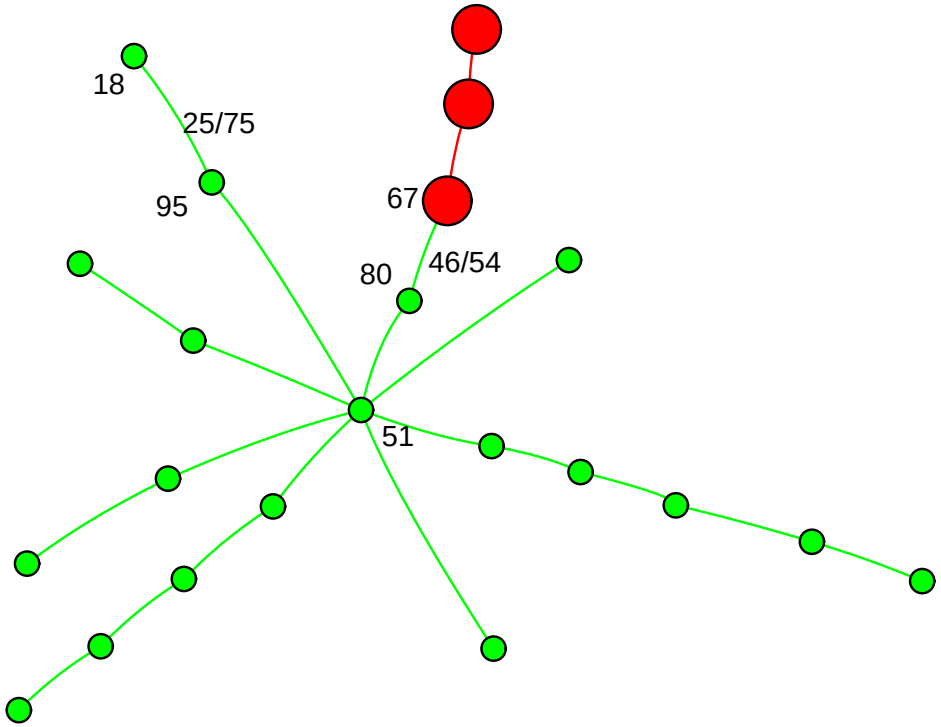
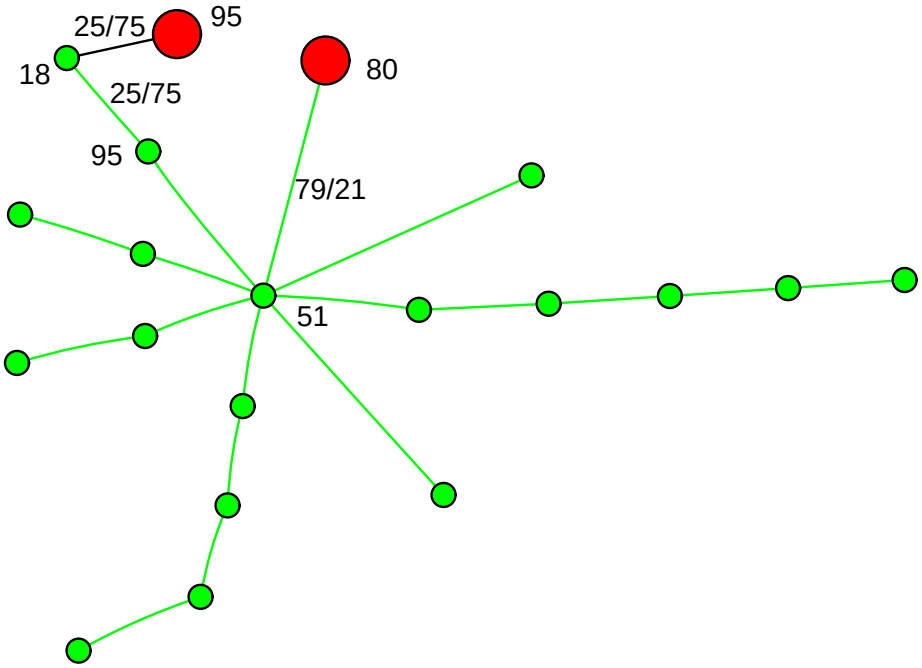
Computational Results: Subgraph Isomorphism

Type & topological isomorphism exists between green vertices



Target



Found

Actual graphs from a 234M edge instance

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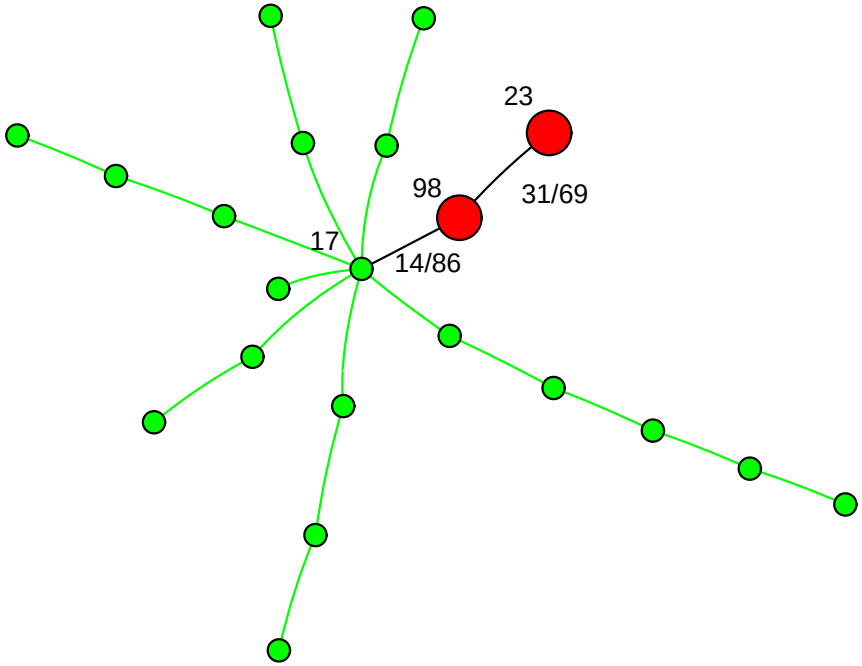
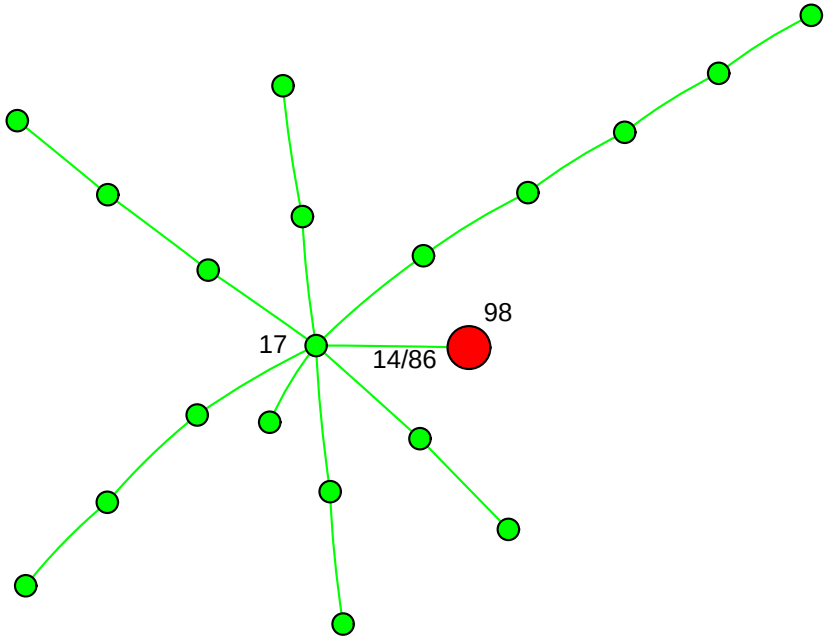
Can try harder if we want a closer match

Type & topological isomorphism exists between green vertices



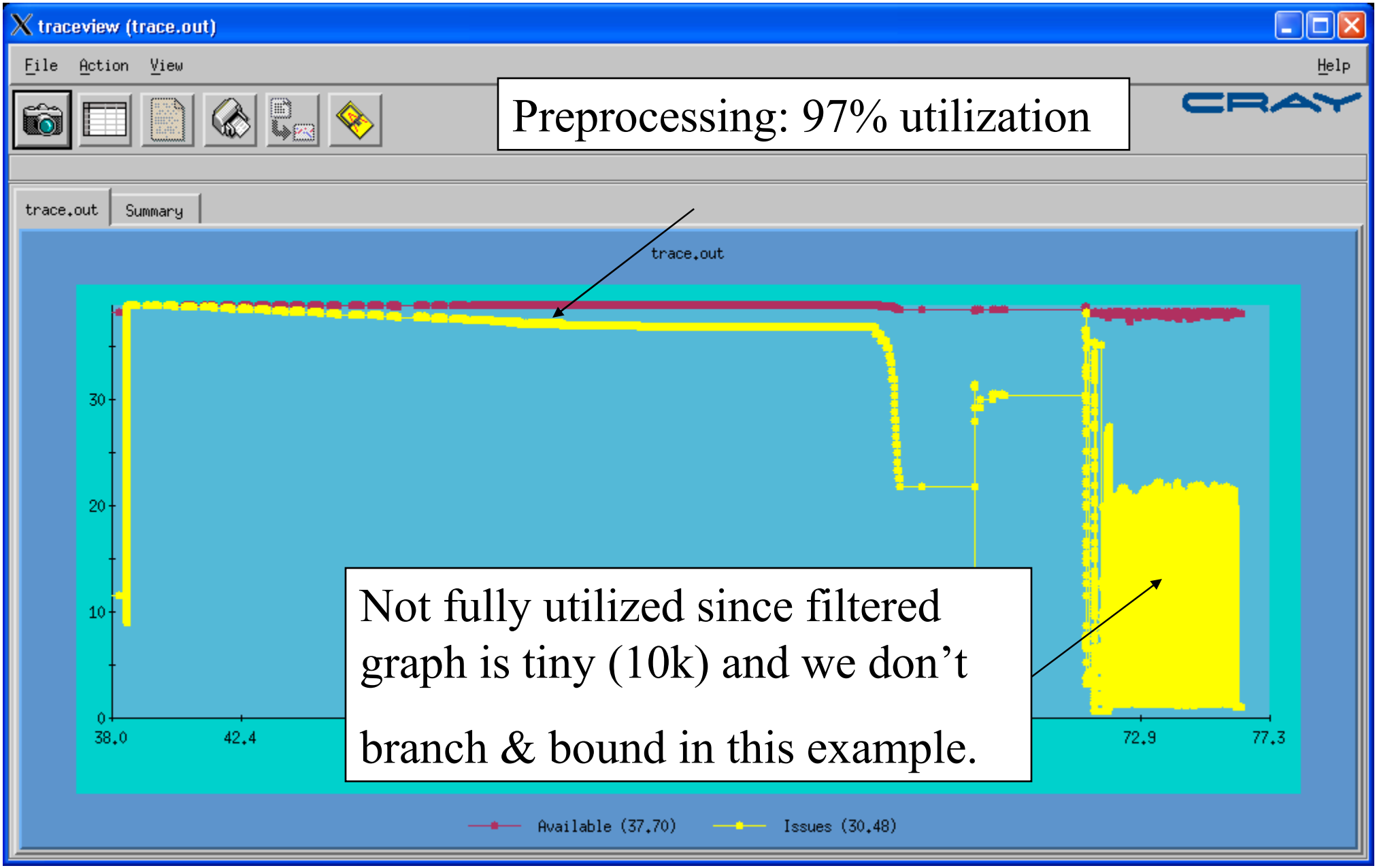
Target



Found

Actual graphs from a 234M edge instance

Traceview Output for Subgraph Isomorphism



Future

- **Massively-multithreaded Graph Algorithm R&D**
- **Open-Sourcing of the MTGL**
- **Run on SMP**
- **Query system with shared, mmapped graphs**

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Acknowledgements

- Bruce Hendrickson (Graph Informatics lead)
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