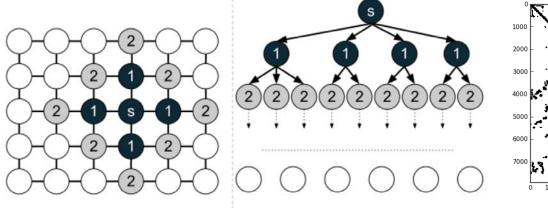
CUDA 6 Breadth-First Search

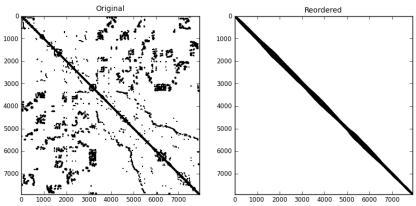
CS121 Parallel Computing Spring 2021



Breadth-first search

- Given a graph, explore it layer by layer.
 - ☐ Go wide, then go deep.
- Large number of applications.
 - Connected components, path finding, Ford-Fulkerson max flow algorithm, Cuthill-McKee ordering, bipartiteness testing, search engine crawlers, garbage collection, etc.
- Used in benchmarks such as Graph500 and Parboil to test parallel computer's memory performance.





Source: http://www.stoimen.com/blog/2012/10/08/computeralgorithms-shortest-path-in-a-graph/

Source: http://dpo.github.io/pyorder/_images/commanche_dual_rcmk.png



Real world graphs

Name	Sparsity Plot	Description	<i>n</i> (10 ⁶)	<i>m</i> (10 ⁶)	d	Avg. Search Depth
europe.osm		European road network	50.9	108.1	2.1	19314
grid5pt.5000		5-point Poisson stencil (2D grid lattice)	25.0	125.0	5.0	7500
hugebubbles-00020		Adaptive numerical simulation mesh	21.2	63.6	3.0	6151
grid7pt.300		7-point Poisson stencil (3D grid lattice)	27.0	188.5	7.0	679
nlpkkt160		3D PDE-constrained optimization	8.3	221.2	26.5	142
audikw1	9	Automotive finite element analysis	0.9	76.7	81.3	62
cage15		Electrophoresis transition probabilities	5.2	94.0	18.2	37
kkt_power		Nonlinear optimization (KKT)	2.1	13.0	6.3	37
coPapersCiteseer		Citation network	0.4	32.1	73.9	26
wikipedia-20070206		Links between Wikipedia pages	3.6	45.0	12.6	20
kron_g500-logn20		Graph500 RMAT (A=0.57, B=0.19, C=0.19)	1.0	100.7	96.0	6
random.2Mv.128Me		G(n, M) uniform random	2.0	128.0	64.0	6
rmat.2Mv.128Me		RMAT (A=0.45, B=0.15, C=0.15)	2.0	128.0	64.0	6

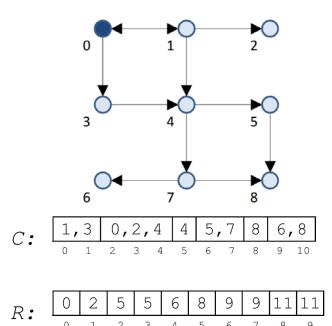
- Hundreds of millions of nodes and edges.
 - Some graphs have billions or trillions of edges. But these don't fit into the memory of a single GPU.
- Low average degree (sparse), but high variation in degree.
 - Some nodes have a few neighbors, some nodes 100K's.
- "Small world" graphs have low diameter (~10).
- Grids and maps have high diameter (~1-10K).

Source: High Performance and Scalable GPU Graph Traversal, Merrill, Garland, Grimshaw



Sequential algorithm

- Assume graph is sparse, and stored in compressed sparse row format.
 - □ R[i] indicates index where node i's neighbors start in C.
 - \square Ex R[1] = 2 means node 1's neighbors (0, 2, 4) are listed starting at C[2].
- Maintain a queue of unvisited nodes.
 - □ Dequeue a node, add its unvisited neighbors to the queue.
- Running time O(|V|+|E|).



Traversal from source vertex v ₀					
BFS Iteration	Vertex frontier	Edge frontier			
1	{0}	{1,3}			
2	{1,3}	{0,2,4,4}			
3	{2,4}	{5,7}			
4	{5,7}	{6,8,8}			
5	{6,8}	{}			
10 if $(dist[j] == \infty)$					
dist[j] := dist[i] + 1;					
12 $Q.Enqueue(j)$					



Parallelizing BFS

- First BFS algorithms for GPUs focused on data parallelism.
- Initially set source distance to 0.
- Run for D rounds, where D is the diameter from s.
 - In round i, distance i nodes are marked.
 - □ Iterate through all the nodes. If a node is marked, mark its unvisited neighbors as distance i+1 nodes.
- Works well in small diameter graphs, e.g. social networks.
- Very inefficient for large diameter graphs, e.g. maps, since only a few nodes marked per round.
- O(|V||E|) running time.

```
parallel for (i in V) :
    dist[i] := ∞

dist[s] := 0
iteration := 0

do :    should add "if dist[j] == ∞" here

    done := true

    parallel for (i in V) :
        if (dist[i] == iteration)
            done := false
        for (offset in R[i] .. R[i+1]-1)
            j := C[offset]
            dist[j] = iteration + 1
        iteration++
while (!done)
```



Parallelizing BFS

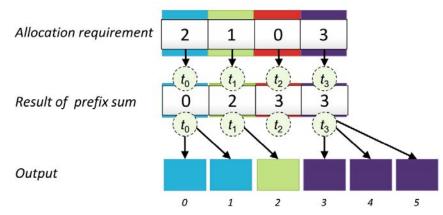
- Linear, i.e. O(|V| + |E|) work parallel BFS algorithms follow the sequential algorithm.
- Two main bottlenecks
 - Maintaining explicit queue of unvisited nodes requires expensive LockedEnqueue operations.
 - □ If nodes have very different degrees (e.g. power law graphs), there's high load imbalance in the main parallel for loop.

```
parallel for (i in V) :
  dist[i] := ∞
dist[s] := 0
iteration := 0
inQ := \{ \}
inQ.LockedEnqueue(s)
while (inQ != \{\}):
  outQ := \{\}
  parallel for (i in inQ) :
     for (offset in R[i] .. R[i+1]-1)
         i := C[offset]
        if (dist[j] == \infty)
           dist[j] = iteration + 1
           outQ. LockedEnqueue ( j)
  iteration++
  inQ := outQ
```



Gathering neighbors

- We use two queues, one for nodes in current layer of BFS, other for nodes in next layer.
 - ☐ After every phase of BFS we swap the queues, to reuse memory.
 - □ To synchronize the layers, use a separate kernel for each layer.
- For each node in first queue, we first add all its neighbors into the second queue (gather).
 - □ Some of the neighbors don't belong in the next BFS layer because they've already been visited.
 - Testing each node explicitly is inefficient.
 - ☐ Also, we may add duplicates into the second queue.
 - □ We'll address both problems later.
- To add neighbors of a node into the queue without expensive locks, we use prefix sum, which is much faster.
 - If node has n_i neighbors, we reserve n_i queue spots for them by adding n_i into the prefix sum.





Load balanced gathering

- To load balance, we assign different numbers of threads to gather the neighbors of a node in parallel.
- If node has moderate number of neighbors, assign a warp of threads to gather its neighbors.
 - □ Each thread in the warp might initially want to gather neighbors of a different node.
 - ☐ The warp votes to find a common node to gather.
 - All threads in warp write to a common location, then read it. The last write "wins". Other threads help gather its node's neighbors.
- If node has large number of neighbors, use entire thread block for gather.
- For remaining nodes, use prefix sum based method.
 - ☐ There's load imbalance, but only for low degree nodes.
- The size of "moderate" and "large" need to be tuned.
- Eliminates most, but not all load imbalance.



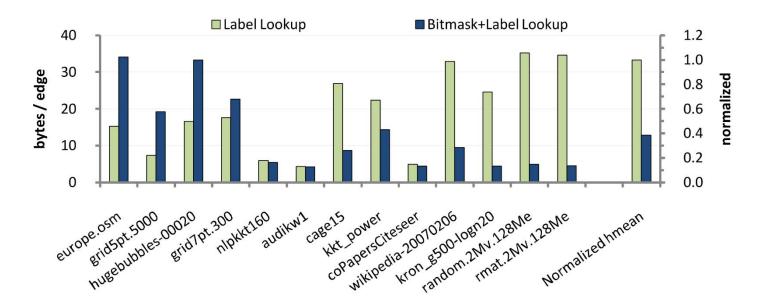
Visited status lookup

- A node should only be added into the frontier queue if it hasn't been visited.
 - □ Before adding a node, look up its visited status.
- To reduce memory traffic, use an integer bitmask to store status of 32 nodes.
- But then two threads might "clobber" each other by setting (different) bits in the same integer.
 - □ Can avoid using atomics, but they're slow.
 - □ Instead, use normal read and write ops, but treat bitmask conservatively.
 - For each node, maintain both a shared bitmask bit, and a private integer label.
 - Usually only access bitmask, saving memory traffic. Occasionally access the label.
 - If bit for a node is set, it's definitely visited.
 - If bit is unset, then not sure about node's visited status, so do another lookup on node's label.



Visited status lookup

- Bitmasks are cached in texture caches.
- This is effective for low diameter graphs.
- Works less well for high diameter graphs, because each layer is processed in separate kernel, and cache flushed after each kernel launch.
- Also doesn't work well for small frontiers, since cached values aren't reused.
- Graphs on left side have high diameter; right ones are low diameter.

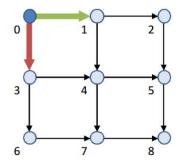


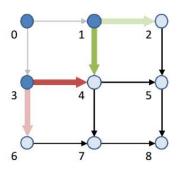


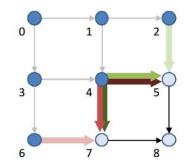
Duplicates in frontier

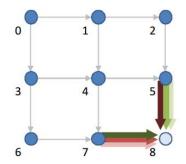
- May add same node into frontier multiple times, due to concurrent discovery.
- Problem especially severe in GPU because of SIMD and high parallelism.
- If duplicates aren't removed, the vertex frontier can grow exponentially.

BFS Iteration	Actual Vertex- frontier	Actual Edge- frontier		
1	0	1,3		
2	1,3	2,4,4,6		
3	2,4,4,6	5,5,7,5,7,7		
4	5,5,7,5,7,7	8,8,8,8,8,8,8		



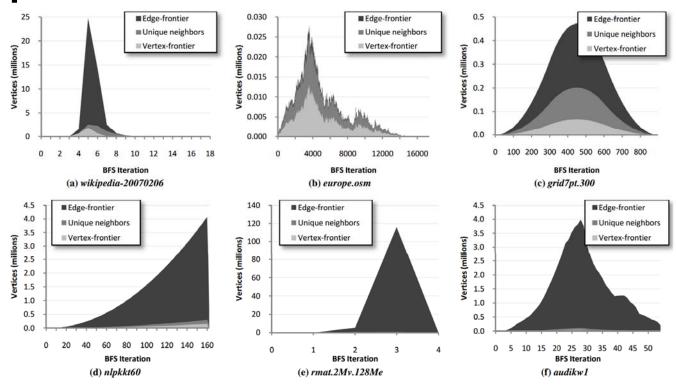






Iteration 1 Iteration 2 Iteration 3 Iteration 4

Duplicates in frontier



- Edge frontier: Number of nodes added to queue, allowing duplicates.
- Unique neighbors: Number of nodes added to queue, removing duplicates, but allowing visited nodes.
- Vertex frontier: Unique neighbors which haven't been visited.
- Allowing duplicates can lead to huge amount of redundant work.



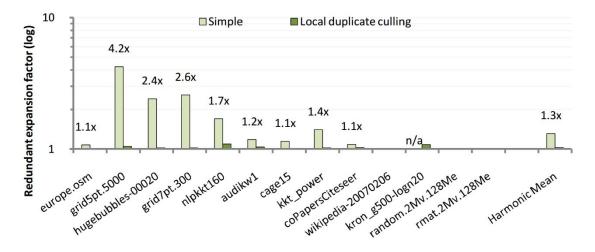
Duplicate culling

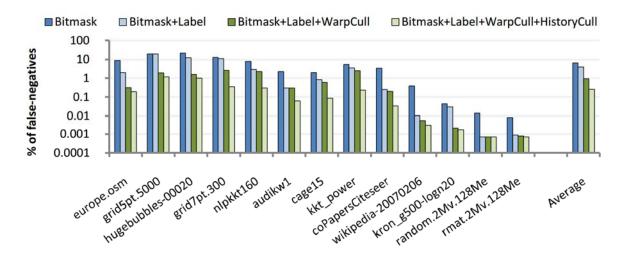
- Try to remove duplicates using hash table.
 - □ Won't remove all duplicates, but quite effective.
- Warp culling
 - □ Each warp allocates a hash table (with 128 entries) in shared memory.
 - □ When inserting a node, hash it into hash table.
 - If table entry empty, store the node in entry, and add node to queue.
 - If table entry filled, then if entry equals the node, don't add node to queue. Otherwise, add it.
- History culling
 - □ Same idea, but use the SM's L1 cache.

M

Duplicate culling

Despite small hash table, culling surprisingly effective.



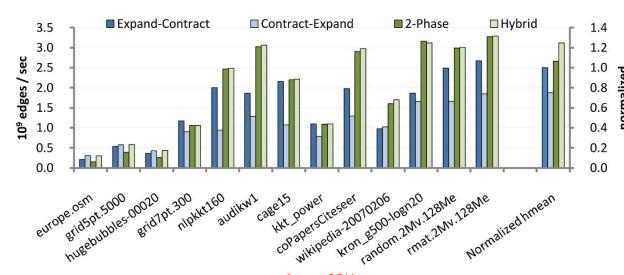




Putting it together

- Each kernel expands one layer of the BFS.
 - □ Input is queue containing last BFS layer (possibly with duplicate nodes).
- Threads assigned nodes from queue.
- A thread first uses warp and history culling to determine if its vertex is a duplicate.
- If not, thread gathers node's neighbors.
 - □ Based on neighbor list size, use a block, warp, or prefix sum gather.
 - Each thread wants to gather neighbors of a different node, and tries to "enlist" a block or warp of threads to help it.
 - Each thread writes into a variable shared by warp or block, then reads it.
 - One thread from the warp / block "wins". All other threads help it.
- Before adding a gathered node to (current layer's) queue, check if it's already visited.
- If not, the thread contributes 1 to a thread block-wide prefix sum.
- Synchronize the block and do a block-wide prefix sum to get number of enqueued nodes for block.
- First thread in block atomically adds sum to global queue index, then shares old global index with block.
- Using old global offset and prefix sum offset, each thread adds its gathered neighbor into queue.





Graph Dataset	Sequential ^T	Parallel	Label Distance		Label Predecessor	
100	10 ⁹ TE/s	10 ⁹ TE/s	10 ⁹ TE/s	Speedup	10 ⁹ TE/s	Speedup
europe.osm	0.029		0.31	11x	0.31	11x
grid5pt.5000	0.081		0.60	7.3x	0.57	7.0x
hugebubbles-00020	0.029		0.43	15x	0.42	15x
grid7pt.300	0.038	0.12**	1.1	28x	0.97	26x
nlpkkt160	0.26	0.47	2.5	9.6x	2.1	8.3x
audikw1	0.65		3.0	4 6x	25	4 0x

8 core CPU **NVIDIA Tesla C2050 (hybrid) CPU CPU** ıp audikw1 4.0x 0.65 3.0 4.6X 2.5 0.23** 0.13 2.2 18x 1.9 15x cage15 0.11** 0.047 1.1 23x 1.0 21x kkt power coPapersCiteseer 0.50 3.0 5.9x 2.5 5.0x 0.19** wikipedia-20070206 0.065 1.4 1.6 25x 22x kron_g500-logn20 2.5 0.24 3.1 13x 11x 0.50*** random.2Mv.128Me 0.10 3.0 29x 2.4 23x 0.70*** 0.15 3.3 2.6 rmat.2Mv.128Me 22x 18x

- Previous algorithm called "contract-expand", because it first takes current layer's edge frontier, contracts it (removes duplicates), then expands into next layer's edge frontier (containing duplicates).
- "Expand-contract", algorithm expands current vertex frontier, then contracts it (removes duplicates) to next laver's vertex frontier.
- 2-phase expands then contracts in two kernels.
- Hybrid combines contractexpand with 2-phase, using 2-phase for iterations with large frontiers.
- Variants differ in amount of memory traffic, latency and parallelism.
- Hybrid's performance is mostly determined by average degree (which generally increases moving down the dataset).

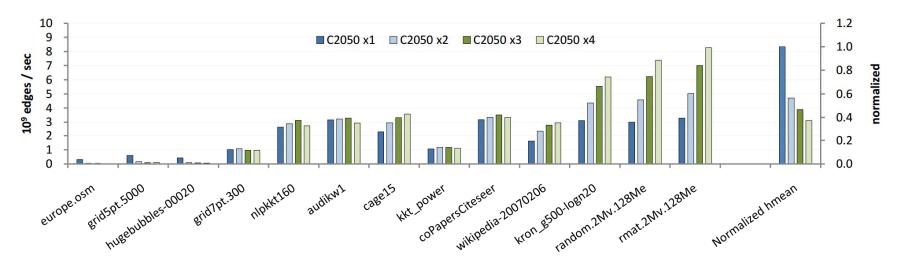


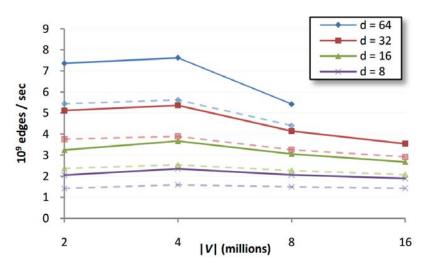
Multi-GPU BFS

- Multiple GPUs can use a single logical address space.
 - □ Communicate through PCI-e 2.0 (6.6 GB/s).
- Given p GPUs, assign n/p vertices and corresponding edges per GPU.
 - Vertices assigned in round robin order for load balancing.
 - □ Poor locality if p large.
- Each GPU expands / contracts its own vertex queue, as in the single GPU algorithm (*).
- Then sort the new frontier into p bins, corresponding to vertices from different GPUs.
- Barrier across all GPUs.
- Run p-1 kernels, where in i'th kernel, the i'th GPU collects bin i from each other GPU.
- Then go back to step (*) to form the next layer. Continue until all nodes visited.



Performance





Performance on uniform random graph. Higher average degree (d) results in better duplicate culling and higher performance.

- Only achieved speedup on graphs with small diameters and large average degrees.
 - Smaller diameter requires less synchronization.
 - Larger degree makes duplicate culling more effective.
 - Max speedups 1.5X, 2.1X and 2.5X on 2, 3, 4 GPUs.
 - Sometimes parallel algorithm performed much worse.