### **Parallel Graph Algorithms**

### Aydın Buluç

ABuluc@lbl.gov http://gauss.cs.ucsb.edu/~aydin/

**Lawrence Berkeley National Laboratory** 

CS267, Spring 2015 March 19, 2015

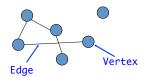
Slide acknowledgments: A. Azad, S. Beamer, J. Gilbert, K. Madduri

### **Lecture Outline**

- Applications
- Designing parallel graph algorithms
- Case studies:
  - A. Graph traversals: Breadth-first search
  - **B. Shortest Paths:** Delta-stepping, Floyd-Warshall
  - C. Maximal Independent Sets: Luby's algorithm
  - **D. Strongly Connected Components**
  - E. Maximum Cardinality Matching

### **Graph Preliminaries**

Define: <u>Graph</u> G = (V,E)
-a set of vertices and a set
of edges between vertices



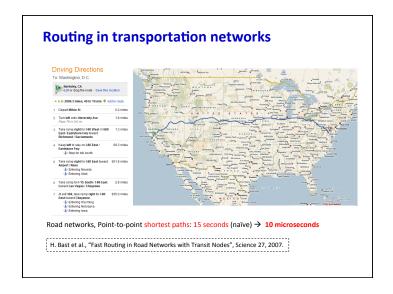
n=|V| (number of vertices)
m=|E| (number of edges)

D=diameter (max #hops between any pair of vertices)

- Edges can be directed or undirected, weighted or not.
- They can even have attributes (i.e. semantic graphs)
- Sequences of edges <u<sub>1</sub>,u<sub>2</sub>>, <u<sub>2</sub>,u<sub>3</sub>>, ..., <u<sub>n-1</sub>,u<sub>n</sub>> is a
  path from u<sub>1</sub> to u<sub>n</sub>. Its length is the sum of its weights.

### **Lecture Outline**

- Applications
- Designing parallel graph algorithms
- Case studies:
  - A. Graph traversals: Breadth-first search
  - B. Shortest Paths: Delta-stepping, Floyd-Warshall
  - C. Maximal Independent Sets: Luby's algorithm
  - **D.** Strongly Connected Components
  - E. Maximum Cardinality Matching

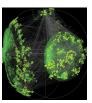


### Internet and the WWW

- The world-wide web can be represented as a directed graph
  - Web search and crawl: traversal
  - Link analysis, ranking: Page rank and HITS
  - Document classification and clustering
- Internet topologies (router networks) are naturally modeled as graphs

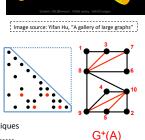






### **Scientific Computing**

- Reorderings for sparse solvers
  - Fill reducing orderings
    - Partitioning, eigenvectors
  - Heavy diagonal to reduce pivoting (matching)
- Data structures for efficient exploitation of sparsity
- Derivative computations for optimization
  - graph colorings, spanning trees
- Preconditioning
  - Incomplete Factorizations
  - Partitioning for domain decomposition
  - Graph techniques in algebraic multigrid
    - Independent sets, matchings, etc.
  - Support Theory
    - Spanning trees & graph embedding techniques



[chordal]

B. Hendrickson, "Graphs and HPC: Lessons for Future Architectures", http://www.er.doe.gov/ascr/ascac/Meetings/Oct08/Hendrickson%20ASCAC.pdf

### Large-scale data analysis

- Graph abstractions are very useful to analyze complex data sets.
- Sources of data: petascale simulations, experimental devices, the Internet, sensor networks
- Challenges: data size, heterogeneity, uncertainty, data quality

Astrophysics: massive datasets,

temporal variations



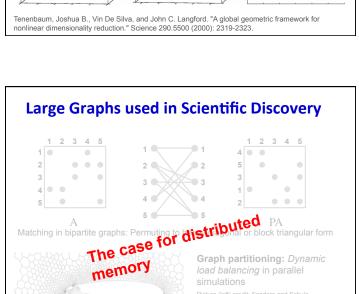


Social Informatics: new analytics challenges, data uncertainty



 $Image \ sources: (1) \ \underline{http://physics.nmt.edu/images/astro/hst\_starfield.jpq} \ (2,3) \ www.visual Complexity.complex$ 

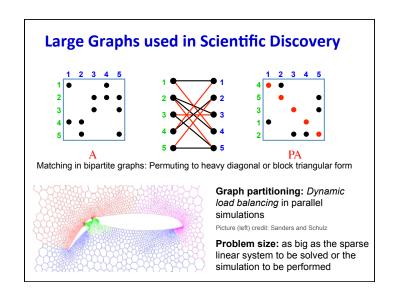
## Isomap (Nonlinear dimensionality reduction): Preserves the intrinsic geometry of the data by using the geodesic distances on manifold between all pairs of points Tools used or desired: - K-nearest neighbors - All pairs shortest paths (APSP) - Top-k eigenvalues Tenenbaum, Joshua B., Vin De Silva, and John C. Langford. "A global geometric framework for nonlinear dimensionality reduction." Science 290.5500 (2000): 2319-2323.

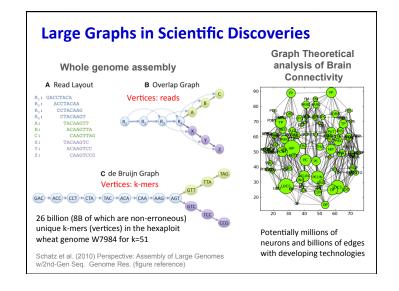


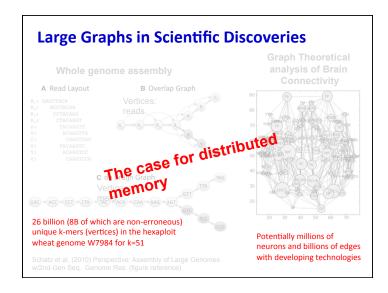
Problem size: as big as the sparse

linear system to be solved or the

simulation to be performed







- Applications
- · Designing parallel graph algorithms
- · Case studies:
  - A. Graph traversals: Breadth-first search
  - B. Shortest Paths: Delta-stepping, Floyd-Warshall
  - C. Maximal Independent Sets: Luby's algorithm
  - **D. Strongly Connected Components**
  - E. Maximum Cardinality Matching

### The PRAM model

- Many PRAM graph algorithms in 1980s.
- Idealized parallel shared memory system model
- Unbounded number of synchronous processors; no synchronization, communication cost; no parallel overhead
- EREW (Exclusive Read Exclusive Write), CREW (Concurrent Read Exclusive Write)
- Measuring performance: space and time complexity; total number of operations (work)

### **PRAM Pros and Cons**

- Pros
  - Simple and clean semantics.
  - The majority of theoretical parallel algorithms are designed using the PRAM model.
  - Independent of the communication network topology.
- Cons
  - Not realistic, too powerful communication model.
  - Communication costs are ignored.
  - Synchronized processors.
  - No local memory.
  - Big-O notation is often misleading.

### **Graph representations** Compressed sparse rows (CSR) = cache-efficient adjacency lists 2 Index into adjacency 6 (row pointers in CSR) array (column ids in CSR) Adjacencies (numerical values in CSR)

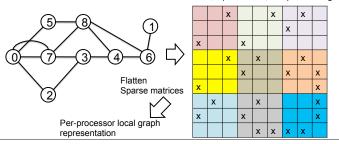
### **Distributed graph representations**

- Each processor stores the entire graph ("full replication")
- Each processor stores n/p vertices and all adjacencies out of these vertices ("1D partitioning")
- How to create these "p" vertex partitions?
  - Graph partitioning algorithms: recursively optimize for conductance (edge cut/size of smaller partition)
  - Randomly shuffling the vertex identifiers ensures that edge count/processor are roughly the same

### 2D checkerboard distribution

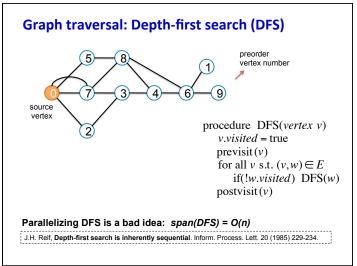
- Consider a logical 2D processor grid (p, \* p, = p) and the matrix representation of the graph
- Assign each processor a sub-matrix (i.e, the edges within the sub-matrix)

9 vertices, 9 processors, 3x3 processor grid

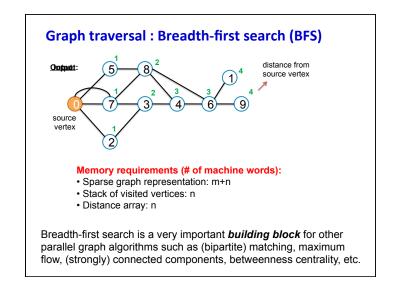


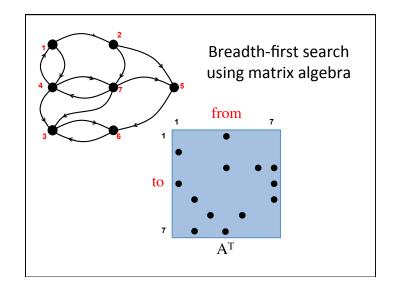
### **Lecture Outline**

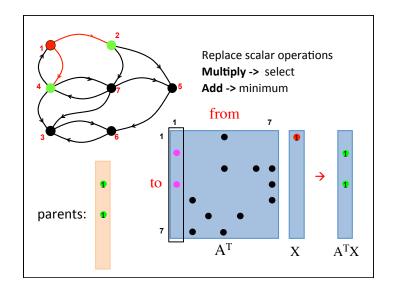
- Applications
- Designing parallel graph algorithms
- Case studies:
  - A. Graph traversals: Breadth-first search
  - B. Shortest Paths: Delta-stepping, Floyd-Warshall
  - C. Maximal Independent Sets: Luby's algorithm
  - **D. Strongly Connected Components**
  - E. Maximum Cardinality Matching

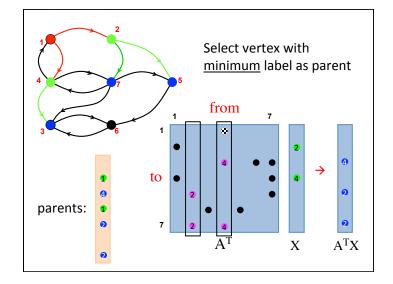


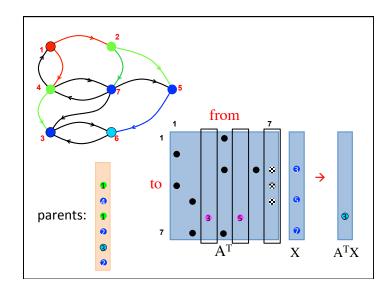
# Parallel BFS Strategies 1. Expand current frontier (level-synchronous approach, suited for low diameter graphs) • O(D) parallel steps • Adjacencies of all vertices in current frontier are visited in parallel 2. Stitch multiple concurrent traversals (Ullman-Yannakakis approach, suited for high-diameter graphs) • path-limited searches from "super vertices" • APSP between "super vertices" • APSP between "super vertices"

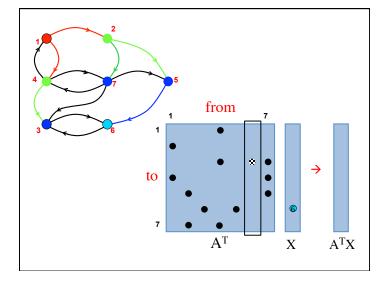










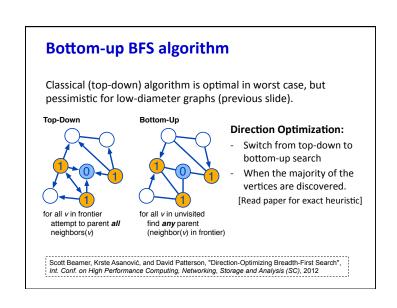


### 1D Parallel BFS algorithm AT frontier ALGORITHM:

- 1. Find owners of the current frontier's adjacency [computation]
- 2. Exchange adjacencies via all-to-all. [communication]
- 3. Update distances/parents for unvisited vertices. [computation]

### 

### 2D Parallel BFS algorithm AT frontier ALGORITHM: 1. Gather vertices in processor column [communication] 2. Find owners of the current frontier's adjacency [computation] 3. Exchange adjacencies in processor row [communication] 4. Update distances/parents for unvisited vertices. [computation]



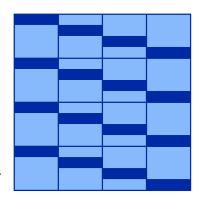
### **Direction optimizing BFS with 2D decomposition**

- Adoption of the 2D algorithm created the first quantum leap
- The second quantum leap comes from the bottom-up search
- Can we just do bottom-up on 1D?
- Yes, if you have *in-network* fast frontier membership queries
  - IBM by-passed MPI to achieve this [Checconi & Petrini, IPDPS'14]
  - · Unrealistic and counter-productive in general
- 2D partitioning reduces the required frontier segment by a factor of p<sub>c</sub> (typically Vp), without fast in-network reductions
- · Challenge: Inner loop is serialized

### **Direction optimizing BFS with 2D decomposition**

**Solution:** Temporally partition the work

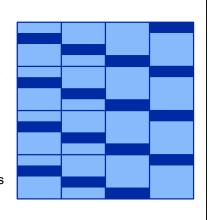
- Temporal Division a vertex is processed by at most one processor at a time
- Systolic Rotation send completion information to next processor so it knows what to skip



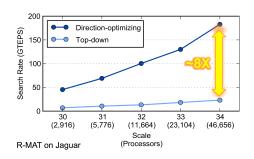
### **Direction optimizing BFS with 2D decomposition**

**Solution:** Temporally partition the work

- Temporal Division a vertex is processed by at most one processor at a time
- Systolic Rotation send completion information to next processor so it knows what to skip



### **Direction optimizing BFS with 2D decomposition**



- ORNL Titan (Cray XK6, Gemini interconnect AMD Interlagos)
- Kronecker (Graph500): 16 billion vertices and 256 billion edges.

Scott Beamer, Aydın Buluç, Krste Asanović, and David Patterson, "Distributed Memory Breadth-First Search Revisited: Enabling Bottom-Up Search", IPDPSW, 2013

### **Parallel De Bruijn Graph Traversal**

### Goal:

- Traverse the de Bruijn graph and find UU contigs (chains of UU nodes), or alternatively
- find the connected components which consist of the UU contigs.



- Main idea:
  - Pick a seed
  - Iteratively extend it by consecutive lookups in the distributed hash table

### **Parallel De Bruijn Graph Traversal**

Assume one of the UU contigs to be assembled is:

CGTATTGCCAATGCAACGTATCATGGCCAATCCGAT

### **Parallel De Bruijn Graph Traversal**

Processor P<sub>i</sub> picks a random k-mer from the distributed hash table as seed:



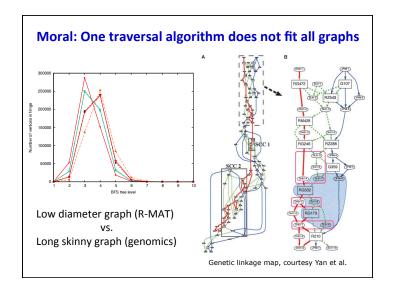
- P<sub>i</sub> knows that forward extension is A
- P<sub>i</sub> uses the last k-1 bases and the forward extension and forms: CAACGTATCA
- P<sub>i</sub> does a lookup in the distributed hash table for CAACGTATCA
- P<sub>i</sub> iterates this process until it reaches the "right" endpoint of the UU contig
- $\mathbf{P}_{\mathrm{i}}$  also iterates this process backwards until it reaches the "left" endpoint of the UU contig

### Multiple processors on the same UU contig



However, processors  ${\rm P_{i\nu}}~{\rm P_{j}}$  and  ${\rm P_{t}}$  might have picked initial seeds from the same UU contig

- Processors P<sub>i</sub>, P<sub>j</sub> and P<sub>t</sub> have to collaborate and concatenate subcontigs in order to avoid redundant work.
- Solution: lightweight synchronization scheme based on a state machine



- Applications
- Designing parallel graph algorithms
- Case studies:
  - A. Graph traversals: Breadth-first search
  - B. Shortest Paths: Delta-stepping, Floyd-Warshall
  - C. Maximal Independent Sets: Luby's algorithm
  - **D. Strongly Connected Components**
  - E. Maximum Cardinality Matching

### Parallel Single-source Shortest Paths (SSSP) algorithms

- · Famous serial algorithms:
  - Bellman-Ford: label correcting works on any graph
  - **Dijkstra**: label setting requires nonnegative edge weights
- No known PRAM algorithm that runs in sub-linear time and O(m+n log n) work
- Ullman-Yannakakis randomized approach
- Meyer and Sanders, Δ stepping algorithm

U. Meyer and P.Sanders, Δ - stepping: a parallelizable shortest path algorithm. Journal of Algorithms 49 (2003)

 Chakaravarthy et al., clever combination of Δ - stepping and direction optimization (BFS) on supercomputer-scale graphs.

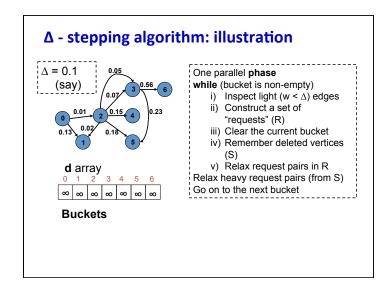
V. T. Chakaravarthy, F. Checconi, F. Petrini, Y. Sabharwal "Scalable Single Source Shortest Path Algorithms for Massively Parallel Systems", IPDPS'14

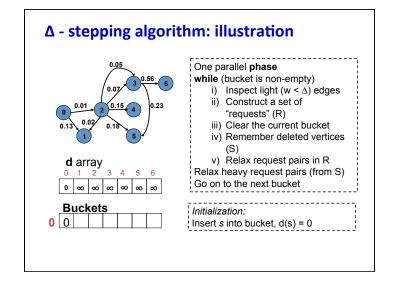
### Δ - stepping algorithm

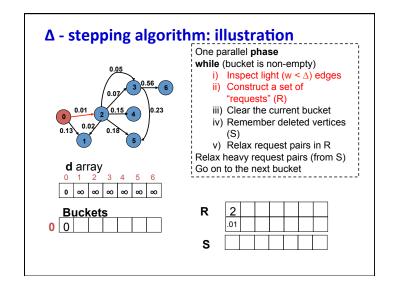
- Label-correcting algorithm: Can relax edges from unsettled vertices also
- "approximate bucket implementation of Dijkstra"
- For random edge weighs [0,1], runs in  $O(n+m+D\cdot L)$  where L = max distance from source to any node
- Vertices are ordered using buckets of width  $\Delta$
- Each bucket may be processed in parallel
- Basic operation: Relax ( e(u,v) )
   d(v) = min { d(v), d(u) + w(u, v) }

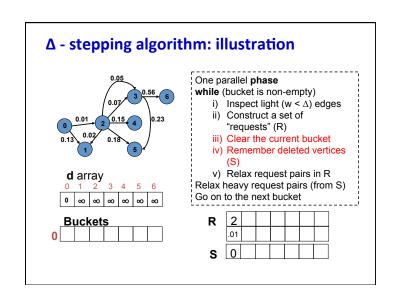
Δ < min w(e) : Degenerates into Dijkstra

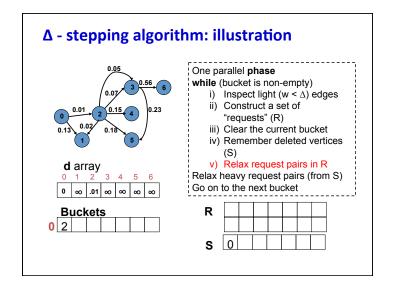
Δ > max w(e): Degenerates into Bellman-Ford

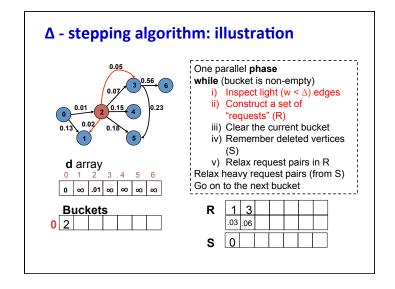


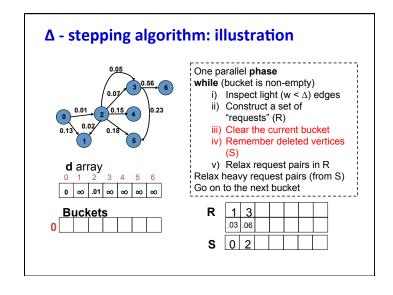


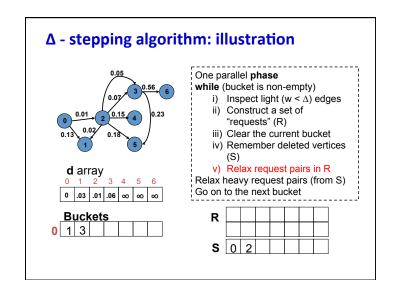


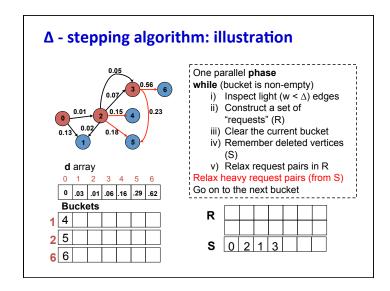


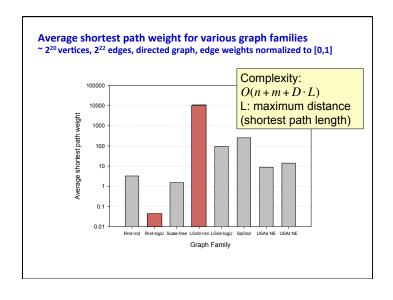


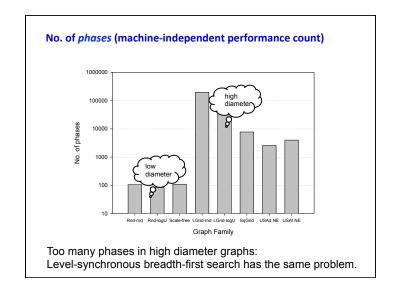










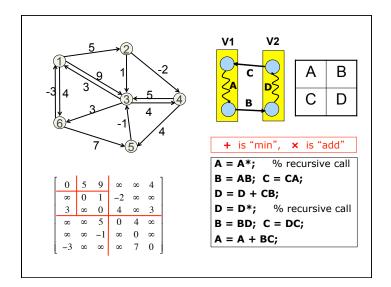


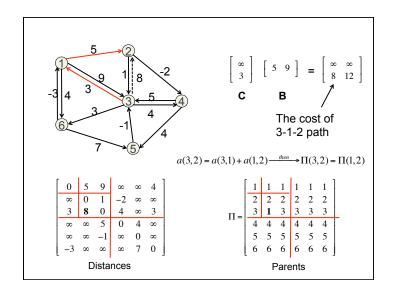
### All-pairs shortest-paths problem

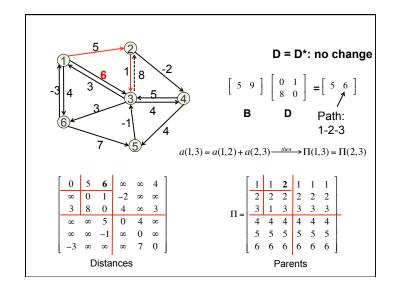
- Input: Directed graph with "costs" on edges
- Find least-cost paths between all reachable vertex pairs
- Classical algorithm: Floyd-Warshall

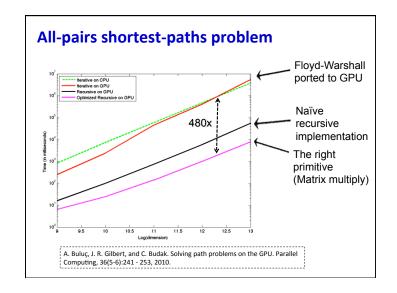
for 
$$k=1$$
:n // the induction sequence  
for  $i=1$ :n  
for  $j=1$ :n  
if  $(w(i\rightarrow k)+w(k\rightarrow j)< w(i\rightarrow j))$   
 $w(i\rightarrow j):=w(i\rightarrow k)+w(k\rightarrow j)$ 

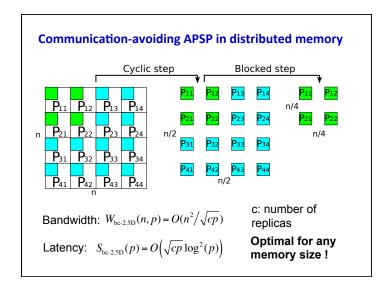
• It turns out a previously overlooked **recursive version** is more parallelizable than the triple nested loop

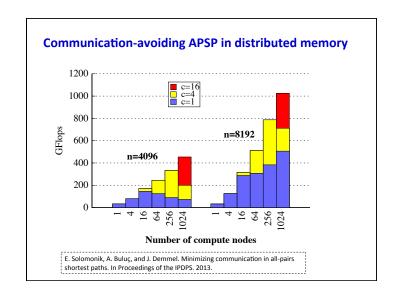








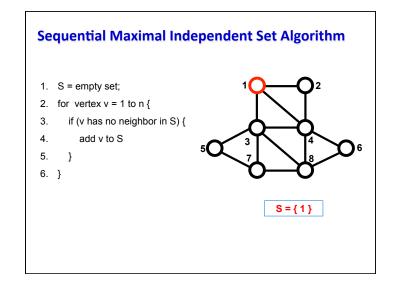




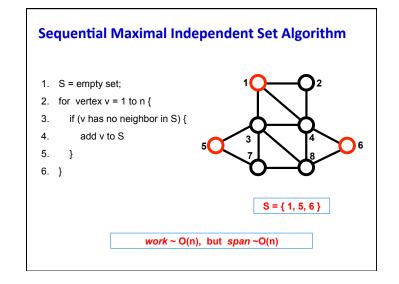
- Applications
- Designing parallel graph algorithms
- Case studies:
  - A. Graph traversals: Breadth-first search
  - B. Shortest Paths: Delta-stepping, Floyd-Warshall
  - C. Maximal Independent Sets: Luby's algorithm
  - **D. Strongly Connected Components**
  - E. Maximum Cardinality Matching

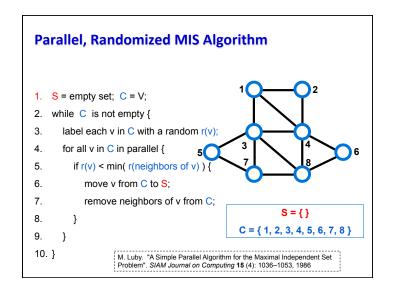
### **Maximal Independent Set** • Graph with vertices V = {1,2,...,n} · A set S of vertices is independent if no two vertices in S are neighbors. • An independent set S is maximal if it is impossible to add another vertex and stay independent · An independent set S is maximum if no other independent set has more • Finding a maximum independent set is The set of red vertices intractably difficult (NP-hard) $S = \{4, 5\}$ is independent and is maximal • Finding a maximal independent set is but not maximum easy, at least on one processor.

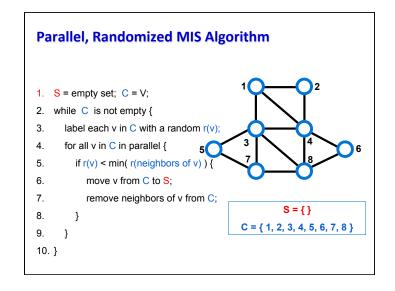
### Sequential Maximal Independent Set Algorithm 1. S = empty set; 2. for vertex v = 1 to n { 3. if (v has no neighbor in S) { 4. add v to S 5. } 6. } S = {}

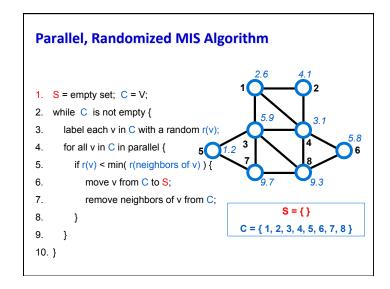


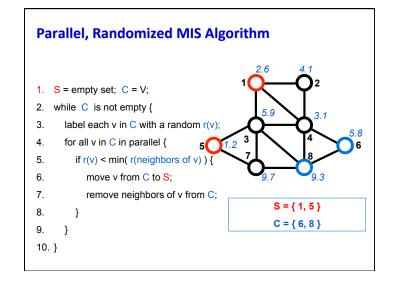
## Sequential Maximal Independent Set Algorithm 1. S = empty set; 2. for vertex v = 1 to n { 3. if (v has no neighbor in S) { 4. add v to S 5. } 6. } S = {1,5}



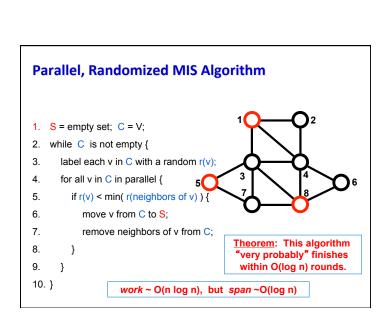








### **Parallel, Randomized MIS Algorithm** 1. S = empty set; C = V; 2. while C is not empty { label each v in C with a random r(v); 4. for all v in C in parallel { 5. if r(v) < min( r(neighbors of v) ) { 6. move v from C to S; 7. remove neighbors of v from C; $S = \{1, 5\}$ 8. $C = \{ 6, 8 \}$ } 10. }

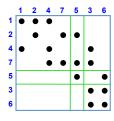


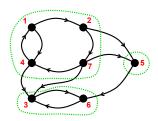
### **Parallel, Randomized MIS Algorithm** 1. S = empty set; C = V; 2. while C is not empty { label each v in C with a random r(v); for all v in C in parallel { 5. if r(v) < min( r(neighbors of 6. move v from C to S; 7. remove neighbors of v from C; $S = \{1, 5, 8\}$ 8. $C = \{\}$ 9. 10.}

### **Lecture Outline**

- Applications
- Designing parallel graph algorithms
- Case studies:
  - A. Graph traversals: Breadth-first search
  - B. Shortest Paths: Delta-stepping, Floyd-Warshall
  - C. Maximal Independent Sets: Luby's algorithm
  - **D. Strongly Connected Components**
  - E. Maximum Cardinality Matching

### **Strongly connected components (SCC)**





- · Symmetric permutation to block triangular form
- · Find P in linear time by depth-first search

Tarjan, R. E. (1972), "Depth-first search and linear graph algorithms", SIAM Journal on Computing 1 (2): 146–160

### Strongly connected components of directed graph

- Sequential: use depth-first search (Tarjan);
   work=O(m+n) for m=|E|, n=|V|.
- DFS seems to be inherently sequential.
- Parallel: divide-and-conquer and BFS (Fleischer et al.); worst-case span O(n) but good in practice on many graphs.

L. Fleischer, B. Hendrickson, and A. Pınar. On identifying strongly connected components in parallel. Parallel and Distributed Processing, pages 505–511, 2000.

### Fleischer/Hendrickson/Pinar algorithm

- Partition the given graph into three disjoint subgraphs
- Each can be processed independently/recursively

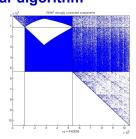
**Lemma:**  $FW(v) \cap BW(v)$  is a unique SCC for any v. For every other SCC s, either

(a)  $s \subseteq FW(v)\backslash BW(v)$ ,

 $\text{(b) s} \subset \mathsf{BW}(\mathsf{v}) \backslash \mathsf{FW}(\mathsf{v}),$ 

(c)  $s \subset V \setminus (FW(v) \cup BW(v))$ .

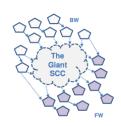
**FW(v):** vertices reachable from vertex v. **BW(v):** vertices from which v is reachable.





### Improving FW/BW with parallel BFS

Observation: Real world graphs have giant SCCs



Finding FW(pivot) and BW(pivot) can dominate the running time with span=O(N)

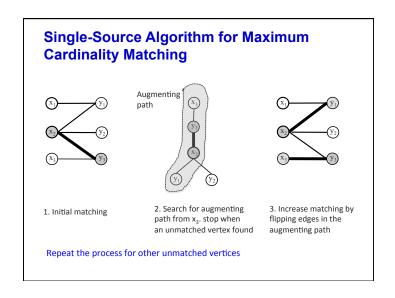
**Solution**: Use *parallel BFS* to limit span to diameter(SCC)

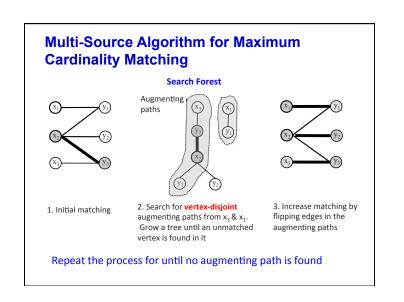
- Remaining SCCs are very small; increasing span of the recursion.
- + Find weakly-connected components and process them in parallel

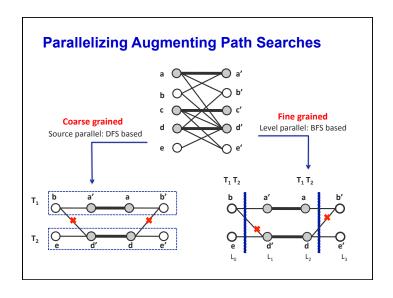
S. Hong, N.C. Rodia, and K. Olukotun. On Fast Parallel Detection of Strongly Connected Components (SCC) in Small-World Graphs. Proc. Supercomputing, 2013

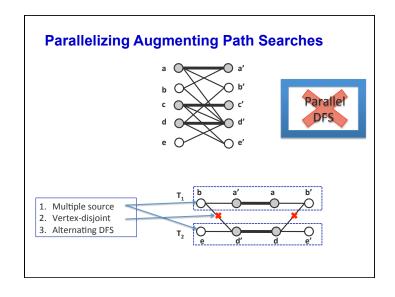
- Applications
- Designing parallel graph algorithms
- Case studies:
  - A. Graph traversals: Breadth-first search
  - **B.** Shortest Paths: Delta-stepping, Floyd-Warshall
  - C. Maximal Independent Sets: Luby's algorithm
  - **D. Strongly Connected Components**
  - E. Maximum Cardinality Matching

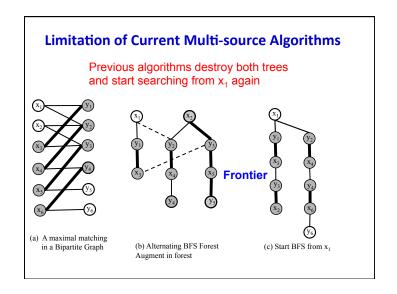
### Bipartite Graph Matching • Matching: A subset M of edges with no common end vertices. - |M| = Cardinality of the matching M Matched vertex — Matched edge Unmatched vertex — Unmatched edge Sylvy A Matching (Maximal cardinality) Maximum Cardinality Matching

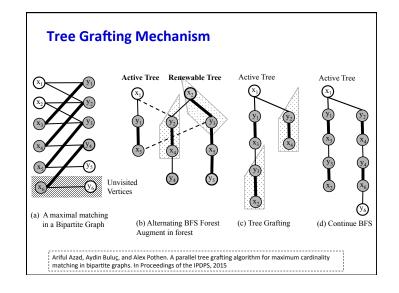






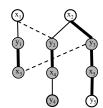






### **Parallel Tree Grafting**

- 1. Parallel direction optimized BFS (Beamer et al. SC 2012)
  - Use bottom-up BFS when the frontier is large

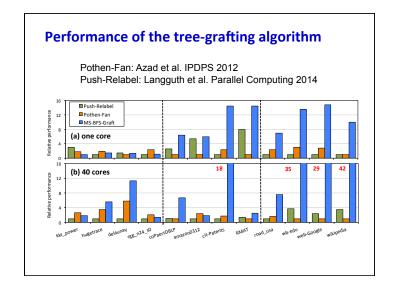


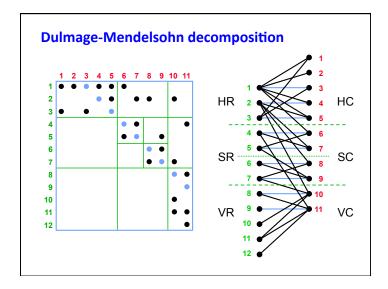
Maintain visited array

To maintain vertex-disjoint paths, a vertex is visited only once in an iteration.

Thread-safe atomics

- 2. Since the augmenting paths are vertex disjoint we can augment them in parallel
- 3. Each renewable vertex tries to attach itself to an active vertex. No synchronization necessary





### **Dulmage-Mendelsohn decomposition**

- 1. Find a "perfect matching" in the bipartite graph of the matrix.
- 2. Permute the matrix to have a zero free diagonal.
- 3. Find the "strongly connected components" of the directed graph of the permuted matrix.

Let M be a maximum-size matching. Define:

VR = { rows reachable via alt. path from some unmatched row }

VC = { cols reachable via alt. path from some unmatched row }

HR = { rows reachable via alt. path from some unmatched col }

HC = { cols reachable via alt. path from some unmatched col }

SR = R - VR - HR

SC = C - VC - HC

### **Applications of D-M decomposition**

- Strongly connected components of directed graphs
- Connected components of undirected graphs
- Permutation to block triangular form for Ax=b
- Minimum-size vertex cover of bipartite graphs
- Extracting vertex separators from edge cuts for arbitrary graphs
- Nonzero structure prediction for sparse matrix factorizations