Parallel Graph Algorithms

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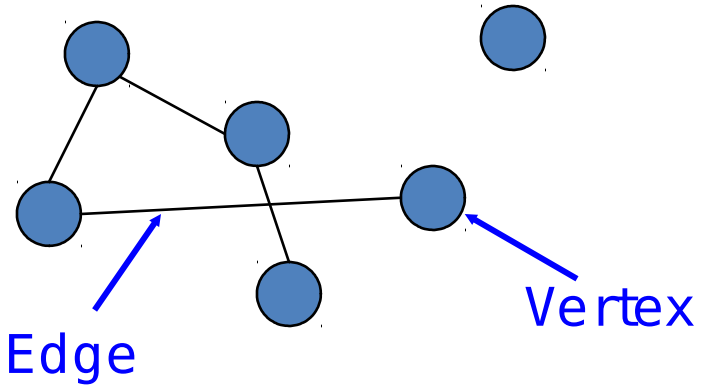
CS267, Spring 2013

April 9, 2013

Slide acknowledgments: K. Madduri, J. Gilbert, D. Delling, S. Beamer

Graph Preliminaries

Define: Graph 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)

Lecture Outline

- Applications
- Designing parallel graph algorithms
- Case studies:
  - **Graph traversals:** Breadth-first search
  - **Shortest Paths:** Delta-stepping, PHAST, Floyd-Warshall
  - **Ranking:** Betweenness centrality
  - **Maximal Independent Sets:** Luby's algorithm
  - **Strongly Connected Components**
- . Wrap-up: challenges on current systems

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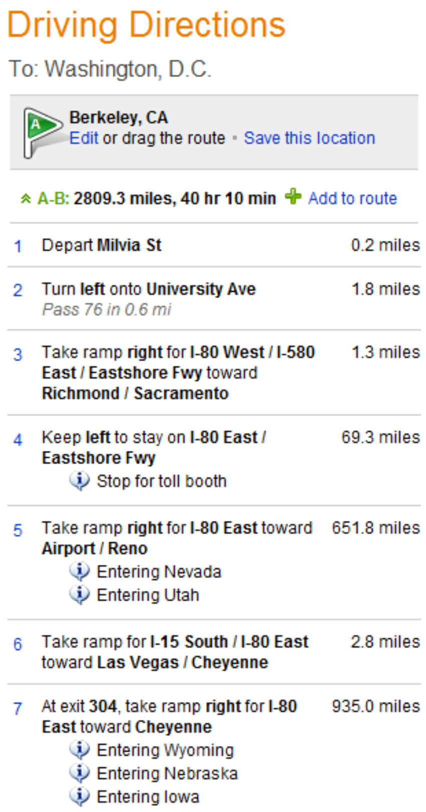
Routing in transportation networks

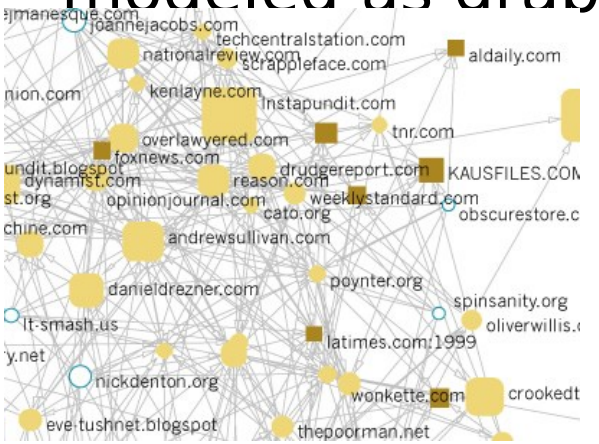


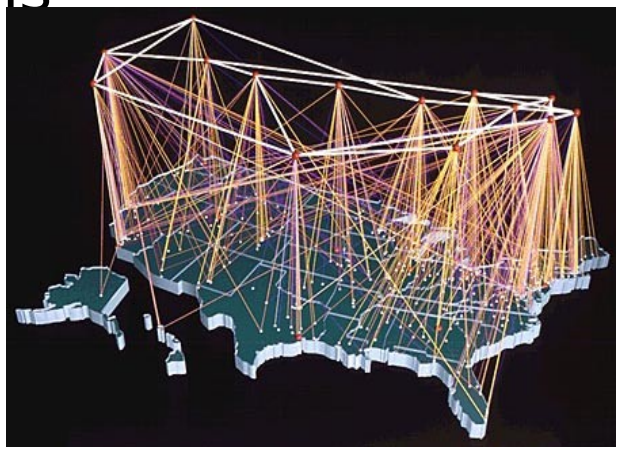
Road networks, Point-to-point shortest paths: 15 seconds (naïve) → **10 microseconds**

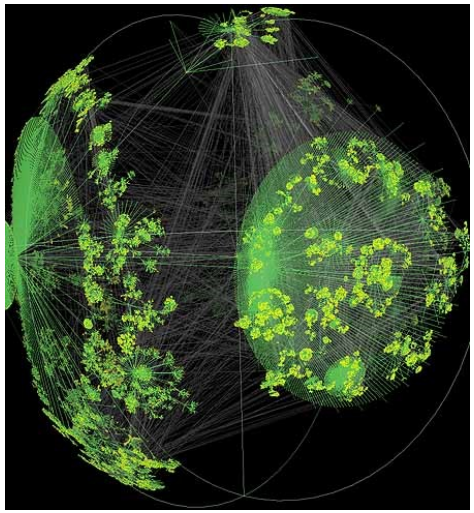
H. Bast et al., “Fast Routing in Road Networks with Transit Nodes”, Science 27, 2007.

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

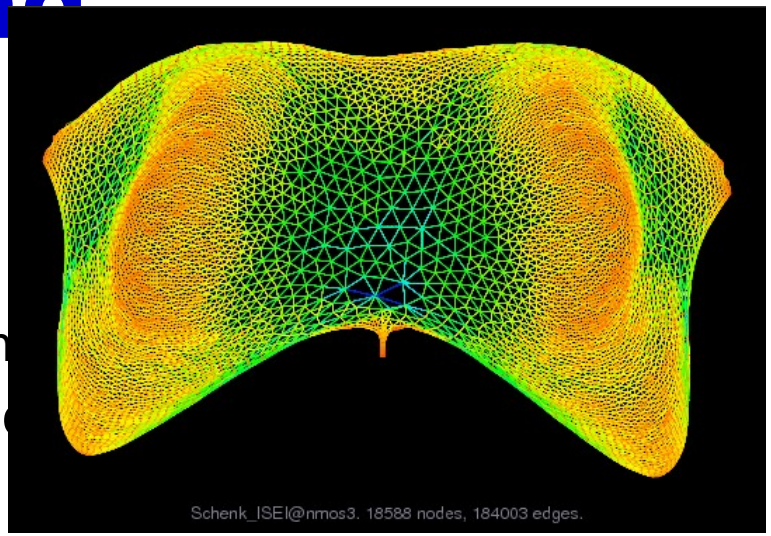
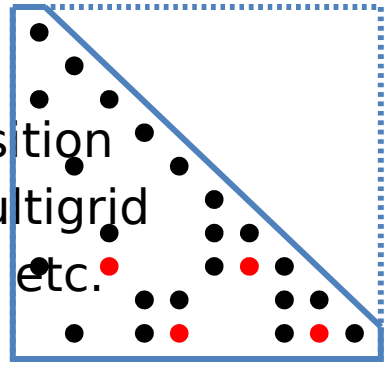
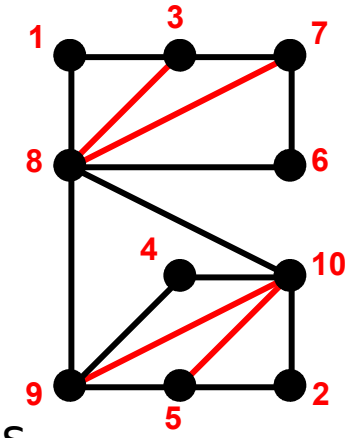


Image source: Yifan Hu, "A gallery of large graphs"

- Reorderings for sparse solvers
  - Fill reducing orderings
    - Partitioning, eigenvectors
  - Heavy diagonal to reduce pivoting (m
- Data structures for efficient exploitati
  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





G+(A)
[chordal]

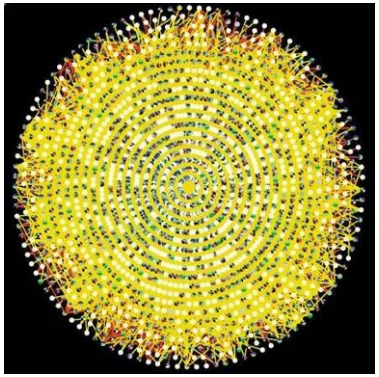
B. Hendrickson, "Graphs and HPC: Lessons for Future Architectures", http://www.er.doe.gov/ascr/ascac/Meetings/Oct08/Hendrickson%20ASCAC.pdf

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 data sets, temporal variations

Bioinformatics: data quality, heterogeneity



Social Informatics: new analytics challenges, data uncertainty

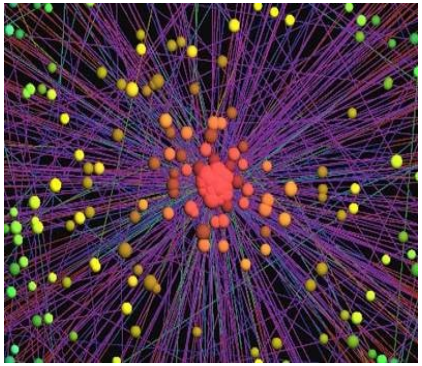


Image sources: (1) http://physics.nmt.edu/images/astro/hst_starfield.jpg (2,3) www.visualComplexity.com

Graph-theoretic problems in social networks

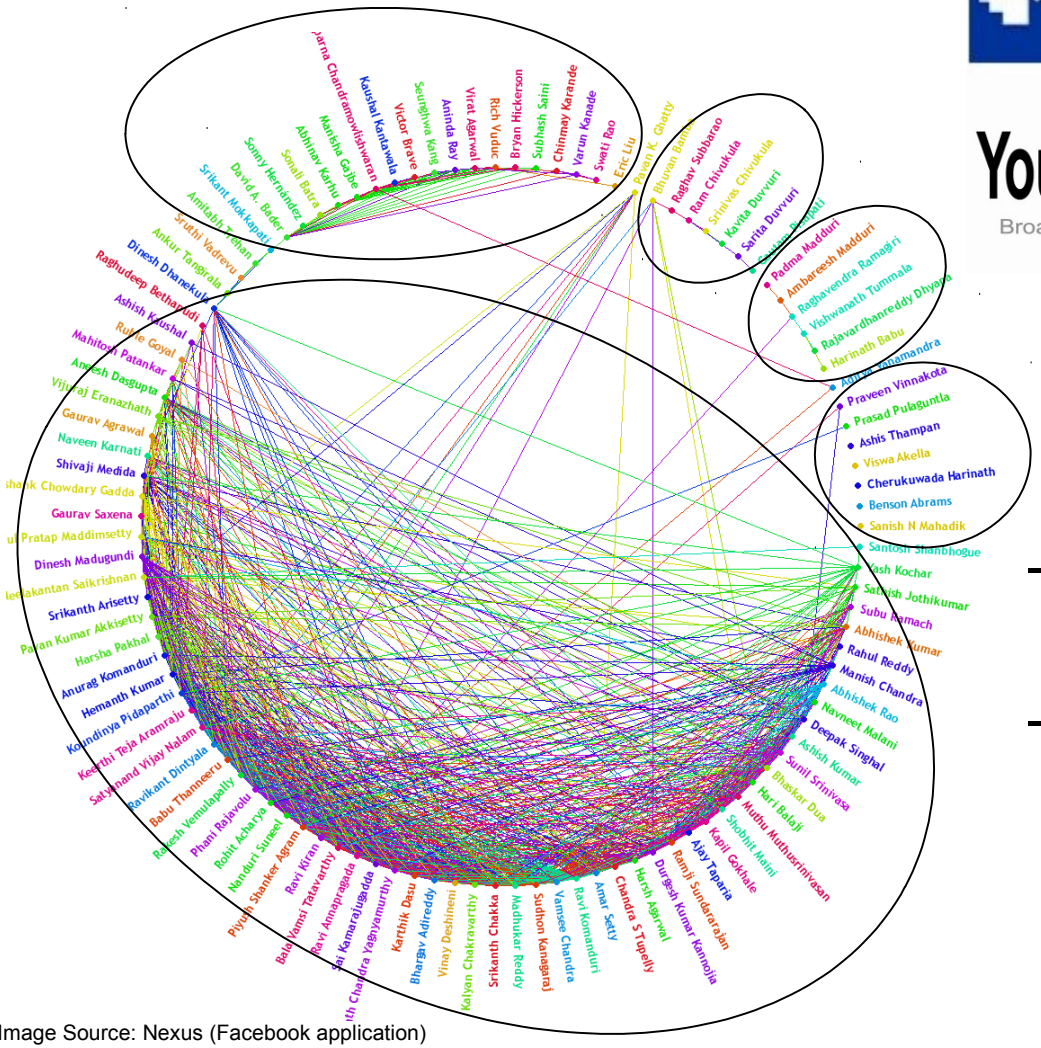


Image Source: Nexus (Facebook application)

myspace.com a place for friends

facebook

YouTube Broadcast Yourself

flickr BETA

LinkedIn

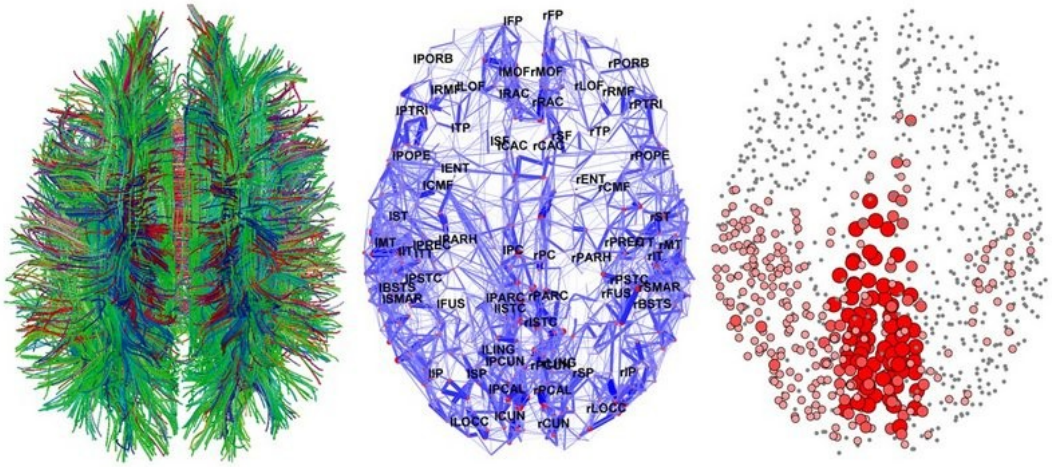
xanga.com THE WEBLOG COMMUNITY

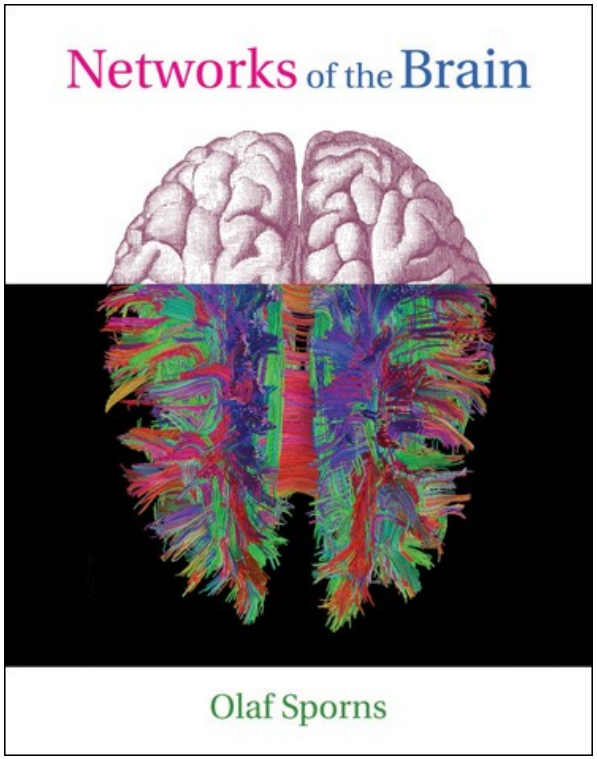
- Targeted advertising: clustering and centrality
- Studying the spread of information

Network Analysis for Neurosciences

Graph-theoretical models are used to predict the course of degenerative illnesses like Alzheimer's.

Vertices: ROI (regions of interest)
Edges: structural/functional connectivity

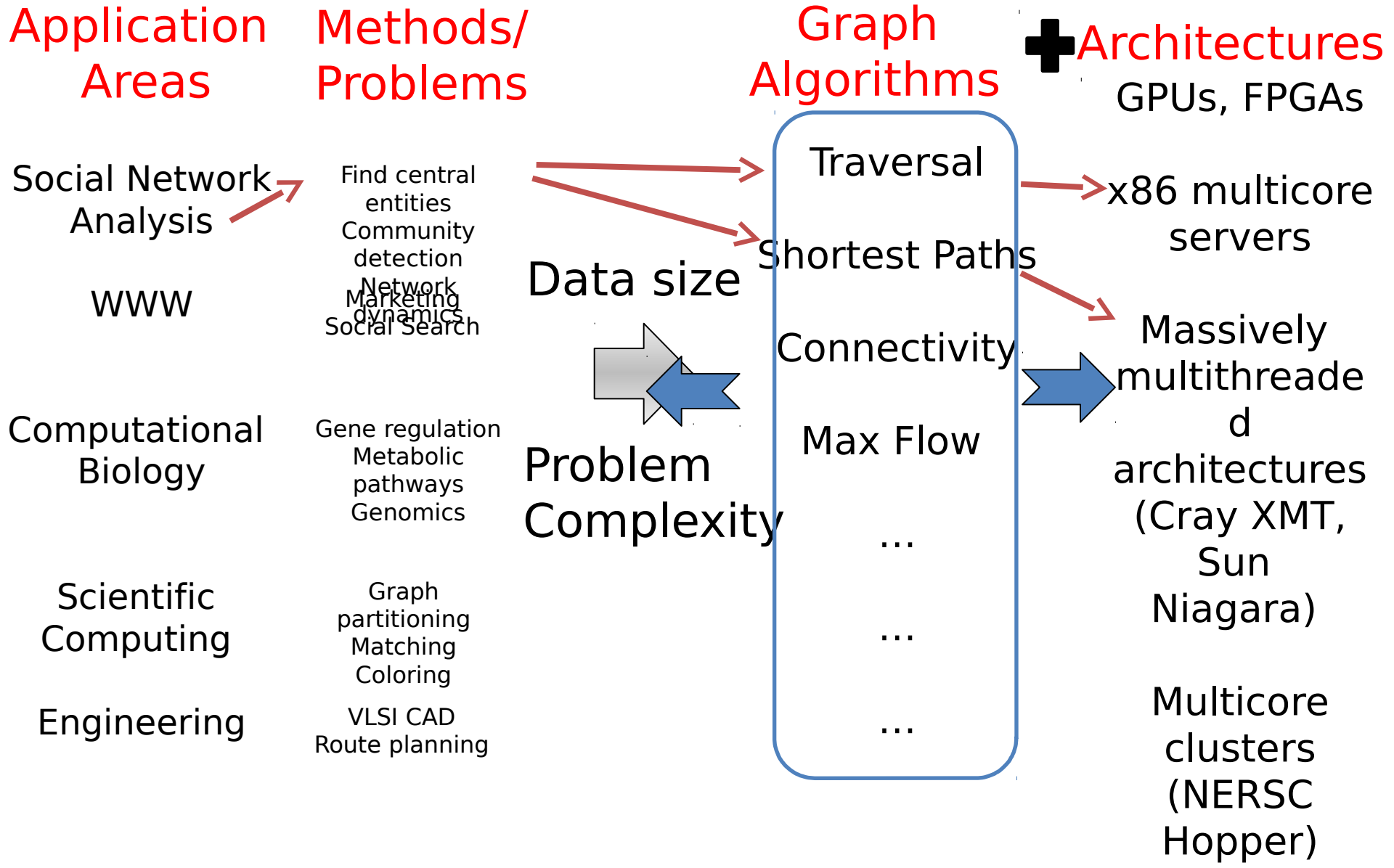




Some disease indicators:

- Deviation from small-world property
- Emergence of "epicenters" with disease-associated patterns

Research in Parallel Graph Algorithms



Characterizing Graph-theoretic computations

Input data

Problem: Find *

- paths
- clusters
- partitions
- matchings
- patterns
- orderings

Graph kernel

- traversal
- shortest path algorithms
- flow algorithms
- spanning tree algorithms
- topological sort

…..

Factors that influence choice of algorithm

- graph sparsity (m/n ratio)
- static/dynamic nature
- weighted/unweighted, weight distribution
- vertex degree distribution
- directed/undirected
- simple/multi/hyper graph
- problem size
- granularity of computation at nodes/edges
- domain-specific characteristics

Graph problems are often recast as sparse linear algebra (e.g., partitioning) or linear programming (e.g., matching) computations

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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

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.

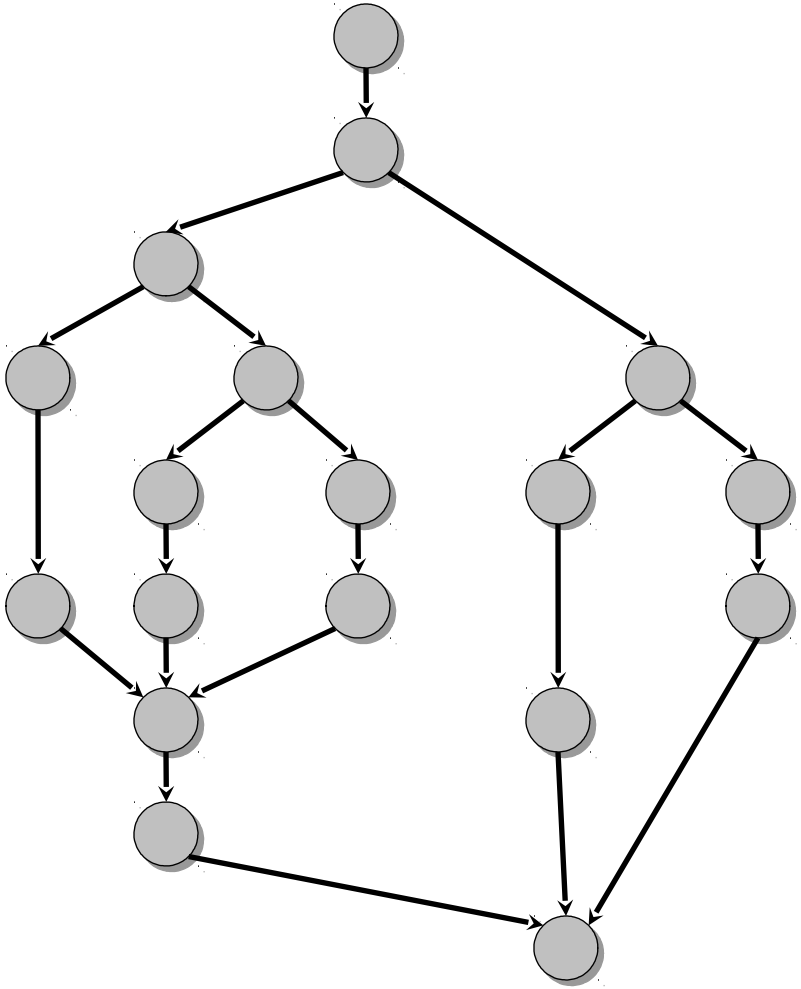
Building blocks of classical PRAM graph algorithms

- Prefix sums
- Symmetry breaking
- Pointer jumping
- List ranking
- Euler tours
- Vertex collapse
- Tree contraction

[some covered in the “Tricks with Trees” lecture]

Work / Span Model

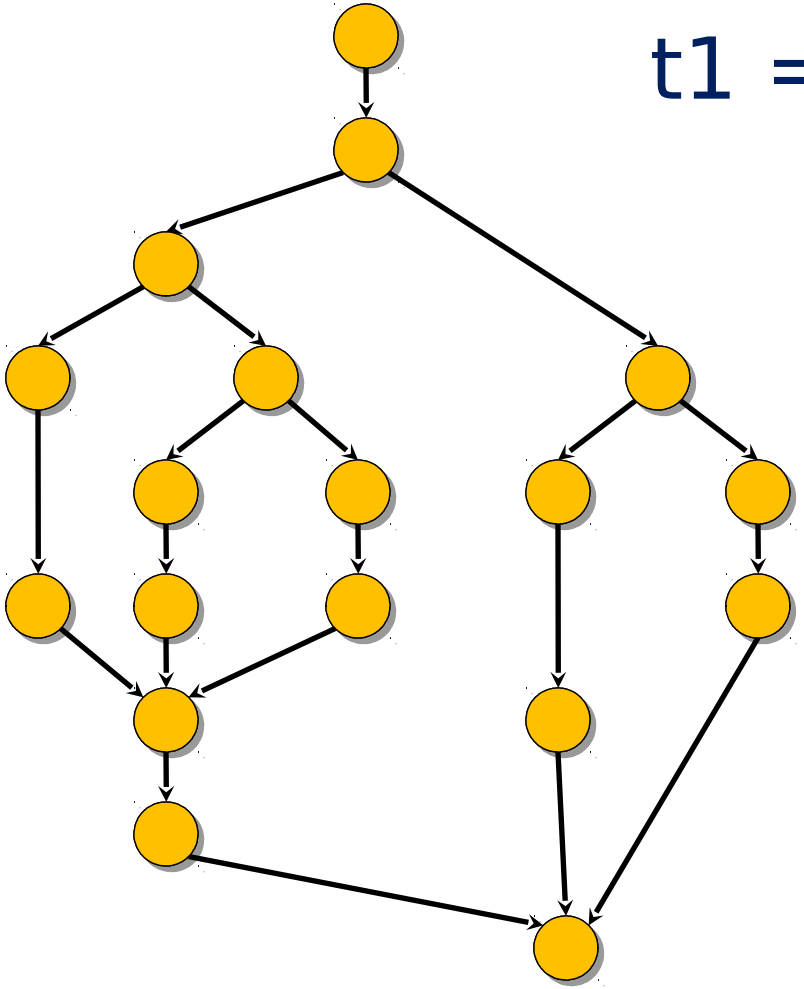
tp = execution time on p processors



Work / Span Model

tp = execution time on p processors

t1 = ***work***



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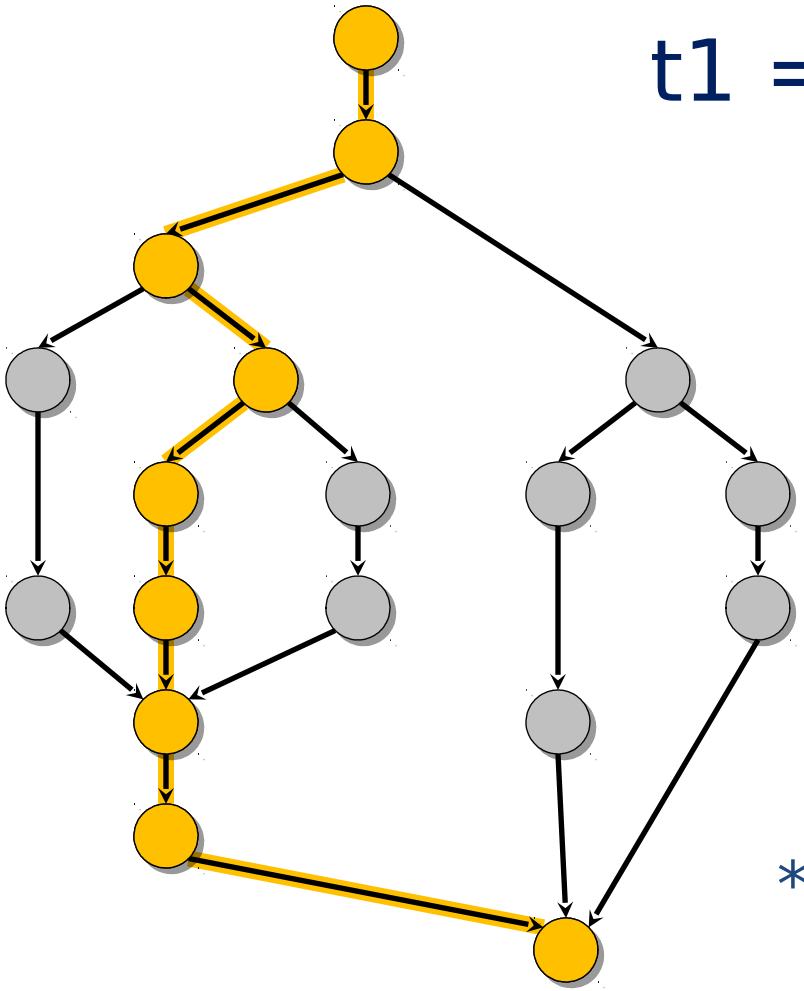


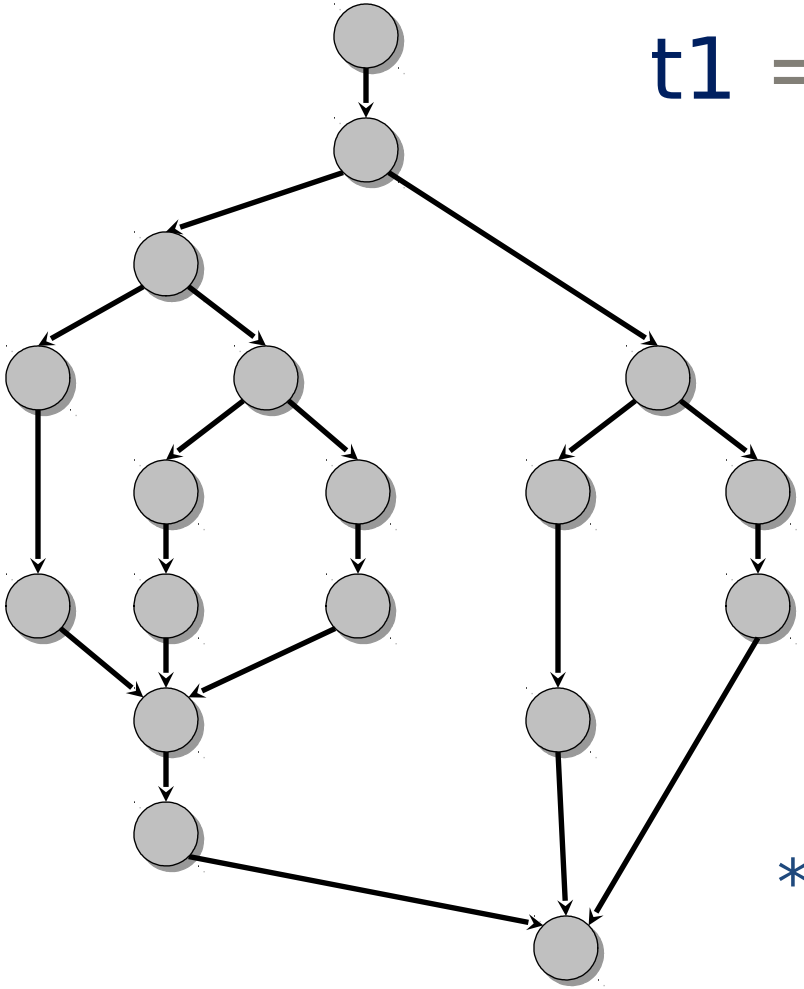
t1 = ***work***

t∞ = ***span*** *

*Also called ***critical-path length*** or ***computational depth***.

Work / Span Model

t_p = execution time on p processors



t_1 = ***work*** t_∞ = ***span***

WORK LAW

- $t_p \geq t_1/p$

SPAN LAW

- $t_p \geq t_\infty$

*Also called ***critical-path length*** or ***computational depth***.

Data structures: graph representation

Static case

- Dense graphs (m = Θ(n2)): adjacency matrix commonly used.
- Sparse graphs: adjacency lists, compressed sparse matrices

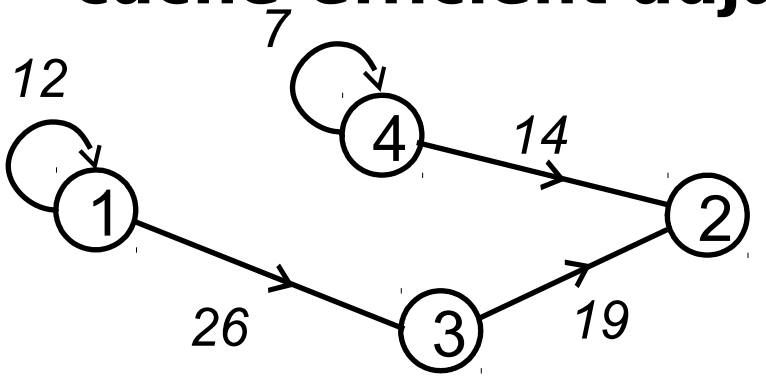
Dynamic

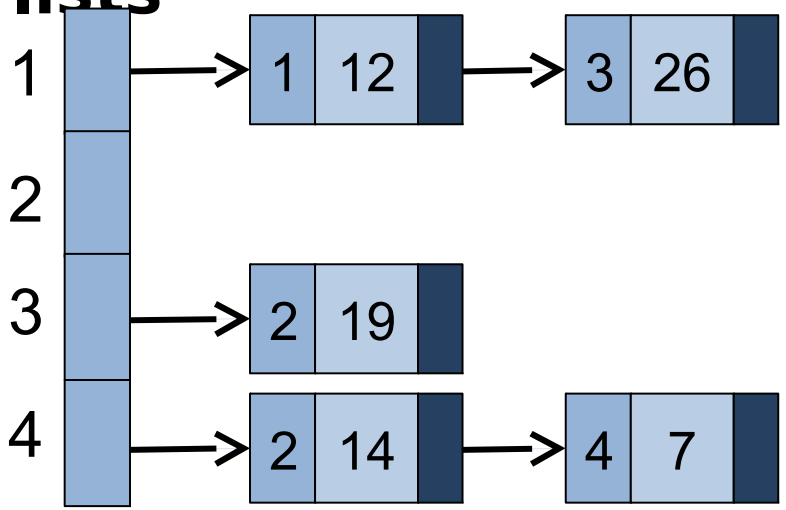
- representation depends on common-case query
- Edge insertions or deletions? Vertex insertions or deletions? Edge weight updates?
- Graph update rate
- Queries: connectivity, paths, flow, etc.

- Optimizing for locality a key design

Graph representations

Compressed sparse rows (CSR) = cache-efficient adjacency lists





Index into adjacency array

1	3	3	4	6

(row pointers in CSR)

Adjacencies	1	3	2	2	4
Weights	12	26	19	14	7

(column ids in CSR)

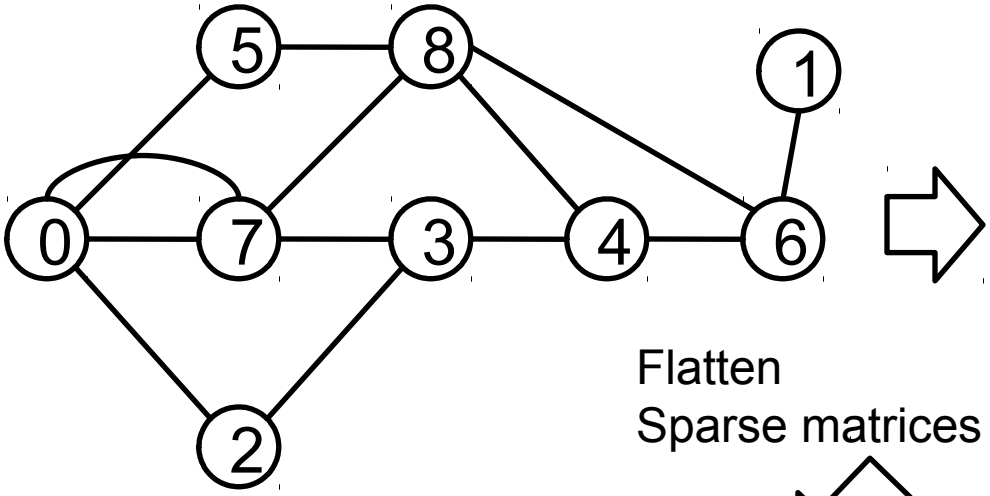
(numerical values in CSR)

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

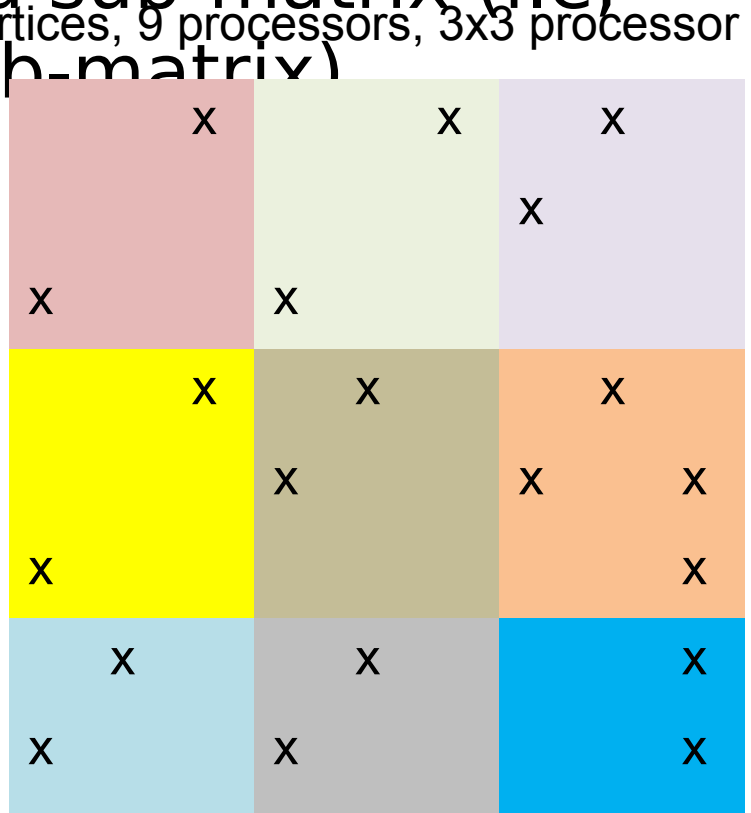
2D checkerboard distribution

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



Flatten Sparse matrices

Per-processor local graph representation



High-performance graph algorithms

- Implementations are typically array-based for performance (e.g. CSR representation).
- Concurrency = minimize synchronization (span)
- Where is the data? Find the distribution that minimizes inter-processor communication.
- Memory access patterns
  - Regularize them (spatial locality)
  - Minimize DRAM traffic (temporal locality)
- Work-efficiency
  - Is (Parallel time) * (# of processors) = (Serial

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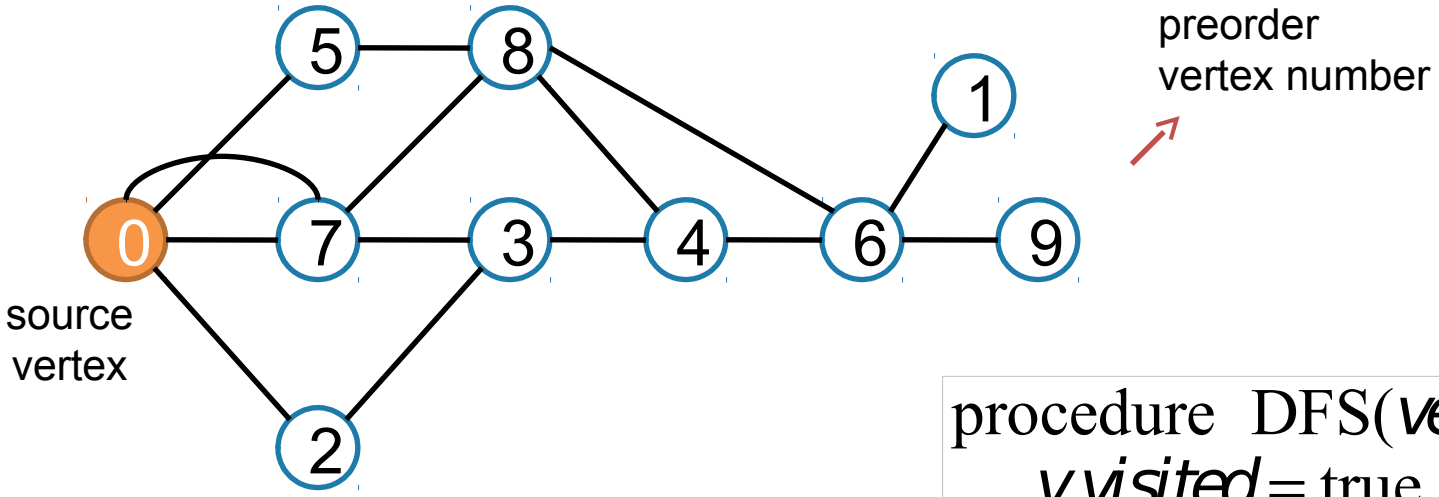
Graph traversal: Depth-first search (DFS)

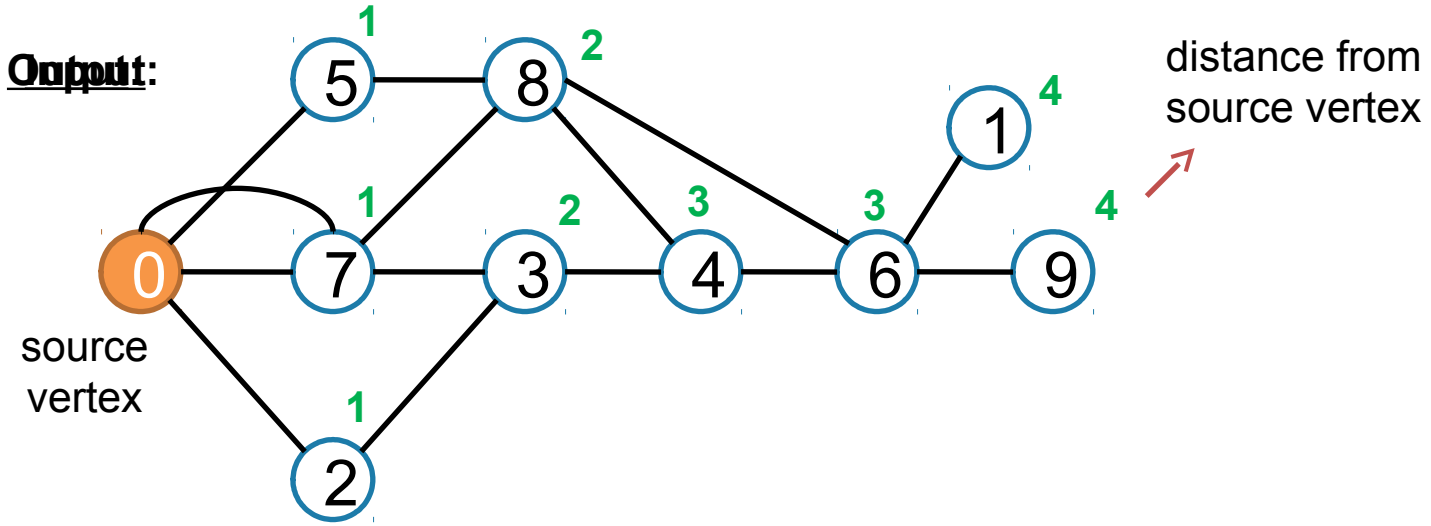



```
procedure DFS(vertex v)
    v.visited = true
    previsit(v)
    for all v s.t. (v, w) ∈ E
        if(!w.visited) DFS(w)
    postvisit(v)
```

Parallelizing DFS is a bad idea: *span(DFS) = O(n)*

J.H. Reif, **Depth-first search is inherently sequential**. Inform. Process. Lett. 20 (1985) 229-234.

Graph traversal : Breadth-first search (BFS)

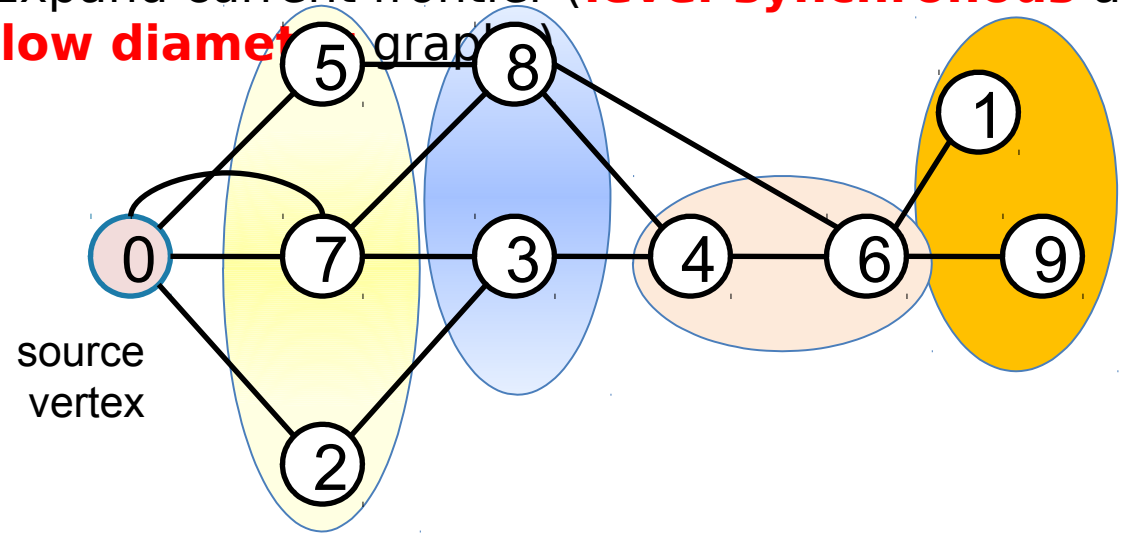


Memory requirements (# of machine words):

- Sparse graph representation: m+n
- Stack of visited vertices: n
- Distance array: n

Parallel BFS Strategies

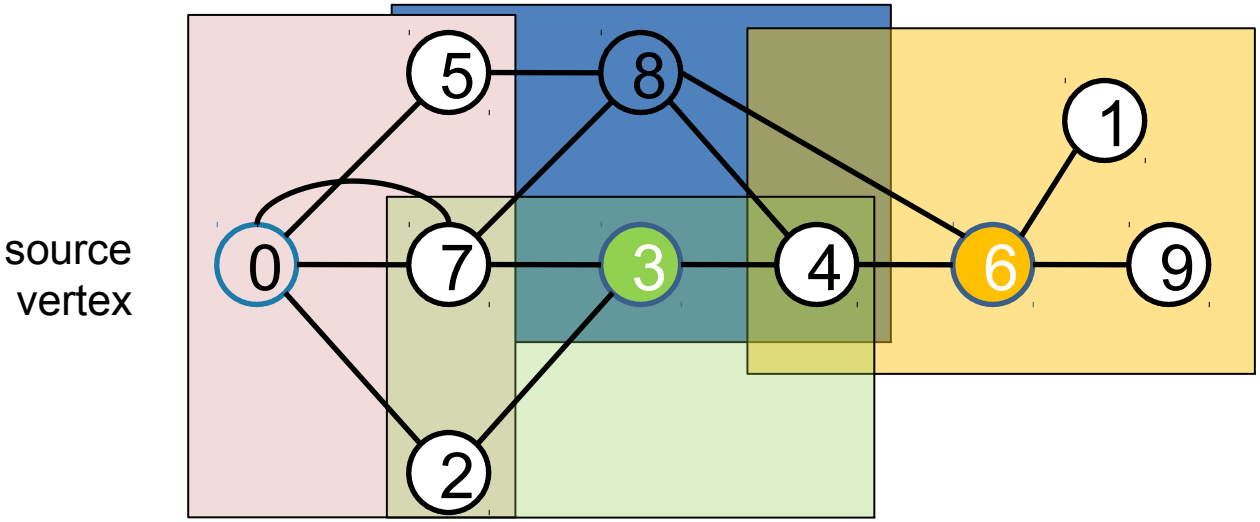
1. Expand current frontier (**level-synchronous** approach, suited for **low diameter** graphs)



- O(D) parallel steps
- Adjacencies of all vertices

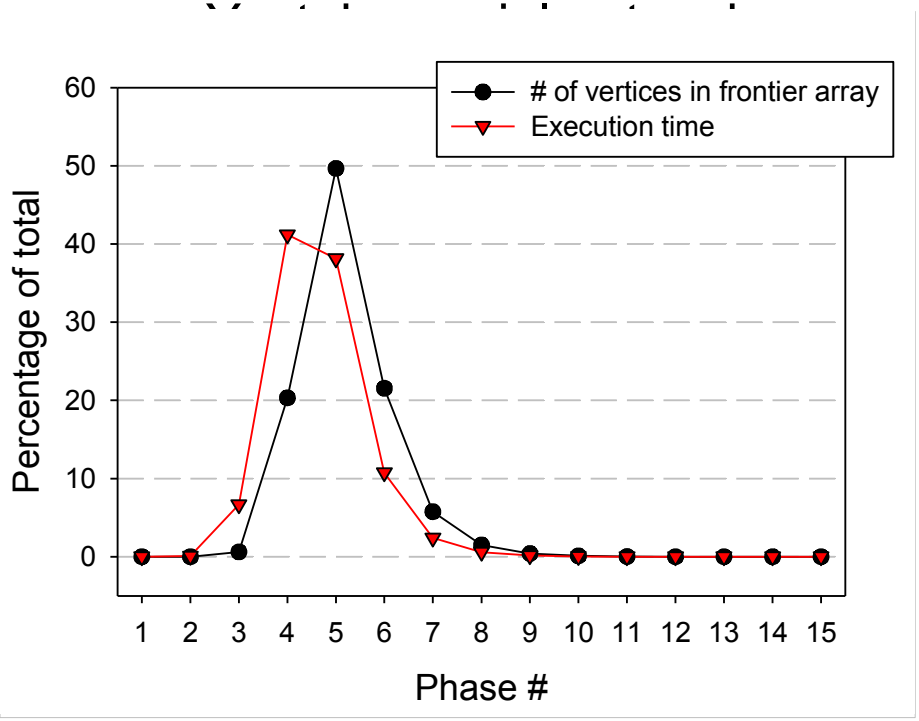
in current frontier are visited in parallel

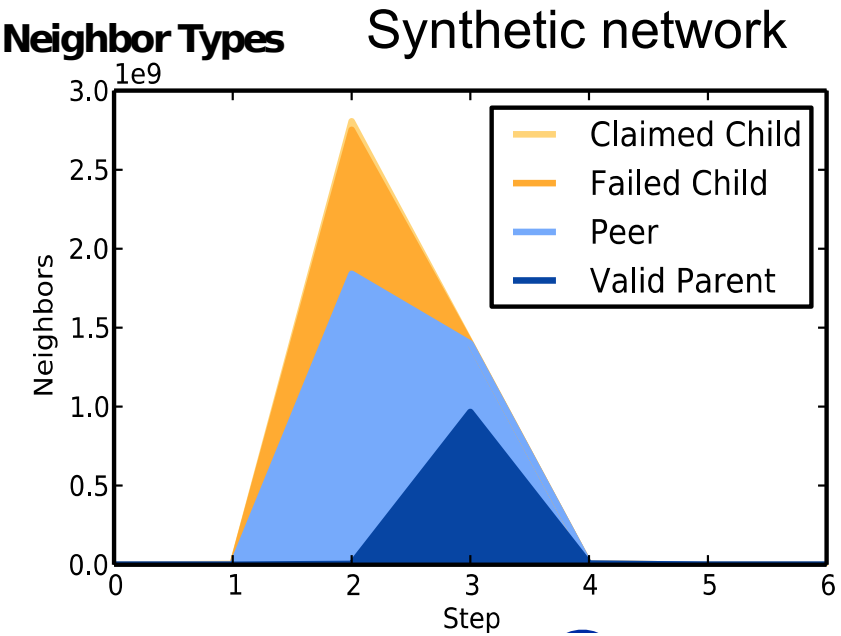
2. Stitch multiple concurrent traversals (Ullman-Yannakakis approach, suited for **high-diameter** graphs)



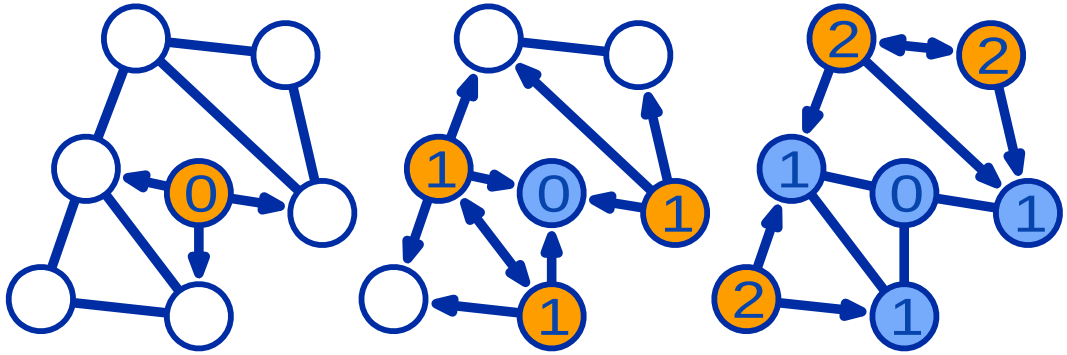
- path-limited searches from “super vertices”
- APSP between “super vertices”

Performance observations of the level-synchronous algorithm





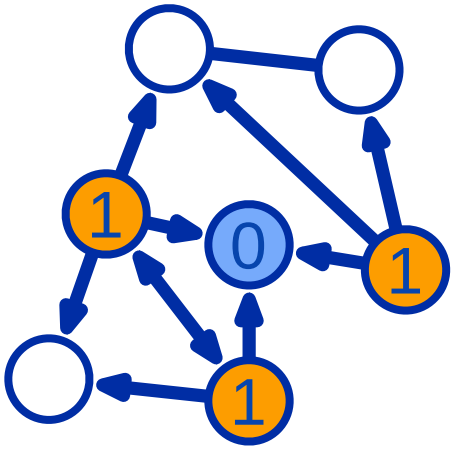
When the frontier is at its peak, almost all edge examinations "fail" to claim a child



Bottom-up BFS algorithm

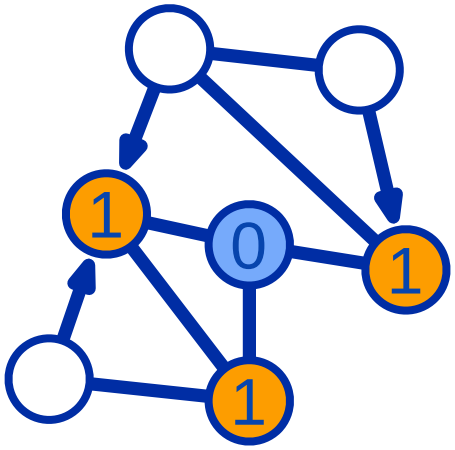
Classical (top-down) algorithm is optimal in worst case, but pessimistic for low-diameter graphs (previous slide)

Top-Down



for all *v* in frontier
attempt to parent ***all*** neighbors(*v*)

Bottom-Up



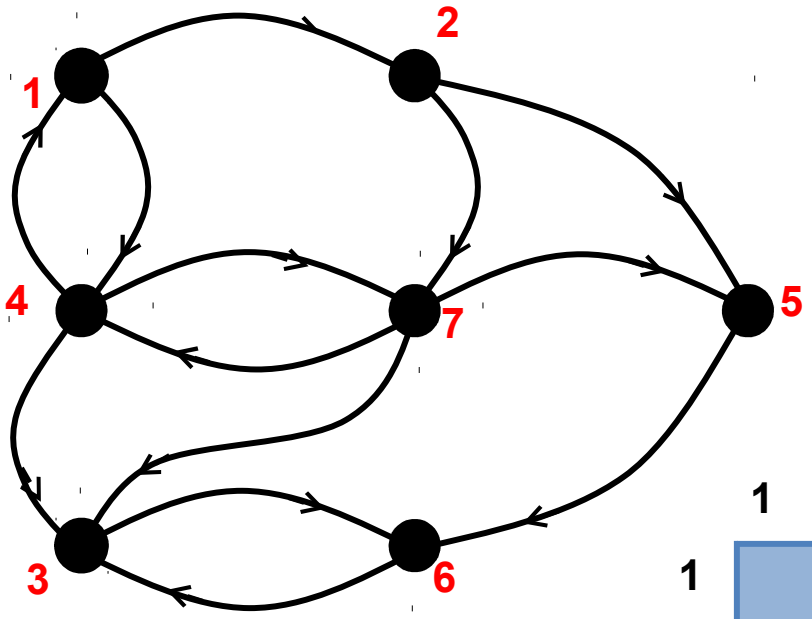
for all *v* in unvisited
find ***any*** parent
(neighbor(*v*) in frontier)

Direction-optimizing approach:

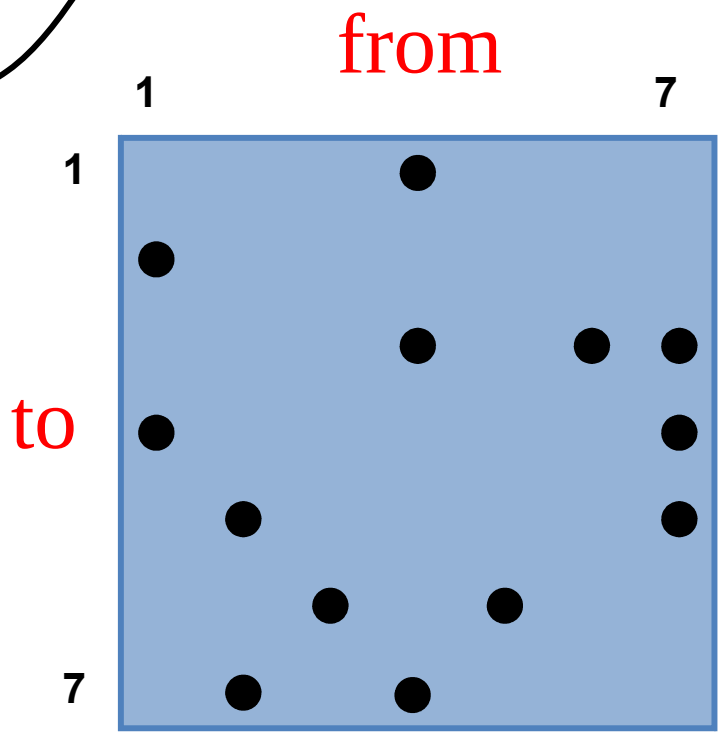
- Switch from top-down to bottom-up search
- When the majority of the vertices are discovered.

[Read paper for exact heuristic]

Scott Beamer, Krste Asanović, and David Patterson, "Direction-Optimizing Breadth-First Search", *Int. Conf. on High Performance Computing, Networking, Storage and Analysis (SC)*, 2012



Breadth-first search in the language of linear algebra



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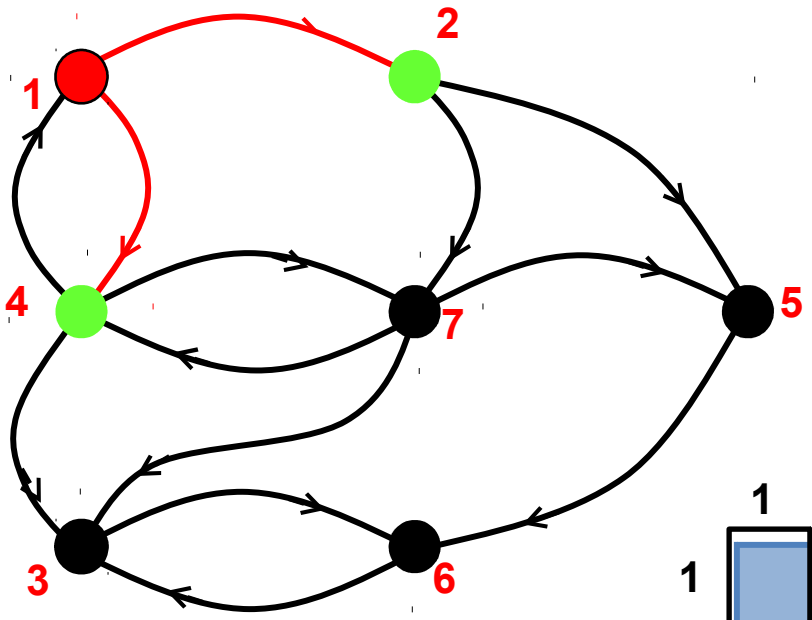
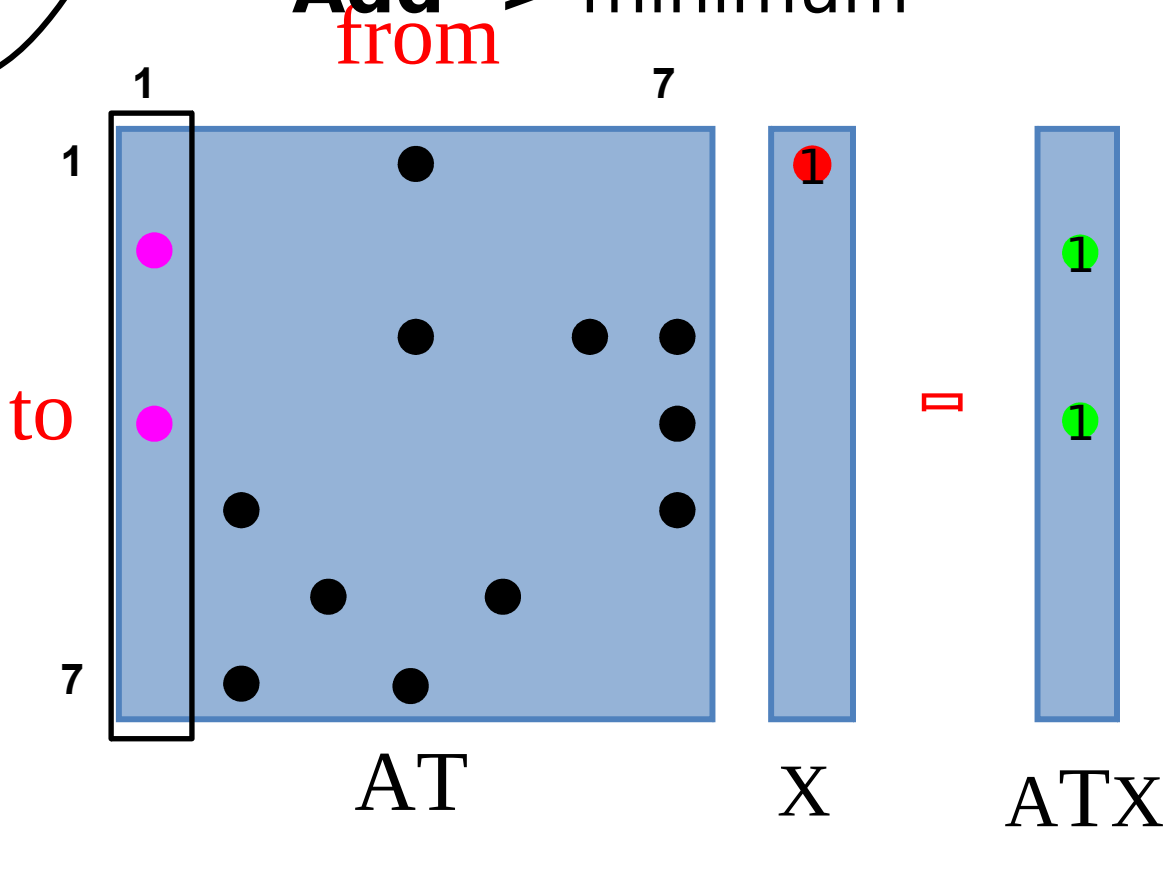


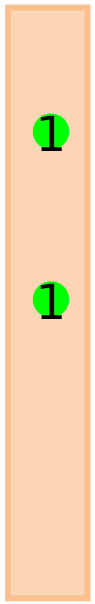
Replace scalar operations

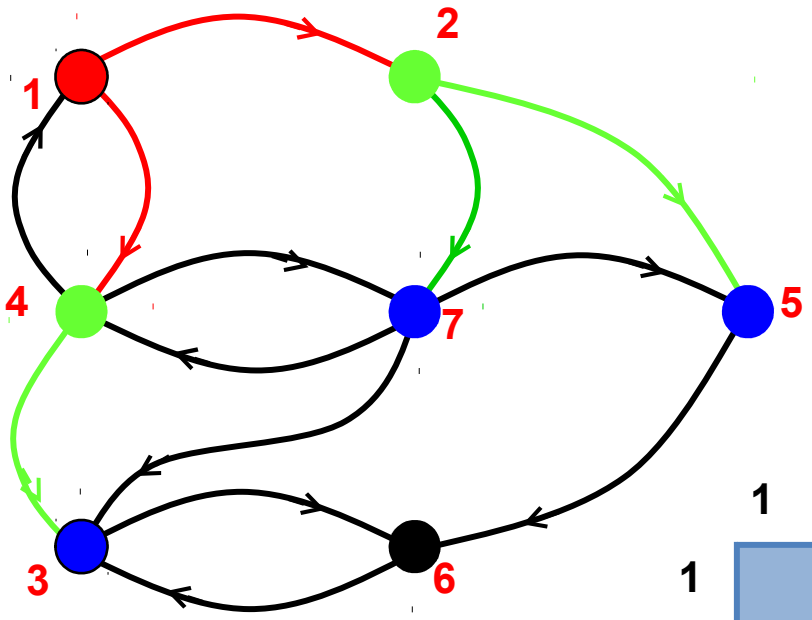
Multiply -> select

Add -> minimum

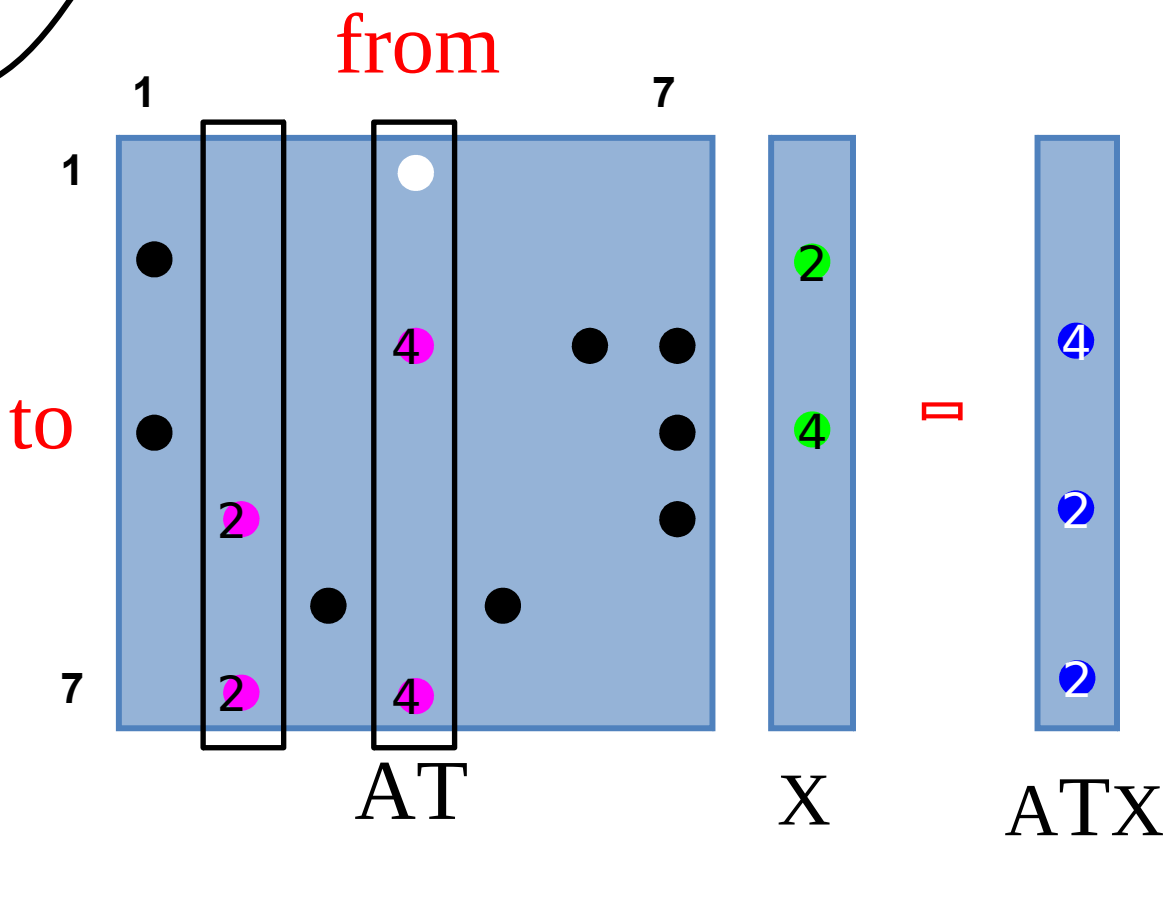


parents:

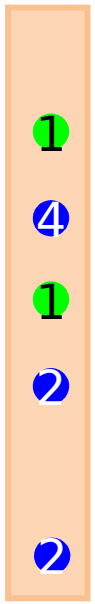


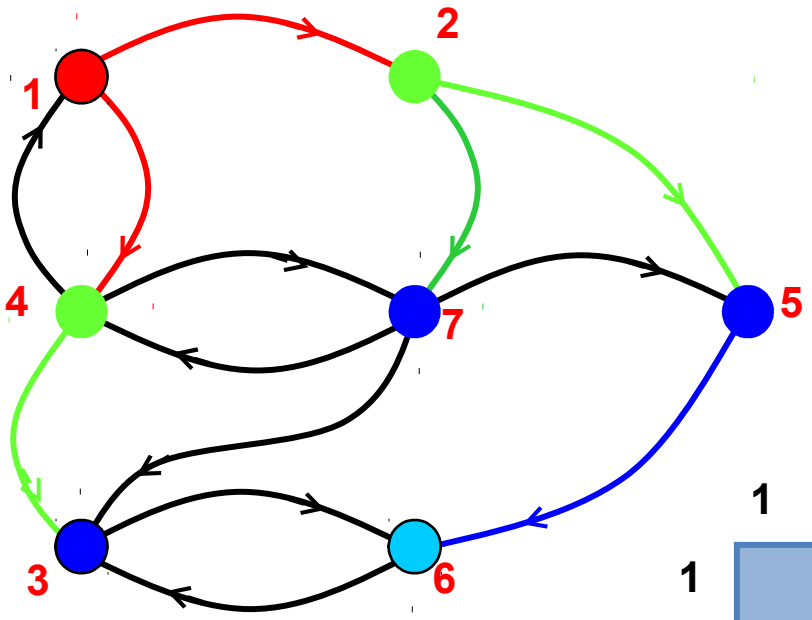


Select vertex with
minimum label as parent

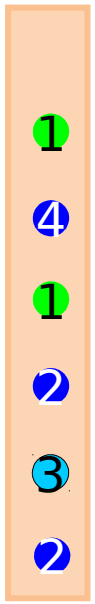


parents:



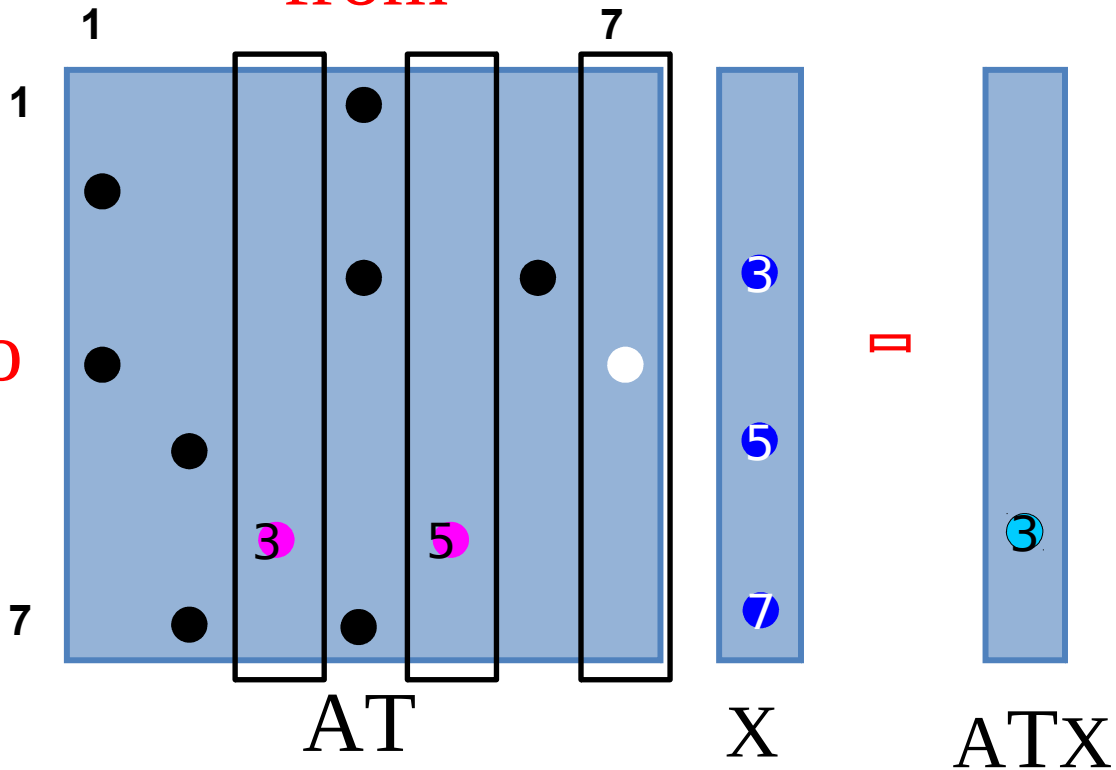


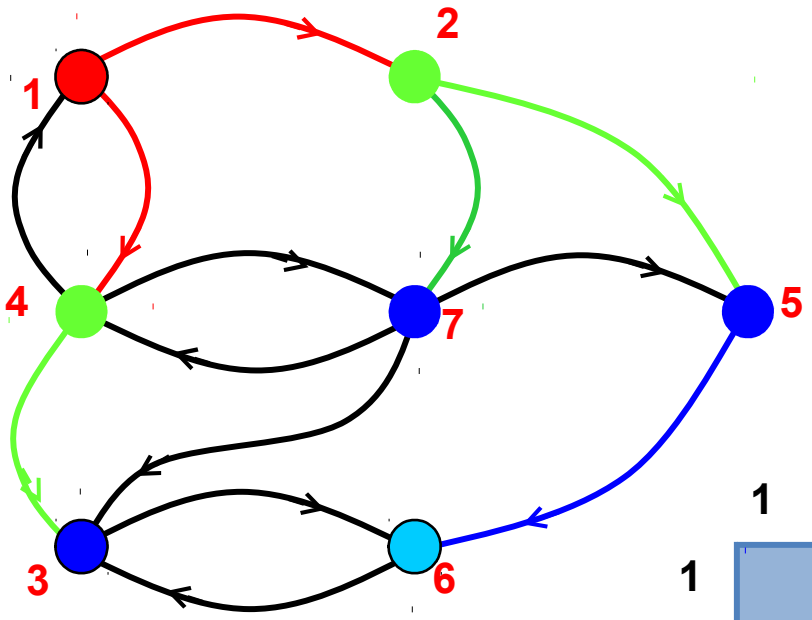
parents:

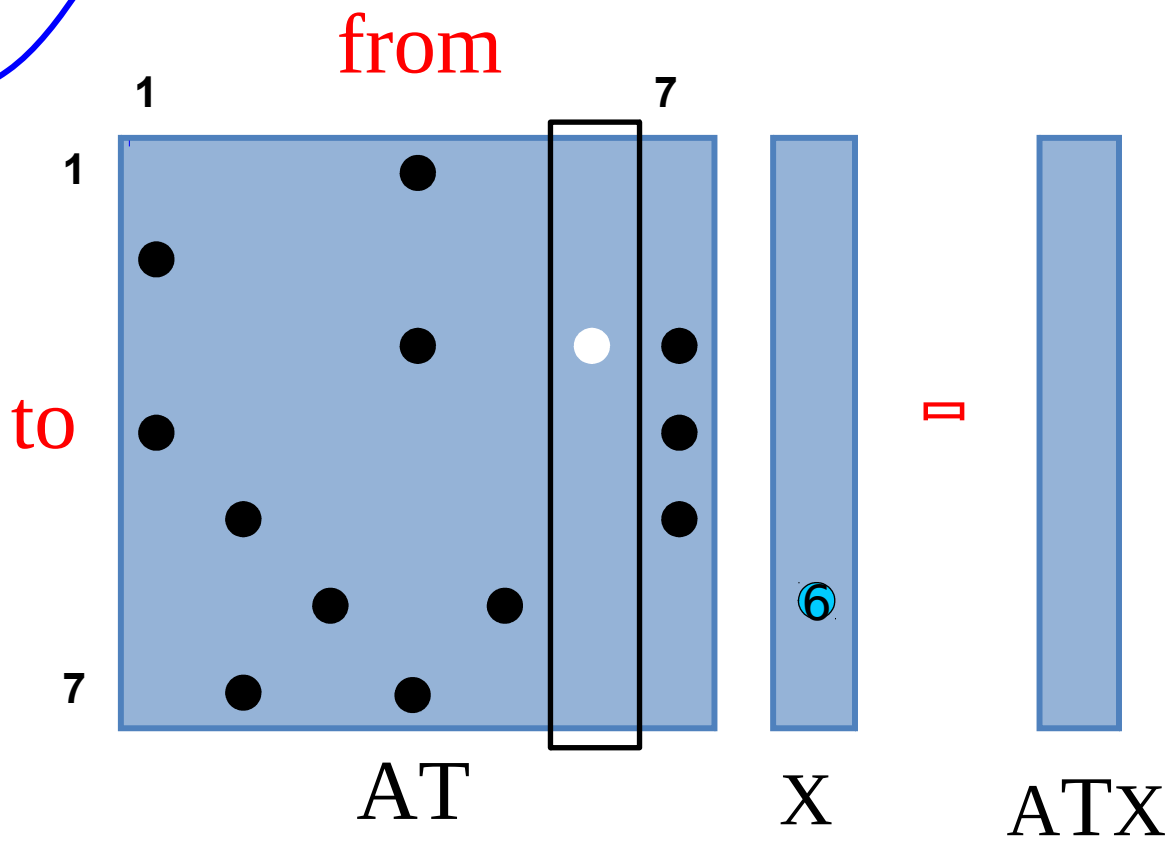


from

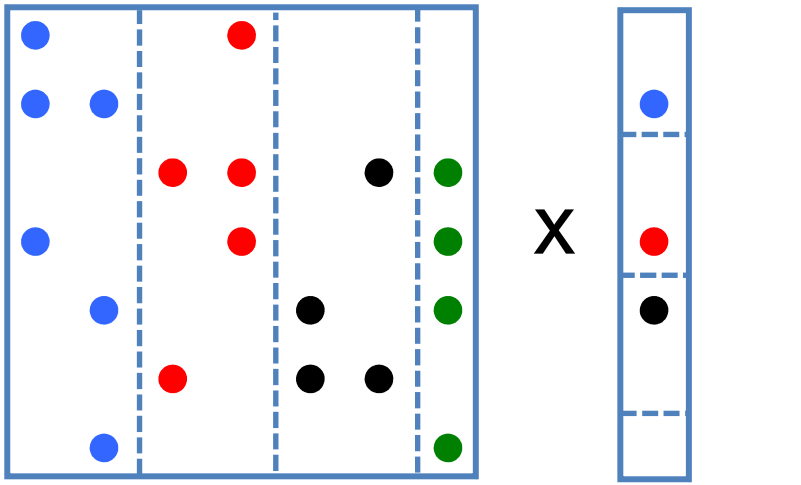
to

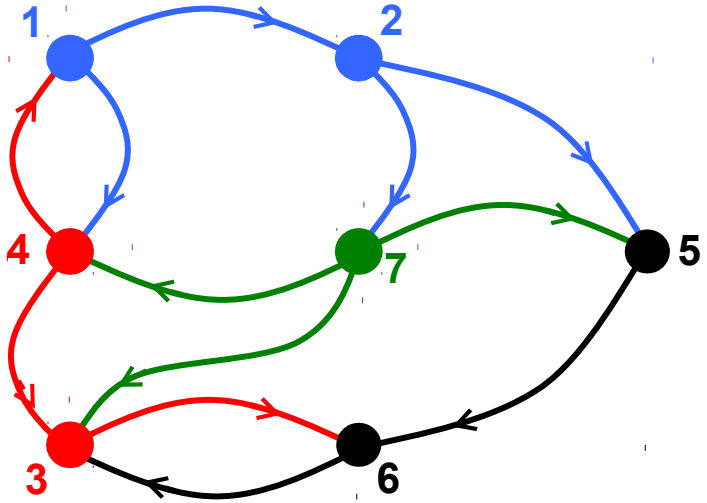



1
2
3
4
5
6
7


from
to
1
7
1
7
6
=
AT
X
ATX

1D Parallel BFS algorithm

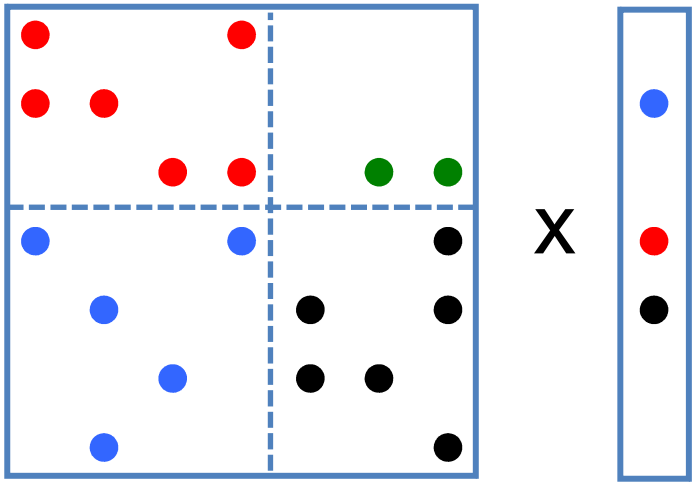


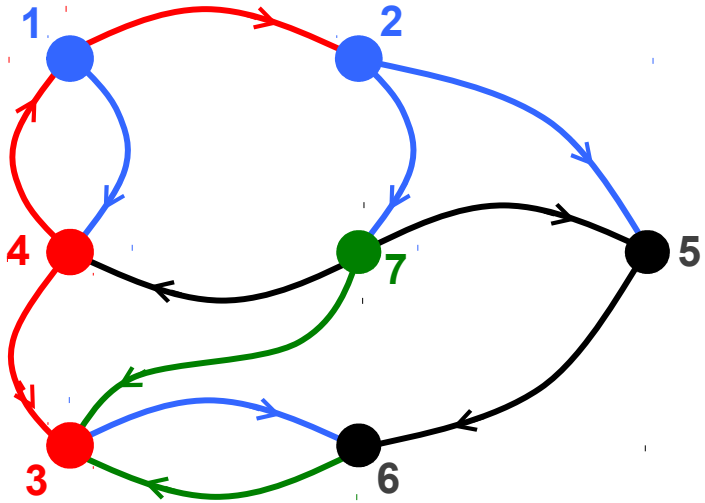


ALGORITHM:

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

2D Parallel BFS algorithm

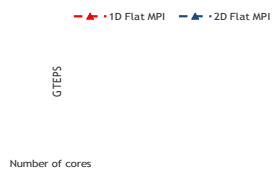


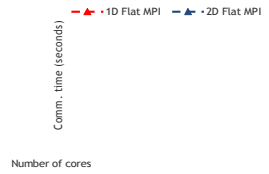


ALGORITHM:

1. Gather vertices in *processor column* **[communication]**
2. Find owners of the current frontier's adjacency [computation]
3. Exchange adjacencies in *processor row* **[communication]**

BFS Strong Scaling

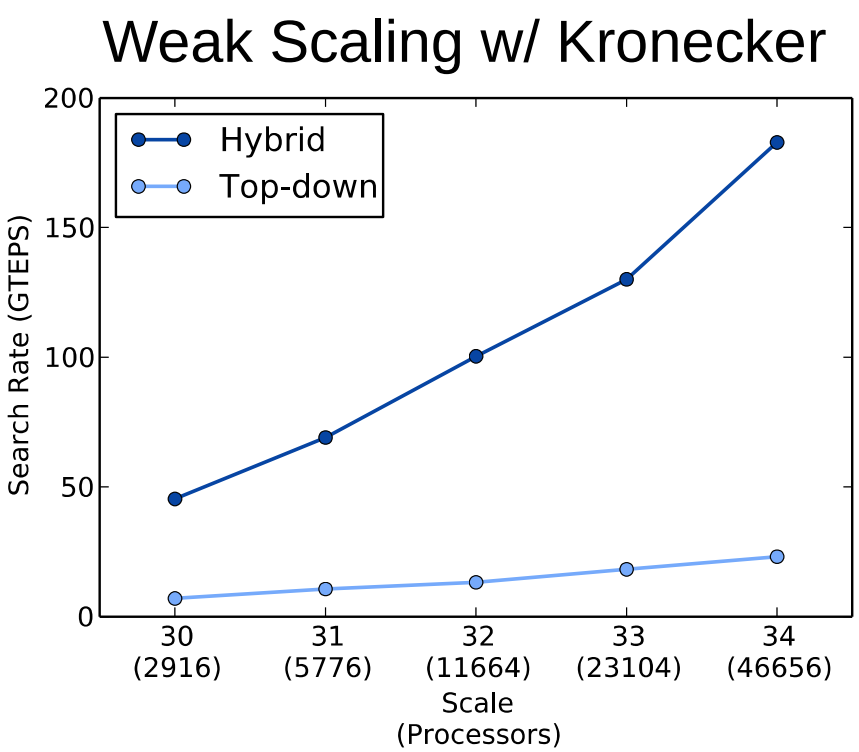


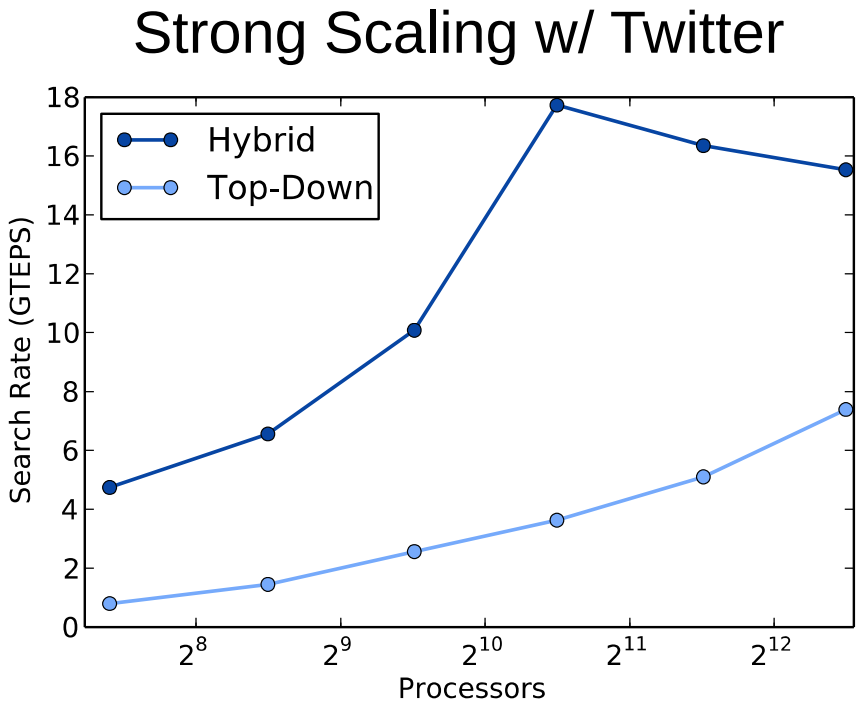


- NERSC Hopper (Cray XE6, Gemini interconnect AMD Magny-Cours)
- Hybrid: In-node 6-way OpenMP multithreading
- Kronecker (Graph500): 4 billion vertices and 64 billion edges

A. Buluç, K. Madduri. Parallel breadth-first search on distributed memory systems. *Proc. Supercomputing*, 2011.

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", *Workshop on Multithreaded Architectures and Applications (MTAAP), at the International Parallel & Distributed Processing Symposium (IPDPS)*, 2013

Lecture Outline

- Applications
- Designing parallel graph algorithms
- Case studies:
  - **Graph traversals:** Breadth-first search
  - **Shortest Paths:** Delta-stepping, PHAST, Floyd-Warshall
  - **Ranking:** Betweenness centrality
  - **Maximal Independent Sets:** Luby's algorithm
  - **Strongly Connected Components**
- . Wrap-up: challenges on current systems

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
- Distributed memory implementations based on graph partitioning
- Heuristics for load balancing and termination detection

K. Madduri, D.A. Bader, J.W. Berry, and J.R. Crobak, "An Experimental Study of A Parallel Shortest Path Algorithm for Solving Large-Scale Graph Instances," *Workshop on Algorithm Engineering and Experiments* (ALENEX), New Orleans, LA, January 6, 2007.

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 $O(n+m+D\times L)$ where L = max distance from source to any node
- Vertices are ordered using buckets of width Δ
- Each bucket may be processed in parallel

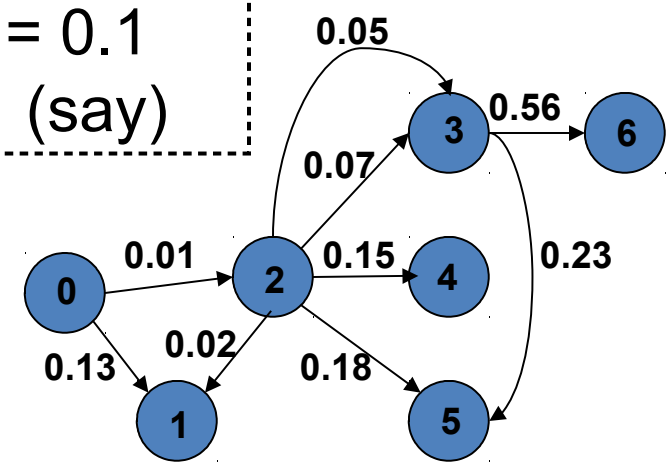
Δ < min w(e) : Degenerates into Dijkstra

Δ > max w(e) : Degenerates into

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

Δ - stepping algorithm: illustration

Δ = 0.1 (say)



d array

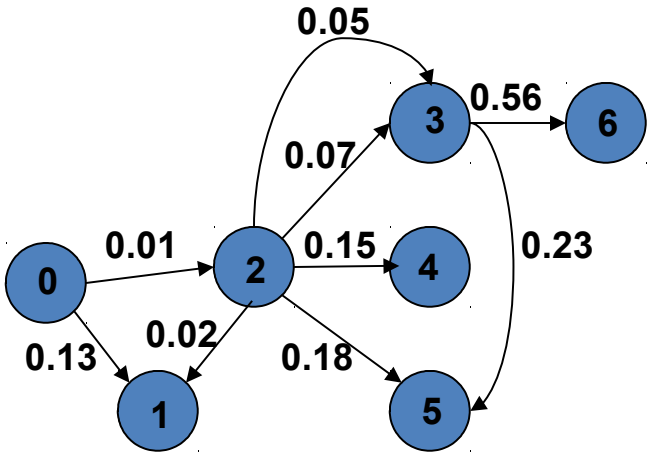
0	1	2	3	4	5	6
∞	∞	∞	∞	∞	∞	∞

Buckets

One parallel **phase**
while (bucket is non-empty)
- Inspect light (w < Δ) edges
- Construct a set of “requests” (R)
- Clear the current bucket
- Remember deleted vertices (S)
- Relax request pairs in R

Relax heavy request pairs (from S)
Go on to the next bucket

Δ - stepping algorithm: illustration



d array

0	1	2	3	4	5	6
0	∞	∞	∞	∞	∞	∞

Buckets

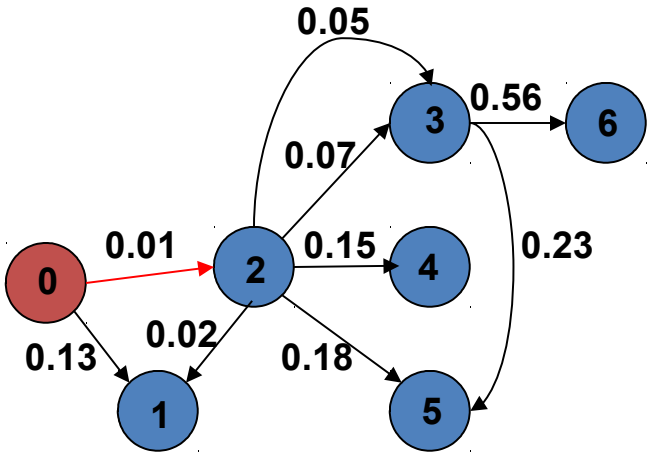
0	0						

One parallel **phase**
while (bucket is non-empty)
- Inspect light (w < Δ) edges
- Construct a set of “requests” (R)
- Clear the current bucket
- Remember deleted vertices (S)
- Relax request pairs in R

Relax heavy request pairs (from S)
Go on to the next bucket

Initialization:
Insert *s* into bucket, d(s) = 0

Δ - stepping algorithm: illustration



One parallel **phase**
while (bucket is non-empty)
- Inspect light (w < Δ) edges
- Construct a set of "requests" (R)
- Clear the current bucket
- Remember deleted vertices (S)
- Relax request pairs in R

Relax heavy request pairs (from S)
Go on to the next bucket

d array

0	1	2	3	4	5	6
0	∞	∞	∞	∞	∞	∞

Buckets

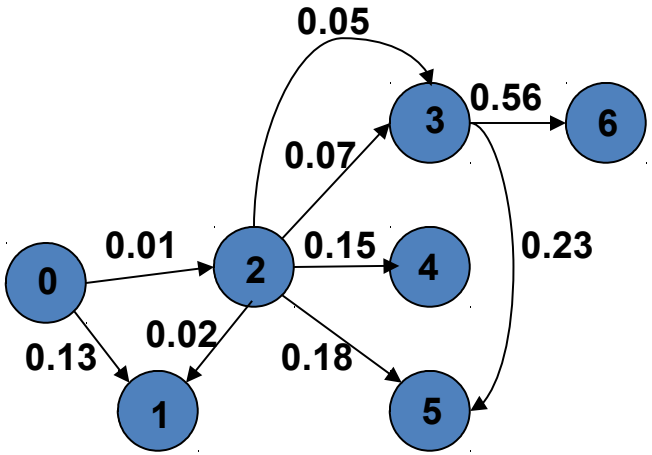
0	0						

R

2						
.01						

S

Δ - stepping algorithm: illustration



d array

0	1	2	3	4	5	6
0	∞	∞	∞	∞	∞	∞

Buckets

0							

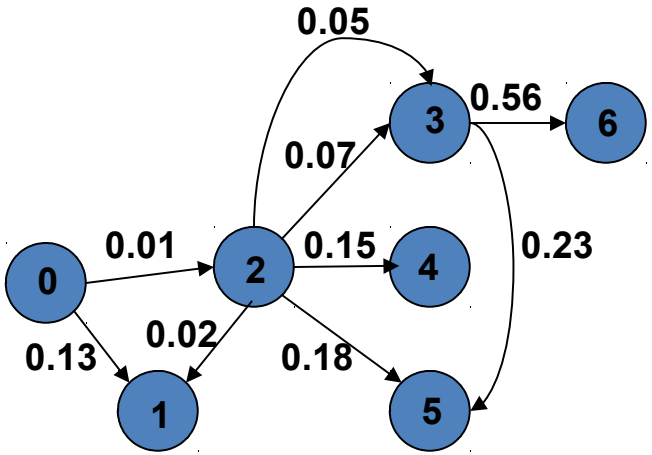
One parallel **phase**
while (bucket is non-empty)
- Inspect light (w < Δ) edges
- Construct a set of “requests” (R)
- Clear the current bucket
- Remember deleted vertices (S)
- Relax request pairs in R

Relax heavy request pairs (from S)
Go on to the next bucket

R	2						
	.01						

S	0						

Δ - stepping algorithm: illustration



d array

0	1	2	3	4	5	6
0	∞	.01	∞	∞	∞	∞

Buckets

0	2						

One parallel **phase**
while (bucket is non-empty)

- Inspect light (w < Δ) edges
- Construct a set of "requests" (R)
- Clear the current bucket
- Remember deleted vertices (S)
- Relax request pairs in R

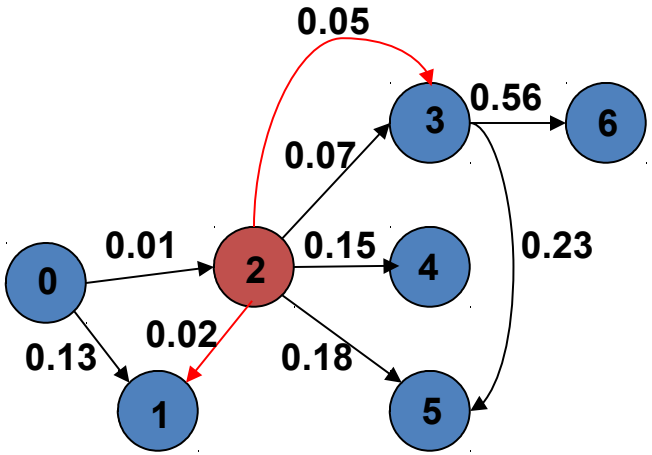
Relax heavy request pairs (from S)
Go on to the next bucket

R

S

0						

Δ - stepping algorithm: illustration



d array

0	1	2	3	4	5	6
0	∞	.01	∞	∞	∞	∞

Buckets

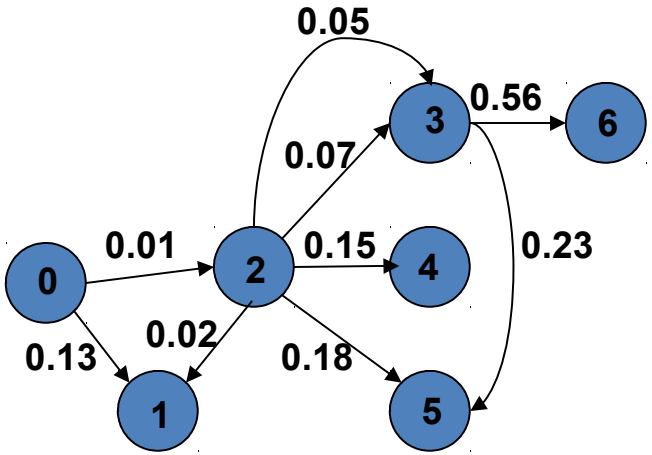
0	2						

One parallel **phase**
while (bucket is non-empty)
- Inspect light (w < Δ) edges
- Construct a set of "requests" (R)
- Clear the current bucket
- Remember deleted vertices (S)
- Relax request pairs in R

Relax heavy request pairs (from S)
Go on to the next bucket

R	1	3					
	.03	.06					
S	0						

Δ - stepping algorithm: illustration



d array

0	1	2	3	4	5	6
0	∞	.01	∞	∞	∞	∞

Buckets

0							

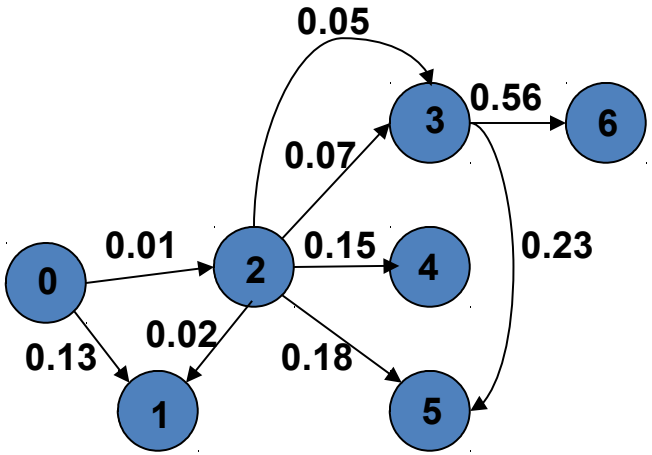
One parallel **phase**
while (bucket is non-empty)
- Inspect light (w < Δ) edges
- Construct a set of "requests" (R)
- Clear the current bucket
- Remember deleted vertices (S)
- Relax request pairs in R

Relax heavy request pairs (from S)
Go on to the next bucket

R	1	3					
	.03	.06					

S	0	2					

Δ - stepping algorithm: illustration



d array

0	1	2	3	4	5	6
0	.03	.01	.06	∞	∞	∞

Buckets

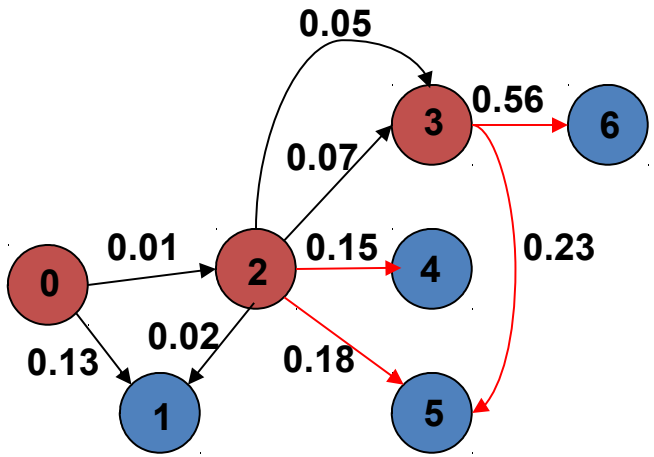
0	1	3					

One parallel **phase**
while (bucket is non-empty)
- Inspect light (w < Δ) edges
- Construct a set of “requests” (R)
- Clear the current bucket
- Remember deleted vertices (S)
- Relax request pairs in R

Relax heavy request pairs (from S)
Go on to the next bucket

R							
S	0	2					

Δ - stepping algorithm: illustration



d array

0	1	2	3	4	5	6
0	.03	.01	.06	.16	.29	.62

Buckets

1	4						
2	5						
6	6						

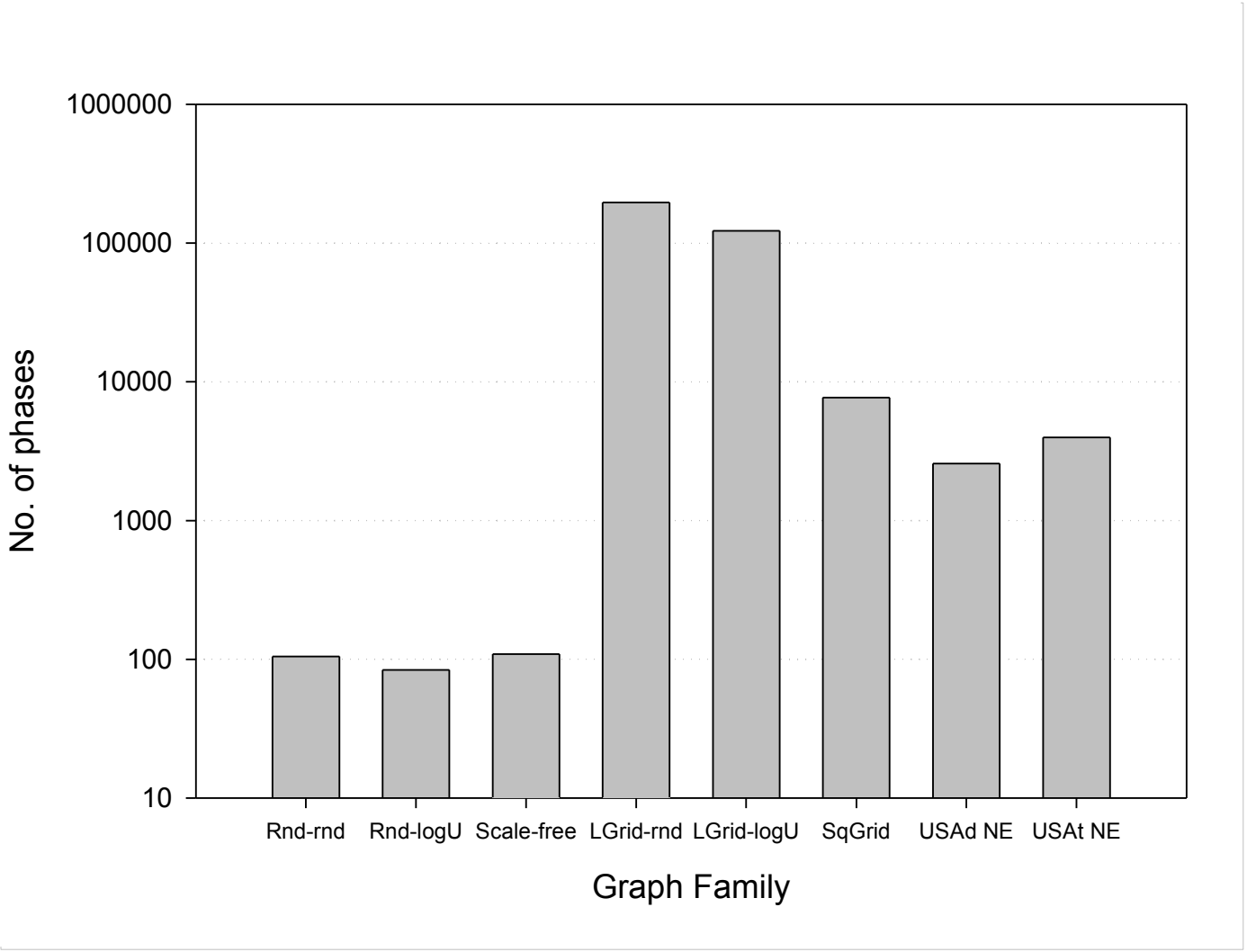
One parallel **phase**
while (bucket is non-empty)

- Inspect light (w < Δ) edges
- Construct a set of “requests” (R)
- Clear the current bucket
- Remember deleted vertices (S)
- Relax request pairs in R

Relax heavy request pairs (from S)
Go on to the next bucket

R							
S	0	2	1	3			

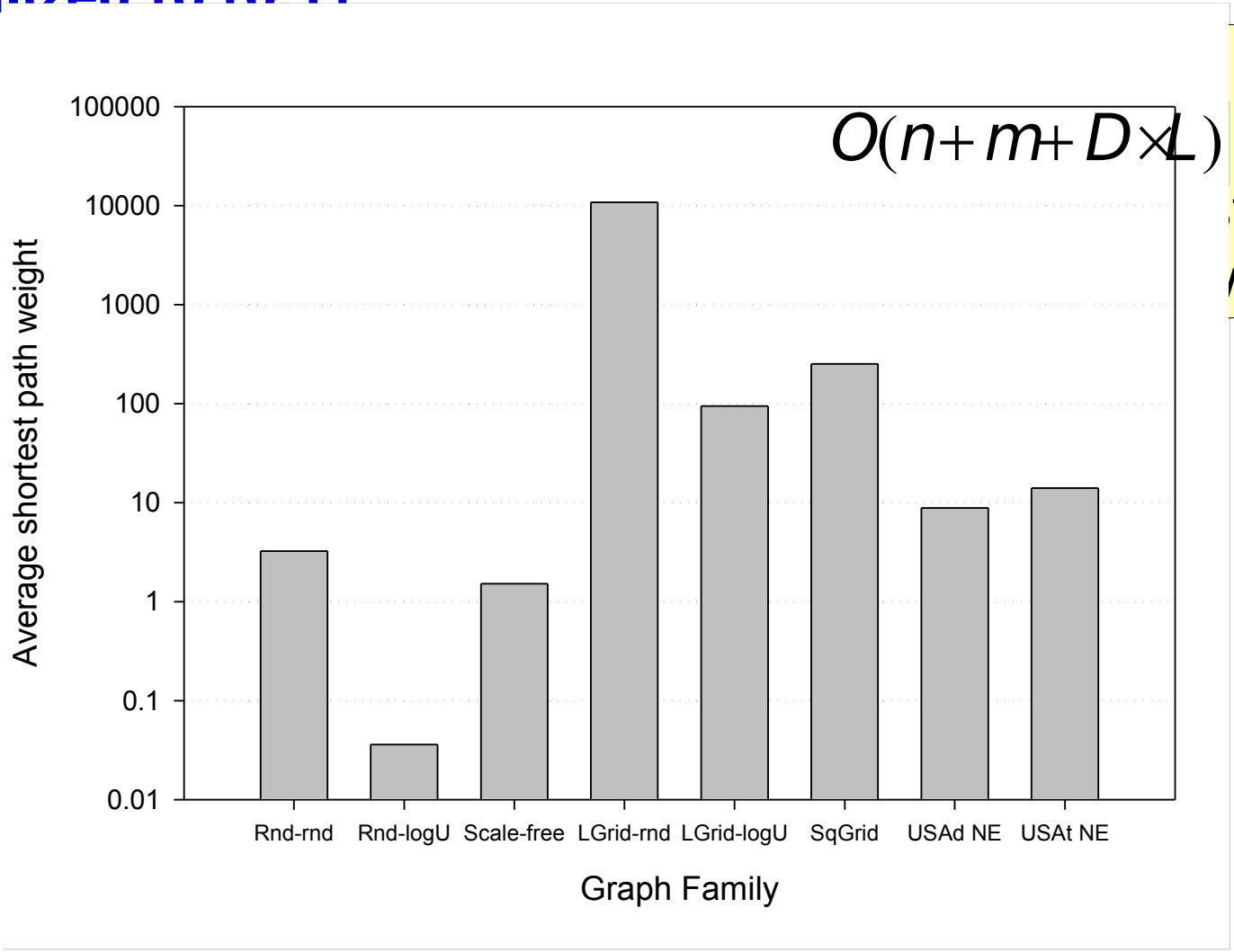
No. of *phases* (machine-independent performance count)



Too many phases in high diameter graphs:
Level-synchronous breadth-first search has the same problem.

Average shortest path weight for various graph families

~ 220 vertices, 222 edges, directed graph, edge weights normalized to [0,1]

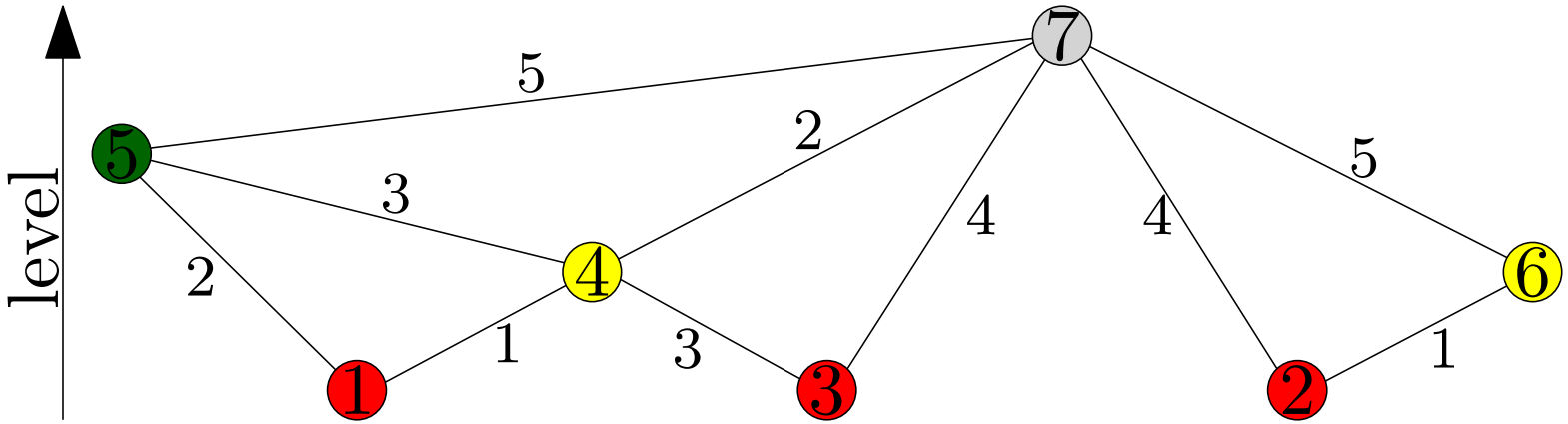


tance
veight)

PHAST – hardware accelerated shortest path trees

Preprocessing: Build a **contraction hierarchy**

- order nodes by importance (*highway dimension*)
- process in order
- add shortcuts to preserve distances
- assign levels (ca. 150 in road networks)
- 75% increase in number of edges (for road networks)

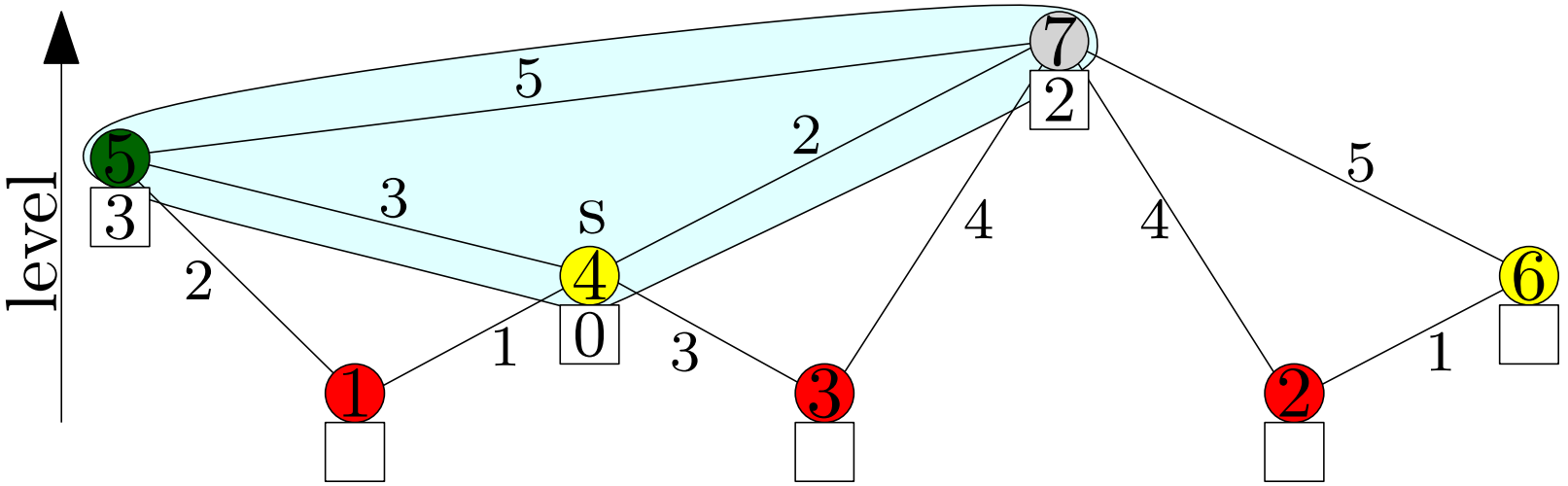


D. Delling, A. V. Goldberg, A. Nowatzyk, and R. F. Werneck. PHAST: Hardware- Accelerated Shortest Path Trees. In IPDPS. IEEE Computer Society, 2011

PHAST – hardware accelerated shortest path trees

One-to-all search from source s:

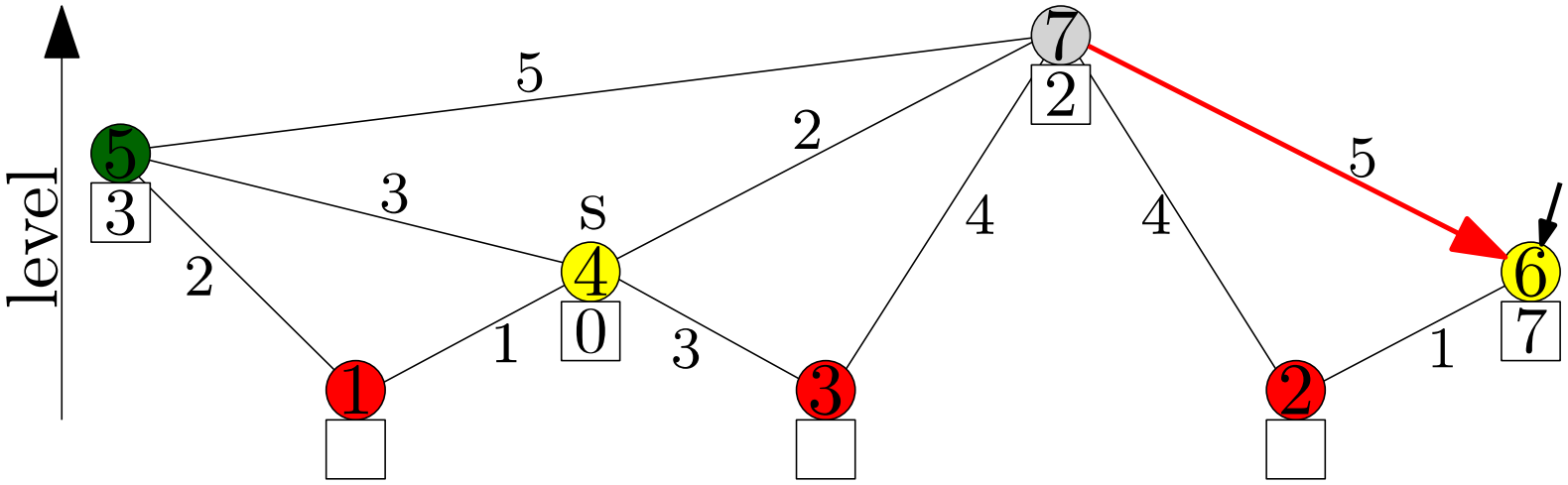
- Run forward search from s
- Only follow edges to more important nodes
- Set distance labels d of reached nodes



PHAST – hardware accelerated shortest path trees

From top-down:

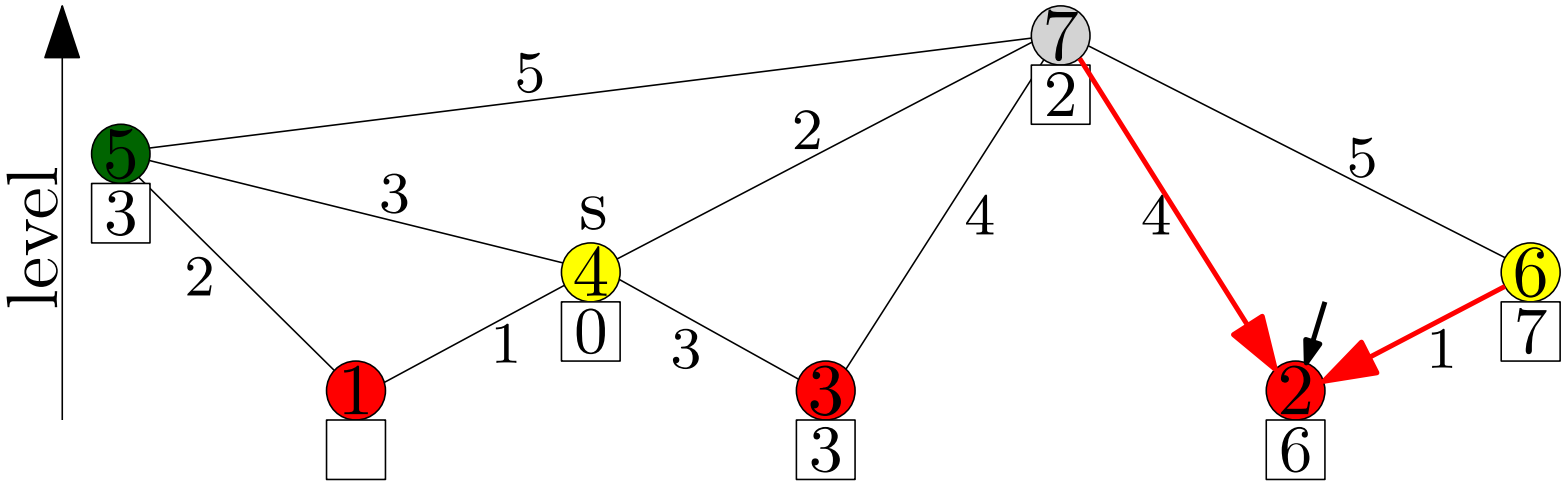
- process all nodes u in reverse level order:
- check incoming arcs (v,u) with lev(v) > lev(u)
- Set d(u)=min{d(u),d(v)+w(v,u)}



PHAST – hardware accelerated shortest path trees

From top-down:

- linear sweep without priority queue
- reorder nodes, arcs, distance labels by level
- accesses to d array becomes contiguous (no jumps)
- parallelize with SIMD (SSE instructions, and/or GPU)

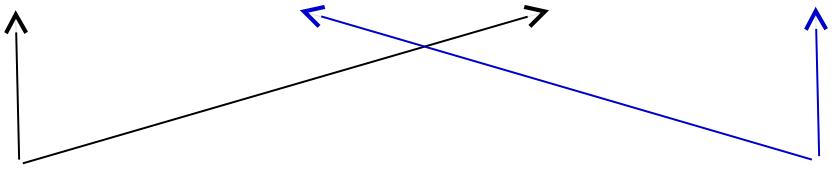


PHAST – performance comparison

Inputs: Europe/USA Road Networks

		Europe		USA	
algorithm	device	time	distance	time	distance
Dijkstra	M1-4	1103.52	618.18	1910.67	1432.35
	M2-6	288.81	177.58	380.40	280.17
	M4-12	168.49	108.58	229.00	167.77
PHAST	M1-4	19.47	23.01	28.22	29.85
	M2-6	7.20	8.27	10.42	10.71
	M4-12	4.03	5.03	6.18	6.58
GPHAST	GTX 480	2.90	4.75	4.49	5.69

GPU implementation



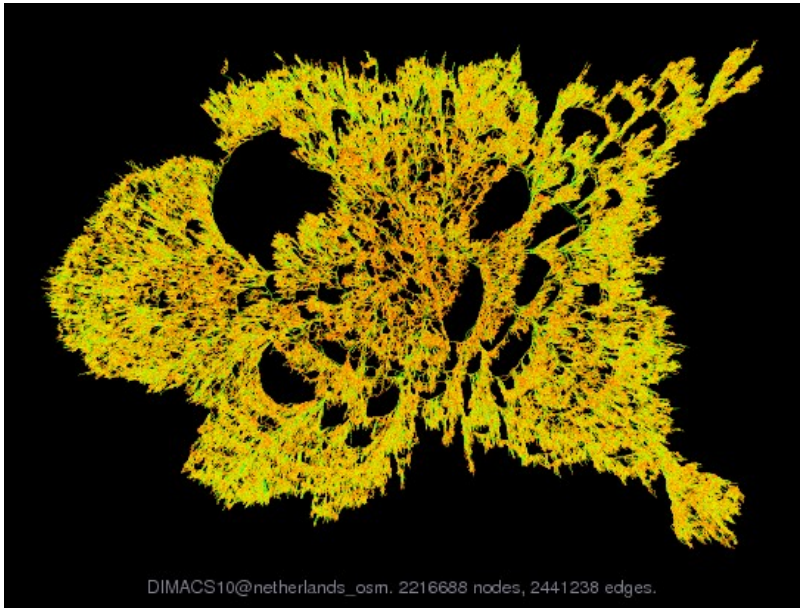
Edge weights:
estimated travel times

Edge weights:
physical distances

PHAST – hardware accelerated shortest path trees

- Specifically designed for **road networks**
- Fill-in can be much higher for other graphs
  (Hint: think about sparse Gaussian Elimination)

- Road networks are (almost) planar.
- Planar graphs have $O(\sqrt{n})$ separators.
- Good separators lead to orderings with minimal fill.

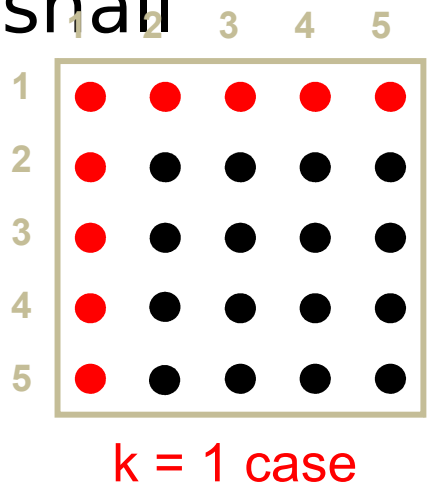


Lipton, Richard J.; Tarjan, Robert E. (1979), "A separator theorem for planar graphs", SIAM Journal on Applied Mathematics 36 (2): 177–189
Alan George. “Nested Dissection of a Regular Finite Element Mesh”. SIAM Journal on Numerical Analysis, Vol. 10, No. 2 (Apr., 1973), 345-363

All-pairs shortest-paths problem

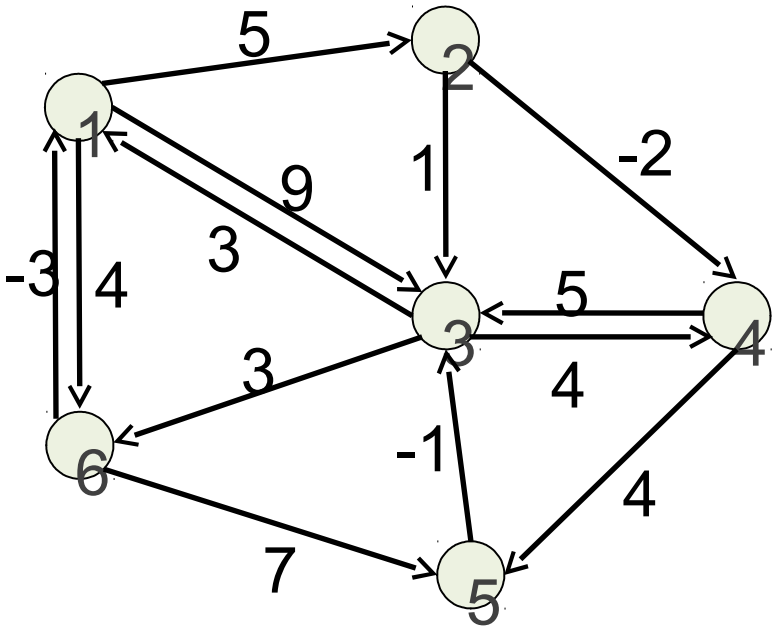
- Input: Directed graph with “costs” on edges
- Find least-cost paths between all reachable vertex pairs
- Classical algorithm: Floyd-Warshall

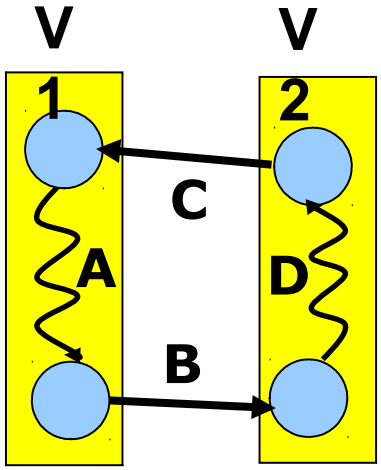
```
for k=1:n        // the induction sequence
    for i = 1:n
        for j = 1:n
            if(w(i→k)+w(k→j) < w(i→j))
                w(i→j):= w(i→k) + w(k→j)
```



k = 1 case

- It turns out a previously overlooked



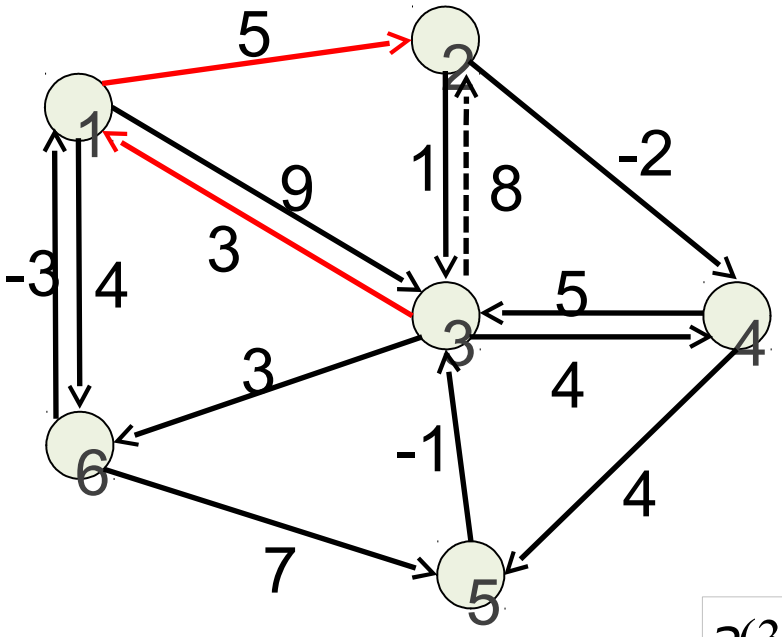


A	B
C	D

+ is "min", **×** is "add"

A = A*; % recursive call
B = AB; C = CA;
D = D + CB;
D = D*; % recursive call
B = BD; C = DC;
A = A + BC;

$$\begin{bmatrix} 0 & 5 & 9 & \infty & \infty & 4 \\ \infty & 0 & 1 & -2 & \infty & \infty \\ 3 & \infty & 0 & 4 & \infty & 3 \\ \infty & \infty & 5 & 0 & 4 & \infty \\ \infty & \infty & -1 & \infty & 0 & \infty \\ -3 & \infty & \infty & \infty & 7 & 0 \end{bmatrix}$$



$$\begin{bmatrix} \infty \\ 3 \end{bmatrix} \quad \begin{bmatrix} 5 & 9 \end{bmatrix} = \begin{bmatrix} \infty & \infty \\ 8 & 12 \end{bmatrix}$$

C **B**

The cost of 3-1-2 path

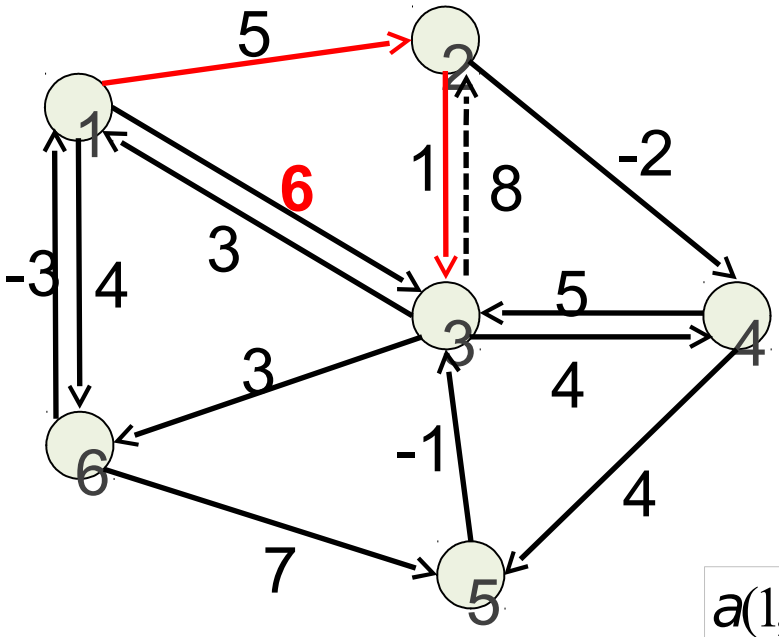
$$a(3,2) = a(3,1) + a(1,2) \xrightarrow{\text{then}} \Pi(3,2) = \Pi(1,2)$$

$$\begin{bmatrix} 0 & 5 & 9 & \infty & \infty & 4 \\ \infty & 0 & 1 & -2 & \infty & \infty \\ 3 & \mathbf{8} & 0 & 4 & \infty & 3 \\ \infty & \infty & 5 & 0 & 4 & \infty \\ \infty & \infty & -1 & \infty & 0 & \infty \\ -3 & \infty & \infty & \infty & 7 & 0 \end{bmatrix}$$

Distances

$$\Pi = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 2 & 2 & 2 & 2 & 2 & 2 \\ 3 & \mathbf{1} & 3 & 3 & 3 & 3 \\ 4 & 4 & 4 & 4 & 4 & 4 \\ 5 & 5 & 5 & 5 & 5 & 5 \\ 6 & 6 & 6 & 6 & 6 & 6 \end{bmatrix}$$

Parents



D = D*: no change

$$\begin{bmatrix} 5 & 9 \end{bmatrix} \quad \begin{bmatrix} 0 & 1 \\ 8 & 0 \end{bmatrix} = \begin{bmatrix} 5 & 6 \end{bmatrix}$$

B **D** Path: 1-2-3

$$a(1,3) = a(1,2) + a(2,3) \xrightarrow{\text{then}} \Pi(1,3) = \Pi(2,3)$$

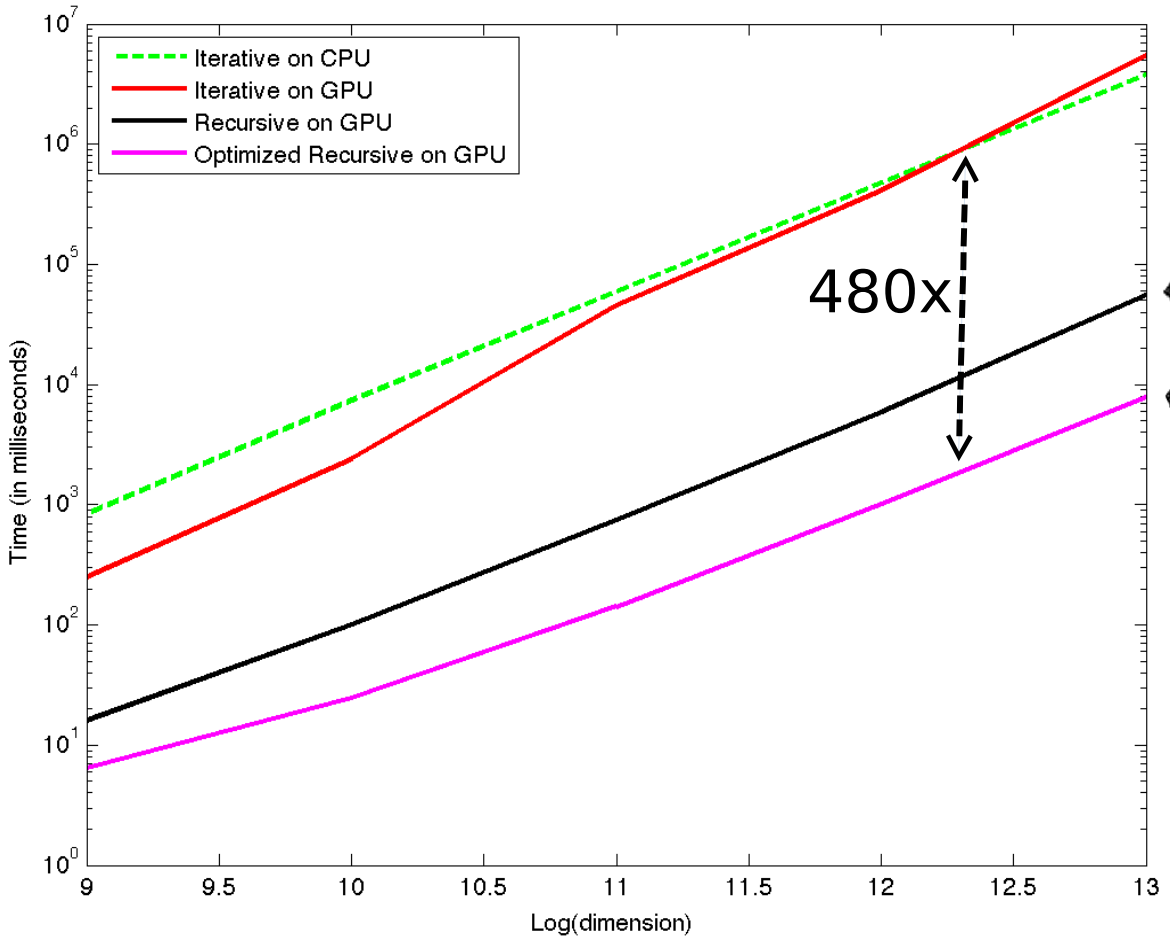
$$\begin{bmatrix} 0 & 5 & \mathbf{6} & \infty & \infty & 4 \\ \infty & 0 & 1 & -2 & \infty & \infty \\ 3 & 8 & 0 & 4 & \infty & 3 \\ \infty & \infty & 5 & 0 & 4 & \infty \\ \infty & \infty & -1 & \infty & 0 & \infty \\ -3 & \infty & \infty & \infty & 7 & 0 \end{bmatrix}$$

Distances

$$\Pi = \begin{bmatrix} 1 & 1 & \mathbf{2} & 1 & 1 & 1 \\ 2 & 2 & 2 & 2 & 2 & 2 \\ 3 & 1 & 3 & 3 & 3 & 3 \\ 4 & 4 & 4 & 4 & 4 & 4 \\ 5 & 5 & 5 & 5 & 5 & 5 \\ 6 & 6 & 6 & 6 & 6 & 6 \end{bmatrix}$$

Parents

All-pairs shortest-paths problem



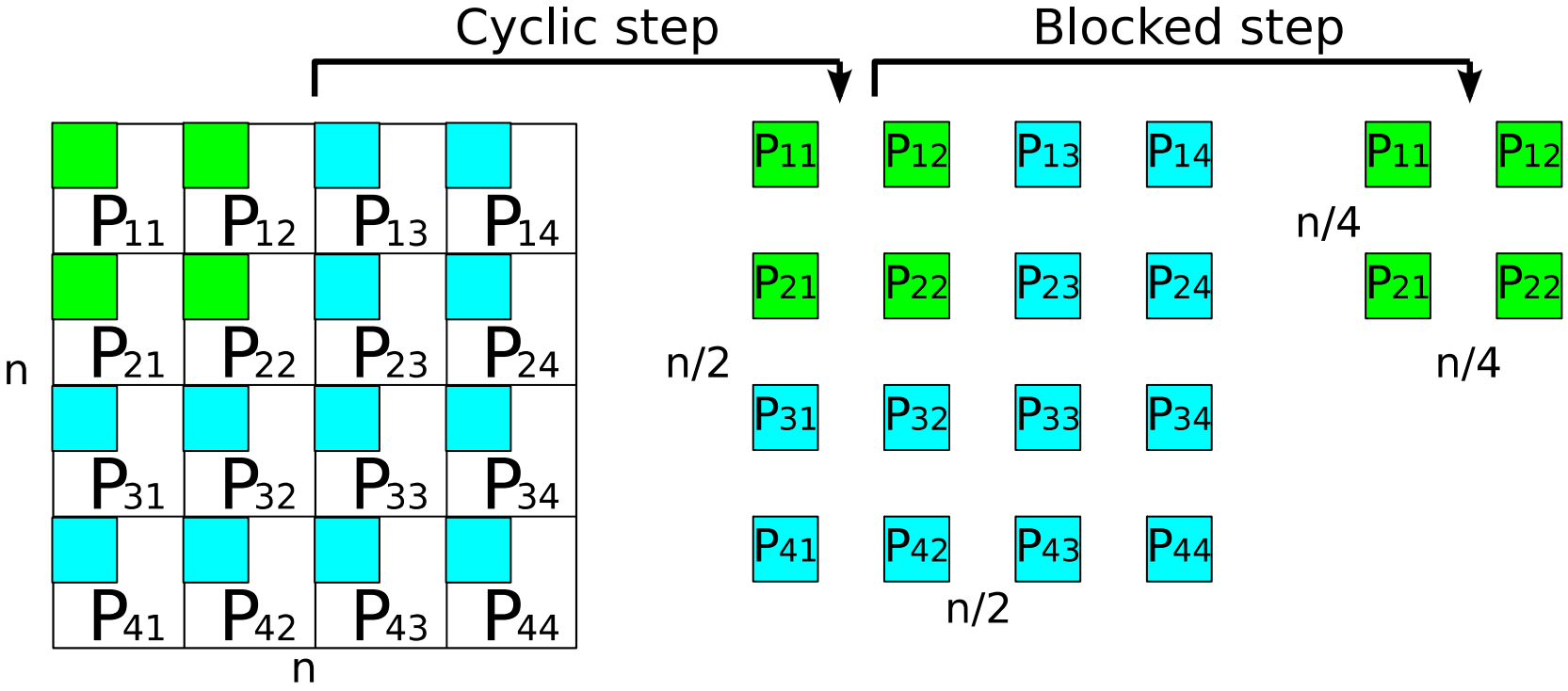
Floyd-Warshall ported to GPU

Naïve recursive implementation

The right primitive (Matrix multiply)

A. Buluç, J. R. Gilbert, and C. Budak. Solving path problems on the GPU. Parallel Computing, 36(5-6):241 - 253, 2010.

Communication-avoiding APSP in distributed memory



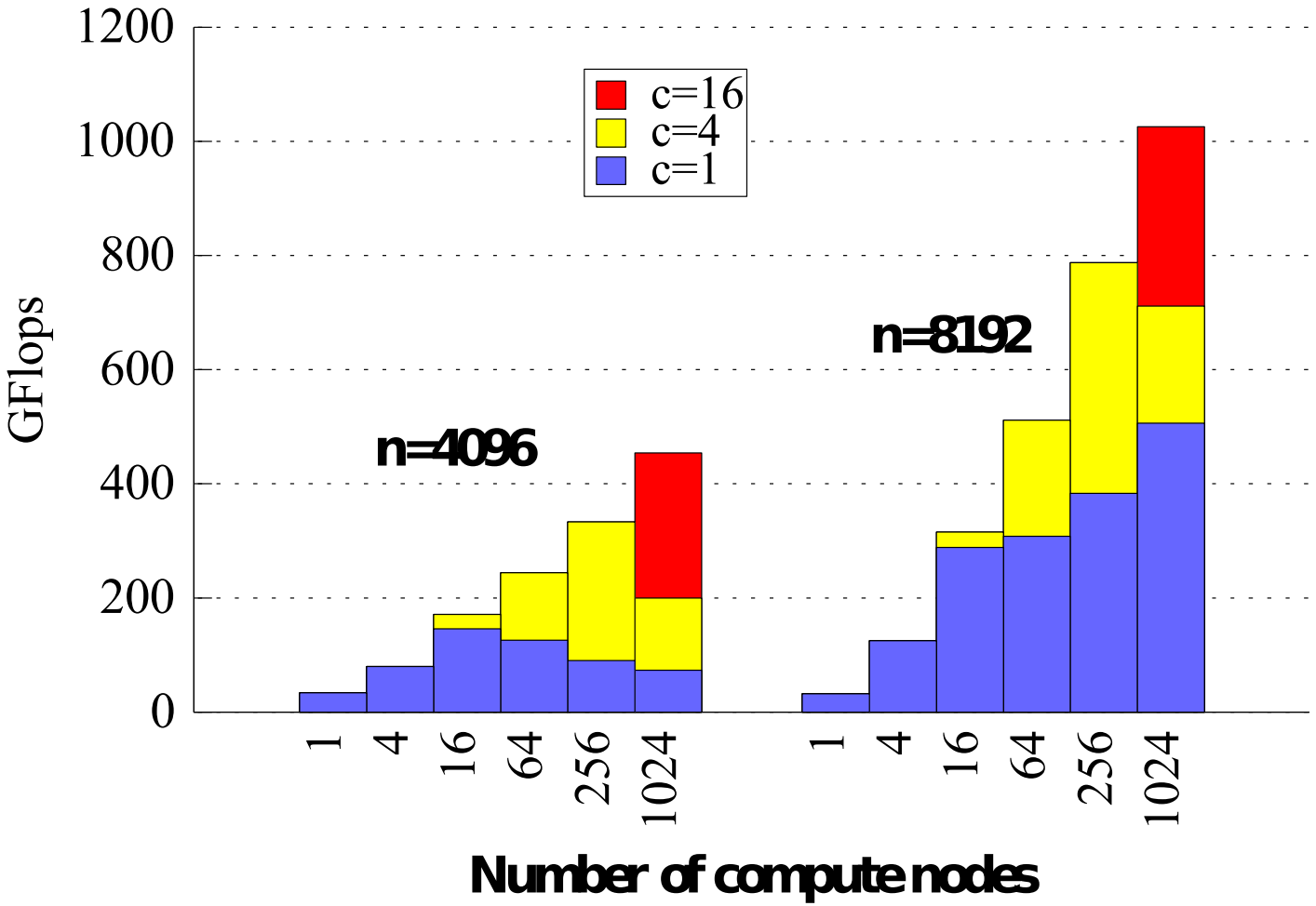
Bandwidth: $W_{\text{bc-2.5D}}(n,p) = O(n^2/\sqrt{cp})$

Latency: $S_{\text{bc-2.5D}}(p) = O(\sqrt{cp}\log^2(p))$

c: number of replicas

Optimal for any memory size !

Communication-avoiding APSP in distributed memory



E. Solomonik, A. Buluç, and J. Demmel. Minimizing communication in all-pairs shortest paths. In Proceedings of the IPDPS. 2013.

Lecture Outline

- Applications
- Designing parallel graph algorithms
- Case studies:
  - **Graph traversals:** Breadth-first search
  - **Shortest Paths:** Delta-stepping, PHAST, Floyd-Warshall
  - **Ranking:** Betweenness centrality
  - **Maximal Independent Sets:** Luby's algorithm
  - **Strongly Connected Components**
- . Wrap-up: challenges on current systems

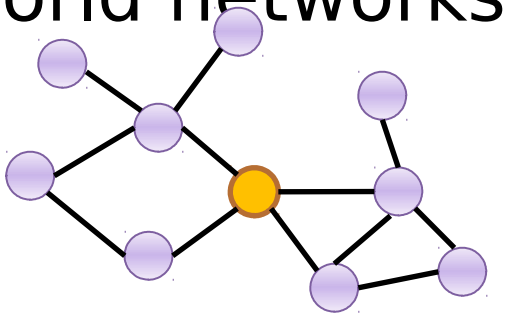
Betweenness Centrality (BC)

- Centrality: Quantitative measure to capture the importance of a vertex/edge in a graph
  - degree, closeness, eigenvalue, betweenness
- Betweenness Centrality

$$BC(v) = \sum_{s \neq v \neq t} \frac{\sigma_{st}(v)}{\sigma_{st}}$$

(σ_{st} : No. of shortest paths between s and t)

- Applied to several real-world networks
  - Social interactions
  - WWW
  - Epidemiology
  - Systems biology



Algorithms for Computing Betweenness

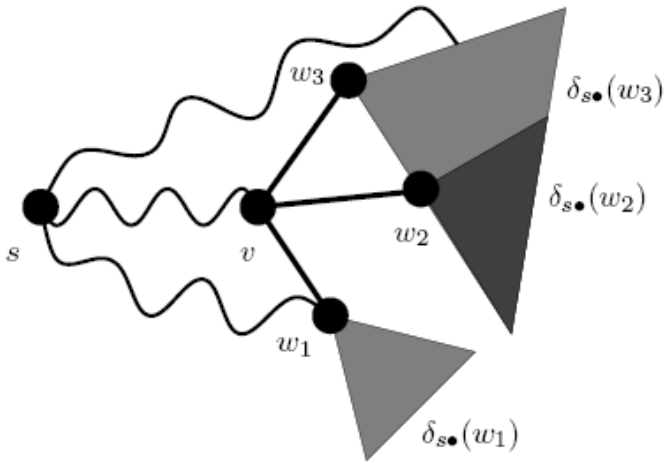
- **All-pairs shortest path approach:** compute the length and number of shortest paths between all s-t pairs (**O(n3)** time), sum up the fractional dependency values (**O(n2)** space).
- **Brandes' algorithm** (2003): Augment a single-source shortest path computation to count paths; uses the Bellman criterion; **O(mn)** work and **O(m+n)** space on unweig

$$\delta(v) = \sum_{w \in adj(v)} \frac{\sigma(v)}{\sigma(w)} \left(1 + \delta(w)\right)$$

Dependency of source on v.

Number of shortest paths from source to w

$$\delta(v) = \sum_{t \in V} \sigma_{st}(v)$$



Parallel BC algorithms for unweighted graphs

- **High-level idea:** Level-synchronous parallel *breadth-first search* augmented to compute centrality scores
- Two steps (both implemented as BFS)
  - traversal and path counting
  - dependency accumulation

Shared-memory parallel algorithms for betweenness centrality

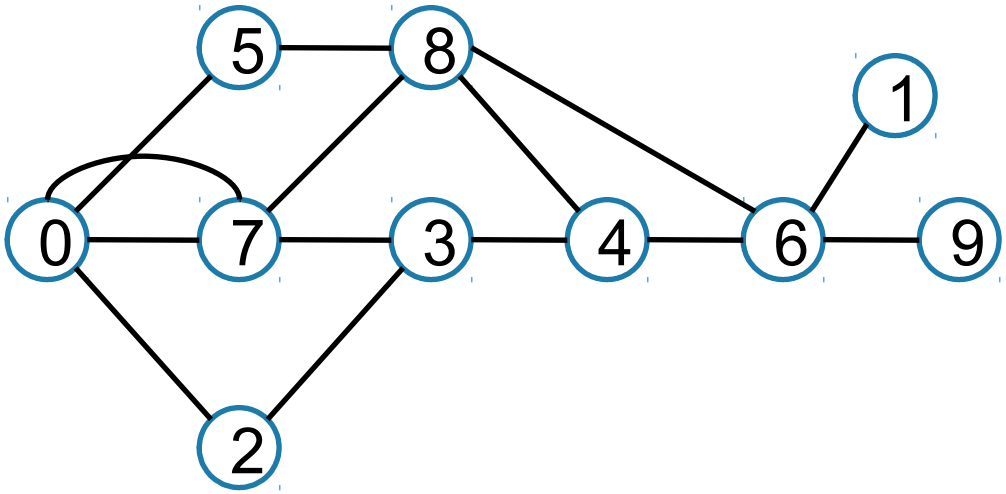
Exact algorithm: **O(mn)** work, **O(m+n)** space, **O(nD+nm/p)** time.

D.A. Bader and K. Madduri. Parallel algorithms for evaluating centrality indices in real-world networks. ICPP'06

Improved with **lower synchronization overhead** and **fewer non-contiguous memory references.**

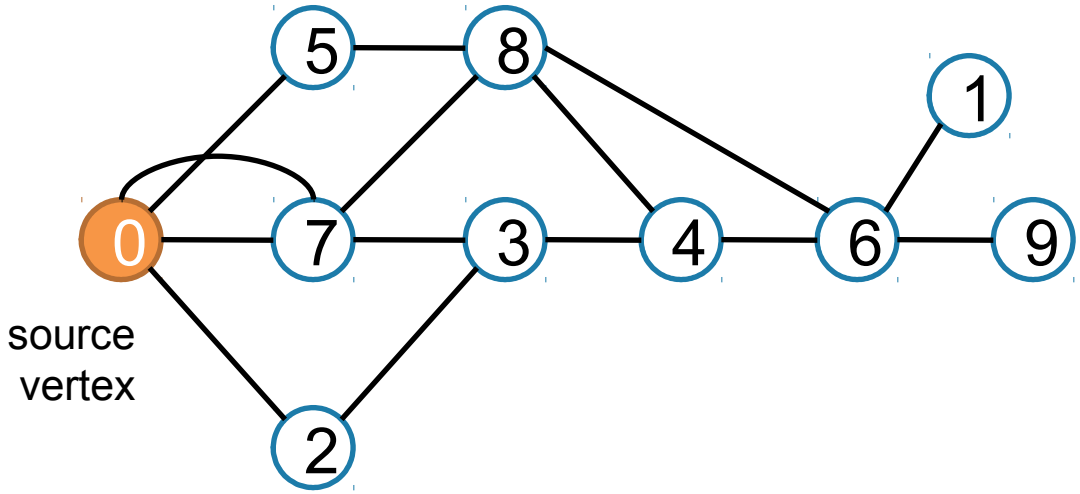
K. Madduri, D. Ediger, K. Jiang, D.A. Bader, and D. Chavarria-Miranda. A faster parallel algorithm and efficient multithreaded implementations for evaluating betweenness centrality on massive datasets. MTAAP 2009

Parallel BC Algorithm Illustration



Parallel BC Algorithm Illustration

1. Traversal step: visit adjacent vertices, update distance and path counts.



Parallel BC Algorithm Illustration

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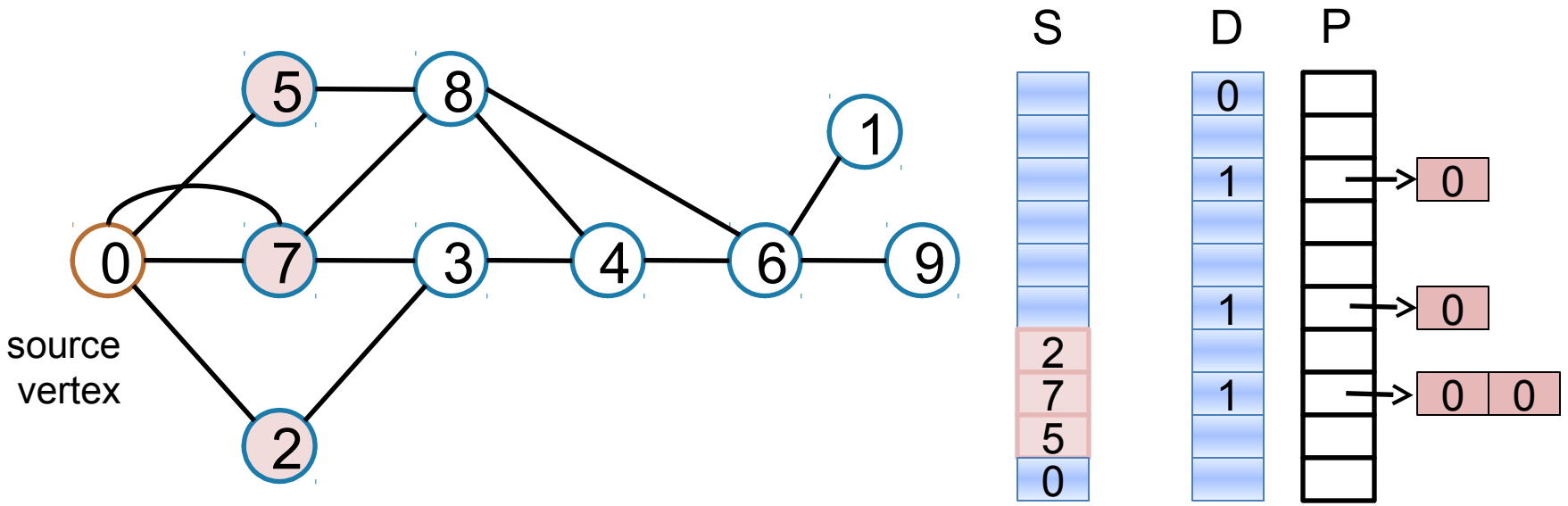
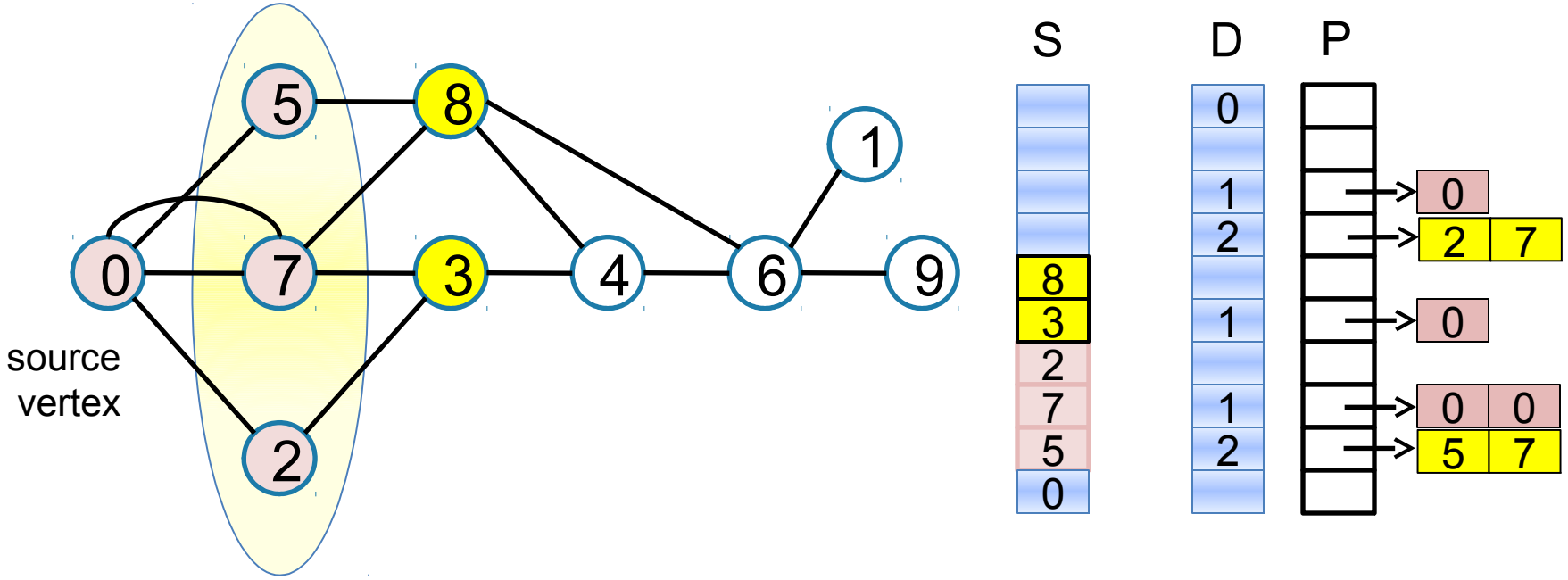


Parallel BC Algorithm Illustration

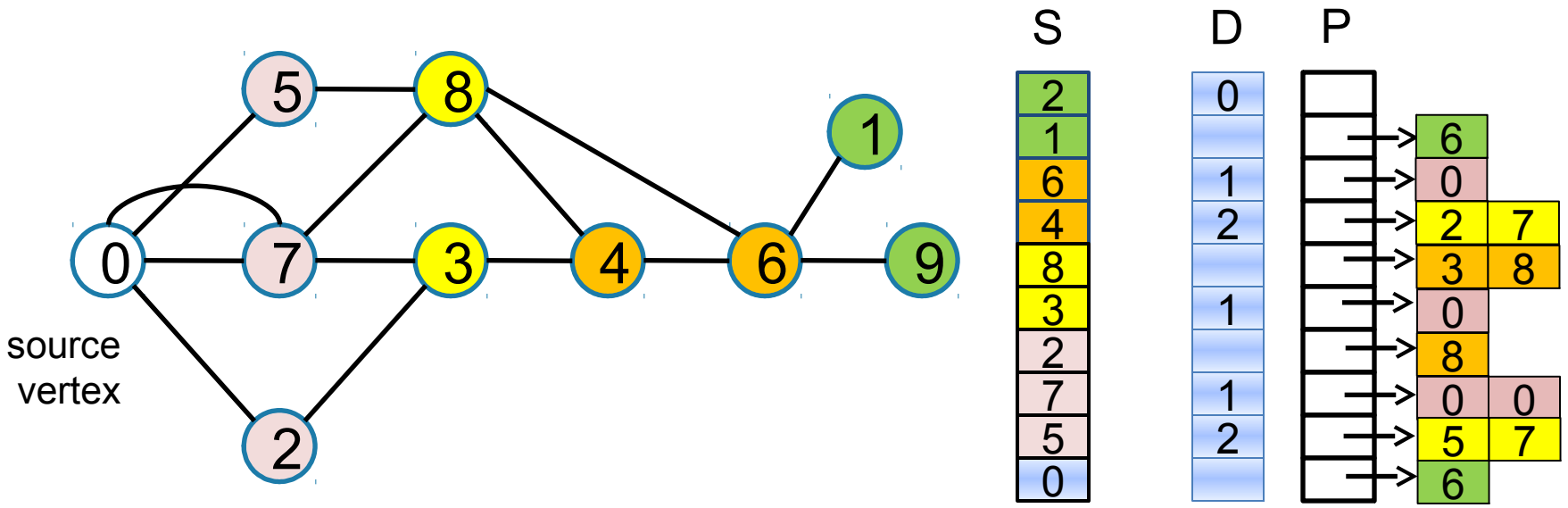
1. Traversal step: visit adjacent vertices, update distance and path counts.



Level-synchronous approach: The adjacencies of all vertices in the current frontier can be visited in parallel

Parallel BC Algorithm Illustration

1. Traversal step: at the end, we have all reachable vertices, their corresponding predecessor multisets, and D values.

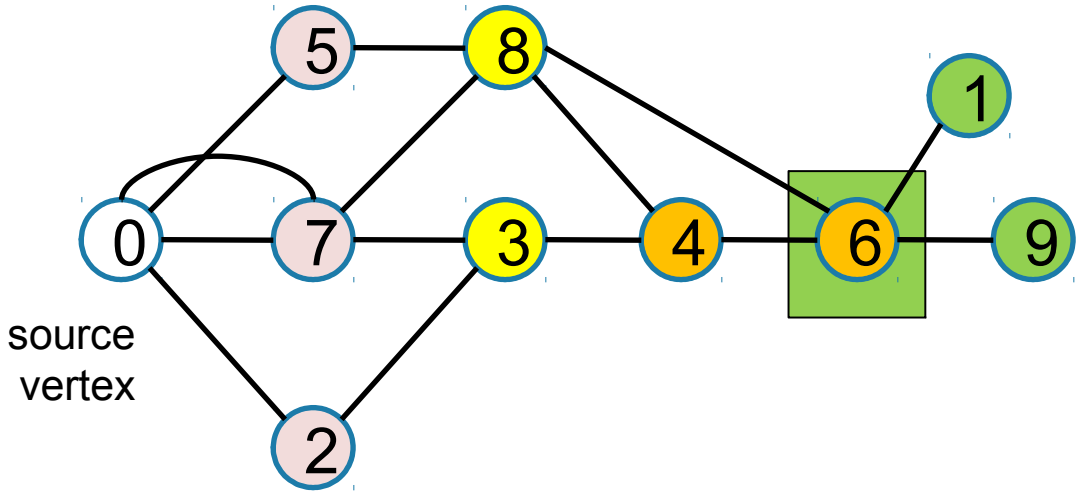


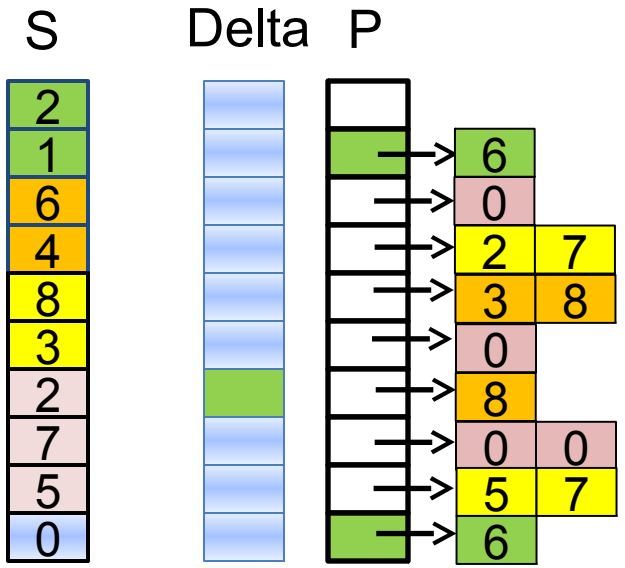
Level-synchronous approach: The adjacencies of all vertices in the current frontier can be visited in parallel

Parallel BC Algorithm Illustration

2. Accumulation step: Pop vertices from stack, update dependence scores.

$$\delta(v) = \sum_{v \in P(w)} \frac{\sigma(v)}{\sigma(w)} (1 + \delta(w))$$

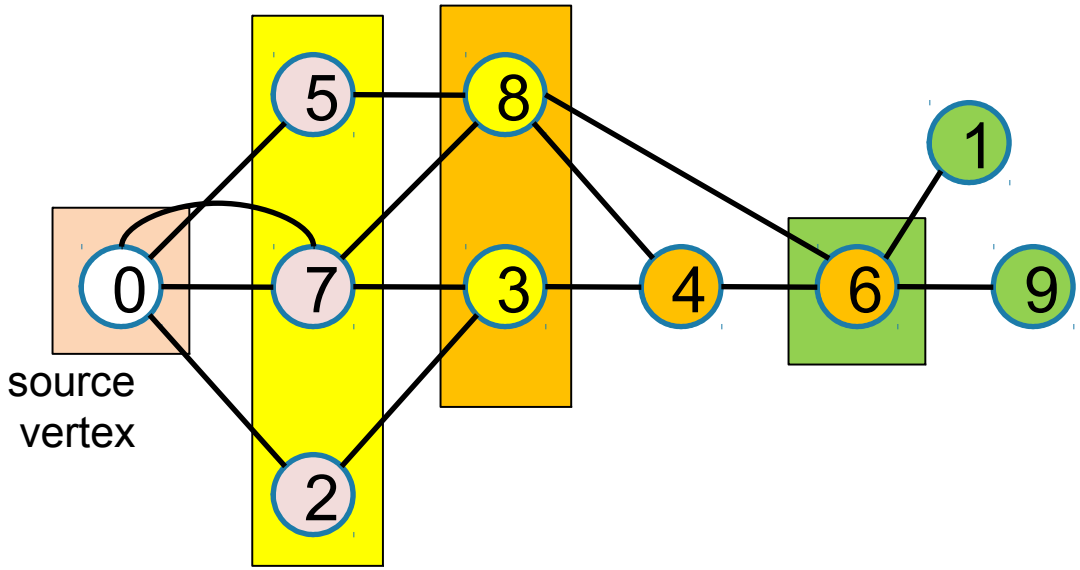


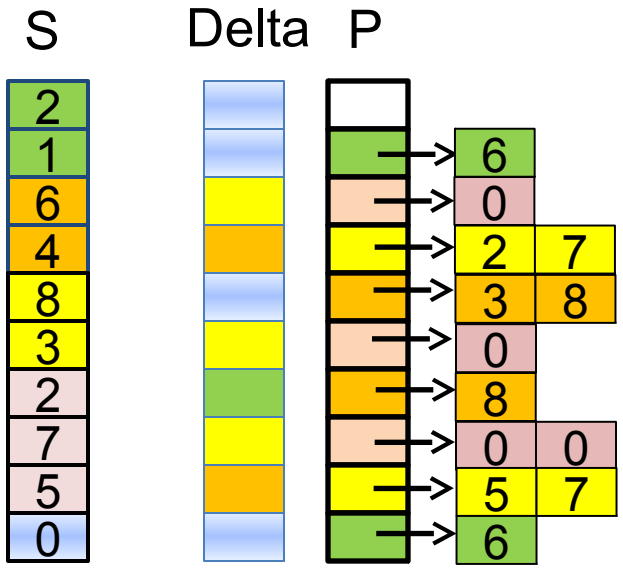


Parallel BC Algorithm Illustration

2. Accumulation step: Can also be done in a level-synchronous manner.

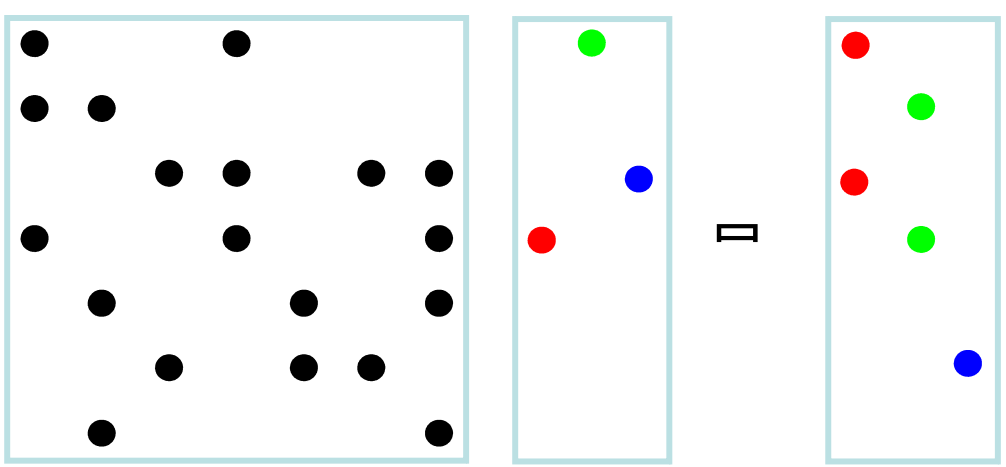
$$\delta(v) = \sum_{w \in adj(v)} \frac{\sigma(v)}{\sigma(w)} \left(1 + \delta(w)\right)$$

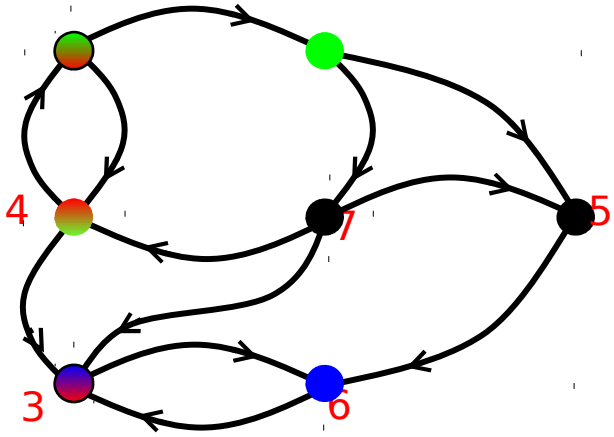




Distributed memory BC algorithm

Work-efficient parallel breadth-first search via **parallel sparse matrix-matrix multiplication over semirings**





Encapsulates three level of parallelism:

1. columns(B): multiple BFS searches in parallel
2. columns(AT)+rows(B): parallel over frontier vertices in each BFS
3. rows(AT): parallel over incident edges of each frontier vertex

A. Buluç, J.R. Gilbert. The Combinatorial BLAS: Design, implementation, and applications. The International Journal of High Performance Computing Applications, 2011.

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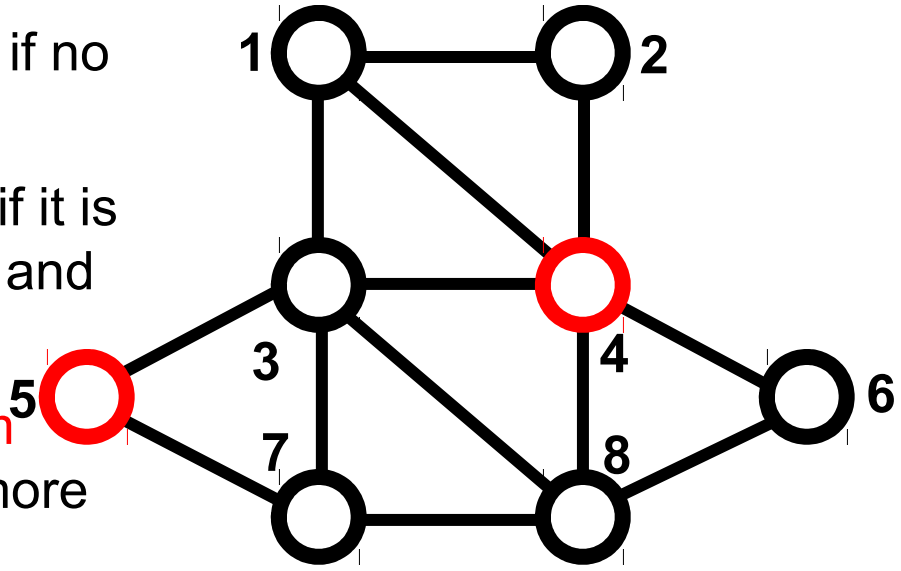
Maximal Independent Set

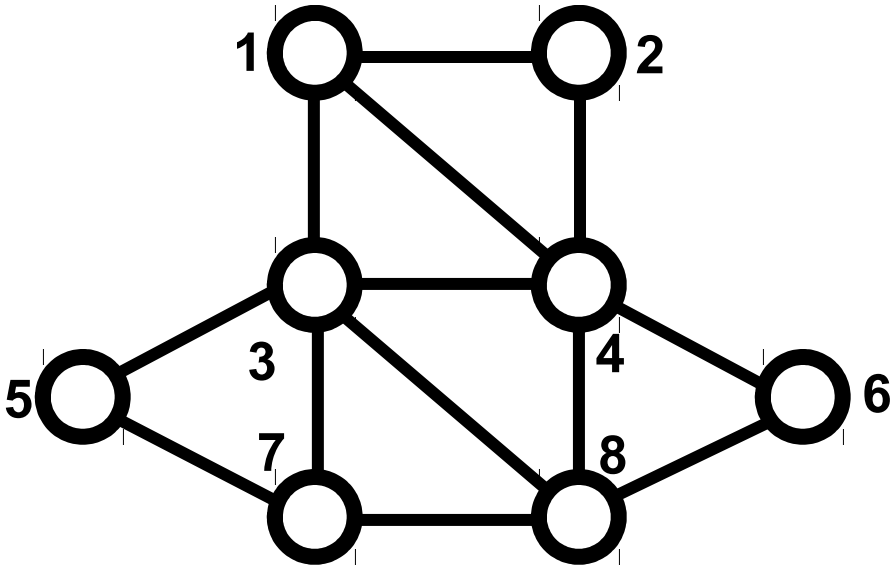
- Graph with vertices V = {1,2,…,n}
- A set S of vertices is independent if no two vertices in S are neighbors.
- An independent set S is maximal if it is impossible to add another vertex and stay independent
- An independent set S is maximum if no other independent set has more vertices
- Finding a *maximum* independent set is intractably difficult (NP-hard)
- Finding a *maximal* independent set is easy, at least on one processor.



The set of red vertices
S = {4, 5} is *independent*
and is *maximal*
but not *maximum*

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

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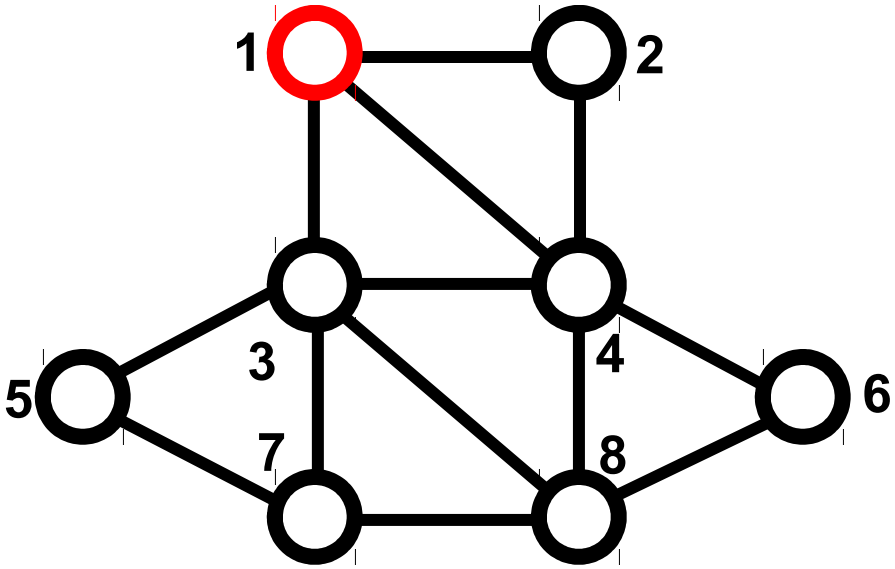
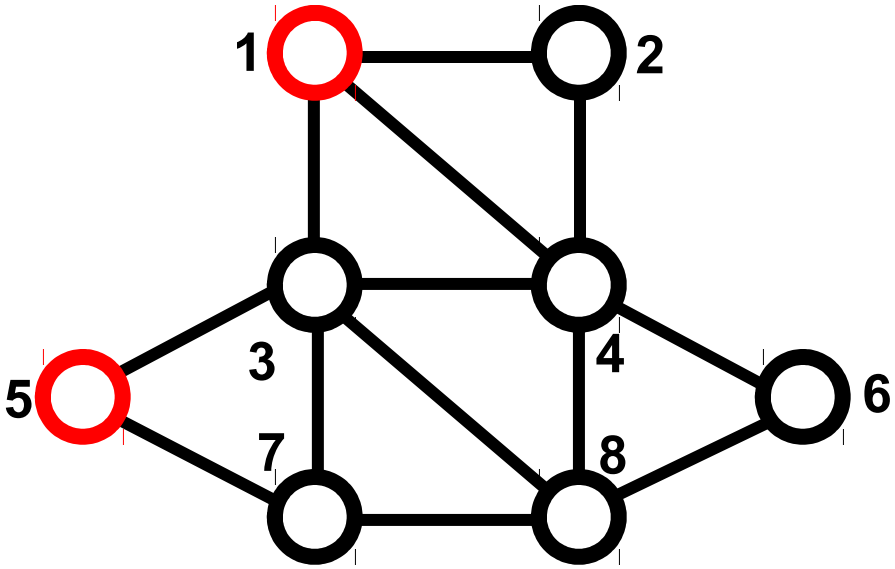


S = { 1 }

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 }

Sequential Maximal Independent Set Algorithm

```
1.  S = empty set;
2.  for  vertex v = 1 to n {
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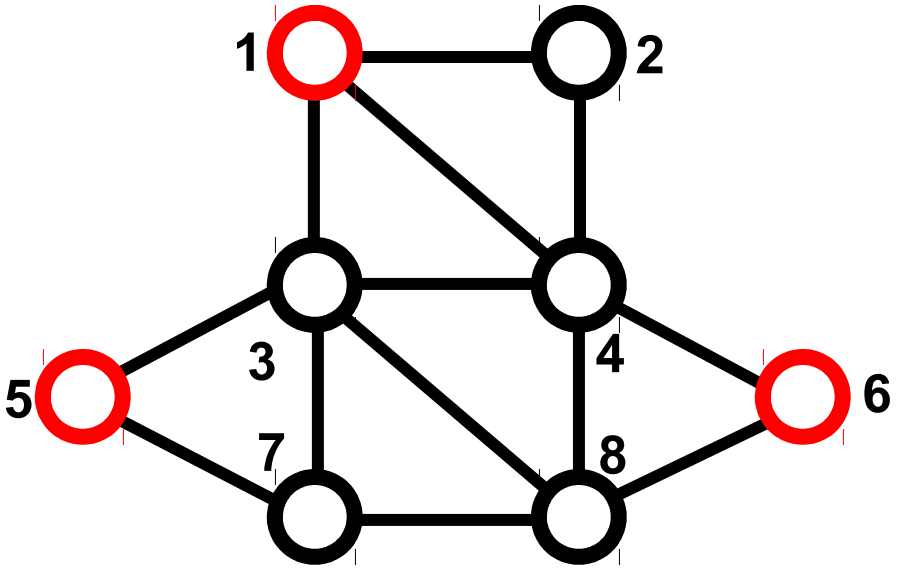
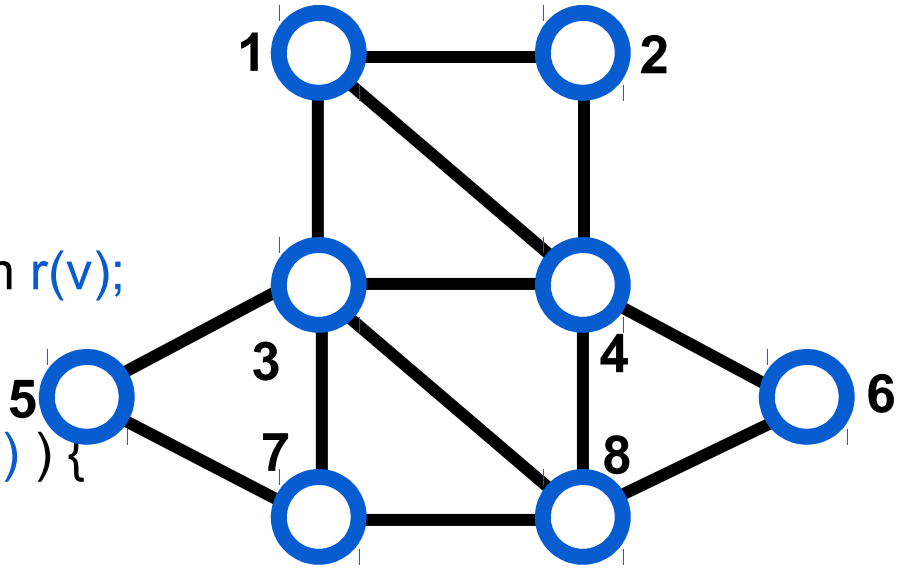


S = { 1, 5, 6 }

work **~ O(n), but** ***span*** **~O(n)**

Parallel, Randomized MIS Algorithm

```
1.  S = empty set;  C = V;
2.  while  C  is not empty {
3.      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;
8.          }
9.      }
10. }
```



S = { }

C = { 1, 2, 3, 4, 5, 6, 7, 8 }

M. Luby. "A Simple Parallel Algorithm for the Maximal Independent Set Problem". *SIAM Journal on Computing* **15** (4): 1036–1053, 1986

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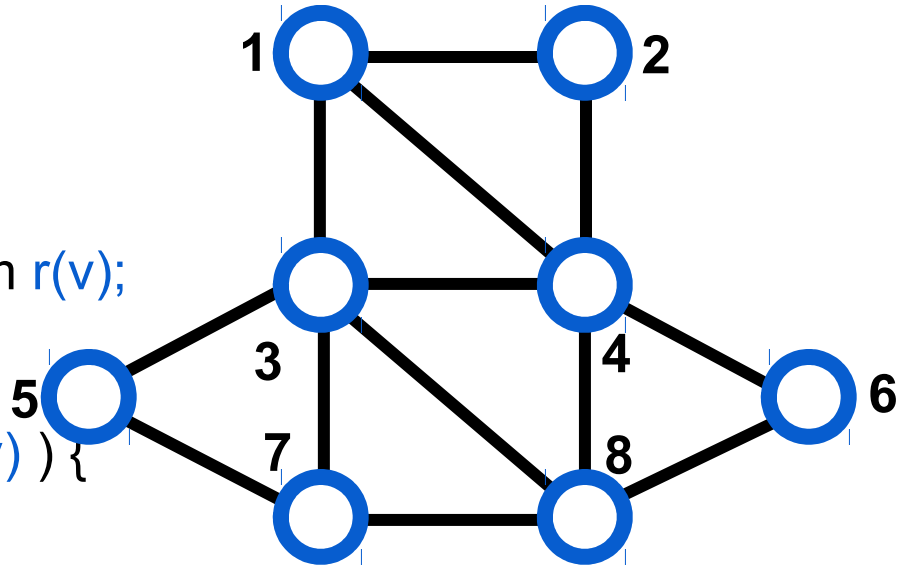

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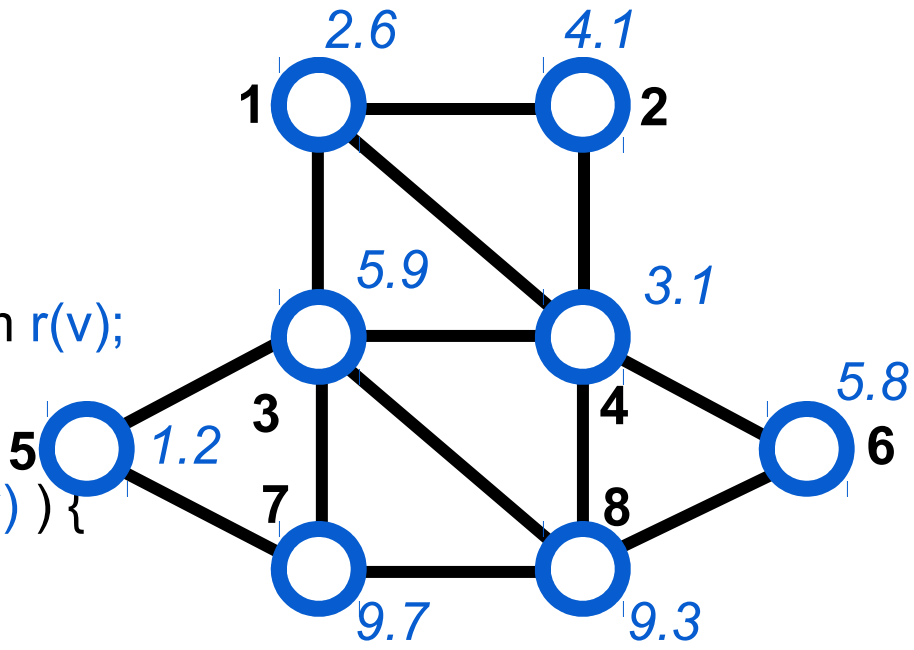

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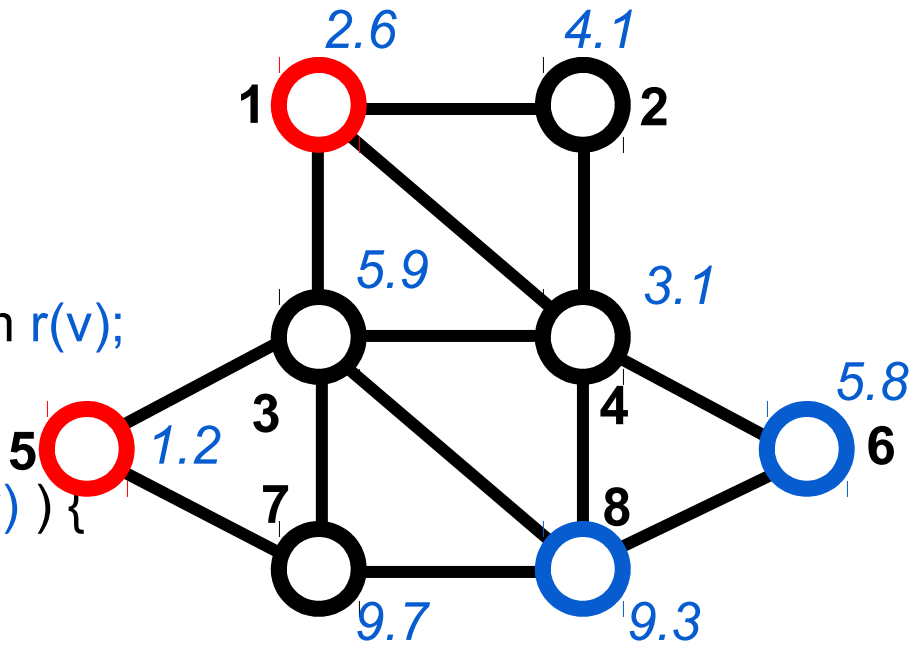

S = { 1, 5 }

C = { 6, 8 }

Parallel, Randomized MIS Algorithm

```
1.  S = empty set;  C = V;
2.  while  C  is not empty {
3.      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) ) {
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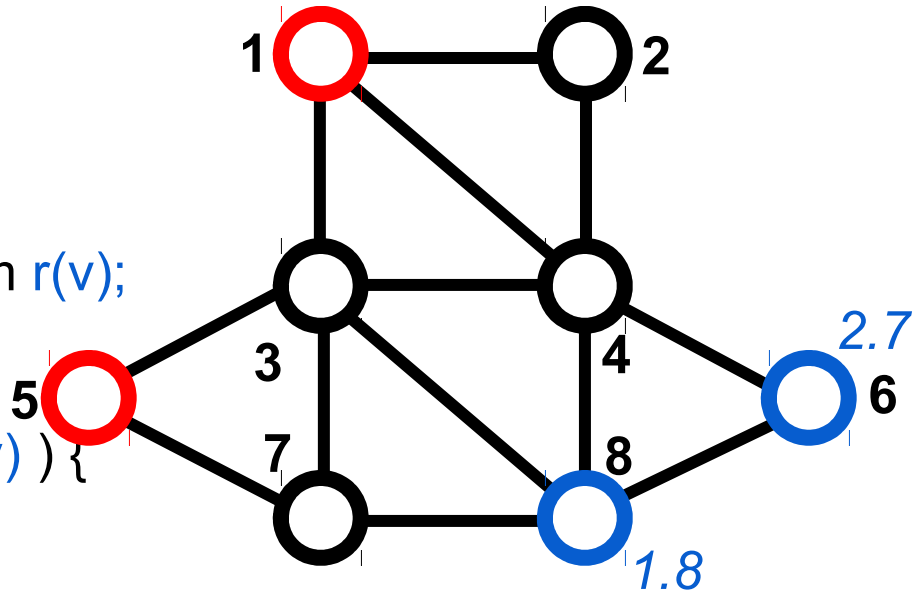

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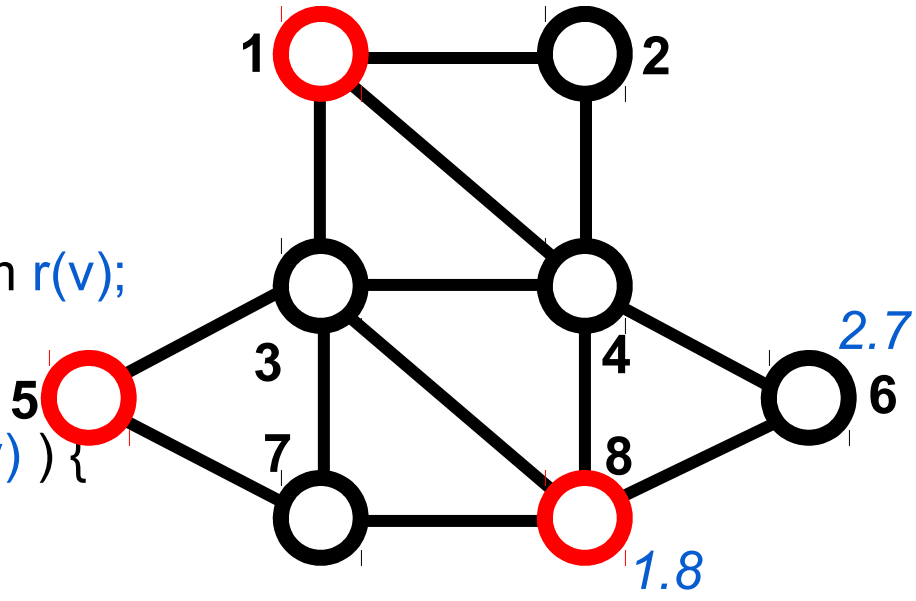

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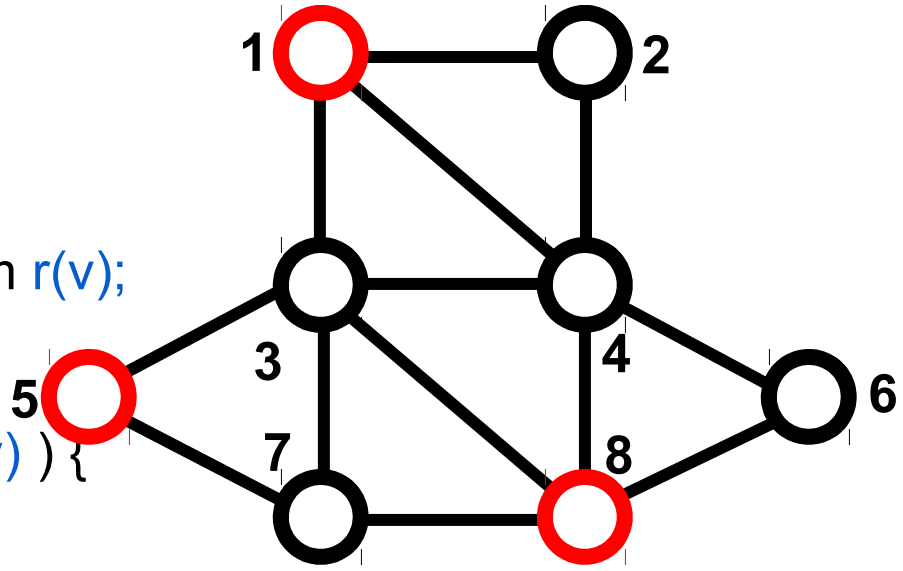


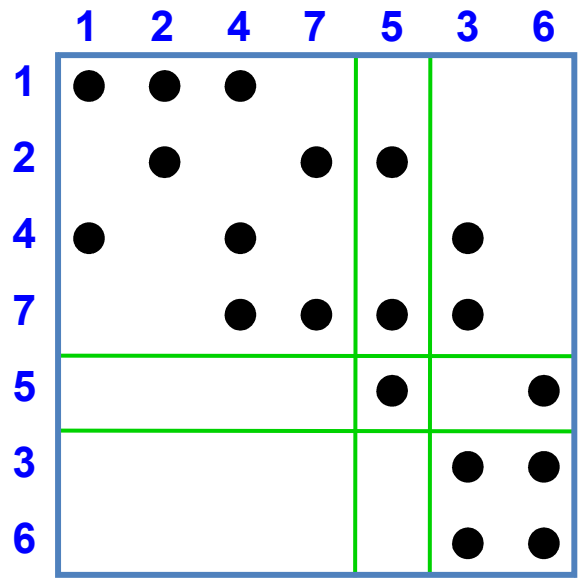
Theorem: This algorithm "very probably" finishes within O(log n) rounds.

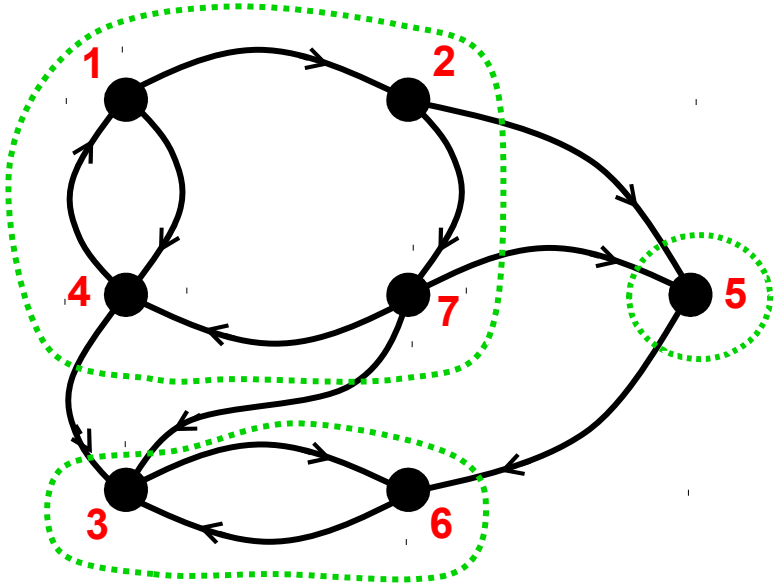
work **~ O(n log n), but** ***span*** **~O(log n)**

Lecture Outline

- Applications
- Designing parallel graph algorithms
- Case studies:
  - **Graph traversals:** Breadth-first search
  - **Shortest Paths:** Delta-stepping, PHAST, Floyd-Warshall
  - **Ranking:** Betweenness centrality
  - **Maximal Independent Sets:** Luby's algorithm
  - **Strongly Connected Components**
- . Wrap-up: challenges on current systems

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|.

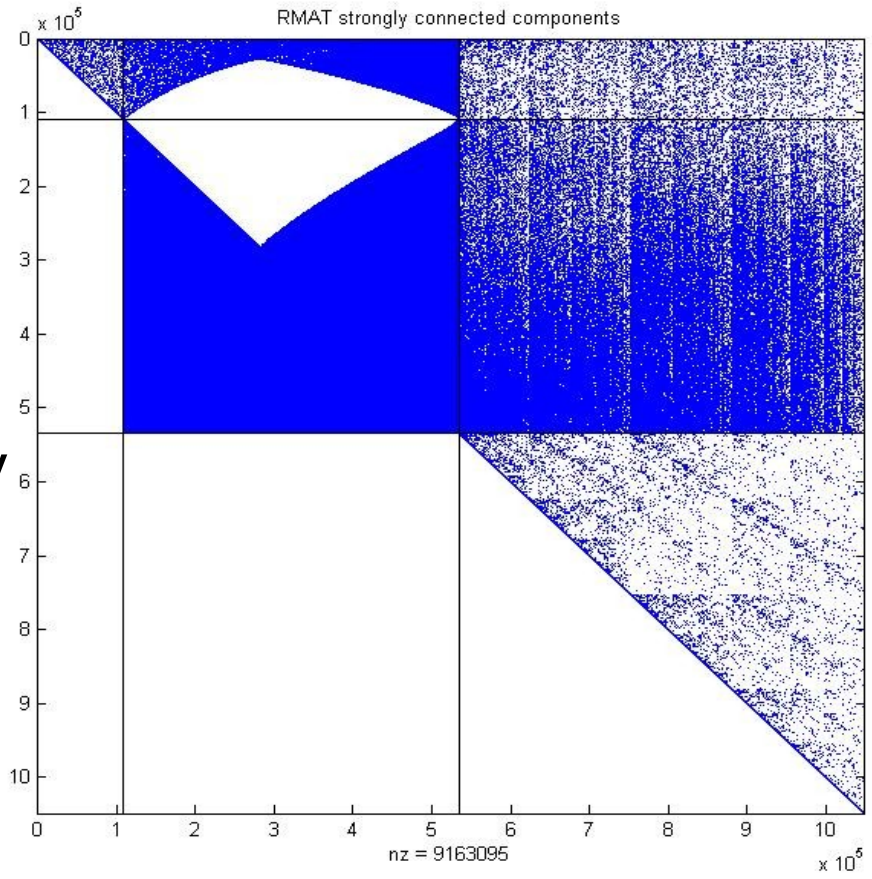
- DFS seems to be inherently sequential.

- 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)∩ BW(v) is a unique SCC for any v. For every other SCC s, either
(a) s ⊂ FW(v)\BW(v),
(b) s ⊂ BW(v)\FW(v),
(c) s ⊂ V \ (FW(v)∪BW(v)).

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

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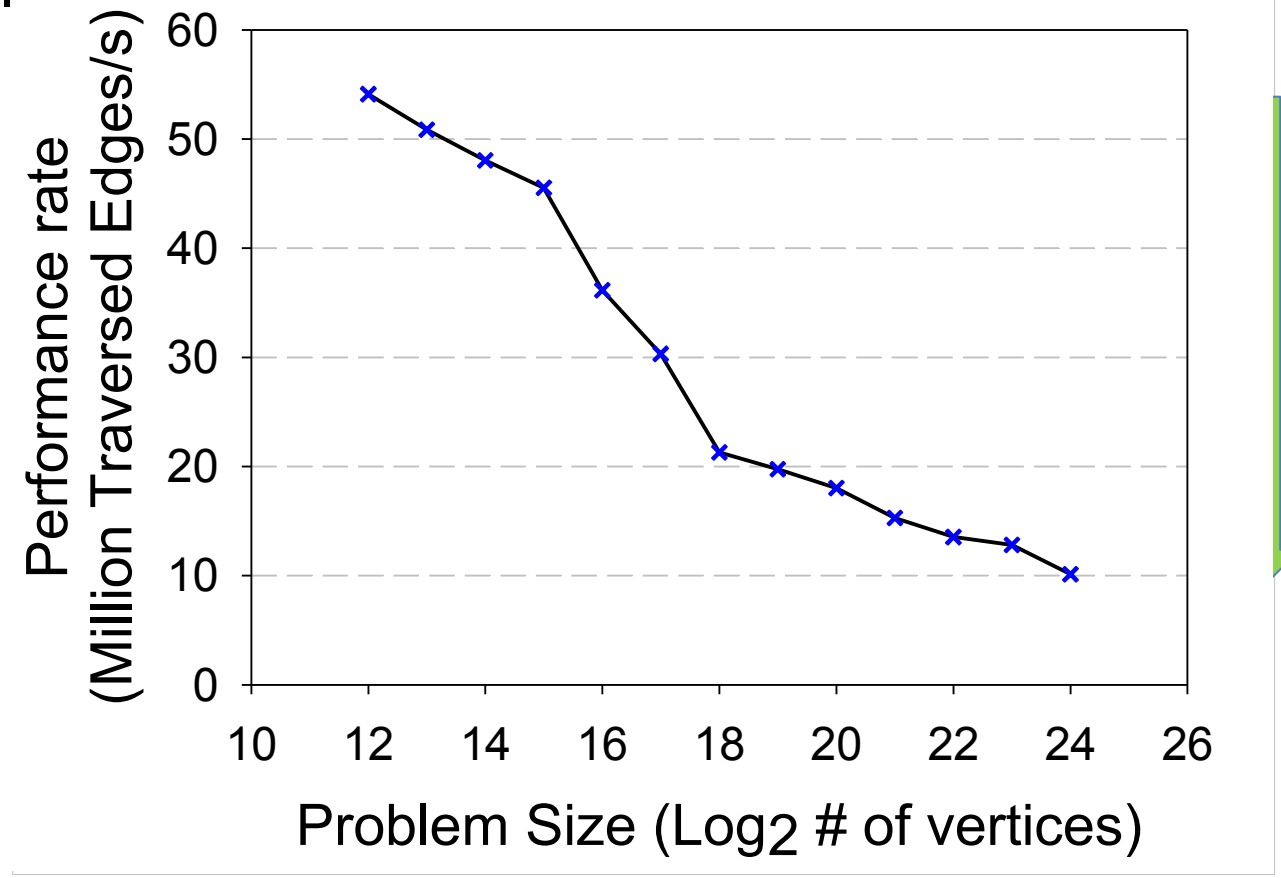
- . Wrap-up: challenges on current systems

The locality challenge

"Large memory footprint, low spatial and temporal locality impede performance"

Serial Performance of "approximate betweenness centrality" on a 2.67 GHz Intel Xeon 5560 (12 GB RAM, 8MB L3 cache)

I



8*n*)

~ 5X drop in performance

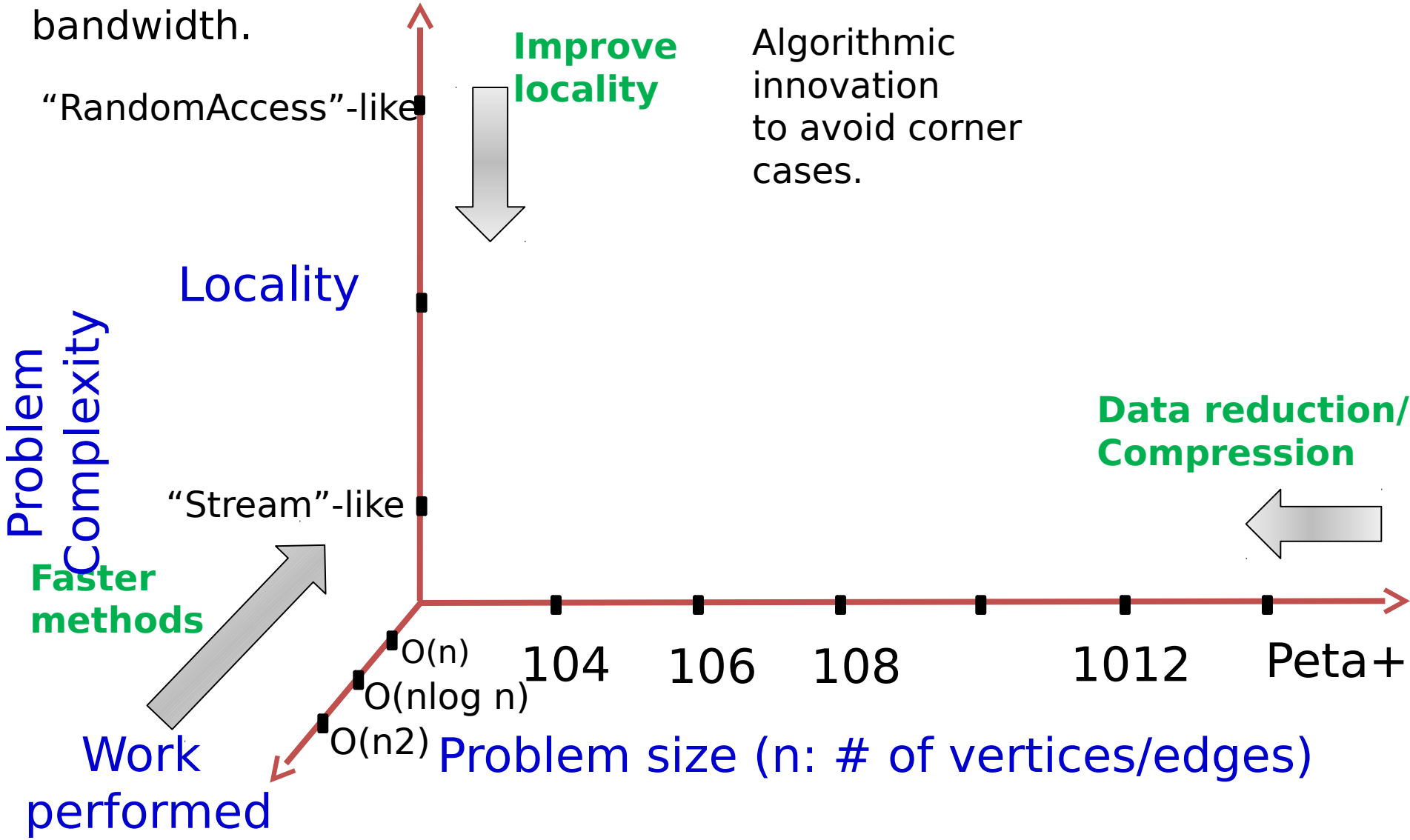
The parallel scaling challenge
"Classical parallel graph algorithms perform poorly on current parallel systems"

- Graph topology assumptions in classical algorithms do not match real-world datasets
- Parallelization strategies at loggerheads with techniques for enhancing memory locality
- Classical "work-efficient" graph algorithms may not fully exploit new architectural features
  - Increasing complexity of memory hierarchy, processor heterogeneity, wide SIMD.
- Tuning implementation to minimize parallel overhead is non-trivial
  - Shared memory: minimizing overhead of locks, barriers.
  - Distributed memory: bounding message buffer sizes, bundling messages, overlapping communication w/ computation.

Designing parallel algorithms for large sparse graph analysis

System requirements: High (on-chip memory, DRAM, network, I/O) bandwidth.

Solution: Efficiently utilize available memory bandwidth.



Conclusions

- Best algorithm depends on the input.
- Communication costs (and hence data distribution) is crucial for distributed memory.
- Locality is crucial for in-node performance.
- Graph traversal (BFS) is fundamental building block for more complex algorithms.
- Best parallel algorithm can be significantly different than the best