## Parallel Graph Algorithms

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## 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: Graph G = (V,E)
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)
- Sequences of edges $\left\langle\mathrm{u}_{1}, \mathrm{u}_{2}>,<\mathrm{u}_{2}, \mathrm{u}_{3}>, \ldots,<\mathrm{u}_{\mathrm{n}-1}, \mathrm{u}_{\mathrm{n}}\right\rangle$ is a path from $u_{1}$ to $u_{n}$. Its length is the sum of its weights.


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## Routing in transportation networks



Road networks, Point-to-point shortest paths: 15 seconds (naiive) $\rightarrow 10$ microseconds H. Bast et al., "Fast Routing in Road Networks with Transit Nodes",

## Large Graphs in Scientific Computing



PA
Matching in bipartite graphs: Permuting to heavy diagonal or block triangular form

## 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



## Large-scale data analysis

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

Astrophysics: massive datasets, temporal variations


Bioinformatics: data quality heterogeneity


Social Informatics: new analytics challenges, data uncertainty


[^0]
## Manifold Learning

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


B


Tenenbaum, Joshua B., Vin De Silva, and John C. Langford. "A global geometric framework for
nonlinear dimensionality reduction." Science 290.5500 (2000): $2319-2323$.


## 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.


## 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


## Graph representations

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


ndex into
array
Adjacencies
Weights

(row pointers in CSR)
(column ids in CSR)
(numerical values in CSR)

## 2D checkerboard distribution

- Consider a logical 2D processor grid ( $p_{r} * p_{c}=p$ ) 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, $3 \times 3$ processor grid


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## Graph traversal : Breadth-first search (BFS)



Memory requirements (\# of machine words):

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

Breadth-first search is a very important building block for other parallel graph algorithms such as (bipartite) matching, maximum flow, (strongly) connected components, betweenness centrality, etc.

Graph traversal: Depth-first search (DFS)


Parallelizing DFS is a bad idea: $\operatorname{span}(D F S)=O(n)$
J.H. Reif, Depth-first search in inherently sequential Inform. Process. Lett. 20 (1985) 229--234

## 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 |
| l | visited in parallel

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




## 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. [computation]

Performance observations of the level-synchronous algorithm


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


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]

## Bottom-up BFS algorithm

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


## 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

- Adoption of the 2 D 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 $p_{c}$ (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



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

Contig 1: GATCTGA


- Main idea:
- Pick a seed
- Iteratively extend it by consecutive lookups in the distributed hash table (vertex $=k$-mer $=$ key, edge $=$ extension = value)


## Parallel De Bruijn Graph Traversal

Assume one of the UU contigs to be assembled is

CGTATTGCCAATGCAACGTATCATGGCCAATCCGAT

## Parallel De Bruijn Graph Traversal

Processor $\mathrm{P}_{\mathrm{i}}$ picks a random k-mer from the distributed hash table as seed:

## CGTATTGCCAATGCAACGTATC GGCCAATCCGAT

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

## Multiple processors on the same UU contig



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

- Processors $P_{i}, P_{j}$ and $P_{t}$ have to collaborate and concatenate subcontigs in order to avoid redundant work.
- Solution: lightweight synchronization scheme based on a state machine


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Moral: One traversal algorithm does not fit all graphs


Low diameter graph (R-MAT)
vs.
Long skinny graph (genomics)


## 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, $\Delta$ - stepping algorithm
U. Meyer and P.Sanders, $\Delta$ - stepping: a parallelizable shortest path algorithm Journal of Algorithms 49 (2003)
- Chakaravarthy et al., clever combination of $\Delta$ - stepping and direction optimization (BFS) on supercomputer-scale graphs.

"Scalable Single Source Shecortest Path Algorithms for Massively Parallel Systems", IPDPS'14


## $\Delta$ - 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))

$$
d(v)=\min \{d(v), d(u)+w(u, v)\}
$$

$\Delta<\boldsymbol{\operatorname { m i n }} \mathbf{w}(\mathrm{e})$ : Degenerates into Dijkstra
$\Delta>\max \boldsymbol{w}(\mathrm{e})$ : Degenerates into Bellman-Ford

## $\Delta$ - stepping algorithm: illustration



One parallel phase while (bucket is non-empty)
i) Inspect light $(w<\Delta)$ edges
ii) Construct a set of
"requests" (R)
iii) Clear the current bucket
iv) Remember deleted vertices (S)
v) Relax request pairs in $R$ Relax heavy request pairs (from $S$ ) Go on to the next bucket

[^1]
## $\Delta$ - stepping algorithm: illustration


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## $\Delta$ - stepping algorithm: illustration

One parallel phase


| d array |
| :--- |
| $\begin{array}{l}0 \\ 0\end{array} 1$ |

Buckets
00

while (bucket is non-empty)
i) Inspect light $(w<\Delta)$ edges
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Relax heavy request pairs (from S) Go on to the next bucket

R


## $\Delta$ - stepping algorithm: illustration


d array


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0 $\square$
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## $\Delta$ - stepping algorithm: illustration


d array

Buckets
02


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


## $\Delta$ - stepping algorithm: illustration



d array |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 0 | 1 | 2 | 3 | 4 | 5 | 6 |
| 0 | $\infty$ | .01 | $\infty$ | $\infty$ | $\infty$ | $\infty$ |

Buckets

02 | |  |  |  |  |
| :--- | :--- | :--- | :--- |

One parallel phase while (bucket is non-empty)
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## $\Delta$ - stepping algorithm: illustration



0 $\square$

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R


## $\Delta$ - stepping algorithm: illustration


d array $\left.\begin{array}{|l|l|l|l|l|l|}\hline 0 & 1 & 2 & 3 & 4 & 5\end{array}\right)$
Buckets
$0 \quad 13$


## One parallel phase

while (bucket is non-empty)
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## $\Delta$ - stepping algorithm: illustration



One parallel phase
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R


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 $\sim 2^{20}$ vertices, $\mathbf{2}^{22}$ edges, directed graph, edge weights normalized to $[0,1]$


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

$\mathrm{k}=1$ case
- It turns out a previously overlooked recursive version is more parallelizable than the triple nested loop




## All-pairs shortest-paths problem



Communication-avoiding APSP in distributed memory


Bandwidth: $W_{\text {bc-.2.5 }}(n, p)=O\left(n^{2} / \sqrt{c p}\right)$
c: number of
Latency: $S_{\text {bc-2.5D }}(p)=O\left(\sqrt{c p} \log ^{2}(p)\right)$
replicas
Optimal for any memory size!

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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 $\mathrm{v}=1$ to $\mathrm{n}\{$
3. if ( $v$ has no neighbor in S ) \{
. add $v$ to $S$
4. \}
5. \}


## Sequential Maximal Independent Set Algorithm

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## Sequential Maximal Independent Set Algorithm

S = empty set;
2. for vertex $\mathrm{v}=1$ to $\mathrm{n}\{$
if ( $v$ has no neighbor in $S$ ) add $v$ to $S$
\}
6. \}

$S=\{1,5,6\}$
work $\sim O(n)$, but span $\sim O(n)$

## Parallel, Randomized MIS Algorithm


10. \}

## Parallel, Randomized MIS Algorithm

$S=$ empty set; C = V;
while $C$ is not empty $\{$
label each $v$ in $C$ with a random $r(v)$
for all v in C in parallel \{
if $r(v)<\min (r($ neighbors of $v))$
move $v$ from $C$ to $S$;
remove neighbors of $v$ from C
\}
\}

10. \}

## Parallel, Randomized MIS Algorithm

```
S = empty set; C = V;
while C is not empty {
    label each v in C with a random r(v)
    for all v in C in parallel {
        if r(v) < min(r(neighbors of v) )
            move v from C to S;
            remove neighbors of v from C;
        }
    }
```

```
remove neighbors of \(v\) from \(C\).
                            \(S=\{1,5\}\)
```

                            \(S=\{1,5\}\)
    ```
10. \}

\section*{Parallel, Randomized MIS Algorithm}
; \(\mathrm{C}=\mathrm{V}\);
while \(C\) is not empty \{
    label each v in C with a random \(\mathrm{r}(\mathrm{v})\);
    for all v in C in parallel \{
        if \(r(v)<\min (r(\) neighbors of \(v))\{\)
            move \(v\) from C to S ;
            remove neighbors of \(v\) from C ;
        \}
\}

10. \}
0.\}

\section*{Parallel, Randomized MIS Algorithm}
    \(S=\) empty set; \(C=V ;\)
while \(C\) is not empty \(\{\)
    label each \(v\) in \(C\) with a random \(r(v)\)
    for all \(v\) in \(C\) in parallel \{
        if \(r(v)<\min (r(\) neighbors of \(v))\{\)
            move \(v\) from \(C\) to \(S\);
            remove neighbors of \(v\) from \(C\);
        \}
    \(\}\)

10. \}

\section*{Parallel, Randomized MIS Algorithm}
\(S=\) empty set; \(C=V\);
while \(C\) is not empty \{
    label each \(v\) in \(C\) with a random \(r(v)\)
    for all \(v\) in \(C\) in parallel \{
        if \(r(v)<\min (r(\) neighbors of \(v))\) \{
            move \(v\) from \(C\) to \(S\);
            remove neighbors of \(v\) from C ;
        \}
                        Theorem: This algorithm "very probably" finishes within \(O(\log n)\) rounds.
10. \}
work \(\sim \mathrm{O}(\mathrm{n} \log \mathrm{n})\), but span \(\sim \mathrm{O}(\log \mathrm{n})\)

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Strongly connected components (SCC)

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

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

\section*{Fleischer/Hendrickson/Pinar algorithm}
- Partition the given graph into three disjoint subgraphs
Each can be processed independently/recursively

Lemma: \(F W(v) \cap B W(v)\) is a unique SCC for any v. For every other SCC s, either
 et al.); worst-case span \(\mathrm{O}(\mathrm{n})\) but good in practice on many graphs.

\footnotetext{
L. Fleischer, B. Hendrickson, and A. Pinar. On identiffing strongly connected components in parallel. Parallel and Distributed Processing, pages 505-511, 2000
}
(a) s \(\subset F W(v) \backslash B W(v)\),
(b) s \(\subset B W(v) \backslash F W(v)\),
(c) \(s \subset V \backslash(F W(v) \cup B W(v))\).

FW(v): vertices reachable from vertex \(v\).
\(B W(v)\) : vertices from which \(v\) is reachable.


\section*{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

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\section*{Single-Source Algorithm for Maximum Cardinality Matching}

1. Initial matching

2. Search for augmenting path from \(x_{3}\). stop when an unmatched vertex found

. Increase matching by fliping edges in the augmenting path

\footnotetext{
Repeat the process for other unmatched vertices
}

\section*{Multi-Source Algorithm for Maximum Cardinality Matching}


Search Forest

1. Initial matching
2. Search for vertex-disjoint augmenting paths from \(x_{3} \& x_{1}\). Grow a tree until an unmatched vertex is found in it

Repeat the process for until no augmenting path is found

\section*{Tree Grafting Mechanism}


\section*{Limitation of Current Multi-source Algorithms}

Previous algorithms destroy both trees and start searching from \(\mathrm{x}_{1}\) again

(a) A maximal matching in a Bipartite Graph


\section*{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

\section*{Performance of the tree-grafting algorithm}

Pothen-Fan: Azad et al. IPDPS 2012
Push-Relabel: Langguth et al. Parallel Computing 2014


\section*{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:
\(\mathrm{VR}=\{\) rows reachable via alt. path from some unmatched row \(\}\)
\(\mathrm{VC}=\{\) cols reachable via alt. path from some unmatched row \(\}\)
\(H R=\{\) rows reachable via alt. path from some unmatched col \(\}\) \(H C=\{\) cols reachable via alt. path from some unmatched col \(\}\)

SR = R - VR - HR
\(\mathrm{SC}=\mathrm{C}-\mathrm{VC}-\mathrm{HC}\)

\section*{Dulmage-Mendelsohn decomposition}


\section*{Applications of D-M decomposition}
- Strongly connected components of directed graphs
- Connected components of undirected graphs
- Permutation to block triangular form for \(\mathrm{Ax}=\mathrm{b}\)
- Minimum-size vertex cover of bipartite graphs
- Extracting vertex separators from edge cuts for arbitrary graphs
- Nonzero structure prediction for sparse matrix factorizations```


[^0]:    

[^1]:    Initialization:
    Insert $s$ into bucket, d(s) $=0$

