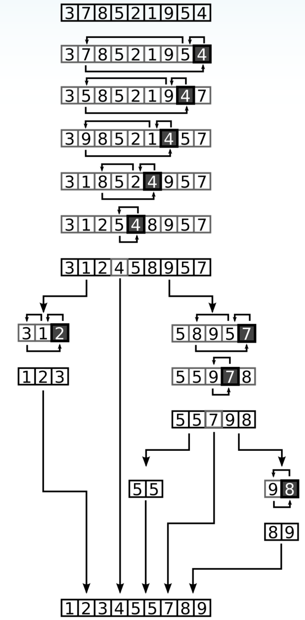
6.506: Algorithm Engineering



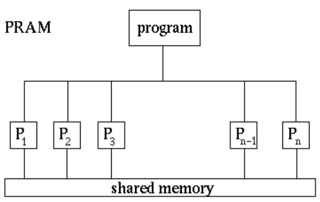
LECTURE 1
Introduction

Julian Shun

February 6, 2024

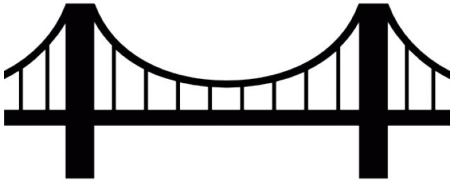
What is Algorithm Engineering?

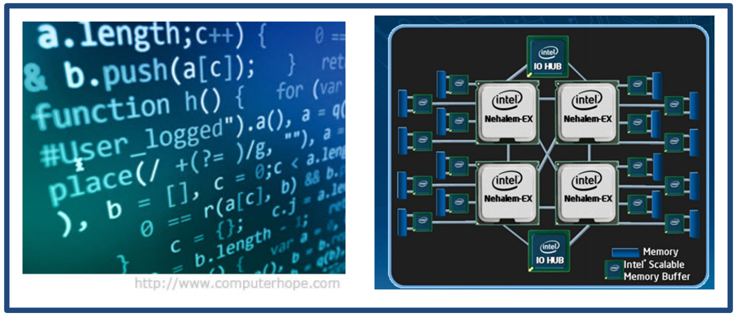
- Algorithm design
- Algorithm analysis
- Algorithm implementation
- Optimization
- Profiling
- Experimental evaluation



O(n log n)
O(n)
O(log n)

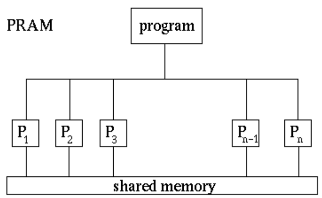
Theory



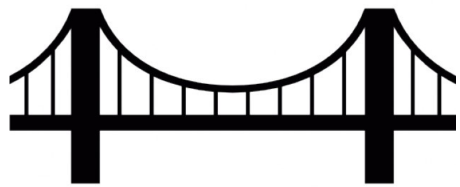


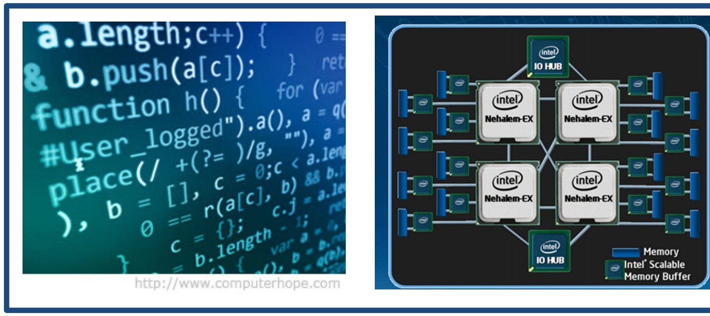
Practice

Bridging Theory and Practice



O(n log n)
O(n)
O(log n)





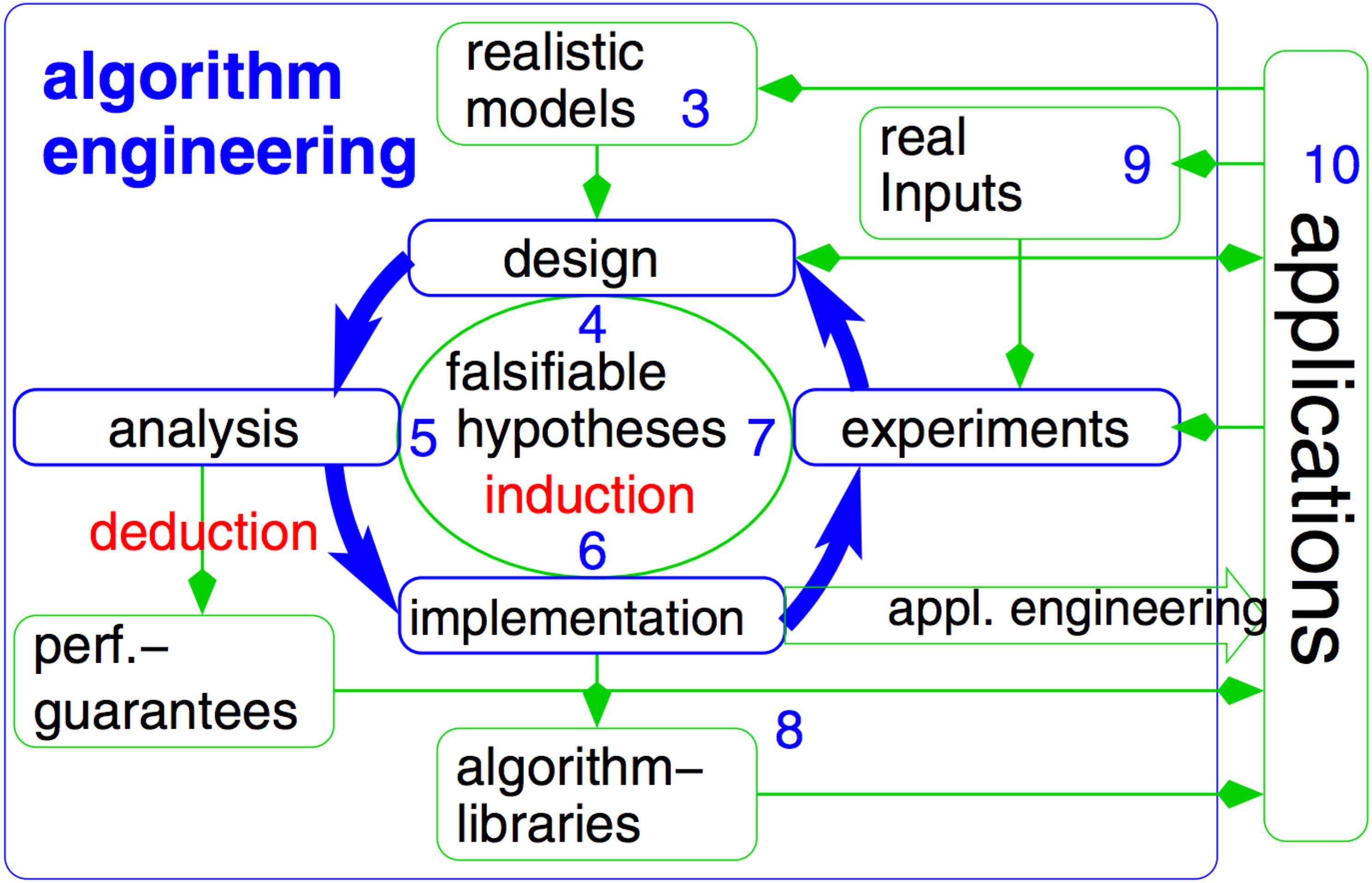
- Good empirical performance
- Confidence that algorithms will perform well in many different settings
- Ability to predict performance (e.g., in real-time applications)
- Important to develop theoretical models to capture properties of technologies

Use theory to inform practice and practice to inform theory.

Brief History

- In early days, implementing algorithms designed was standard practice
- 1970s–1980s: Algorithm theory is a subdiscipline in CS mostly devoted to ”paper and pencil” work
- Late 1980s–1990s: Researchers began noticing gaps between theory and practice
- 1997: First Workshop on Algorithm Engineering (WAE) by P. Italiano (now part of ESA)
- 1998: Meeting on Algorithm Engineering & Experiments (ALENEX)
- 2003: annual Workshop on Experimental Algorithms (WEA), now Symposium on Experimental Algorithms (SEA)
- Nowadays many conferences have papers on algorithm engineering

What is Algorithm Engineering?



Source: “Algorithm Engineering – An Attempt at a Definition”, Peter Sanders

Models of Computation

- Random-Access Machine (RAM)
  - Infinite memory
  - Arithmetic operations, logical operations, and memory accesses take O(1) time
  - Most sequential algorithms are designed using this model (6.006/6.046)
- Nowadays computers are much more complex
  - Deep cache hierarchies
  - Instruction level parallelism
  - Multiple cores
  - Disk if input doesn't fit in memory
  - Read and write costs are not necessary the same

Algorithm Design & Analysis

	Algorithm 1	Algorithm 2
Complexity	$N \log_2 N$	$1000\ N$

- Constant factors matter!
- Avoid unnecessary computations
- Simplicity improves applicability and can lead to better performance
- Think about locality and parallelism
- Think both about worst-case and real-world inputs
- Use theory as a guide to find practical algorithms
- Time vs. space tradeoffs
- Work vs. parallelism tradeoffs

Implementation

- Write clean, modular code
  - Easier to experiment with different methods, and can save a lot of development time
- Write correctness checkers
  - Especially important in numerical and geometric applications due to floating-point arithmetic, possibly leading to different results
- Save previous versions of your code!
  - Version control helps with this

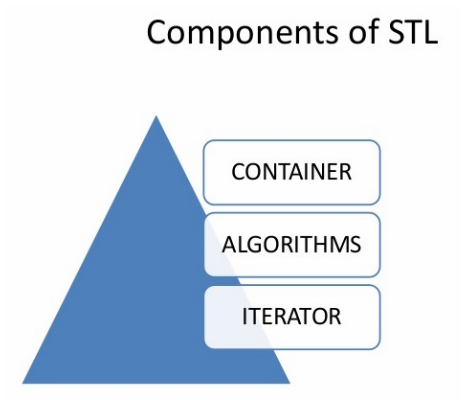
Experimentation

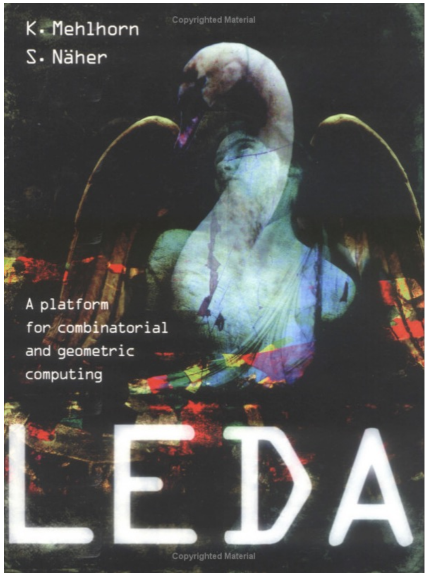
- Instrument code with timers and use performance profilers (e.g., perf, gprof, valgrind)
- Use large variety of inputs (both real-world and synthetic)
  - Use different sizes
  - Use worst-case inputs to identify correctness or performance issues
- Reproducibility
  - Document environmental setup
  - Fix random seeds if needed
- Run multiple times to deal with variance

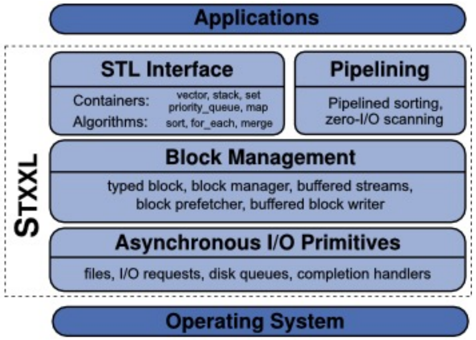
Experimentation II

- For parallel code, test on varying number of processors to study scalability
- Compare with best serial code for problem
- For reproducibility, write deterministic parallel code if possible
  - Or make it easy to turn off non-determinism
- Use numactl to control NUMA effects on multi-socket machines
- Useful tools: Cilkscale, Cilksan

Libraries and Frameworks

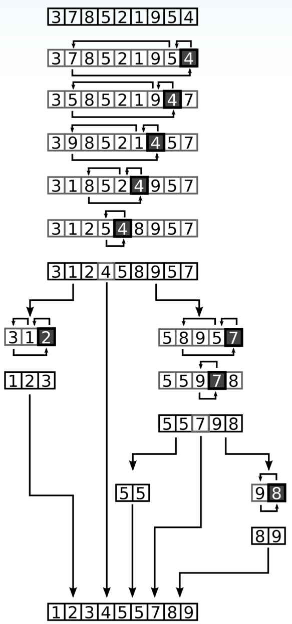






- Use efficient building blocks from existing libraries/frameworks when appropriate
- Contribute to existing libraries/frameworks or develop your own to help others and improve applicability

COURSE INFORMATION



Course Information

- Graduate-level class
  - Undergraduates who have taken 6.122 (6.046) and 6.106 (6.172) are welcome
- Lectures: Tuesday/Thursday 11am-12:30pm ET in 3-370
- Instructor:
  - Julian Shun (jshun@mit.edu)
- TA
  - Amy Hu (amyhu@mit.edu)
- Units: 3-0-9
- We will use Piazza for communication
- Office hours by appointment

Course Website

https://people.csail.mit.edu/jshun/6506-s24/

Date	Topic	Speaker	Required Reading	Optional Reading
Tuesday 2/6	Course Introduction	Julian Shun	Algorithm Engineering - An Attempt at a Definition A Theoretician's Guide to the Experimental Analysis of Algorithms	Algorithm Engineering: Bridging the Gap Between Algorithm Theory and Practice A Guide to Experimental Algorithmics Algorithm engineering: an attempt at a definition using sorting as an example Algorithm Engineering for Parallel Computation Distributed Algorithm Engineering Experimental algorithmics Programming Pearls Smoothed analysis of algorithms: Why the simplex algorithm usually takes polynomial time
Thursday 2/8	Parallel Algorithms	Julian Shun	Parallel Algorithms Thinking in Parallel: Some Basic Data-Parallel Algorithms and Techniques (Chapters 4-8) CLRS Chapter 26 (Parallel Algorithms)	Prefix Sums and Their Applications Algorithm Design: Parallel and Sequential Introduction to Parallel Algorithms Scheduling Multithreaded Computations by Work Stealing Thread Scheduling for Multiprogrammed Multiprocessors Multidimensional Included and Excluded Sums Work-Efficient Parallel Algorithms for Accurate Floating-Point Prefix Sums Problem Based Benchmark Suite
Tuesday 2/13	Parallel Graph Traversal		Direction-Optimizing Breadth-First Search The More the Merrier: Efficient Multi-Source Graph Traversal	A Work-Efficient Parallel Breadth-First Search Algorithm (or How to Cope with the Nondeterminism of Reducers) Internally Deterministic Parallel Algorithms Can Be Fast SlimSell: A Vectorizable Graph Representation for Breadth-First Search

Grading

Grading Breakdown	
Paper Reviews	20%
Problem Set	10%
Paper Presentations	15%
Research Project	45%
Class Participation	10%

You must complete all assignments to pass the class.

Paper Presentations

- Cover content from 2 research papers each lecture
- 25-30 minute student presentation + Q&A per paper
  - Discuss motivation for the problem solved
  - Key technical ideas
  - Theoretical/experimental results
  - Related work
  - Strengths/weaknesses
  - Directions for future work
  - Include several questions for discussion
  - Presentation should cover necessary background to understand paper (you may have to read related papers)
  - Make slides but may use the whiteboard for theory
- Student presentations begin next Tuesday
- Sign-up sheet will be released soon
- Please sign up even if you are a listener

Paper Reviews

- Submit one paper review for each lecture
  - Starting next week
  - Cover motivation, key ideas, results, novelty, strengths/weaknesses, your ideas for improving the techniques or evaluation, any open problems or directions for further work
  - Submit on Canvas by 10am ET on the day of each lecture (before we cover the papers)

Problem Set

- Complete a problem set on parallel algorithms
  - To be released this week and due on Monday 3/4

Research Project

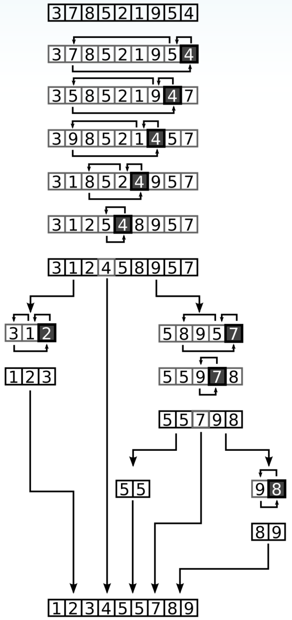
- Open-ended research project to be done in groups of 1-3 people
- Some ideas
  - Implementation of non-trivial algorithms
  - Analyzing/optimizing performance of existing algorithms
  - Designing new theoretically and/or practically efficient algorithms
  - Applying algorithms in the context of larger applications
  - Improving or designing algorithm frameworks or libraries, parallel runtime systems, or software productivity tools
  - Any topic may involve parallelism, cache-efficiency, I/O-efficiency, and memory-efficiency
- Must contain an implementation component
- Can be related to research that you are doing

Project Timeline

Assignment	Due Date
Pre-proposal meeting	3/5
Proposal	3/15
Weekly progress reports	3/22, 4/5, 4/12, 4/19, 4/26, 5/3, 5/10
Mid-term report	4/16
Project presentations	5/14
Final report	5/14

- Pre-proposal meeting
  - 15-minute meeting to run ideas by instructors
- Computing resources for the project
  - Sign up for Google Cloud Platform for free cloud computing credits
  - Talk to instructor if you need additional credits

Parallelism



Parallelism

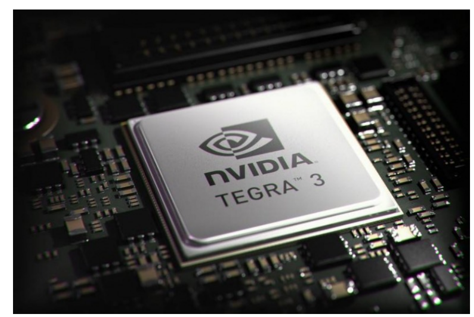
Data is becoming very large!

41 million vertices
1.5 billion edges
(6.3 GB)

1.4 billion vertices
6.6 billion edges
(38 GB)

3.5 billion vertices
128 billion edges
(540 GB)

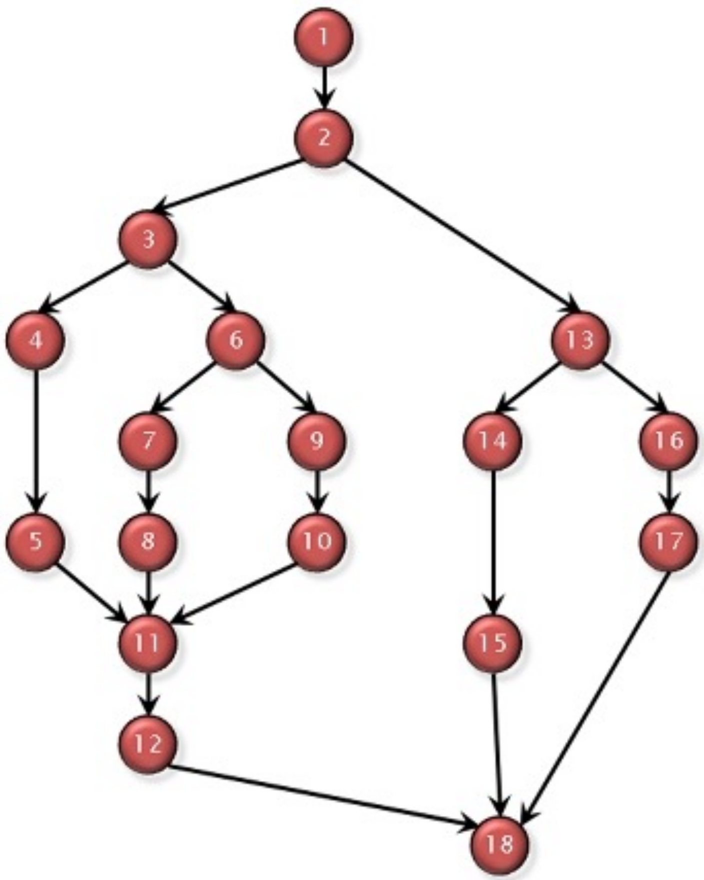
Parallel machines are everywhere!



Can rent machines on AWS with up to 224 cores (448 hyper-threads) and 24TB of RAM

Parallelism Models

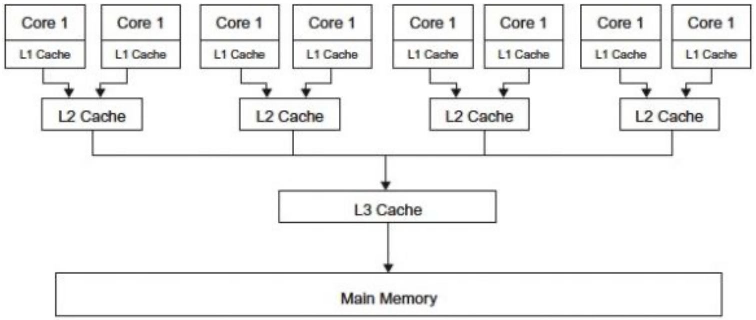
Computation graph



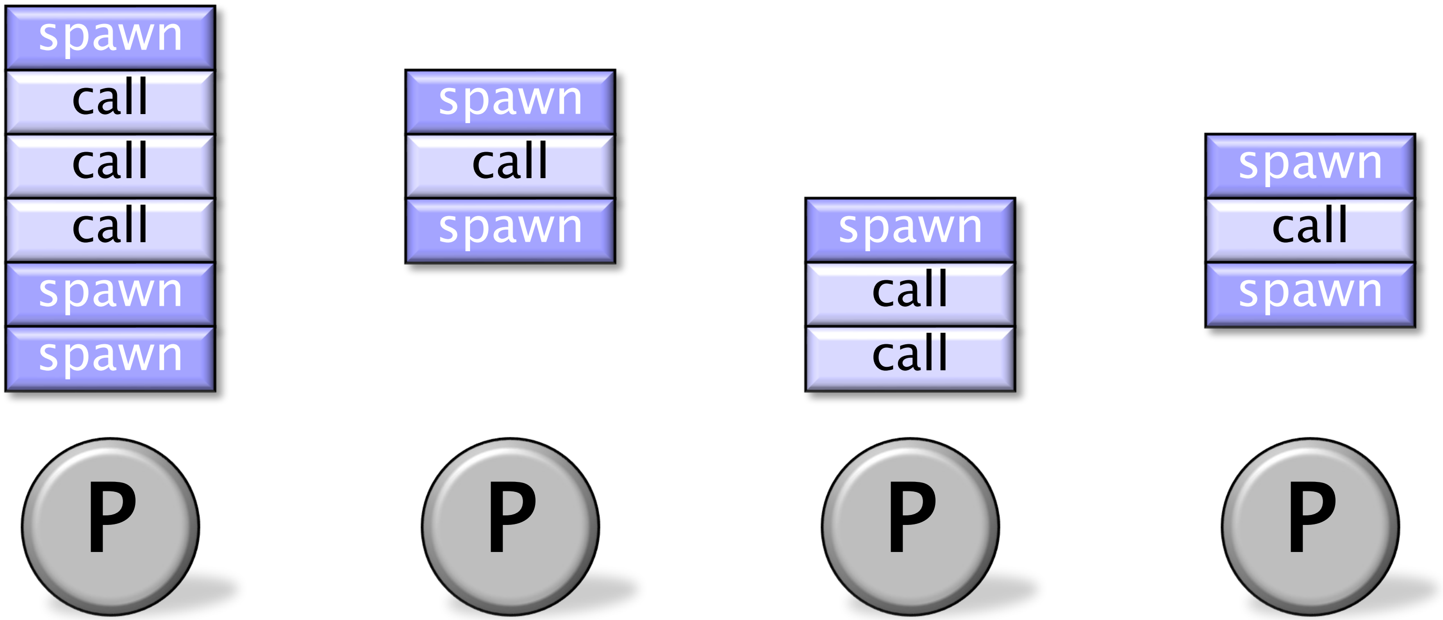
- Work = number of vertices in graph (number of operations)
- Span (depth) = longest directed path in graph (dependence length)
- Running time ≤ (Work/#processors) + O(Span)
- A **work-efficient** parallel algorithm has work that asymptotically matches that of the best sequential algorithm for the problem

Goal 1: work-efficient and low (polylogarithmic) span algorithms

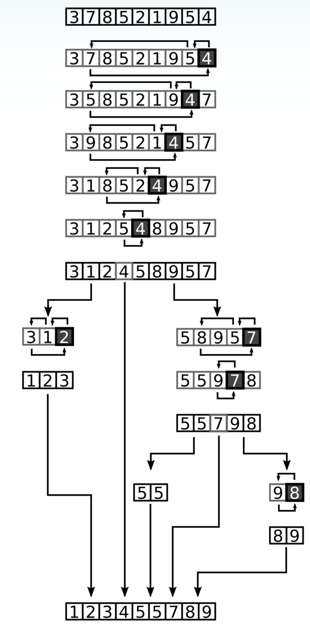
Goal 2: simple, practical, and cache-friendly



Cilk Scheduling



- Manually scheduling threads is difficult
- Cilk work-stealing scheduler
  - How can we translate work and depth bounds into efficient parallel running times in theory and practice?



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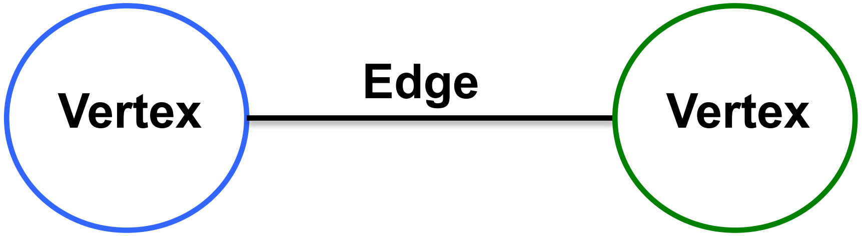
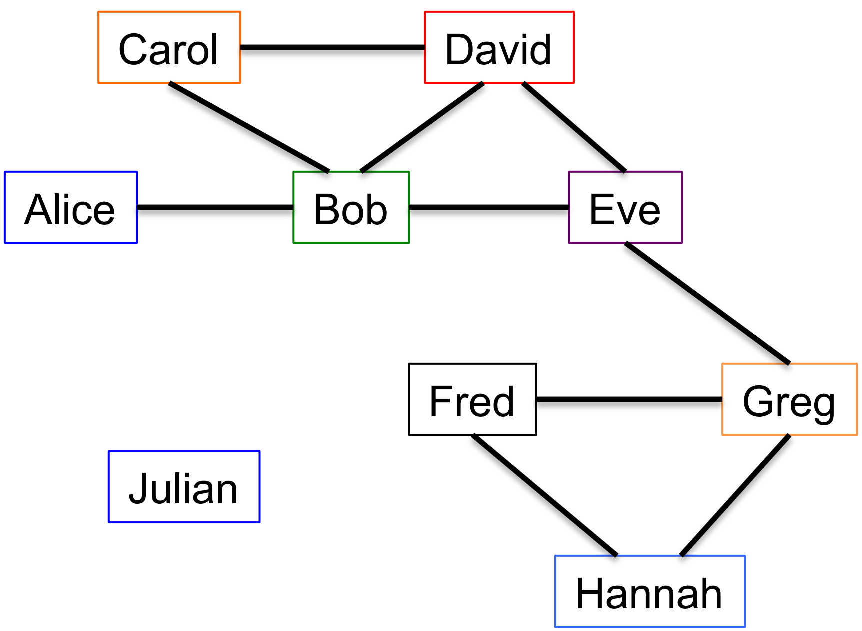
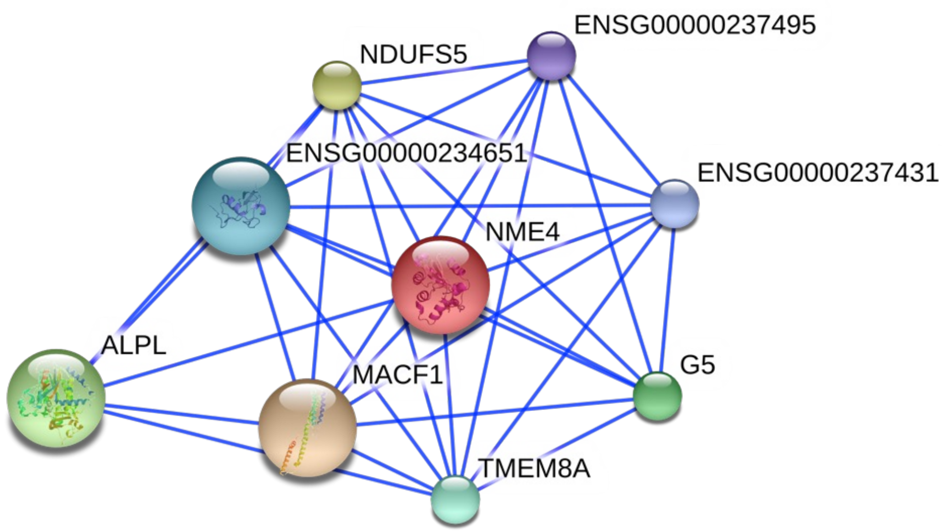
GRAPHS

What is a graph?



- **Vertices** model objects
- **Edges** model relationships between objects





https://commons.wikimedia.org/wiki/File:Protein_Interaction_Network_for_TMEM8A.png

Graph Representations

- Graph has n vertices and m edges
- Vertices labeled from 0 to n−1

	0	1	2	3	4
0	0	1	0	0	0
1	1	0	0	1	1
2	0	0	0	1	0
3	0	1	1	0	0
4	0	1	0	0	0

Adjacency matrix
("1" if edge exists,
"0" otherwise)

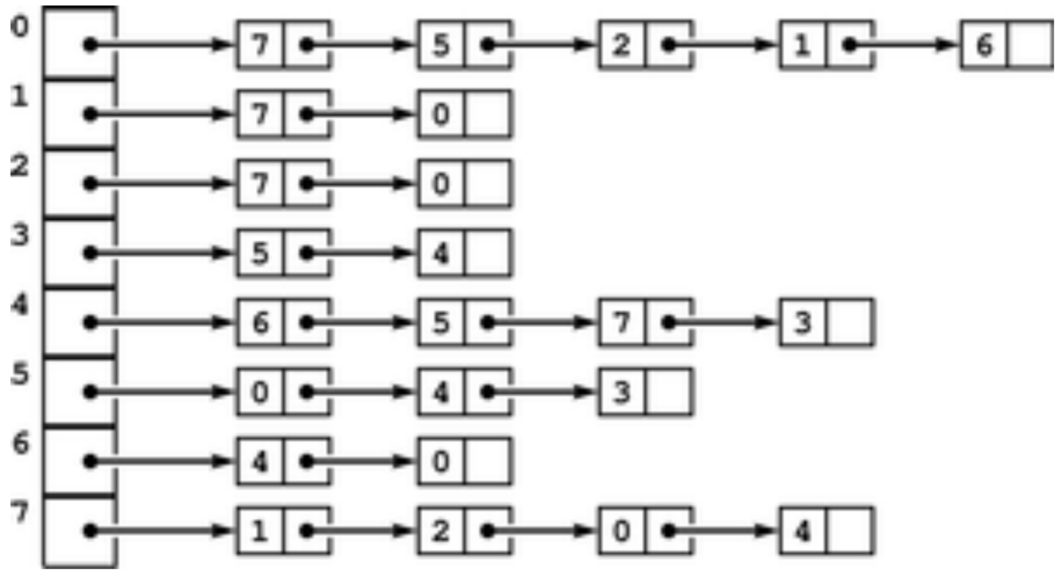
(0,1)
(1,0)
(1,3)
(1,4)
(2,3)
(3,1)
(3,2)
(4,1)

Edge list

- $O(n^2)$ space for adjacency matrix
- $O(m)$ space for edge list

Graph Representations

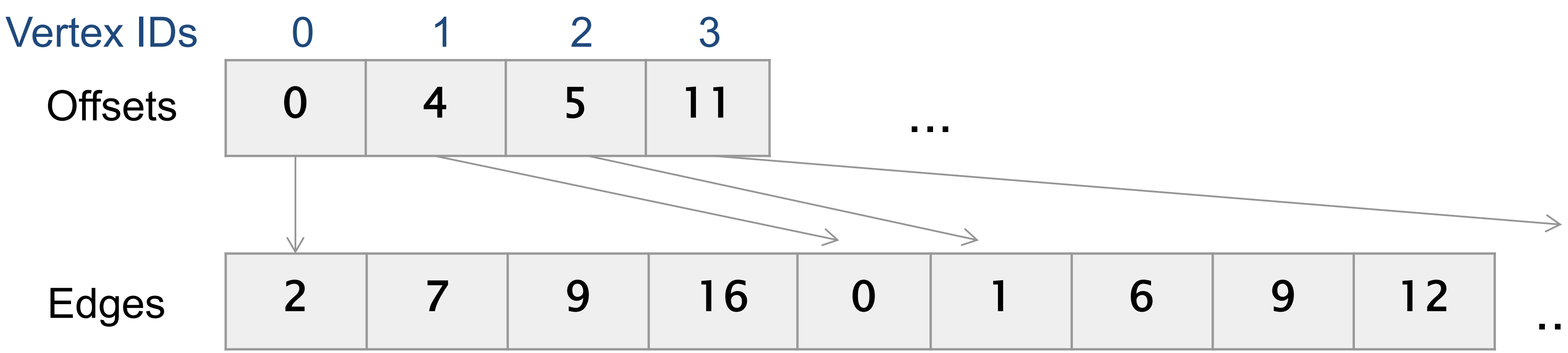
- Adjacency list
  - Array of pointers (one per vertex)
  - Each vertex has an unordered list of its edges



- Space requirement is O(n+m)
- Can substitute linked lists with arrays for better cache performance
  - Tradeoff: more expensive to update graph

Graph Representations

- Compressed sparse row (CSR)
  - Two arrays: Offsets and Edges
  - Offsets[i] stores the offset of where vertex i's edges start in Edges



- How do we know the degree of a vertex?
- Space usage is O(n+m)
- Can also store weights on the edges with an additional array or interleaved with Edges

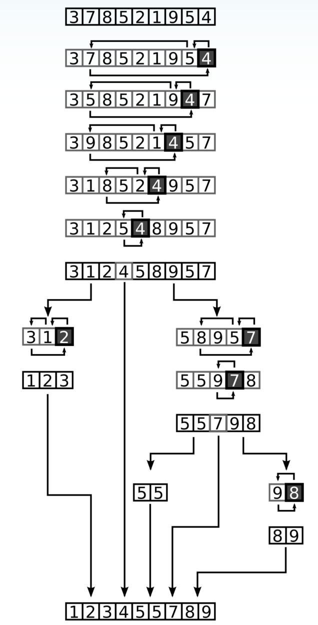
Tradeoffs in Graph Representations

- What is the cost of different operations?

	Adjacency matrix	Edge list	Adjacency list (linked list)	Compressed sparse row
Storage cost / scanning whole graph	$O(n^2)$	O(m)	O(m+n)	O(m+n)
Add edge	O(1)	O(1)	O(1)	O(m+n)
Delete edge from vertex v	O(1)	O(m)	O(deg(v))	O(m+n)
Finding all neighbors of a vertex v	O(n)	O(m)	O(deg(v))	O(deg(v))
Finding if w is a neighbor of v	O(1)	O(m)	O(deg(v))	O(deg(v))

- There are variants/combinations of these representations

BREADTH-FIRST SEARCH



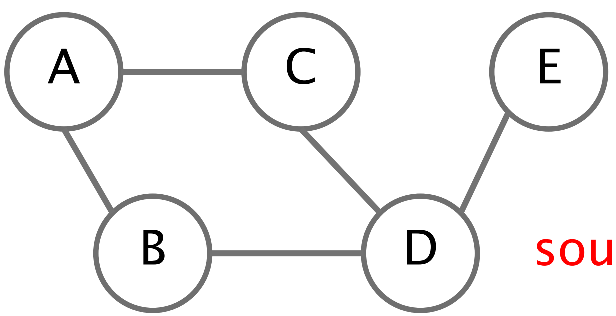
Breadth-First Search (BFS)

- Given a source vertex s, visit the vertices in order of distance from s
- Possible outputs:
  - Vertices in the order they were visited
    - D, B, C, E, A
  - The distance from each vertex to s

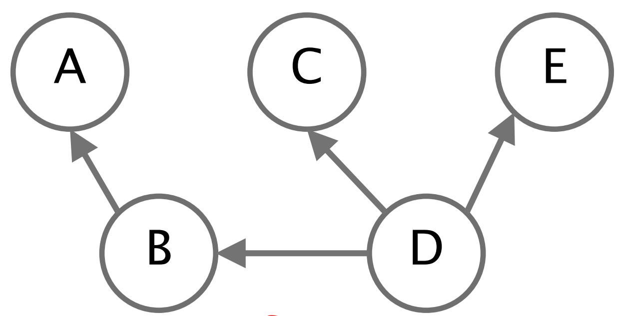
A	B	C	D	E
2	1	1	0	1

  - A BFS tree, where each vertex has a parent to a neighbor in the previous level

Applications
Betweenness centrality
Eccentricity estimation
Maximum flow
Web crawlers
Network broadcasting
Cycle detection
…



source = D



BFS tree

Sequential BFS Algorithm

```
procedure BFS(G, root) is
    let Q be a queue
    label root as explored
    Q.enqueue(root)
    while Q is not empty do
        v := Q.dequeue()


        for all edges from v to w in G.adjacentEdges(v) do
            if w is not labeled as explored then
                label w as explored
                Q.enqueue(w)
```

Source: https://en.wikipedia.org/wiki/Breadth-first_search

- What is the running time of BFS?
  - Each node is enqueued and dequeued once: O(n)
  - Each edge is visited once in each direction: O(m)
- Total: O(n+m)

Sequential BFS Algorithm

- Assume graph is given in compressed sparse row format
  - Two arrays: Offsets and Edges
  - n vertices and m edges (assume Offsets[n] = m)

```
int* parent =
 (int*) malloc(sizeof(int)*n);
int* queue =
 (int*) malloc(sizeof(int)*n);

for(int i=0; i<n; i++) {
   parent[i] = -1;
}

queue[0] = source;
parent[source] = source;

int q_front = 0, q_back = 1;
```

```
//while queue not empty
while(q_front != q_back) {
   int current = queue[q_front++]; //dequeue
   int degree =
        Offsets[current+1]-Offsets[current];
   for(int i=0;i<degree; i++) {
        int ngh = Edges[Offsets[current]+i];
        //check if neighbor has been visited
        if(parent[ngh] == -1) {
            parent[ngh] = current;
            //enqueue neighbor
            queue[q_back++] = ngh;
        }
   }
}
```

Total of m random accesses

- What is the most expensive part of the code?
  - Random accesses cost more than sequential accesses

Analyzing the program

```
int* parent =
 (int*) malloc(sizeof(int)*n);
int* queue =
 (int*) malloc(sizeof(int)*n);

for(int i=0; i<n; i++) {
   parent[i] = -1;
}

queue[0] = source;
parent[source] = source;

int q_front = 0; q_back = 1;
```

```
//while queue not empty
while(q_front != q_back) {
    int current = queue[q_front++]; //dequeue
    int degree =
          Offsets[current+1]-Offsets[current];
    for(int i=0;i<degree; i++) {
          int ngh = Edges[Offsets[current]+i];
          //check if neighbor has been visited
          if(parent[ngh] == -1) {
               parent[ngh] = current;
               //enqueue neighbor
               queue[q_back++] = ngh;
          }
    }
}
```

Check bitvector first before accessing parent array

n cache misses instead of m

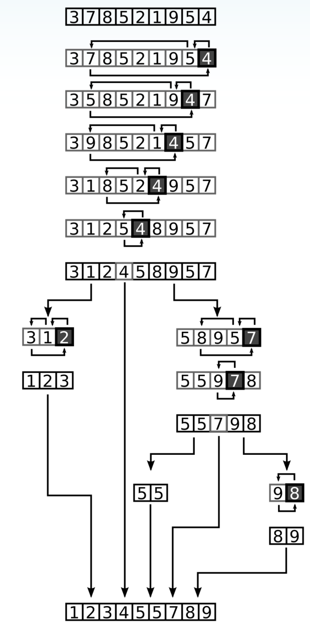
- What if we can fit a bitvector of size n in cache?
  - Might reduce the number of cache misses
  - More computation to do bit manipulation

BFS with bitvector

```
int* parent =
  (int*) malloc(sizeof(int)*n);
int* queue =
  (int*) malloc(sizeof(int)*n);
int nv = 1+n/32;
int* visited =
  (int*) malloc(sizeof(int)*nv);

for(int i=0; i<n; i++) {
   parent[i] = -1;
}

for(int i=0; i<nv; i++) {
   visited[i] = 0;
}

queue[0] = source;
parent[source] = source;
visited[source/32]
   = (1 << (source % 32));

int q_front = 0; q_back = 1;
```

```
//while queue not empty
while(q_front != q_back) {
    int current = queue[q_front++]; //dequeue
    int degree =
         Offsets[current+1]-Offsets[current];
    for(int i=0;i<degree; i++) {
        int ngh = Edges[Offsets[current]+i];
        //check if neighbor has been visited
        if(!((1 << ngh%32) & visited[ngh/32])){
           visited[ngh/32] |= (1 << (ngh%32));
           parent[ngh] = current;
           //enqueue neighbor
           queue[q_back++] = ngh;
        }
    }
}
```

- Bitvector version is faster for large enough values of m

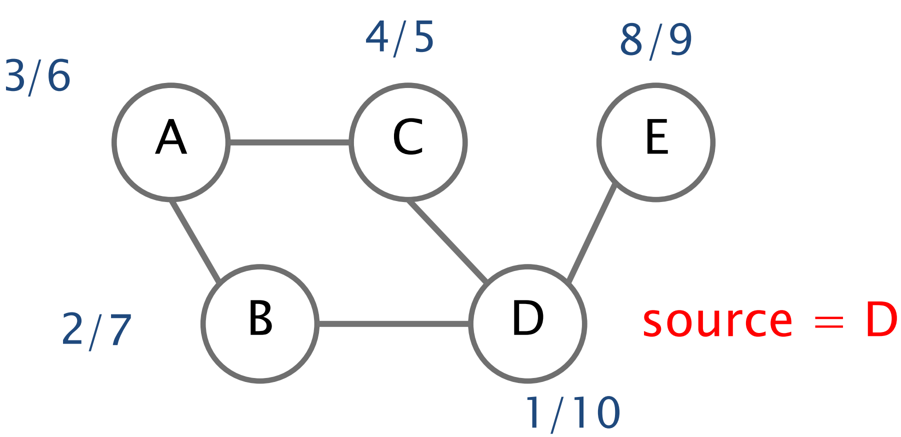


DEPTH-FIRST SEARCH

Depth-First Search (DFS)

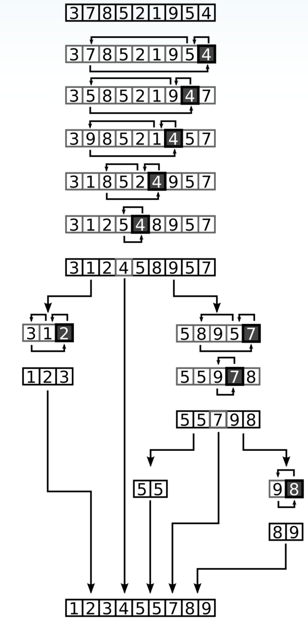
- Explores edges out of the most recently discovered vertex
- Possible outputs:
  - Depth-first forest
  - Vertices in the order they were first visited (preordering)
  - Vertices in the order they were last visited (postordering)
  - Reverse postordering

Applications
Topological sort
Solving mazes
Biconnected components
Strongly connected components
Cycle detection
...



Preorder: D, B, A, C, E
Postorder: C, A, B, E, D
Reverse postorder: D, E, B, A, C

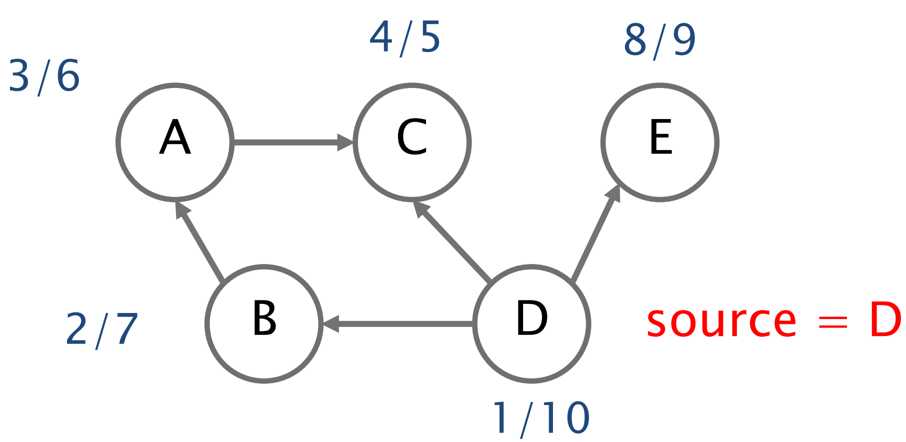
DFS requires O(n+m) work on n vertices and m edges



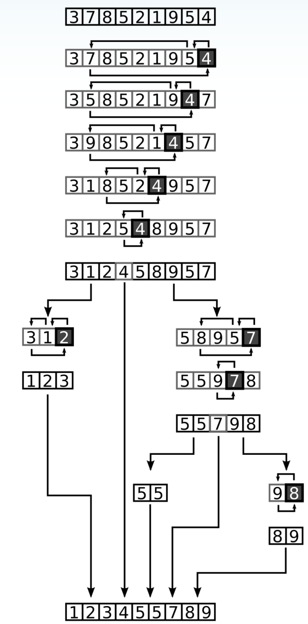
TOPOLOGICAL SORT

Topological Sort

- Given a directed acyclic graph, output the vertices in an order such that all predecessors of a vertex appear before it
  - Application: scheduling tasks with dependencies (e.g., parallel computing, Makefile)
- Solution: output vertices in reverse postorder in DFS



Reverse postorder: D, E, B, A, C



SHORTEST PATHS

Single-Source Shortest Paths

- Given a weighted graph and a source vertex, output the distance from the source vertex to every vertex

- Non-negative weights
  - Dijkstra's algorithm
  - O(m + n log n) work using Fibonacci heap

- General weights
  - Bellman-Ford algorithm
  - O(mn) work

Dijkstra's Algorithm

```
function Dijkstra(Graph, source):
    dist[source] ← 0                                         // Initialization

    create vertex set Q

```

- O((m+n)log n) work using normal heap
- O(m + n log n) work using Fibonacci heap
  - Extract-min takes O(log n) work but decreasing priority only takes O(1) work (amortized)

Bellman-Ford Algorithm

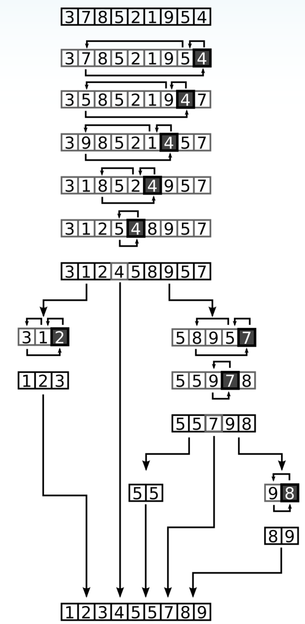
```
Bellman-Ford(G, source):
    ShortestPaths = {∞, ∞, …, ∞}    //size n; stores shortest path distances
    ShortestPaths[source] = 0
    for i=1 to n:
        for each vertex v in G:
            for each w in neighbors(v):
                if(ShortestPaths[v] + weight(v,w) < ShortestPaths[w]):
                    ShortestPaths[w] = ShortestPaths[v] + weight(v,w)
        if no shortest paths changed:
            return ShortestPaths
    report "negative cycle"
```

- At most O(n) rounds, each doing O(n+m) work
- Total work = O(mn)

More Graph Algorithms

- We will study algorithms for particular problems
  - Parallelism, cache-efficiency, dynamic updates

Breadth-first search	Betweenness centrality
PageRank	Spanning forest
Low-diameter decomposition	Maximal independent set
Connected components	Graph clustering
Graph neural networks	Subgraph matching



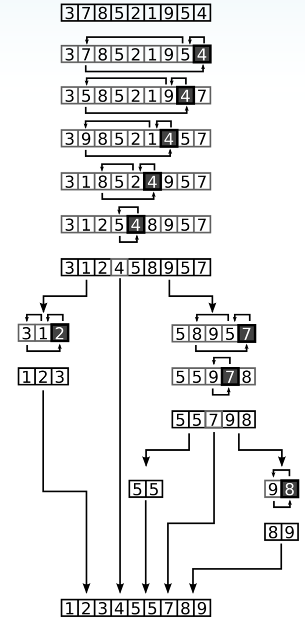
GRAPH PROCESSING FRAMEWORKS

Graph Processing Frameworks

- Provides high-level primitives for graph algorithms
- Reduce programming effort of writing efficient parallel graph programs

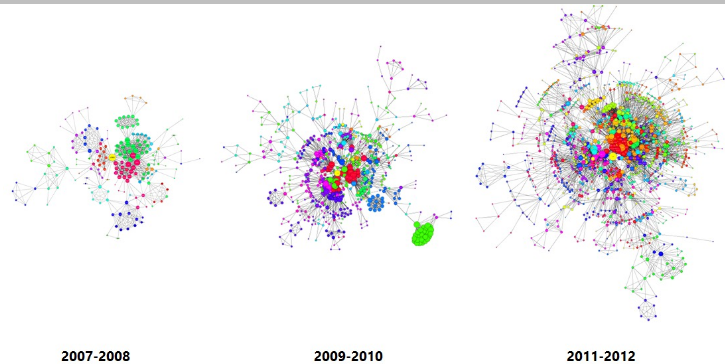
Graph processing frameworks/libraries

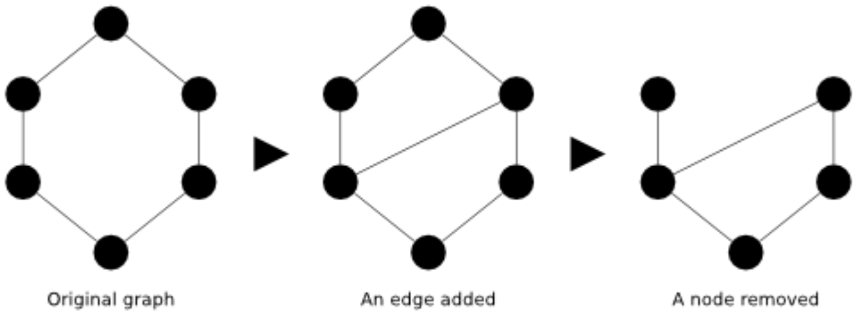
Pregel, Giraph, GPS, GraphLab, PowerGraph, PRISM, Pegasus, Knowledge Discovery Toolbox, CombBLAS, GraphChi, GraphX, Galois, X-Stream, Gunrock, GraphMat, Ringo, TurboGraph, TurboGraph++, FlashGraph, Grace, PathGraph, Polymer, GPSA, GoFFish, Blogel, LightGraph, MapGraph, PowerLyra, PowerSwitch, Imitator, XDGP, Signal/Collect, PrefEdge, EmptyHeaded, Gemini, Wukong, Parallel BGL, KLA, Grappa, Chronos, Green-Marl, GraphHP, P++, LLAMA, Venus, Cyclops, Medusa, NScale, Neo4J, Trinity, GBase, HyperGraphDB, Horton, GSPARQL, Titan, ZipG, Cagra, Milk, Ligra, Ligra+, Julienne, GraphPad, Mosaic, BigSparse, Graphene, Mizan, Green-Marl, PGX, PGX.D, Wukong+S, Stinger, cuStinger, Distinger, Hornet, GraphIn, Tornado, Bagel, KickStarter, Naiad, Kineograph, GraphMap, Presto, Cube, Giraph++, Photon, TuX2, GRAPE, GraM, Congra, MTGL, GridGraph, NXgraph, Chaos, Mmap, Clip, Floe, GraphGrind, DualSim, ScaleMine, Arabesque, GraMi, SAHAD, Facebook TAO, Weaver, G-SQL, G-SPARQL, gStore, Horton+, S2RDF, Quegel, EAGRE, Shape, RDF-3X, CuSha, Garaph, Totem, GTS, Frog, GBTL-CUDA, Graphulo, Zorro, Coral, GraphTau, Wonderland, GraphP, GraphIt, GraPu, GraphJet, ImmortalGraph, LA3, CellIQ, AsyncStripe, Cgraph, GraphD, GraphH, ASAP, RStream, and many others…



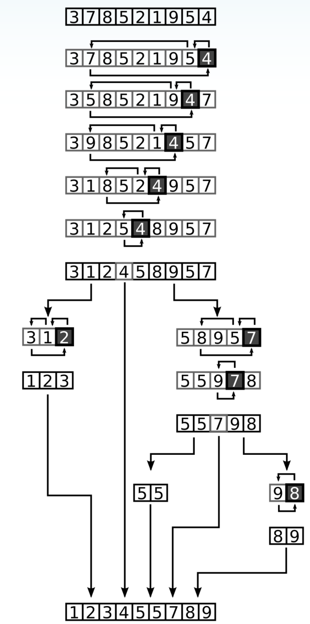
Dynamic Graphs

Dynamic Graphs



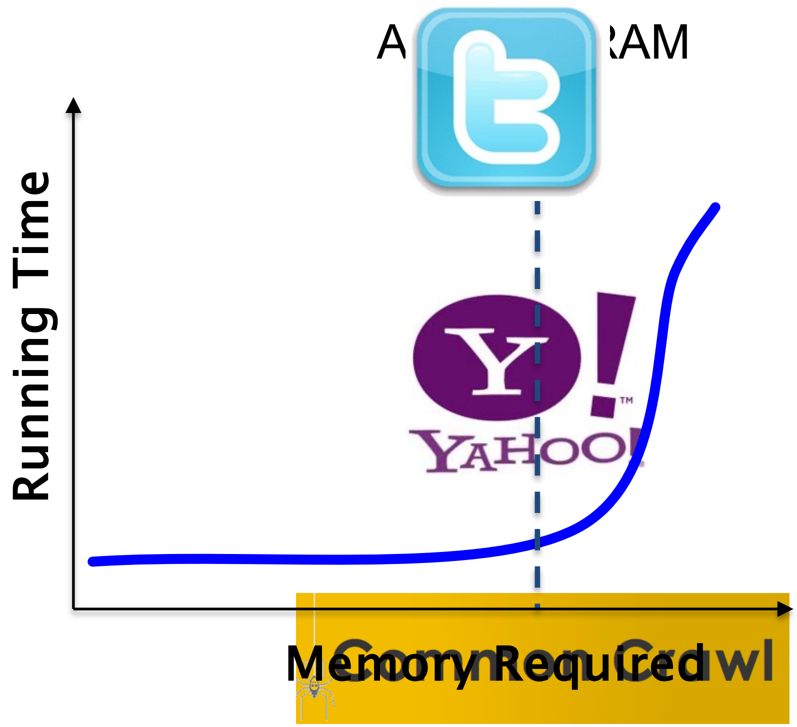


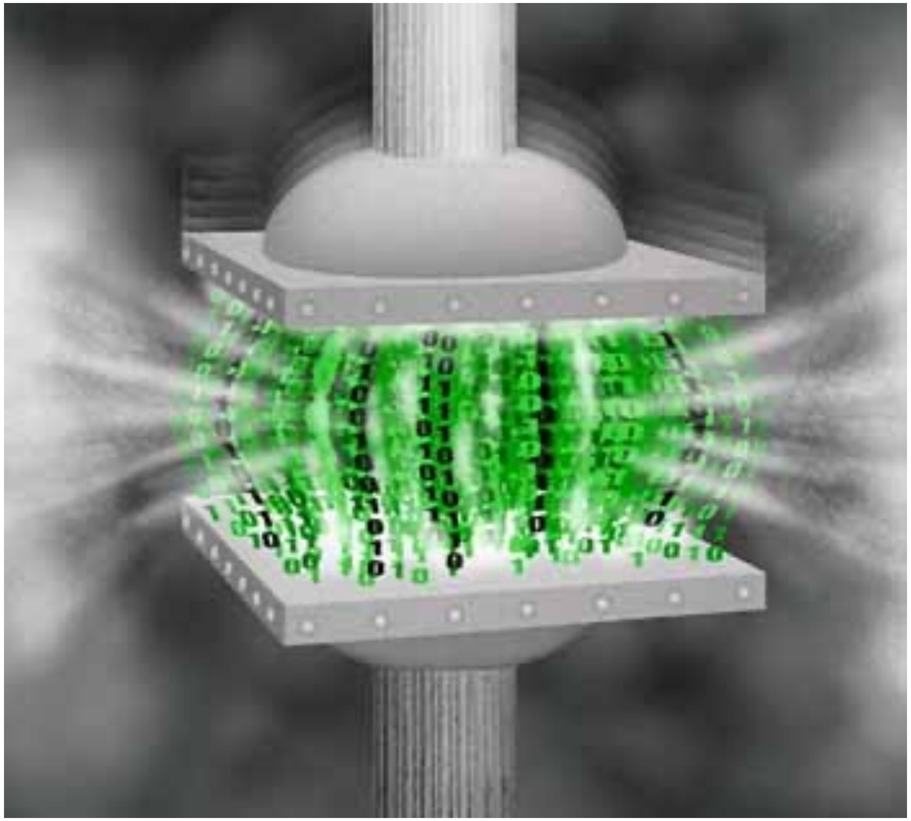
- Many graphs are changing over time
  - Adding/deleting connections on social networks
  - Traffic conditions changing
  - Communication networks (email, IMs)
  - World Wide Web
  - Content sharing (Youtube, Flickr, Pinterest)
- Need graph data structures that allow for efficient updates (in parallel)
- Need (parallel) algorithms that respond to changes without re-computing from scratch



Compression

Large Graphs

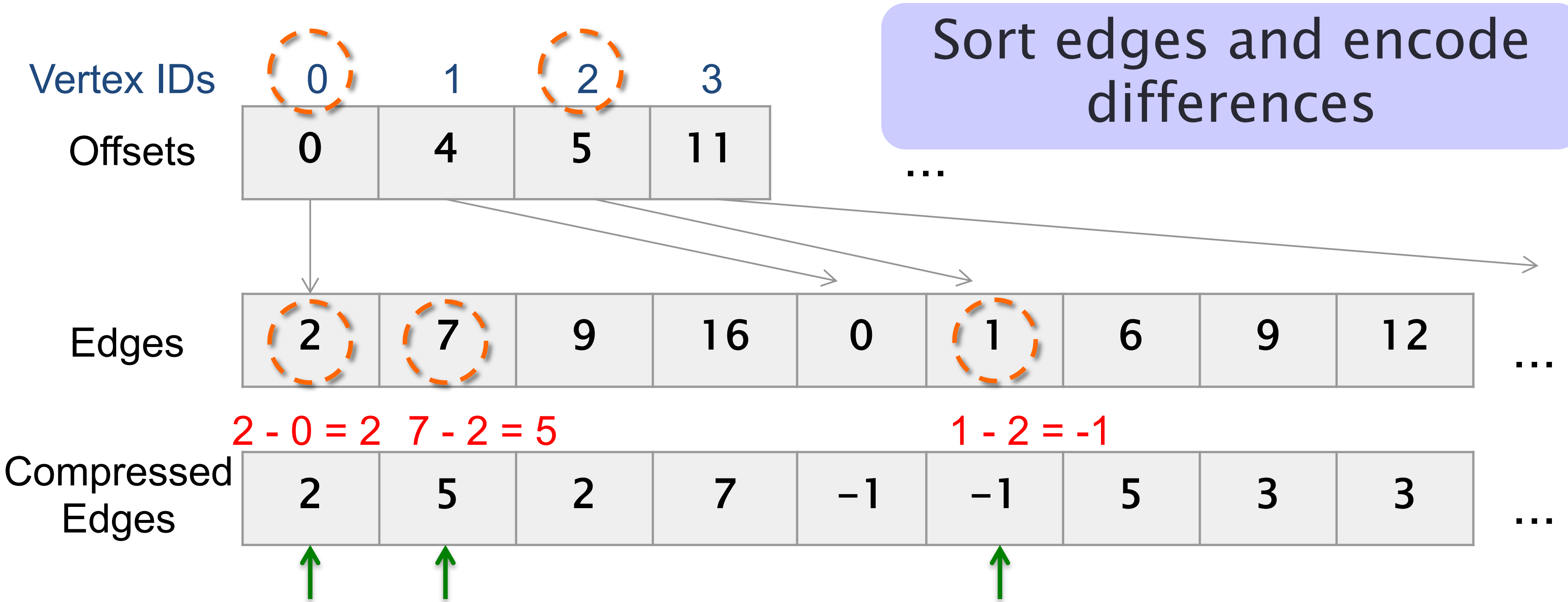




- What if you cannot fit a graph on your machine?
- Cost of machines increases with memory size

Graph Compression

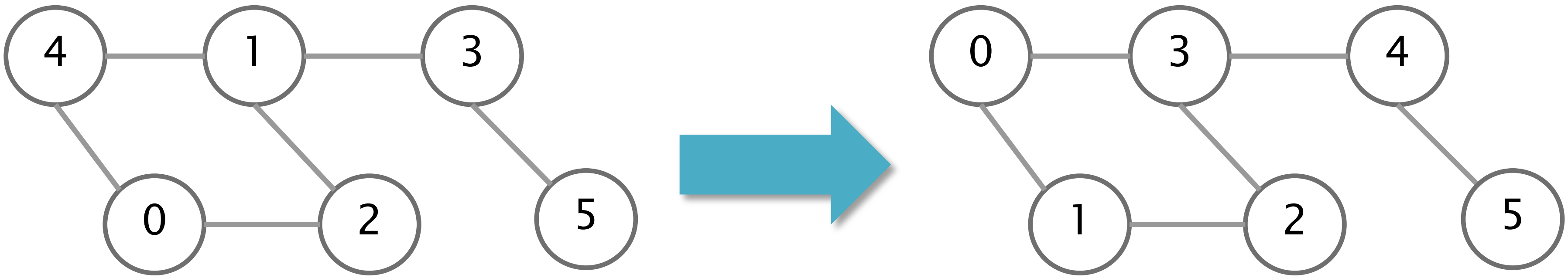
Graph Compression on CSR



- For each vertex v:
  - First edge: difference is Edges[Offsets[v]]−v
  - i’th edge (i>1): difference is Edges[Offsets[v]+i]−Edges[Offsets[v]+i−1]
- Want to use fewer than 32 or 64 bits per value
- Compression can improve running time

Graph Reordering

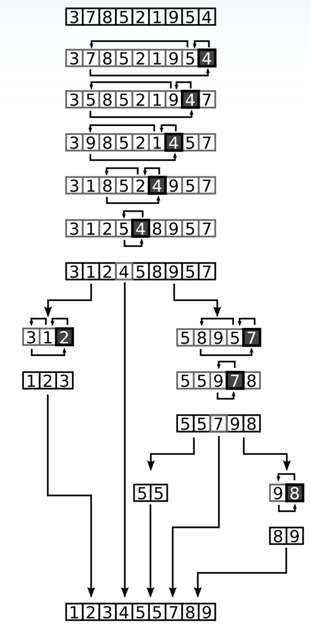
- Reassign IDs to vertices to improve locality
  - Goal: Make vertex IDs close to their neighbors' IDs and neighbors' IDs close to each other



Sum of differences = 23

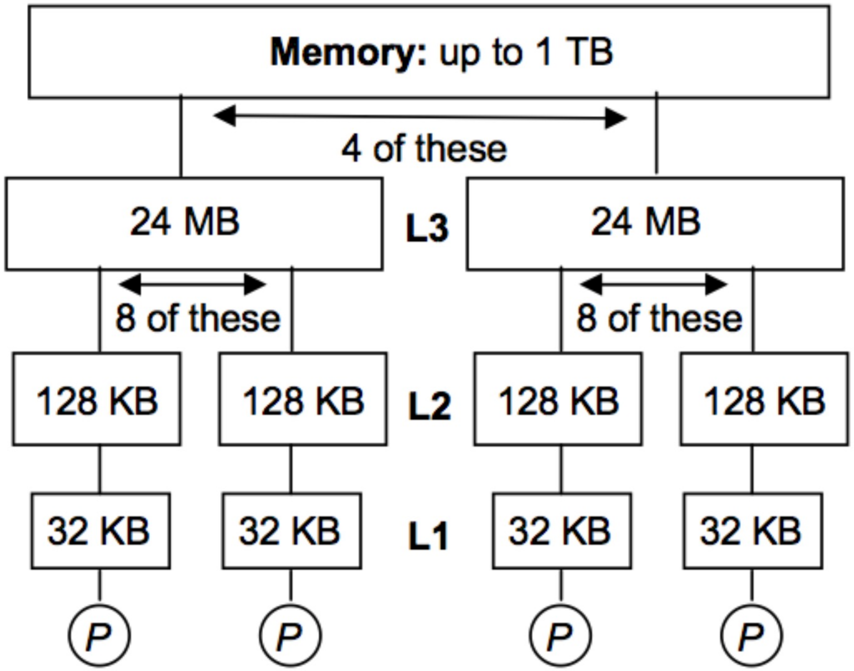
Sum of differences = 20

- Can improve compression rate due to smaller "differences"
- Can improve performance due to higher cache hit rate
- Various methods: BFS, DFS, METIS, degree, etc.



CACHE-EFFICIENCY AND I/O-EFFICIENCY

Cache Hierarchies



Design cache-efficient and cache-oblivious algorithms to improve locality

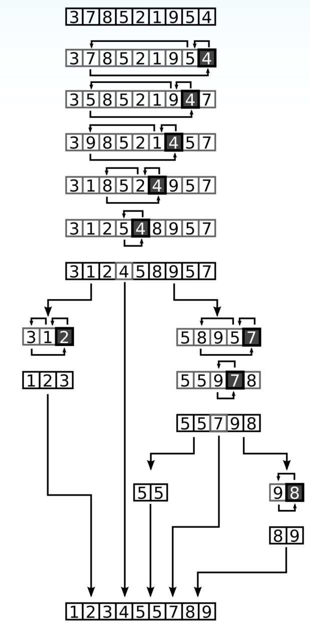
Memory level	Approx latency
L1 Cache	1–2ns
L2 Cache	3–5ns
L3 cache	12–40ns
DRAM	60–100ns

I/O Efficiency

- Need to read input from disk at least once
- May need to read many more times if input doesn't fit in memory

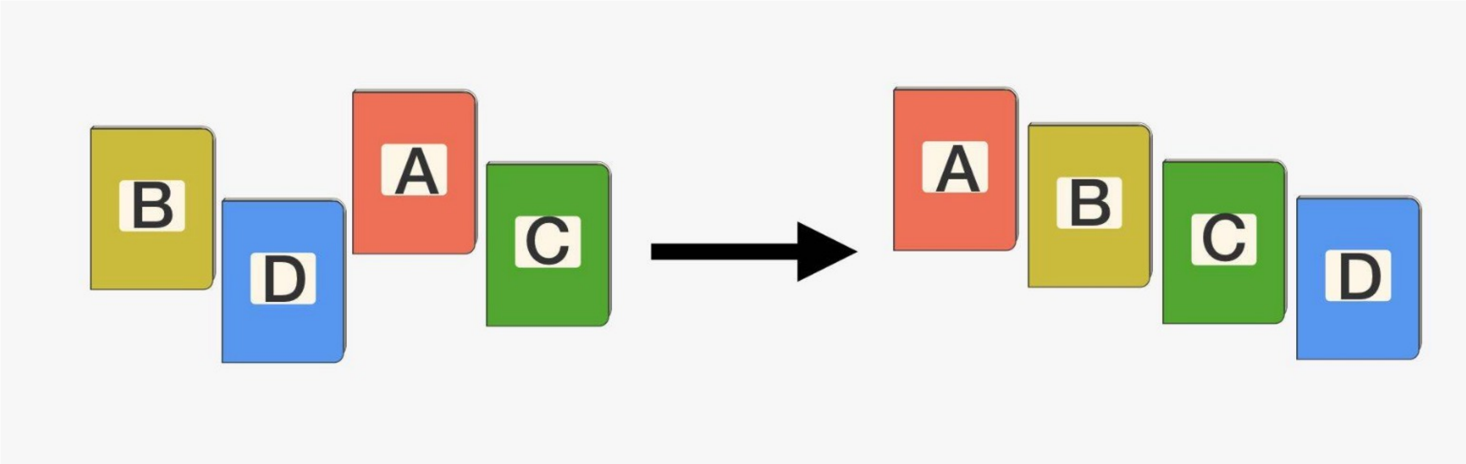
Memory	Latency	Throughput
DRAM	60-100 ns	Tens of GB/s
SSD	Tens of μs	500 MB-2 GB/s (seq), 50-200 MB/s (rand)
HDD	Tens of ms	200 MB/s (seq), 1 MB/s (rand)

Source: https://www.pcgamer.com/hard-drive-vs-ssd-performance/2/



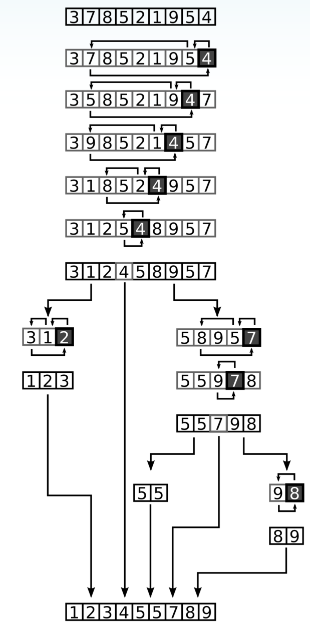
SORTING ALGORITHMS

Sorting

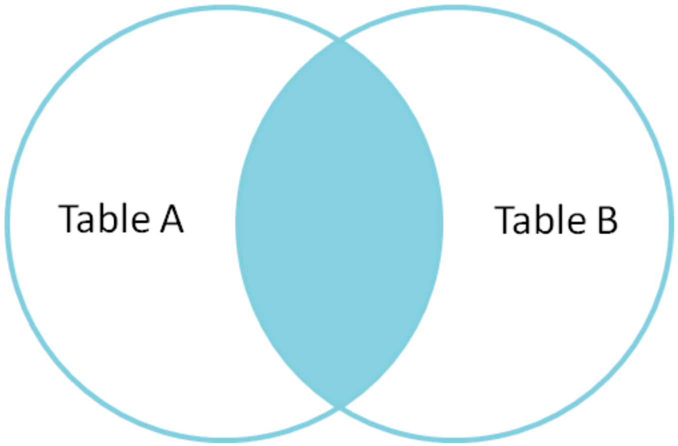


- Lots of research on engineering sorting algorithms
- Will study parallel comparison sorting and integer sorting algorithms
- http://sortbenchmark.org/

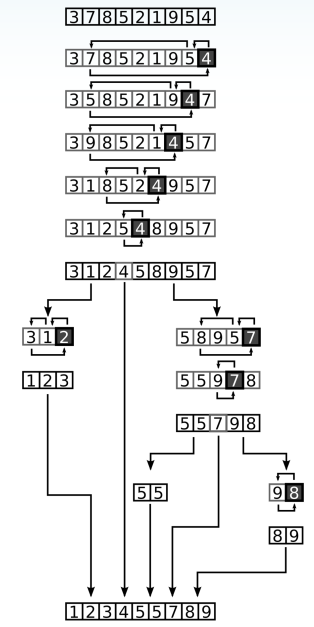
JOINS AND AGGREGATION



Joins and Aggregation



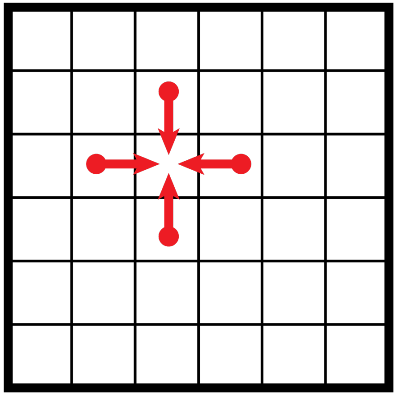
- JOIN and GROUPBY are two of the most expensive operations in database systems
- We will study algorithms and optimizations for these operations (in main-memory)

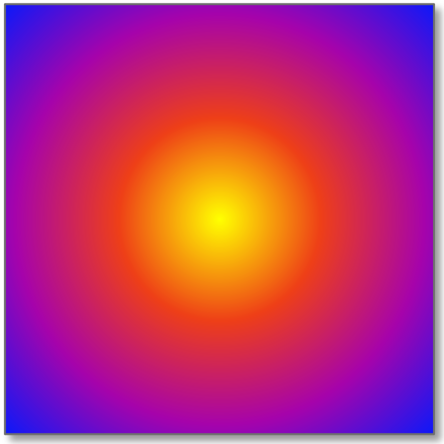


STENCIL COMPUTATIONS

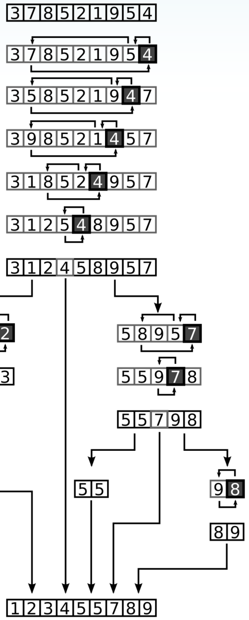
Stencil Computations

- Computations that iteratively update data based on a fixed pattern (stencil)
  - For example, can be used to approximately solve heat equation
- We will study algorithms for stencil computations that improve on work, parallelism, and cache-efficiency over standard approaches





Source: https://en.wikipedia.org/wiki/Iterative_Stencil_Loops



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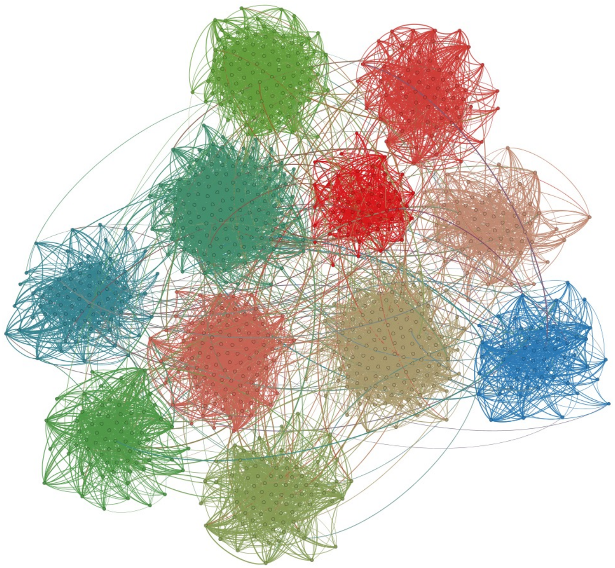
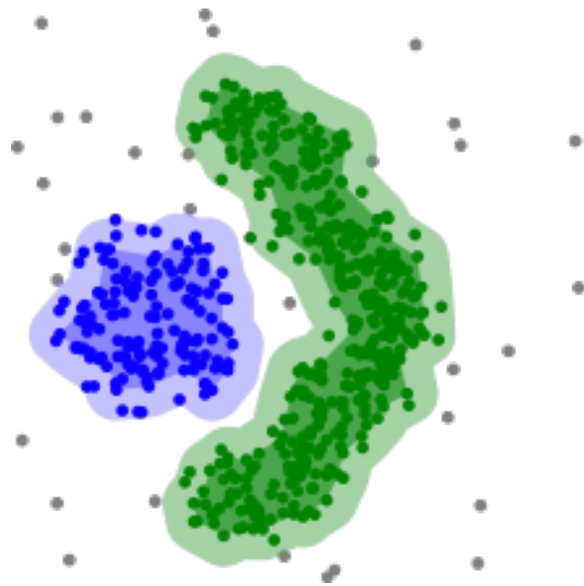
312548957
312458957
312
58957
123
55978
55798
55
98
89
123455789

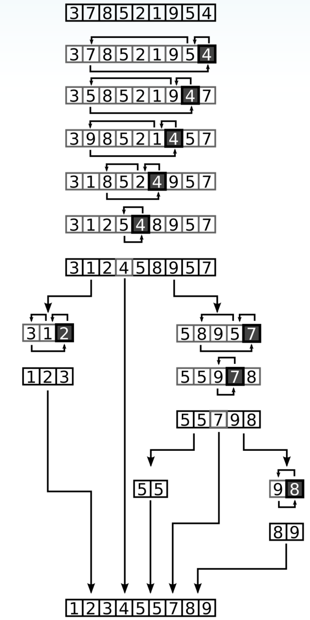
CLUSTERING

Clustering

- Group “similar” objects together, and separate “dissimilar” objects
- Can be applied to graph data and spatial data
- Applications: Community detection, bioinformatics, parallel/distributed processing, visualization, image segmentation, anomaly detection, document analysis, machine learning, etc.



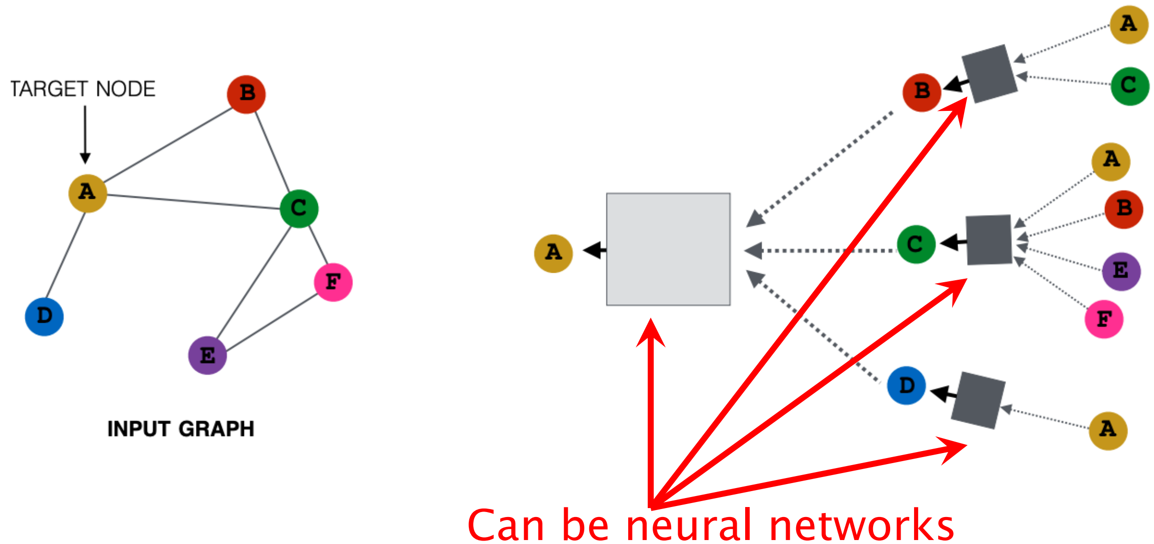




Graph Neural Networks

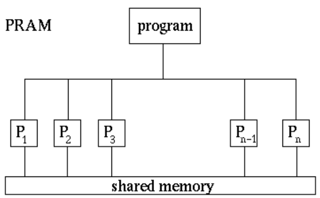
Graph Neural Networks (GNNs)

Source: https://snap-stanford.github.io/cs224w-notes/machine-learning-with-networks/graph-neural-networks

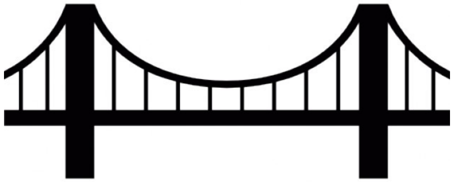


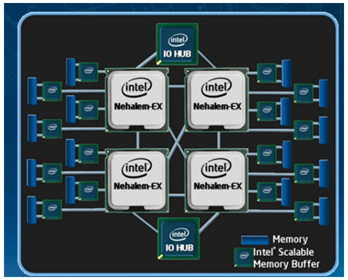
- Traditional neural networks have a fixed topology, but in GNNs the topology is the graph
  - Repeatedly pass messages to neighbors, and aggregate messages received to update node
  - Each node has a different computation graph!
  - Many different graph neural networks, based on how they pass and aggregate messages
  - We'll study some high-performance GNN approaches

Summary



O(n log n)
O(n)
O(log n)





- Lots of exciting research going on in algorithm engineering!
- Take this course to learn about latest results and try out research in the area