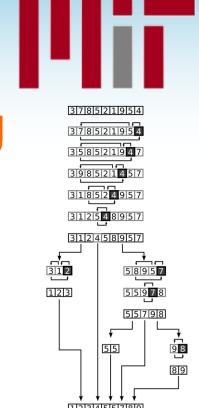
# 6.886: Algorithm Engineering

LECTURE 1
Introduction

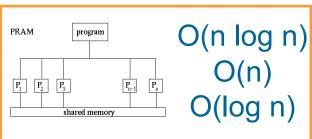
Julian Shun February 5, 2019



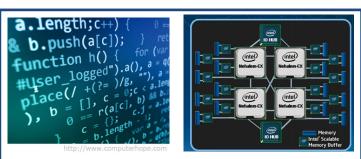


# What is Algorithm Engineering?

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



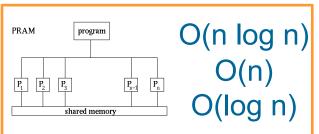




**Theory** 

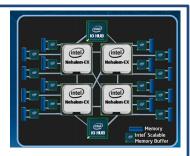
**Practice** 

# **Bridging Theory and Practice**









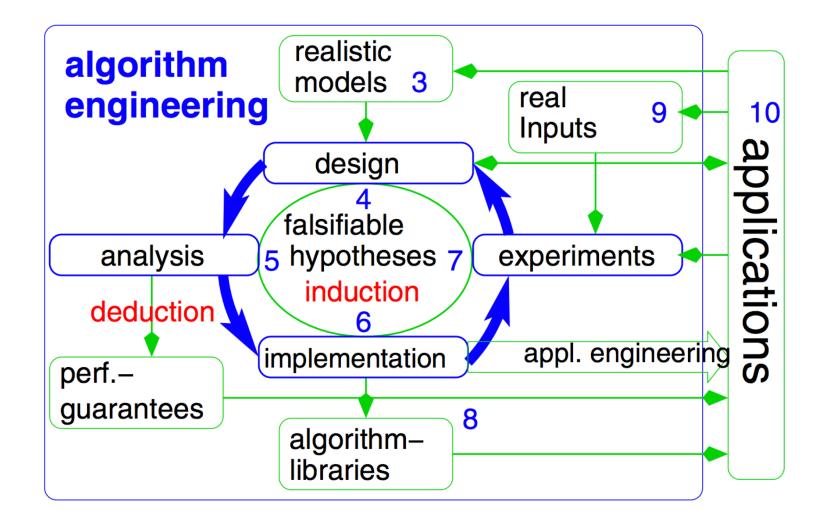
- Good empirical performance
- Confidence that algorithms will perform well in many different settings
- Ability to predict performance (e.g. in real-time applications)
- Important to develop theoretical models to capture properties of technologies

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?



# **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

# Algorithm Design & Analysis

Complexity

Algorithm 1 N log<sub>2</sub> N

Algorithm 2 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 realworld inputs
- Use theory as a guide to find practical algorithms
- Time vs. space 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

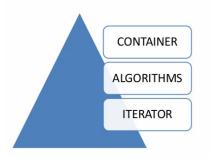
- Instrument code with timers and use performance profilers (e.g., perf, gprof, valgrind)
- Use large variety of inputs (both real-world and synthetic)
  - Use different sizes
  - Use worst-case inputs to identify correctness or performance issues
- Reproducibility
  - Document environmental setup
 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

# **Experimentation II**

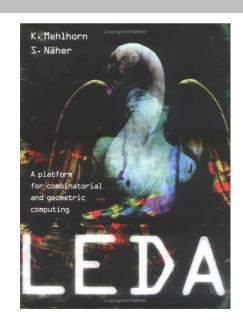
- For parallel code, test on varying number of processors to study scalability
- Compare with best serial code for problem
- For reproducibility, write deterministic code if possible
  - Or make it easy to turn off non-determinism
- Use numactl to control NUMA effects on multi-socket machines
- · Useful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

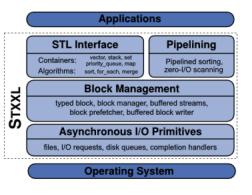
## Libraries and Frameworks

#### Components of STL









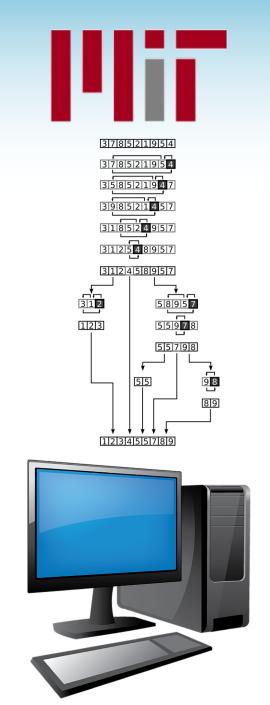


**Problem Based Benchmark Suite** 

Home Benchmarks/Code Inputs License People Publications

- Use efficient building blocks from existing library/frameworks when appropriate
- Develop your own to help others and improve applicability

#### **COURSE INFORMATION**



#### **Course Information**

- Graduate-level class
  - Undergraduates who have taken 6.046 and 6.172 are welcome
- Lectures: Tuesday and Thursday 2:30–4pm
- Instructor: Julian Shun
- Units: 3-0-9
- We will use Piazza for communication

 This course will cover various ideas in algorithm engineering, with an emphasis on parallelism and graph problems

# **Course Website**

#### https://people.csail.mit.edu/jshun/6886-s19/

#### **Schedule (tentative)**

Date	Topic	Speaker	Required Reading	Optional Reading
Tuesday 2/5	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 2/7	Parallel Algorithms	Julian Shun	Parallel Algorithms Thinking in Parallel: Some Basic Data- Parallel Algorithms and Techniques (Chapters 4-8) CLRS Chapter 27	Prefix Sums and Their Applications  Algorithm Design: Parallel and Sequential  Introduction to Parallel Algorithms
				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  Chapter 3.6 of Networks, Crowds, and Markets (describes Betweenness Centrality with an example)
Tuesday 2/12	Parallel Graph Traversal		Direction-Optimizing Breadth-First Search* A Faster Algorithm for Betweenness Centrality The More the Merrier: Efficient Multi- Source Graph Traversal*	Better Approximation of Betweenness Centrality  ABRA: Approximating Betweenness Centrality in Static and Dynamic Graphs with Rademacher Averages  KADABRA is an ADaptive Algorithm for

# Grading

Grading Breakdown	
Paper Reviews	15%
Paper Presentations	20%
Research Project	60%
Class Participation	5%

You must complete all assignments to pass the class.

# **Paper Presentations**

- This is a research-oriented course
- Cover content from 2–3 research papers each lecture
- 25–30 minute student presentation 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 board for theoretical proofs
- Sign up for presentations this week in Google doc
- Would be helpful to sign up even if listening

# **Paper Reviews**

- Submit one paper review each week on a paper that will be covered that 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 Learning Modules by Monday 11:59pm each week (before we cover the papers)
  - Reviews will be made viewable to class (anonymously)
  - Read them before the lecture to help prepare for the discussions

# 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 new algorithm frameworks or libraries
  - Any topic may involve parallelism, cache-efficiency, I/Oefficiency, and memory-efficiency
- Must contain an implementation component
- Can be related to research that you are doing
- On Tuesday 3/5, you can pitch any project ideas you have and find group members

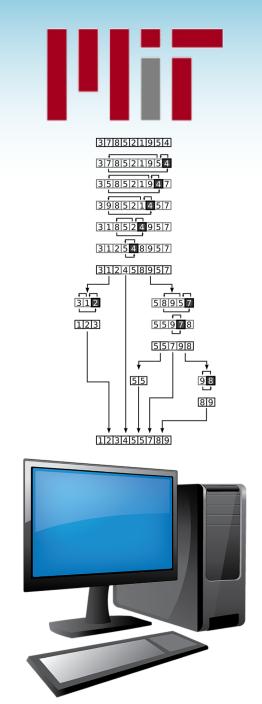
# **Project Timeline**

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

- Pre-proposal meeting
  - 15-minute meeting to run idea by instructor
- Talk to instructors if you need computing resources for the project
  - We may have some AWS credits

\*You can submit it 3 days later if you go to the Comm Lab at least one day before original deadline.

#### **PARALLELISM**



## **Parallelism**

#### Data is becoming very large!



41 million vertices
1.5 billion edges
(6.3 GB)



1.4 billion vertices6.6 billion edges(38 GB)



3.5 billion vertices128 billion edges(540 GB)

#### Parallel machines are everywhere!





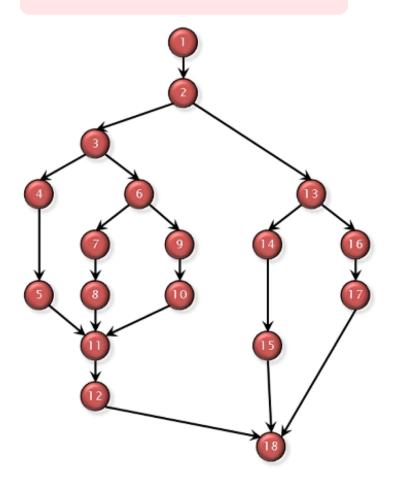




Can rent machines on AWS with 72 cores (144 hyper-threads) and 4TB of RAM

### Parallelism Models

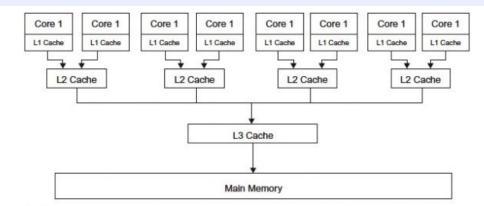
#### Computation graph



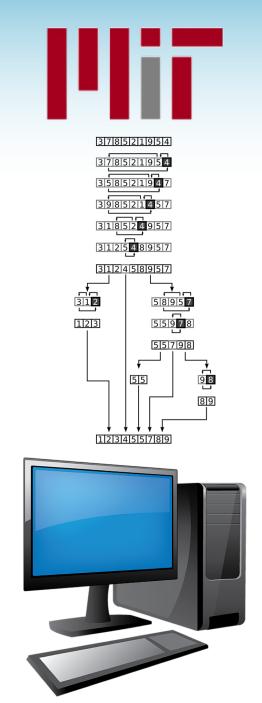
- Work = number of vertices in graph (number of operations)
- Depth (Span) = longest directed path in graph (dependence length)
- Parallelism = Work / Depth

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

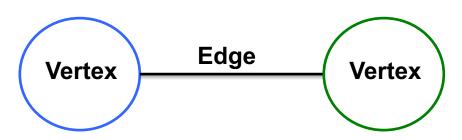
# Goal 2: simple, practical, and cache-friendly



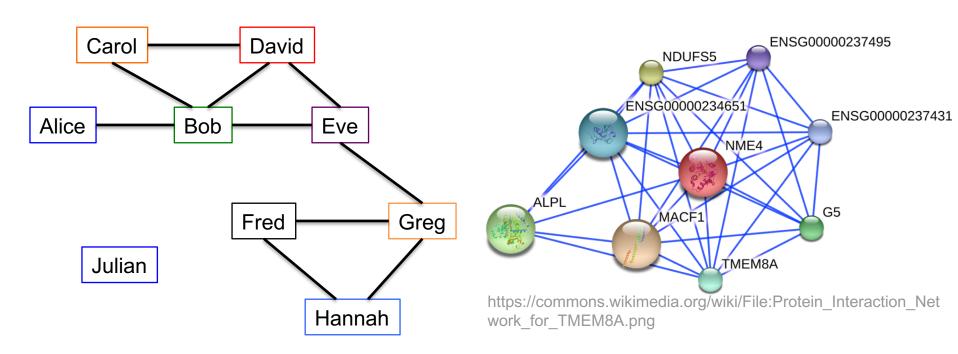
#### **GRAPHS**



# What is a graph?

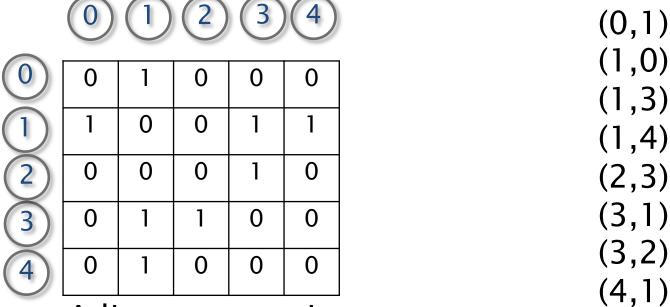


- Vertices model objects
- Edges model relationships between objects



# **Graph Representations**

Vertices labeled from 0 to n-1



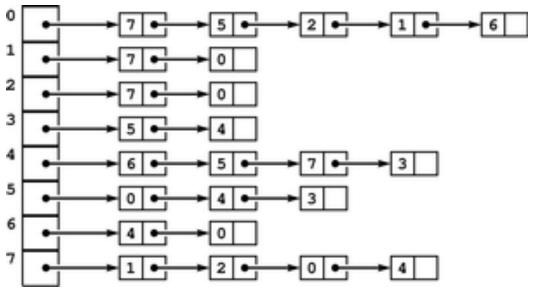
Adjacency matrix ("1" if edge exists, "0" otherwise)

Edge list

- O(n²) 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

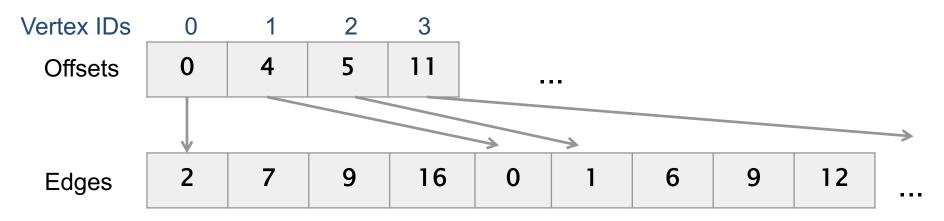


- Space requirement is O(n+m)
- Can substitute linked lists with arrays for better cache performance

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 values on the edges with an additional array or interleaved with Edges

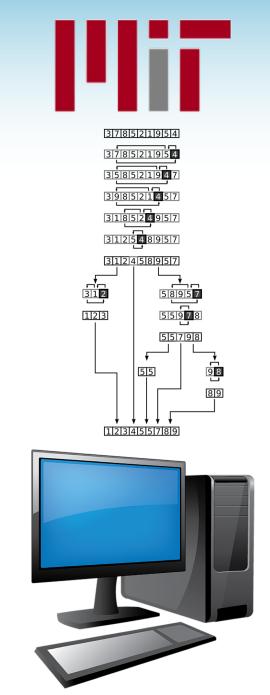
# Tradeoffs in Graph Representations

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 <sup>2</sup> )	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

Α	В	C	D	Ε	
2	1	1	0	1	

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



Betweenness centrality

**Eccentricity** estimation

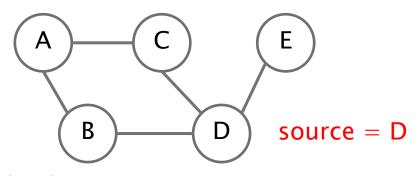
Maximum flow

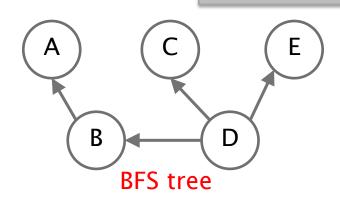
Web crawlers

Network broadcasting

Cycle detection

. . .





# Sequential BFS Algorithm

```
Breadth-First-Search(Graph, root):
     for each node n in Graph:
         n.distance = INFINITY
         n.parent = NIL
Source: https://en.wikipedia.org/wiki/Breadth-first_search
```

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

# 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)

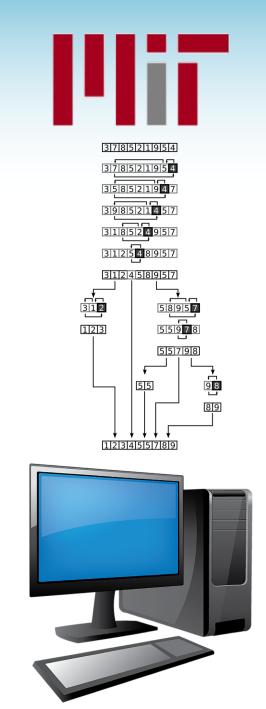
```
int* parent =
  (int*) malloc(sizeof(int)*n);
int* queue =
  (int*) malloc(sizeof(int)*n);

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

queue[0] = source;
parent[source] = source;
int q_front = 0, q_back = 1;</pre>
```

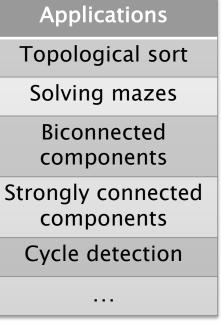
- What is the most expensive part of the code?
  - Random accesses cost more than sequential accesses

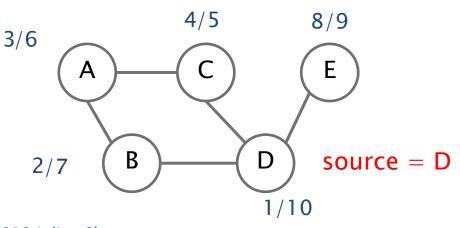
#### **DEPTH-FIRST SEARCH**



# 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

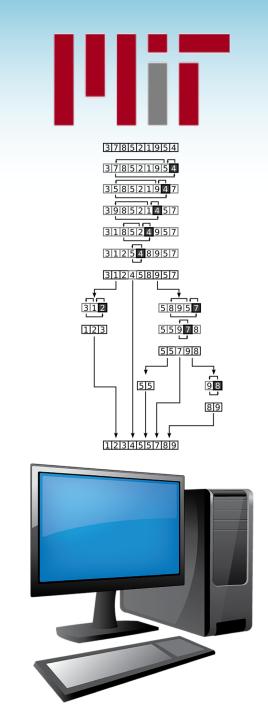




Preorder: D, B, A, C, E Postorder: C, A, B, E, D Reverse postorder: D, E, B, A, C

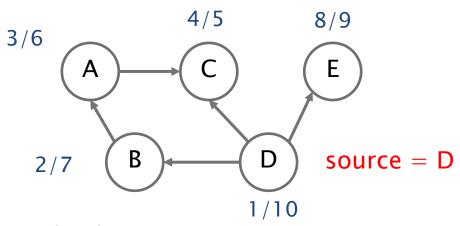
source = D DFS requires O(n+m) work on n vertices and m edges

#### **TOPOLOGICAL SORT**



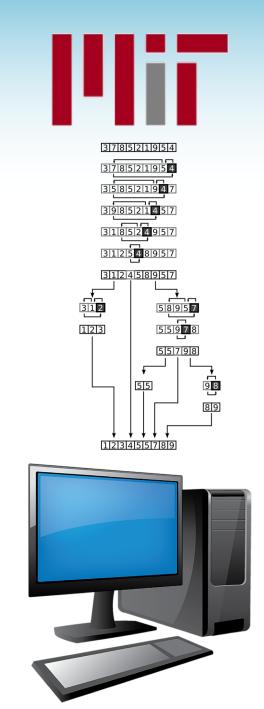
# **Topological Sort**

- 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 Fibonnaci 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 + nlog 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 = \{\infty, \infty, ..., \infty\}
                                    //size n; stores shortest path distances
   ShortestPaths[source] = 0
   for i=1 to n-1:
       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"
```

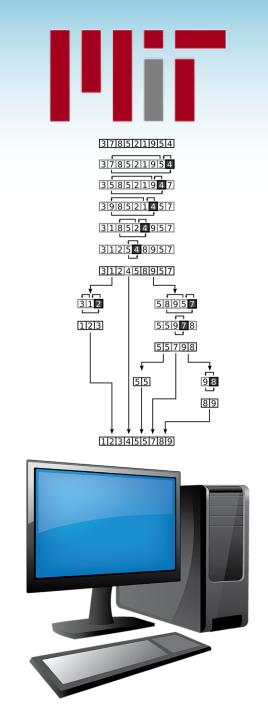
- At most n rounds, each doing O(n+m) work
- Total work = O(mn)

## More Graph Algorithms

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

Breadth-first search	Betweenness centrality	
PageRank	Triangle Computations	
Low-diameter decomposition	SSSP	
Connected components	Maximal independent set	
K-core decomposition	Multi-BFS	
Minimum spanning forest	Spanning forest	
Maximal matching	Set cover	
Eccentricity estimation	Subgraph matching	

## GRAPH PROCESSING FRAMEWORKS



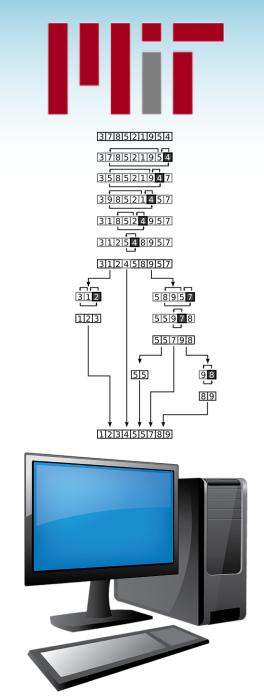
## **Graph Processing Frameworks**

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

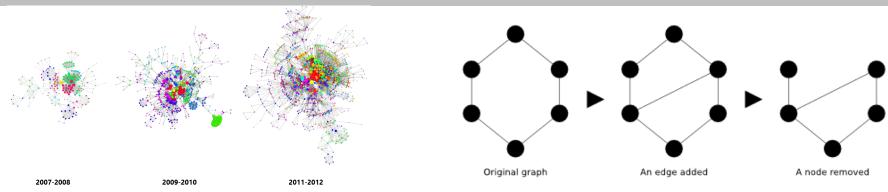
#### **Graph processing frameworks/libraries**

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**

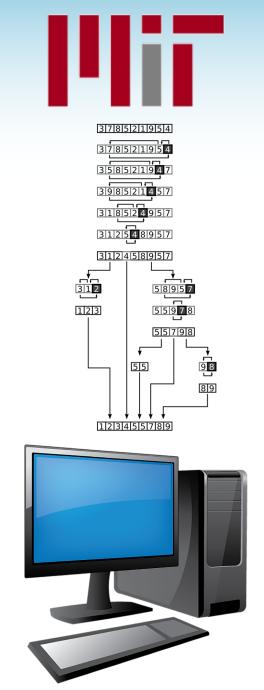


## **Dynamic Graphs**

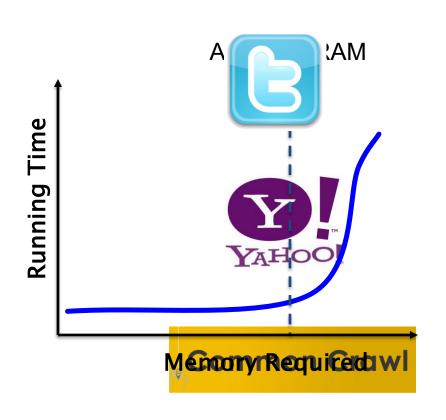


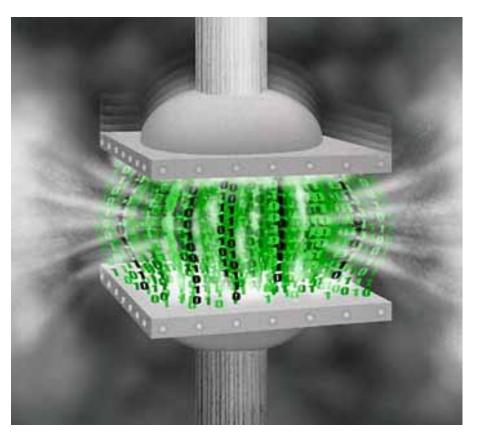
- Many graphs are changing over time
  - Adding/deleting connections on social networks
  - Traffic conditions changing
  - Communication networks (email, IMs)
  - World Wide Web
  - Content sharing (Youtube, Flickr, Pinterest)
- Need graph data structures that allow for efficient updates (in parallel)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

#### **COMPRESSION**



## Large Graphs

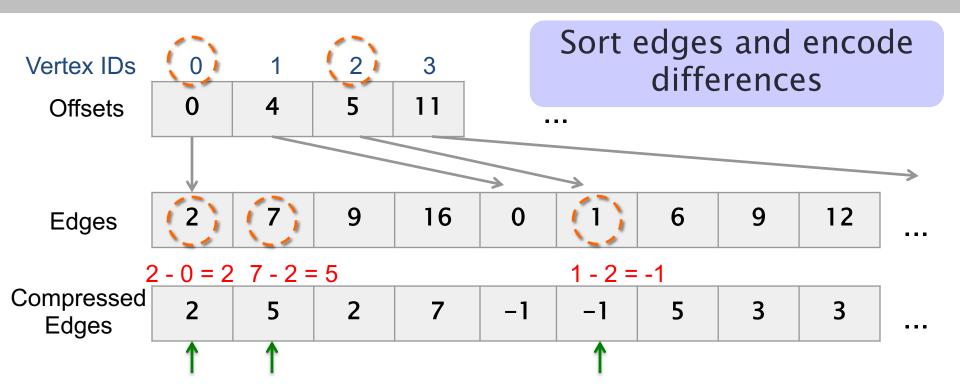




- What if you cannot fit a graph on your machine?
- · Cost of machines increases with memory size

Graph Compression

## **Graph Compression on CSR**



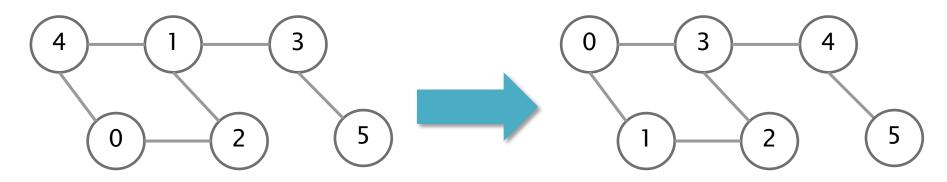
- For each vertex v:
  - First edge: difference is Edges[Offsets[v]]-v
  - i'th edge (i>1): difference is Edges[Offsets[v]+i] Edges[Offsets[v]+i-1]
- Want to use fewer than 32 or 64 bits per value
- Compression can improve running time

#### **Fast Compression Schemes**

- Study speed and space tradeoffs in compression schemes for integer sequences
- Study how compression has been used to speed up sparse matrix-vector multiplication and graph processing
- Also useful in storing inverted lists for information retrieval

## **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

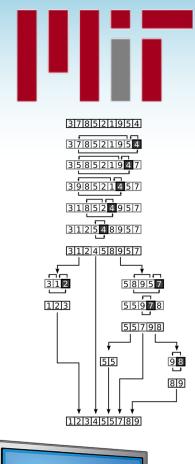


Sum of differences = 21

Sum of differences = 19

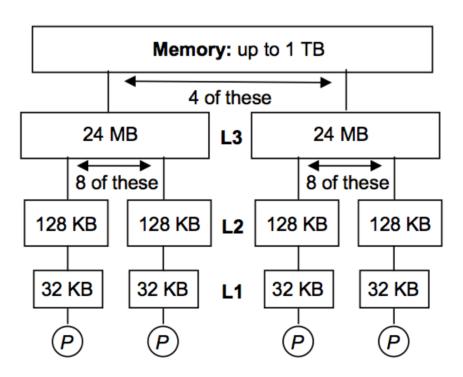
- Can improve compression rate due to smaller "differences"
- Can improve performance due to higher cache hit rate
- Various methods: BFS, DFS, METIS, degree, etc.

#### CACHING AND NON-UNIFORM MEMORY ACCESS





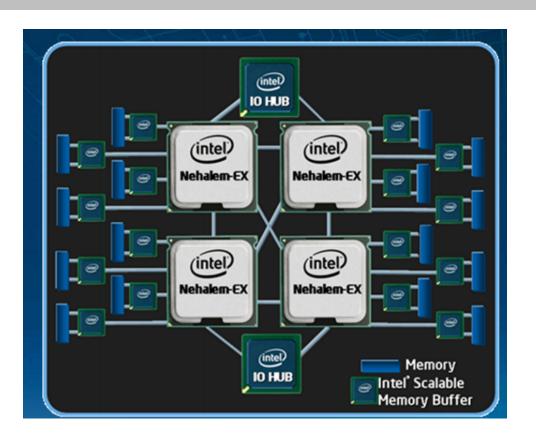
#### **Cache Hierarchies**



Design cacheefficient and cacheoblivious algorithms to improve locality

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

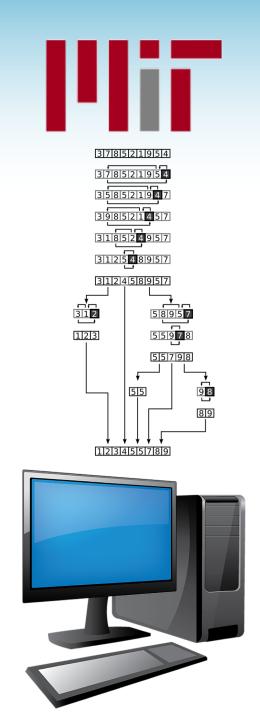
#### Non-uniform Memory Access (NUMA)



Design NUMA-aware algorithms to improve locality

- Accessing remote memory is more expensive than accessing local memory of a socket
  - Latency depends on the number of hops

#### I/O EFFICIENCY



## I/O Efficiency





- Need to read input from disk at least once
- 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)

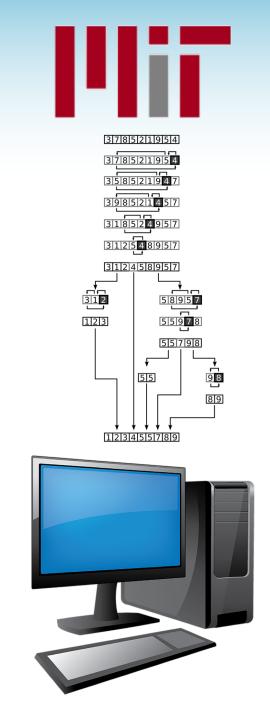
#### I/O Efficiency

- For graphs larger than main memory, diskbased computing can be competitive with distributed clusters
- GraphChi: Large-Scale Graph Computation on Just a PC (OSDI 2012)

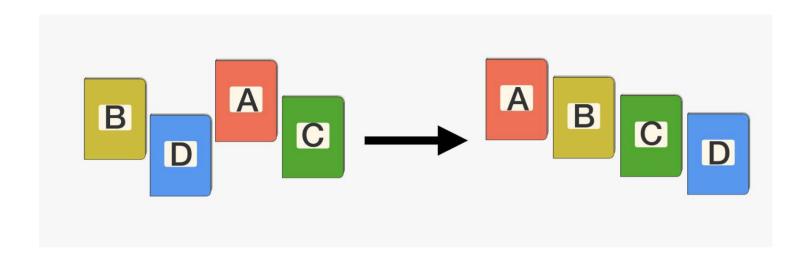
Application & Graph	Iter.	Comparative result	GraphChi (Mac Mini)	Ref
Pagerank & domain	3	GraphLab[30] on AMD server (8 CPUs) 87 s	132 s	-
Pagerank & twitter-2010	5	Spark [45] with 50 nodes (100 CPUs): 486.6 s	790 s	[38]
Pagerank & V=105M, E=3.7B	100	Stanford GPS, 30 EC2 nodes (60 virt. cores), 144 min	approx. 581 min	[37]
Pagerank & V=1.0B, E=18.5B	1	Piccolo, 100 EC2 instances (200 cores) 70 s	approx. 26 min	[36]
Webgraph-BP & yahoo-web	1	Pegasus (Hadoop) on 100 machines: 22 min	27 min	[22]
ALS & netflix-mm, D=20	10	GraphLab on AMD server: 4.7 min	<b>9.8 min</b> (in-mem)	
			40 min (edge-repl.)	[30]
Triangle-count & twitter-2010	-	Hadoop, 1636 nodes: <b>423 min</b>	60 min	[39]
Pagerank & twitter-2010	1	PowerGraph, 64 x 8 cores: 3.6 s	158 s	[20]
Triange-count & twitter- 2010	-	PowerGraph, 64 x 8 cores: <b>1.5 min</b>	60 min	[20]

- Lots of follow-up work on disk-based computing that we will study
- External-memory algorithms to minimize I/O's

#### **SORTING ALGORITHMS**

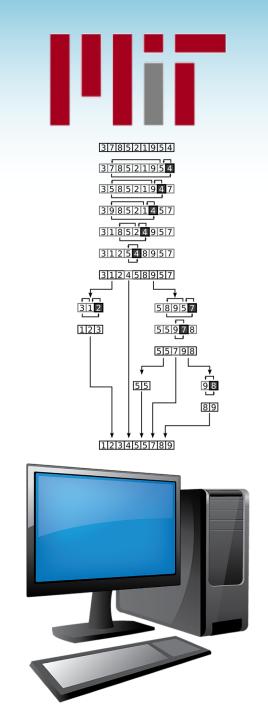


#### Sorting

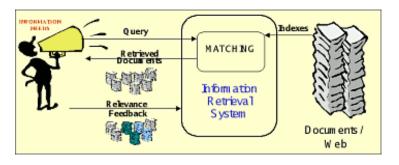


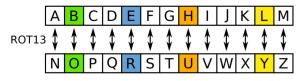
- Lots of research on engineering sorting algorithms
- Will study parallel comparison sorting and radix sorting algorithms
- http://sortbenchmark.org/

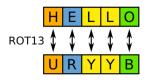
#### **STRING ALGORITHMS**



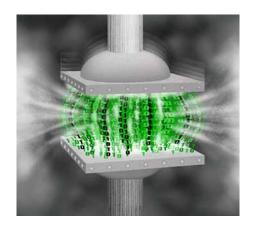
#### **String Algorithms**





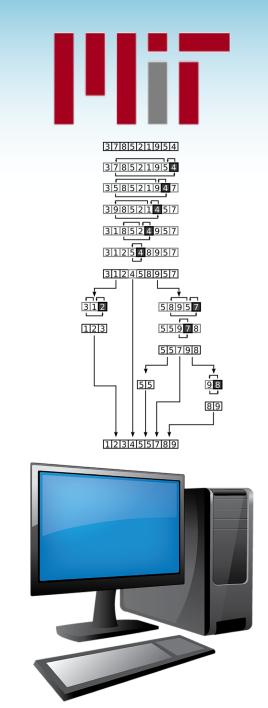




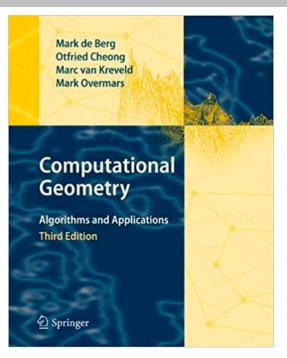


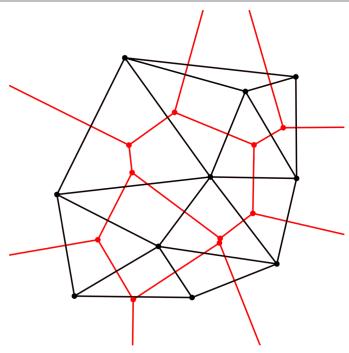
- We will study algorithms for efficiently constructing suffix arrays and suffix trees
- Many other interesting problems (edit distance, Lempel-Ziv compression, approximate string matching, alignment, etc.)

#### **GEOMETRY ALGORITHMS**



## **Computational Geometry**

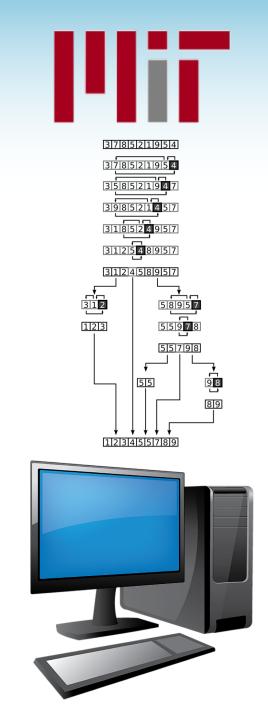




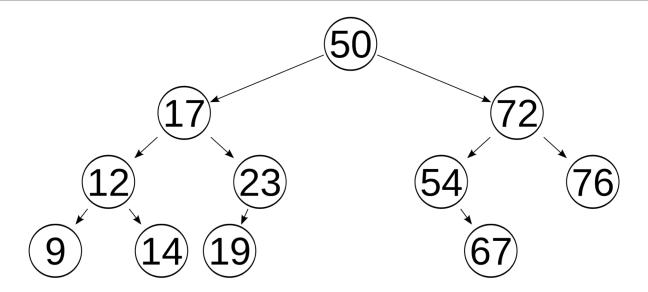
- We will study how to efficiently triangulate a mesh (Delaunay triangulation)
- Many other interesting problems (convex hull, linear programming, segment intersection, point location, space partitions, etc.)

Be careful with numerical issues

#### **BINARY SEARCH TREES**

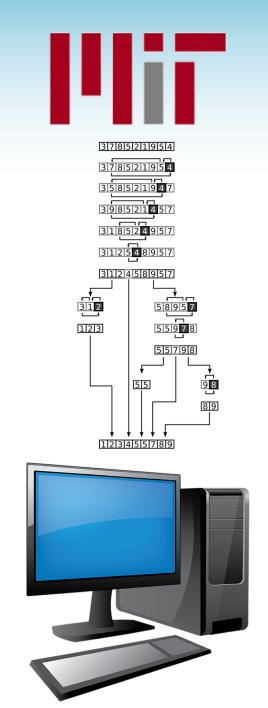


#### **Binary Search Trees**



- We will study different types of binary trees
- We will study how to efficiently construct and update binary search trees in parallel
- We will look at applications such as range trees, interval trees, segment and rectangle queries

#### **JOINS AND AGGREGATION**

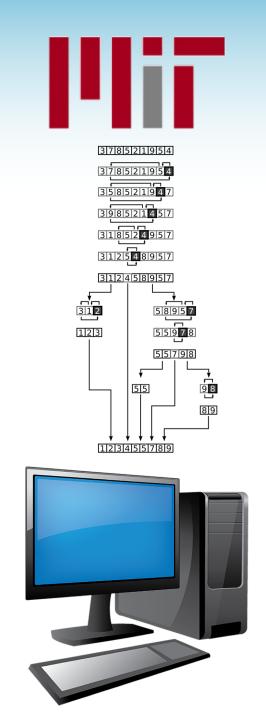


## Joins and Aggregation

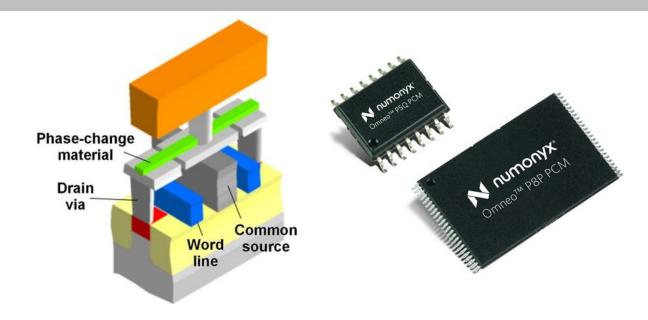


- JOIN and GROUPBY are two of the most expensive operations in database systems
- We will study algorithms and optimizations for these operations (in main-memory)

# WRITE-EFFICIENT ALGORITHMS

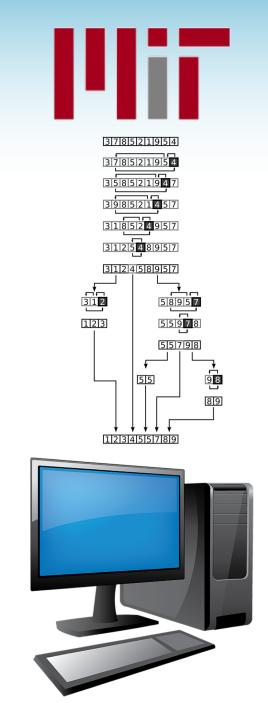


## **Emerging Memory Technologies**

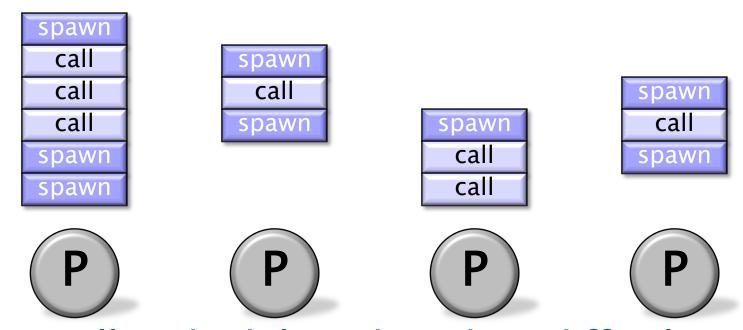


- Non-volatile memories projected to become a dominant form of main memory
- Significant gap in cost for reads vs. writes (energy and latency)
- Need to design models and algorithms that take read-write asymmetry into account

#### PARALLEL SCHEDULING



## **Parallel 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?
- Space-bounded scheduler
  - How can we get efficient running times and cacheefficiency?

## Relevant Topics Not Covered

- GPUs, other accelerators, and special-purpose hardware
- Networking
- Matrix computations
- Linear and integer programming
- Optimizing NP-hard problems
- Succinct data structures
- Concurrent data structures
- Transactional memory
- Performance of different programming languages
- Deep learning

#### Summary



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