Lecture 22:

Domain-specific programming on graphs

Parallel Computer Architecture and Programming
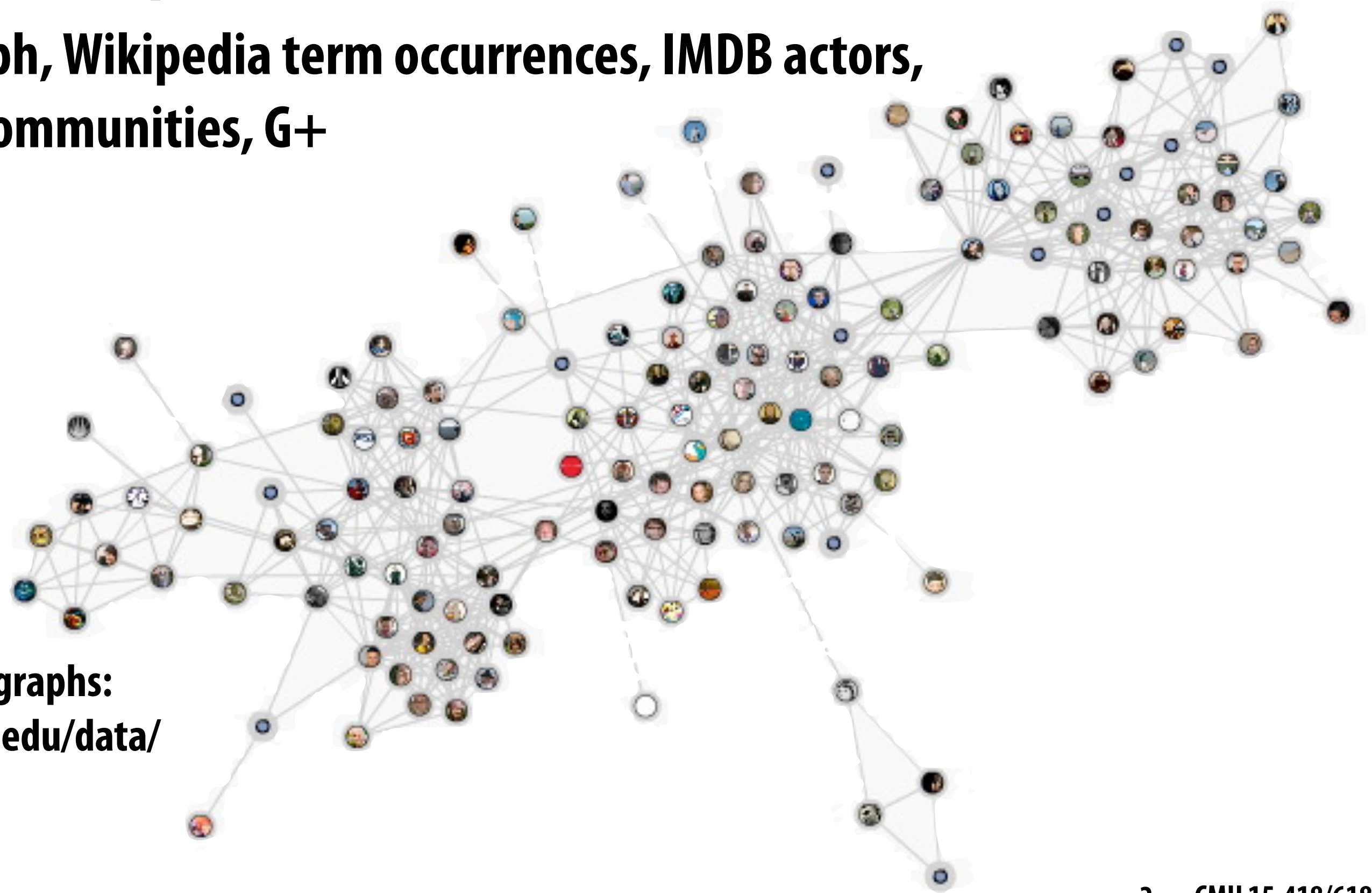**CMU 15-418/15-618, Fall 2023**

Today's topic: analyzing big graphs

- **Many modern applications:**
  - Web search results, recommender systems, influence determination, advertising, anomaly detection, etc.

- **Public dataset examples:**

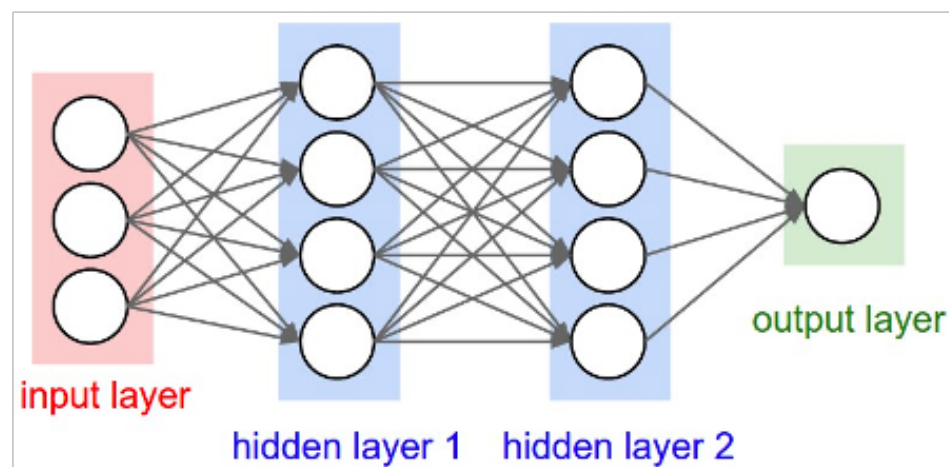 Twitter social graph, Wikipedia term occurrences, IMDB actors, Netflix, Amazon communities, G+

  Good source of public graphs:
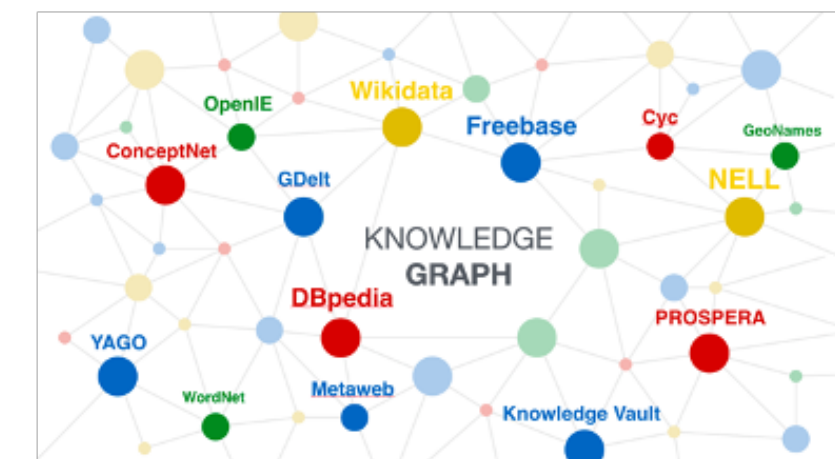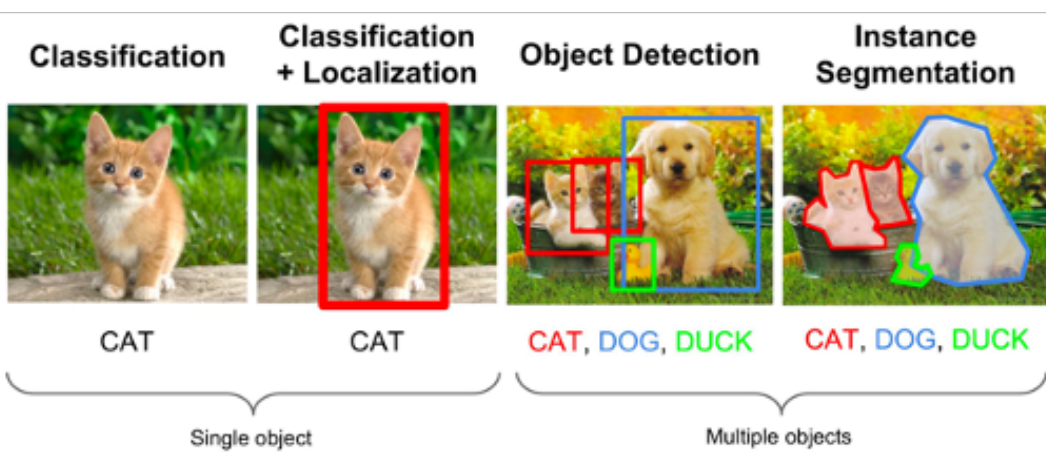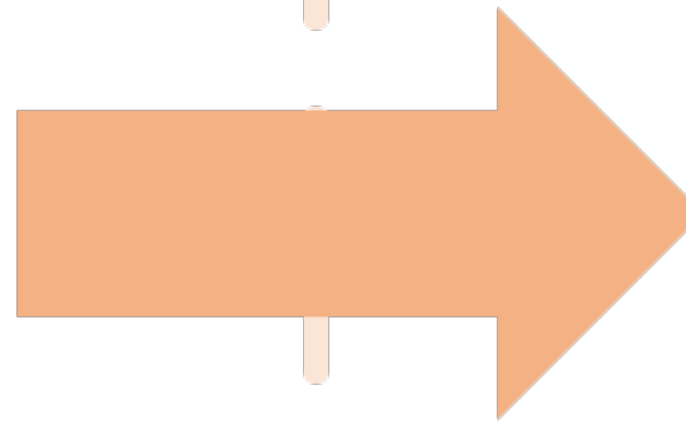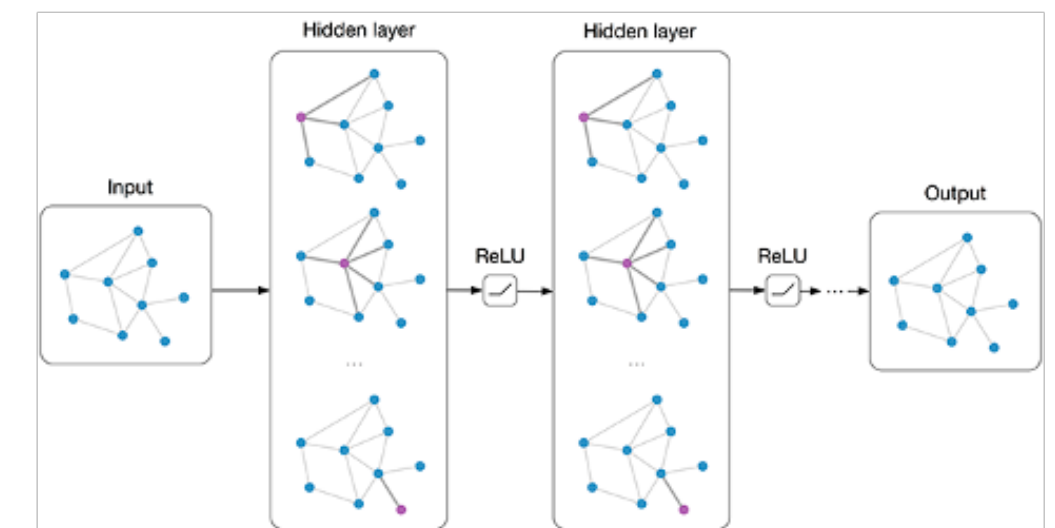 **https://snap.stanford.edu/data/**

Today's topic: analyzing big graphs

- **Emerging interests in machine learning on graphs**

We plan to design a DSL for computing on graphs.

Where might we begin?

What abstractions do we need?

Whenever I'm trying to assess the importance of a new programming system, I ask two questions:

- **"What tasks/problems does the system take off the hands of the programmer?**
  - (are these problems challenging or tedious enough that I feel the system is adding sufficient value for me to want to use it?)"

- **"What problems does the system leave as the responsibility for the programmer?"**
  - (likely because the programmer is better at these tasks)

Halide:

Programmer's responsibility:
- Describing image processing algorithm as pipeline of operations on images
- Describing the schedule for executing the pipeline (e.g., "block this loop, "parallelize this loop", "fuse these stages")

Halide system's responsibility:
- Implementing the schedule using mechanisms available on the target machine (spawning pthreads, allocating temp buffers, emitting vector instructions, loop indexing code)

A good exercise: carry out this evaluation for another programming system: like OpenGL, SQL, MapReduce, etc.

Programming system design questions:

- **What are the fundamental operations we want to be easy to express and efficient to execute?**

- **What are the key optimizations performed by the best implementations of these operations?**
    - high-level abstractions should not prevent these
    - maybe even allow system to perform them for the application

Example graph computation: Page Rank

Page Rank: iterative graph algorithm
Graph nodes = web pages
Graph edges = links between pages

discount

$$R[i] = \frac{1 - \alpha}{N} + \alpha \sum_{j \text{ links to } i} \frac{R[j]}{\text{Outlinks}[j]}$$

Rank of page *i*

Weighted combination of
rank of pages that link to it
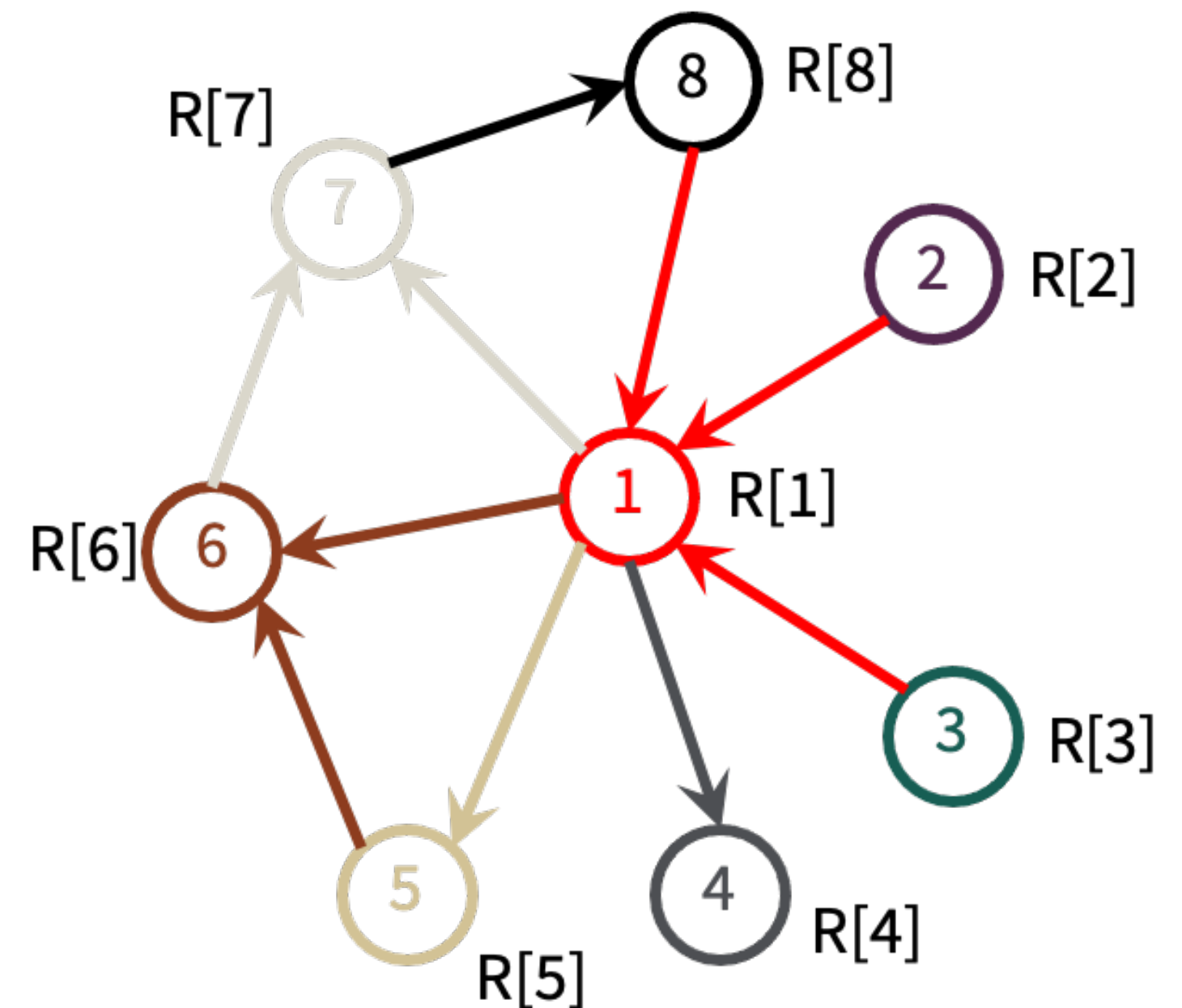
GraphLab

- **A system for describing <u>iterative</u> computations on graphs**

- **Implemented as a C++ runtime**

- **Runs on shared memory machines or distributed across clusters**

  - **GraphLab runtime takes responsibility for scheduling work in parallel, partitioning graphs across clusters of machines, communication between master, etc.**

GraphLab programs: state

- **The graph: G = (V, E)**

  - Application defines **data blocks** on each vertex and directed edge

  - D_v = **data associated with vertex** v

  - $D_{u \rightarrow v}$ = **data associated with directed edge** $u \rightarrow v$

- **Read-only global data**

  - Can think of this as per-graph data, rather than per vertex or per-edge data)

GraphLab operations: the vertex program

- **Defines per-vertex operations on the vertex's local neighborhood**

- **Neighborhood (aka "scope") of vertex:**

  - **The current vertex**

  - **Adjacent edges**

  - **Adjacent vertices**
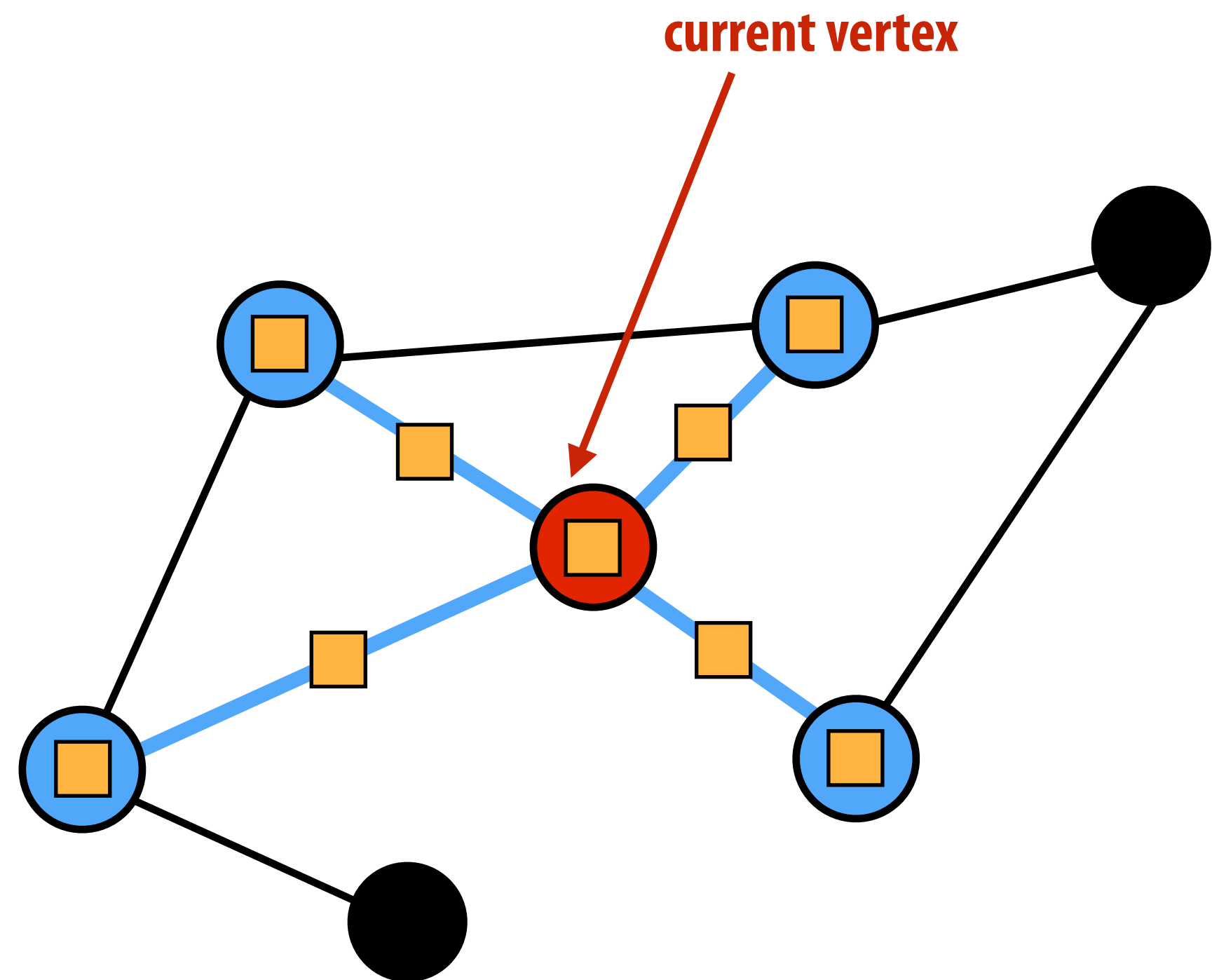
current vertex

= vertex or edge data "in scope" of red vertex
(graph data that can be accessed when executing a
vertex program at the current (red) vertex)

Gather-Apply Scatter (GAS)
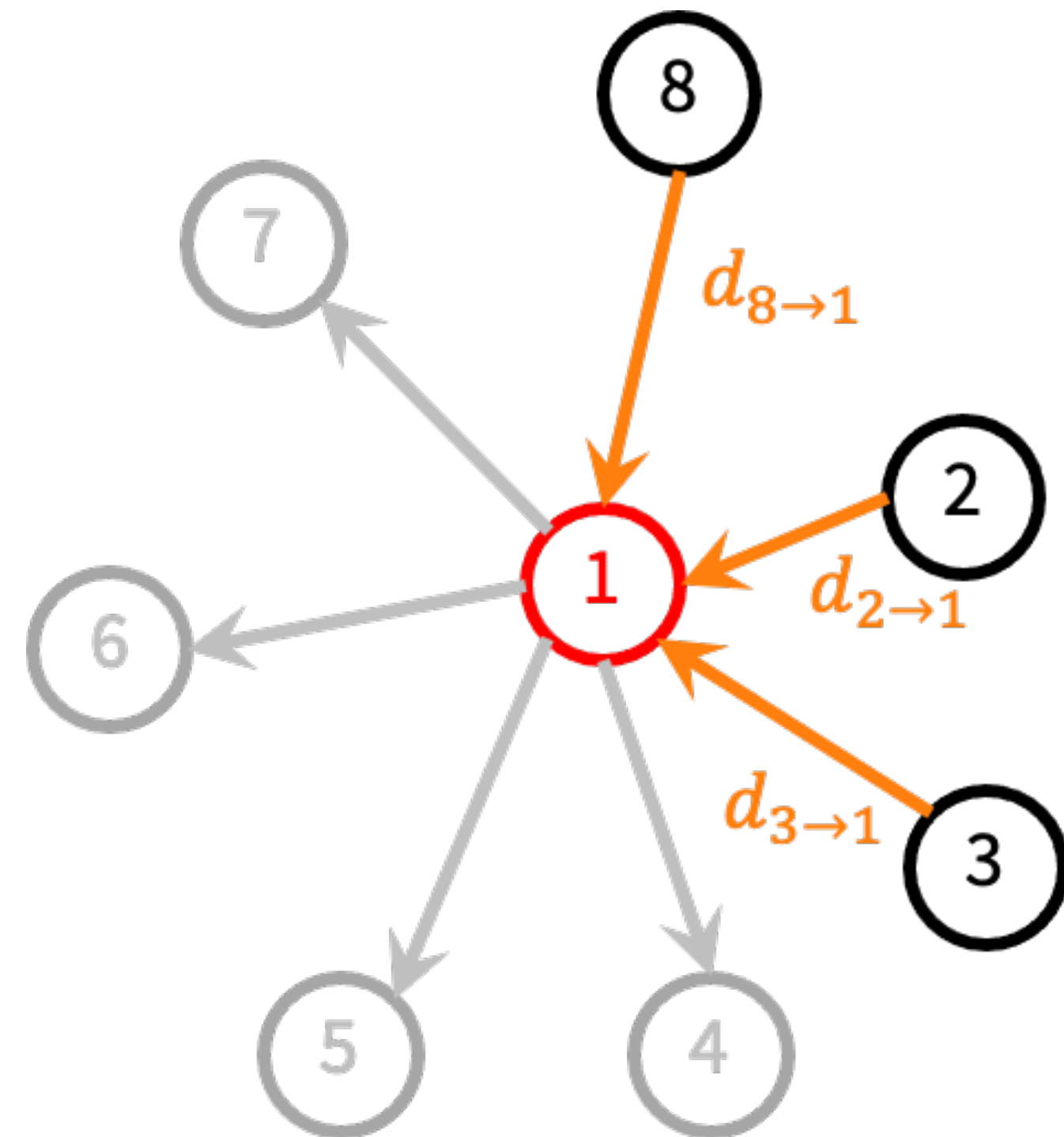
- **Gather: accumulate information from neighbors** $\quad a_u = \sum\limits_{v \in Nbrs} d_{v \to v}$

Gather-Apply Scatter (GAS)

- **Gather: accumulate information from neighbors** $a_u = \sum_{v \in Nbrs} d_{v \to v}$

- **Apply: update the value of the central vertex** $d_u^{new} = update(d_u, a_u)$

$d_{8 \to 1}$

$d_{2 \to 1}$

$d_{3 \to 1}$
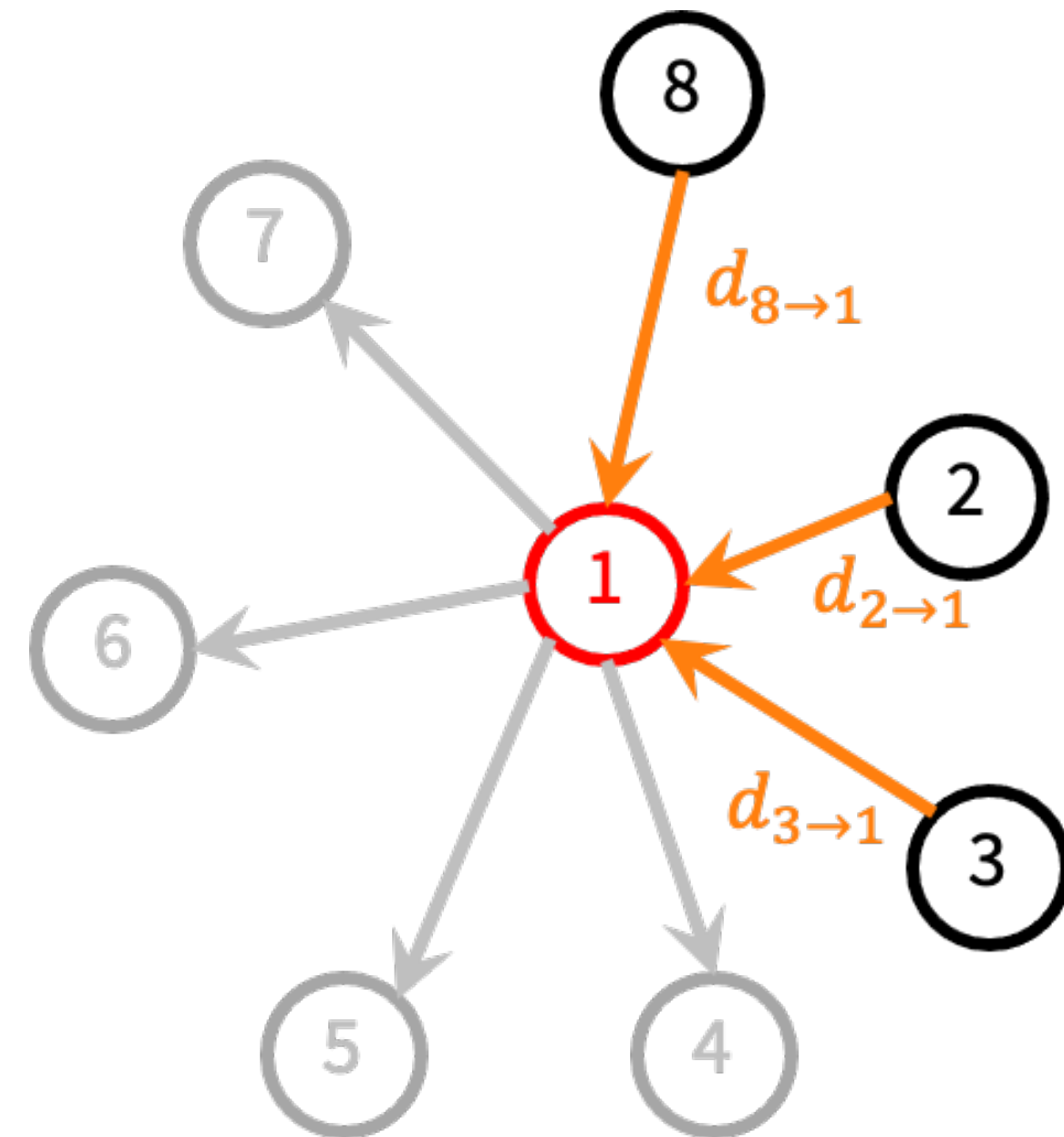
Gather-Apply Scatter (GAS)

- **Gather: accumulate information from neighbors** $\quad a_u = \sum\limits_{v \in Nbrs} d_{v \to v}$

- **Apply: update the value of the central vertex** $\quad d_u^{new} = update(d_u, a_u)$

- **Scatter: use the new value of the central vertex to update the data on adjacent edges**
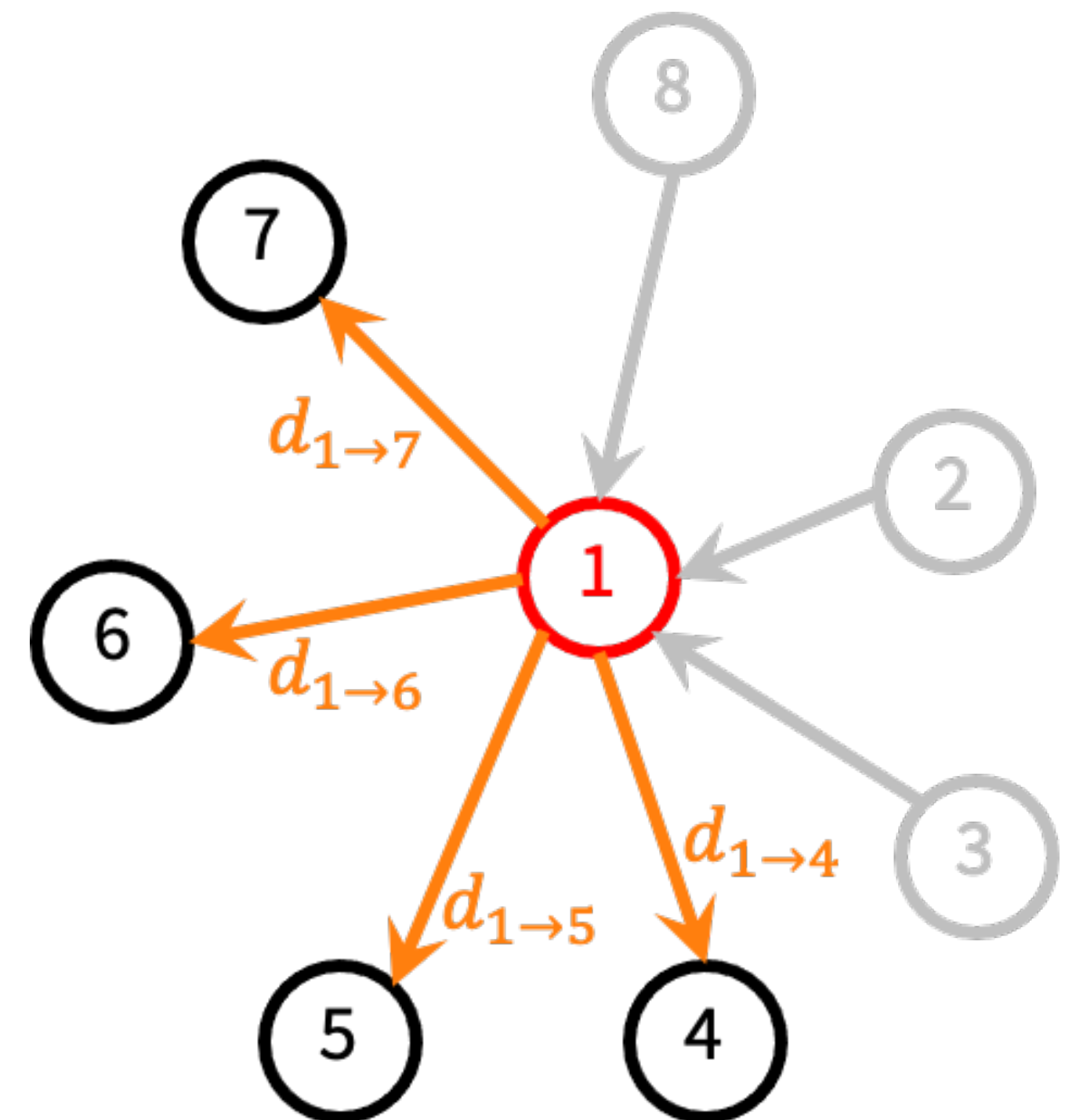
Simple example: PageRank *

$$R[i] = \frac{1 - \alpha}{N} + \alpha \sum_{j \text{ links to } i} \frac{R[j]}{\text{Outlinks}[j]}$$

```
PageRank_vertex_program(vertex i) {

  // (Gather phase) compute the sum of my neighbors rank
  double sum = 0;
  foreach(vertex j : in_neighbors(i)) {
    sum = sum + j.rank / num_out_neighbors(j);
  }

  // (Apply phase) Update my rank (i)
  i.rank = (1-0.85)/num_graph_vertices() + 0.85*sum;
}
```

Let alpha = 0.85

Programming in GraphLab amounts to defining how to update graph state at each vertex. The system takes responsibility for scheduling and parallelization.

* This is made up syntax for slide simplicity: actual syntax is C++, as we'll see on the next slide

GraphLab: data access

- **The application's vertex program executes per-vertex**

- **The vertex program defines:**

  - **What adjacent edges are inputs to the computation**

  - **What computation to perform per edge**

  - **How to update the vertex's value**

  - **What adjacent edges are modified by the computation**

  - **How to update these output edge values**

- **Note how GraphLab requires the program to tell it all data that will be accessed, and whether it is read or write access**

PageRank: GraphLab vertex program (C++ code)

```cpp
struct web_page {
  std::string pagename;
  double      pagerank;
  web_page(): pagerank(0.0) { }
}

typedef graphlab::distributed_graph<web_page, graphlab::empty> graph_type;

class pagerank_program:
            public graphlab::ivertex_program<graph_type, double>,
            public graphlab::IS_POD_TYPE {
public:
  // we are going to gather on all the in-edges
  edge_dir_type gather_edges(icontext_type& context,
                             const vertex_type& vertex) const {
    return graphlab::IN_EDGES;
  }

  // for each in-edge gather the weighted sum of the edge.
  double gather(icontext_type& context, const vertex_type& vertex,
                edge_type& edge) const {
    return edge.source().data().pagerank / edge.source().num_out_edges();
  }

  // Use the total rank of adjacent pages to update this page
  void apply(icontext_type& context, vertex_type& vertex,
             const gather_type& total) {
    double newval = total * 0.85 + 0.15;
    vertex.data().pagerank = newval;
  }

  // No scatter needed. Return NO_EDGES
  edge_dir_type scatter_edges(icontext_type& context,
                              const vertex_type& vertex) const {
    return graphlab::NO_EDGES;
  }
};
```

Graph has record of type web_page per vertex, and no data on edges

Define edges to gather over in "gather phase"

Compute value to accumulate for each edge

Update vertex rank

PageRank example performs no scatter

Running the program

```
graphlab::omni_engine<pagerank_program> engine(dc, graph, "sync");
engine.signal_all();
engine.start();
```

GraphLab runtime provides "engines" that manage scheduling of vertex programs

`engine.signal_all()` marks all vertices for execution

You can think of the GraphLab runtime as a work queue scheduler.
And invoking a vertex program on a vertex as a task that is placed in the work queue.

So it's reasonable to read the code above as: "place all vertices into the work queue"
Or as: "foreach vertex" run the vertex program.

Vertex signaling: GraphLab's mechanism for generating new work

$$R[i] = \frac{1 - \alpha}{N} + \alpha \sum_{j \text{ links to } i} \frac{R[j]}{\text{Outlinks}[j]}$$

Iterate update of all R[i]'s 10 times

Uses generic "signal" primitive (could also wrap code on previous slide in a for loop)

```
struct web_page {
  std::string pagename;
  double      pagerank;
  int         counter;
  web_page(): pagerank(0.0),counter(0) { }
}

 // Use the total rank of adjacent pages to update this page
  void apply(icontext_type& context, vertex_type& vertex,
             const gather_type& total) {
    double newval = total * 0.85 + 0.15;
    vertex.data().pagerank = newval;
    vertex.data().counter++;
    if (vertex.data().counter < 10)
      vertex.signal();
  }
```

Per-vertex "counter"

If counter < 10, signal to scheduler to run the vertex program on the vertex again at some point in the future

Signal: general primitive for scheduling work

Parts of graph may converge at different rates
(iterate PageRank until convergence, but only for vertices that need it)

```cpp
class pagerank_program:
      public graphlab::ivertex_program<graph_type, double>,
      public graphlab::IS_POD_TYPE {

private:
  bool perform_scatter;              ⊦— Private variable set during apply phase,
                                         used during scatter phase

public:

  // Use the total rank of adjacent pages to update this page
  void apply(icontext_type& context, vertex_type& vertex,
             const gather_type& total) {
    double newval = total * 0.85 + 0.15;
    double oldval = vertex.data().pagerank;
    vertex.data().pagerank = newval;
    perform_scatter = (std::fabs(oldval - newval) > 1E-3);    ⊦— Check for convergence
  }


  // Scatter now needed if algorithm has not converged
  edge_dir_type scatter_edges(icontext_type& context,
                              const vertex_type& vertex) const {
    if (perform_scatter) return graphlab::OUT_EDGES;
    else return graphlab::NO_EDGES;
  }


  // Make sure surrounding vertices are scheduled
  void scatter(icontext_type& context, const vertex_type& vertex,    ⊦— Schedule update of
               edge_type& edge) const {                                  neighbor vertices
    context.signal(edge.target());
  }
};
```

Synchronizing parallel execution

Local neighborhood of vertex (vertex's "scope") can be read and written to by a vertex program

current vertex
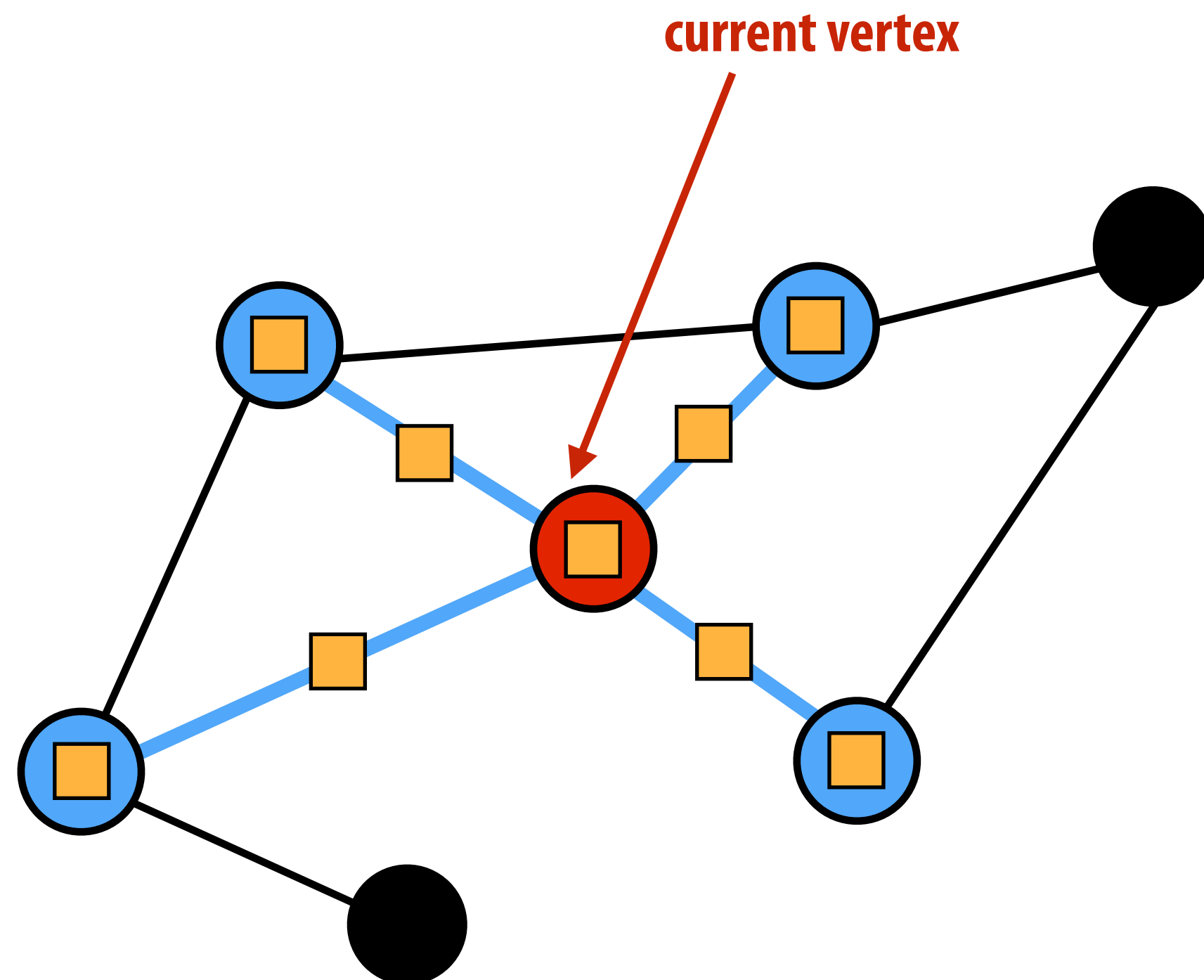
■ = vertex or edge data in scope of red vertex

Programs specify what granularity of atomicity ("consistency") they want GraphLab runtime to provide: this determines amount of available parallelism

- "**Full consistency**": implementation ensures no other execution reads or writes to data in scope of v when vertex program for v is running.

- "**Edge consistency**": no other execution reads or writes any data in v or in edges adjacent to v

- "**Vertex consistency**": no other execution reads or writes to data in v ...

GraphLab: job scheduling order

GraphLab implements several work scheduling policies

- **Synchronous**: update all scheduled vertices "simultaneously" (vertex programs observe no updates from programs run on other vertices in same "round")

Graph
(stored in data structure A)

Updated graph
(stored in data structure B)

Updated graph
(stored in data structure A)

Run vertex programs for all
scheduled vertices.
(output to copy of graph structure)

Run vertex programs for all
scheduled vertices.
(output to copy of graph structure)
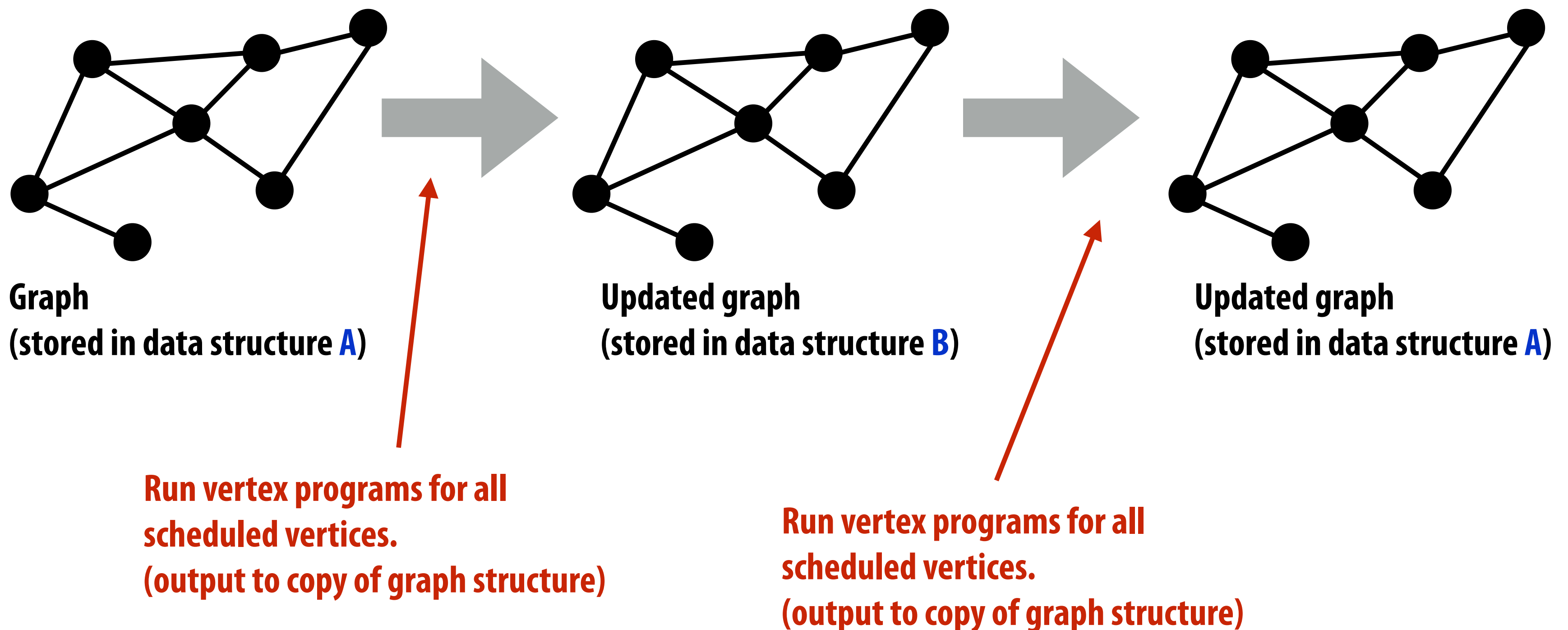
GraphLab: job scheduling order

- **GraphLab implements several work scheduling policies**

  - **Synchronous**: update all vertices simultaneously (vertex programs observe no updates from programs run on other vertices in same "round")

  - **Round-robin**: vertex programs observe most recent updates

  - **Graph coloring**

  - **Dynamic**: based on new work created by `signal`

    - Several implementations: fifo, priority-based, "splash" ...

- **Application developer has flexibility for choosing consistency guarantee and scheduling policy**

  - <u>Implication</u>: **choice of schedule impacts program's correctness/output**

Summary: GraphLab concepts

- **Program state**: data on graph vertices and edges + globals

- **Operations**: per-vertex update programs and global reduction functions (reductions not discussed today)

  - Simple, intuitive description of work (follows mathematical formulation)

  - Graph restricts data access in vertex program to local neighborhood

  - Asynchronous execution model: application creates work dynamically by "signaling vertices" (enable lazy execution, work efficiency on real graphs)

- **Choice of scheduler and consistency implementation**

  - In this domain, the order in which nodes are processed can be critical property for both performance and quality of result

  - Application responsible for choosing right scheduler for its needs

Graph Framework Taxonomy

(a) A sample graph   (b) Vertex-centric (edge-cut) approach   (c) Edge-centric (vertex-cut) approach   (d) Component-centric approach
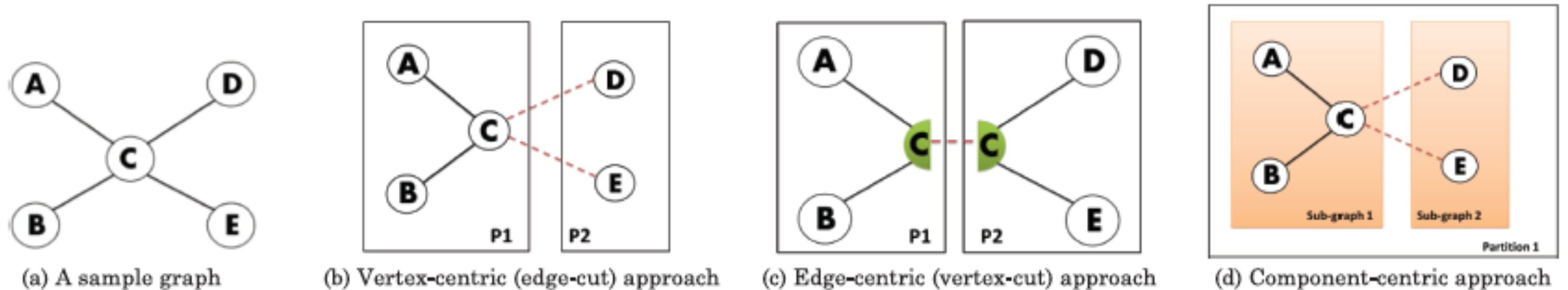
Figure: Safiollah Heidari, Yogesh Simmhan, Rodrigo N. Calheiros, and Rajkumar Buyya. 2018. Scalable Graph Processing Frameworks: A Taxonomy and Open Challenges. ACM Comput. Surv. 51, 3, Article 60 (June 2018).

- **Vertex** centric: GraphLab, Pregel, GPS

- **Edge** centric: Chaos, X-Stream

- **Sub-graph** centric: Giraph++, GoFFish

If you are going to implement GraphLab, will you choose shared-memory or message passing?

PageRank in Pregel

```cpp
class PageRankVertex
    : public Vertex<double, void, double> {
public:
  virtual void Compute(MessageIterator* msgs) {
    if (superstep() >= 1) {
      double sum = 0;
      for (; !msgs->Done(); msgs->Next())
        sum += msgs->Value();
      *MutableValue() = 0.15 / NumVertices() + 0.85 * sum;
    }

    if (superstep() < 30) {
      const int64 n = GetOutEdgeIterator().size();
      SendMessageToAllNeighbors(GetValue() / n);
    } else {
      VoteToHalt();
    }
  }
};
```

Gather Phase

Apply Phase

Satter Phase
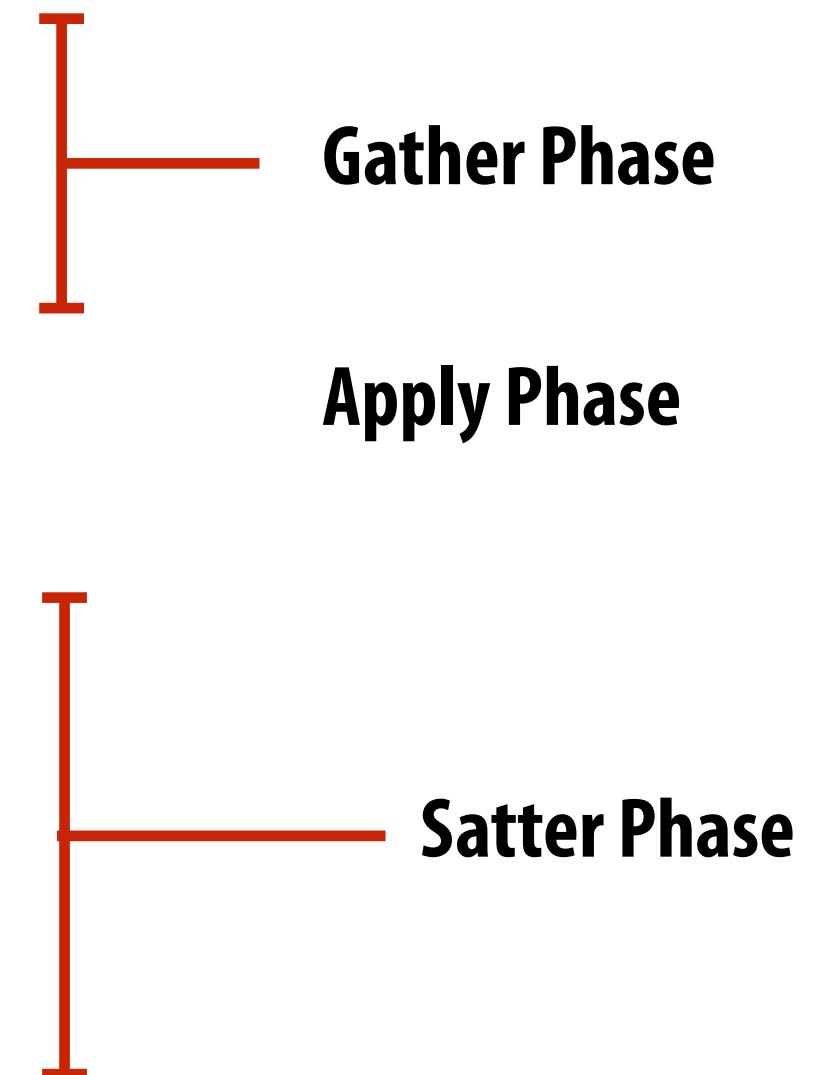
Elements of good domain-specific programming system design

#1: good systems identify the most important cases, and provide most benefit in these situations

- **Structure of code should mimic natural structure of problems in the domain**
    - e.g., graph processing algorithms are designed in terms of per-vertex operations

- **Efficient expression: common operations are easy and intuitive to express**

- **Efficient implementation: the most important optimizations in the domain are performed by the system for the programmer**
    - Our experience: a parallel programming system with "convenient" abstractions that precludes best-known implementation strategies will almost always fail

#2: good systems are usually simple systems

- **They have a small number of key primitives and operations**
  - GraphLab: run computation per vertex, trigger new work by signaling
    - But GraphLab's design gets messy with all the scheduling options
  - Halide: only a few scheduling primitives
  - Hadoop: map + reduce

- **Allows compiler/runtime to focus on optimizing these primitives**

  - Provide parallel implementations, utilize appropriate hardware

- **Common question that good architects ask: "do we really need that?"** (can this concept be reduced to a primitive we already have?)
  - For every domain-specific primitive in the system: there better be a strong performance or expressivity justification for its existence

#3: good primitives compose

- **Composition of primitives allows for wide application scope, even if scope remains limited to a domain**
  - e.g., frameworks discussed today support a wide variety of graph algorithms

- **Composition often allows for generalizable optimization**

- **Sign of a good design:**
  - System ultimately is used for applications original designers never anticipated

- **Sign that a new feature should not be added (or added in a better way):**
  - The new feature does not compose with all existing features in the system
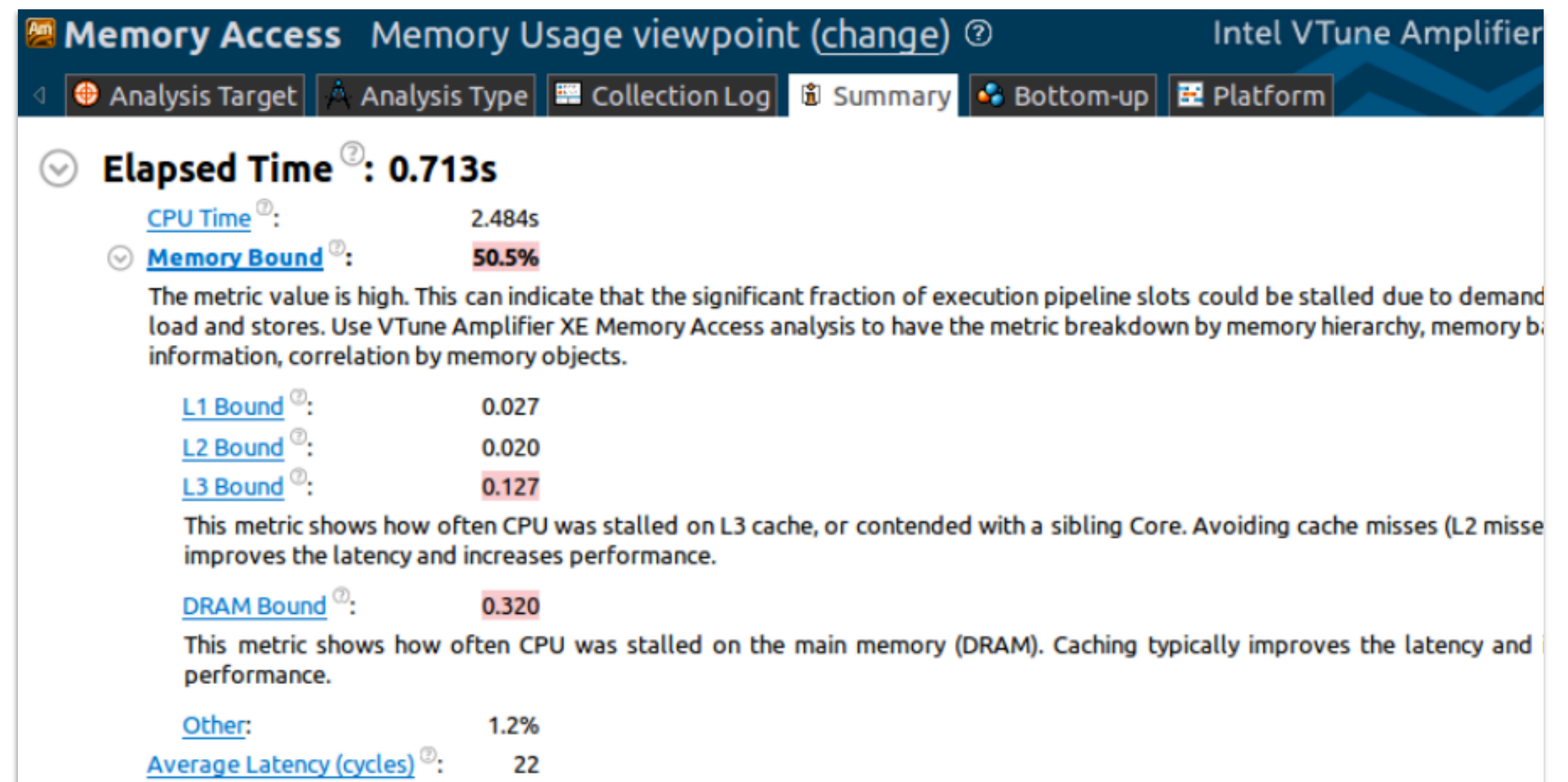
Optimizing graph computations

(now we are talking about implementation)

Wait a minute…

- So far in this lecture, we've discussed issues such as parallelism, synchronization …

- But graph processing typically has **low arithmetic intensity**

VTune profiling results: Memory bandwidth bound!

Walking over edges accesses information from "random" graph vertices

Or just consider PageRank: ~ 1 multiply-accumulate per iteration of summation loop

$$R[i] = \frac{1 - \alpha}{N} + \alpha \sum_{j \text{ links to } i} \frac{R[j]}{\text{Outlinks}[j]}$$

# Two ideas to increase the performance of operations on large graphs *

1. Reorganize graph structure to **increase locality**

2. **Compress** the graph

* Both optimizations might be performed by a framework without application knowledge

Directed graph representation

Vertex Id	1		2		3				4		5				6	
Outgoing Edges	2	3	3	5	2	4	5	6	1	5	1	2	3	6	2	4

Vertex Id	1		2				3			4		5			6	
Incoming Edges	4	5	1	3	5	6	1	2	5	3	6	2	3	4	3	6
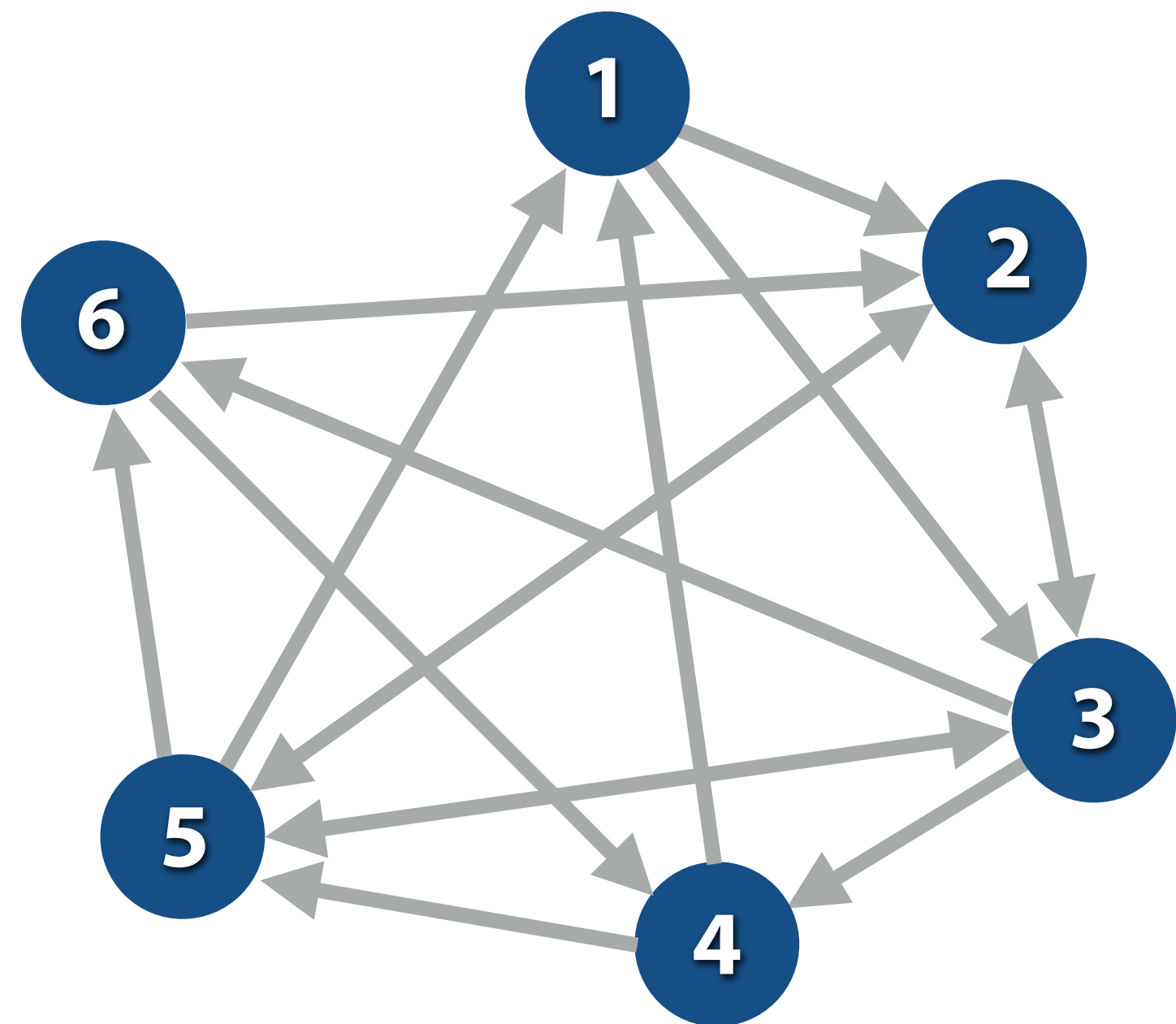
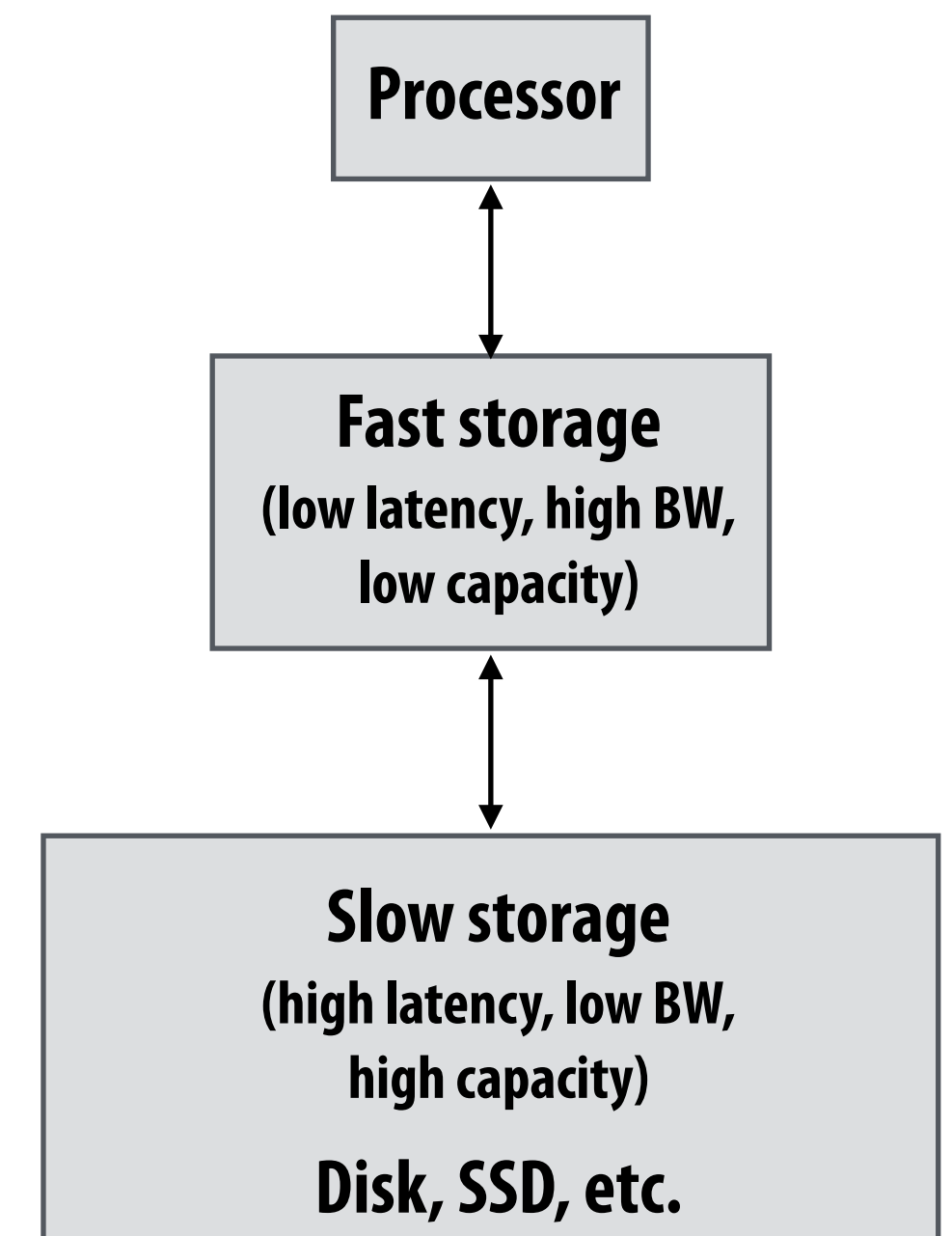# Memory footprint challenge of large graphs

- **Challenge: cannot fit all edges in memory for large graphs (graph vertices may fit)**

    - From example graph representation:

        - Each edge represented twice in graph structure (as incoming/outgoing edge)

        - 8 bytes per edge to represent adjacency

    - May also need to store per-edge values (e.g., 4 bytes for a per-edge weight)

    - **1 billion edges** (modest): **~12 GB** of memory for edge information

    - Algorithm may need multiple copies of per-edge structures (current, prev data, etc.)

- **Could employ cluster of machines to store graph in memory**

    - Rather than store graph on disk

- **Would prefer to process large graphs on a single machine**

    - Managing clusters of machines is difficult

    - Partitioning graphs is expensive (also needs a lot of memory) and difficult

"Streaming" graph computations

- **Graph operations make "random" accesses to graph data (edges adjacent to vertex *v* may distributed arbitrarily throughout storage)**
  - Single pass over graph's edges might make billions of fine-grained accesses to disk

- **Streaming data access pattern**
  - Make large, predictable data accesses to slow storage (achieve high bandwidth data transfer)
  - Load data from slow storage into fast storage*, then reuse it as much as possible before discarding it (achieve high arithmetic intensity)
  - Can we restructure graph data structure so that data access requires only a small number of efficient bulk loads/stores from slow storage?

Processor

↕

Fast storage (low latency, high BW, low capacity)

↕

Slow storage (high latency, low BW, high capacity) **Disk, SSD, etc.**

* By fast storage, in this context I mean DRAM. However, techniques for streaming from disk into memory would also apply to streaming from memory into a processor's cache
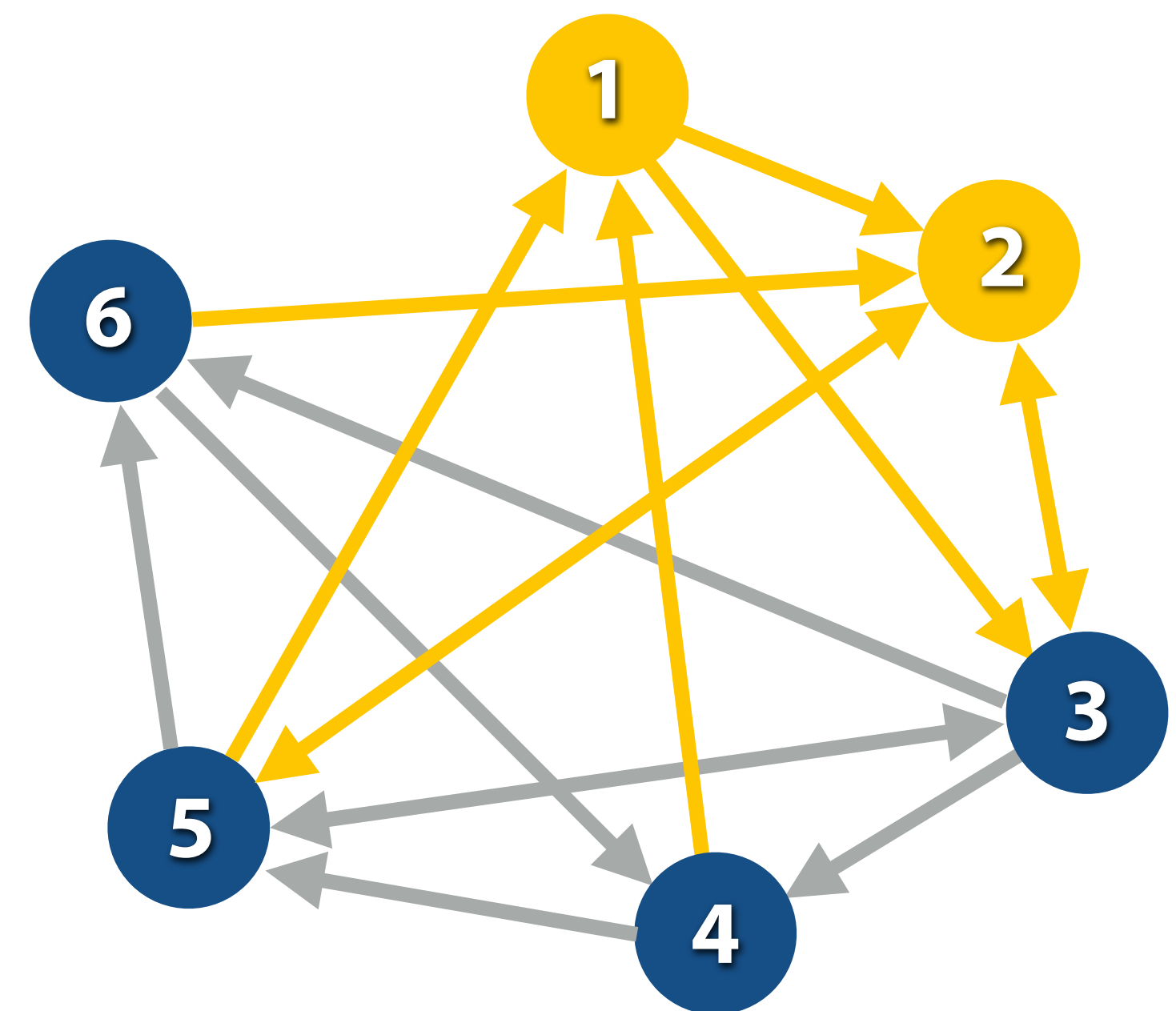
Sharded graph representation

- **Partition** graph vertices into intervals (sized so that subgraph for interval fits in memory)
- Store vertices and only __incoming edges__ to these vertices are stored together in a shard
- **Sort** edges in a shard by source vertex id

Shard 1:
vertices (1-2)

src	dst	value
1	2	0.3
3	2	0.2
4	1	0.8
5	1	0.25
	2	0.6
6	2	0.1

Shard 2:
vertices (3-4)

src	dst	value
1	3	0.4
2	3	0.9
3	4	0.15
5	3	0.2
6	4	0.9

Shard 3:
vertices (5-6)

src	dst	value
2	5	0.6
3	5	0.9
	6	0.85
4	5	0.3
5	6	0.2

Yellow = data required to process subgraph
containing vertices in shard 1

Notice: to construct subgraph containing vertices in shard 1 and their incoming and
outgoing edges, only need to load contiguous information from other P-1 shards
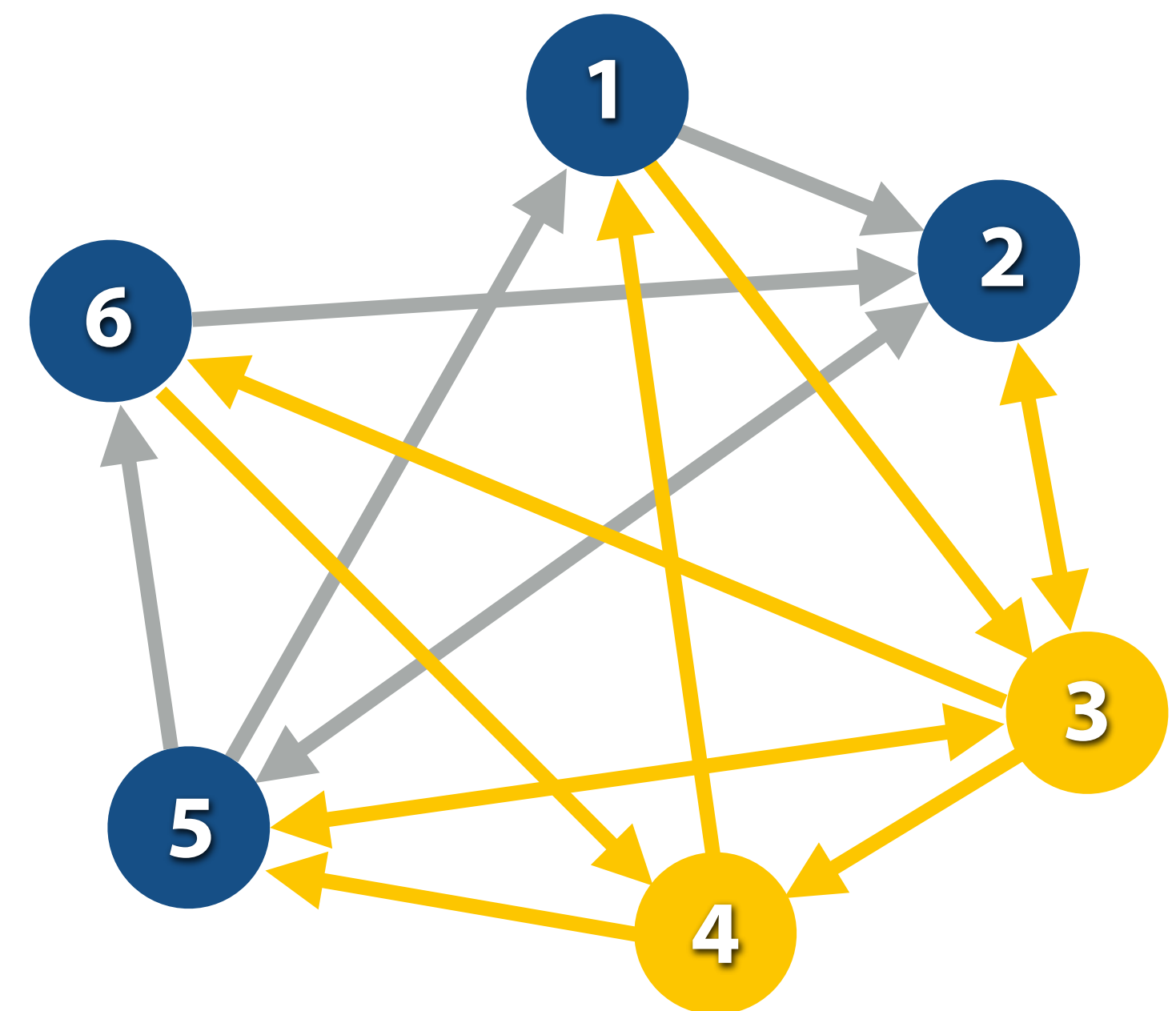
Writes to updated outgoing edges require P-1 bulk writes

Sharded graph representation

- **Partition** graph vertices into intervals (sized so that subgraph for interval fits in memory)
- Store vertices and only <u>incoming edges</u> to these vertices are stored together in a shard
- **Sort** edges in a shard by source vertex id

Shard 1:
vertices (1-2)

src	dst	value
1	2	0.3
3	2	0.2
4	1	0.8
5	1	0.25
	2	0.6
6	2	0.1

Shard 2:
vertices (3-4)

src	dst	value
1	3	0.4
2	3	0.9
3	4	0.15
5	3	0.2
6	4	0.9

Shard 3:
vertices (5-6)

src	dst	value
2	5	0.6
3	5	0.9
	6	0.85
4	5	0.3
5	6	0.2

Yellow = data required to process subgraph
containing vertices in shard 2

Sharded graph representation

- **Partition** graph vertices into intervals (sized so that subgraph for interval fits in memory)
- Store vertices and only <u>incoming edges</u> to these vertices are stored together in a shard
- **Sort** edges in a shard by source vertex id

Shard 1: vertices (1-2)

src	dst	value
1	2	0.3
3	2	0.2
4	1	0.8
5	1	0.25
	2	0.6
6	2	0.1

Shard 2: vertices (3-4)

src	dst	value
1	3	0.4
2	3	0.9
3	4	0.15
5	3	0.2
6	4	0.9

Shard 3: vertices (5-6)

src	dst	value
2	5	0.6
3	5	0.9
	6	0.85
4	5	0.3
5	6	0.2

Yellow = data required to process subgraph containing vertices in shard 3

Observe: due to sort of incoming edges, iterating over all intervals results in contiguous sliding window over the shards

Putting it all together: looping over all graph edges

For each `partition i` of vertices:

- `Load shard i  (contains all incoming edges)`

- `For each other shard s`

  - `Load section of s containing data for edges leaving i and entering s`

- `Construct subgraph in memory`

- `Do processing on subgraph`

Note: a good implementation could hide disk I/O by prefetching data for next iteration of loop

PageRank in GraphChi

GraphChi is a system that implements the out-of-core sliding window approach

PageRank in GraphChi:

```
1  typedef: VertexType float
2  Update(vertex)  begin
3  │    var sum ← 0
4  │    for e in vertex.inEdges() do
5  │    │    sum += e.weight * neighborRank(e)
6  │    end
7  │    vertex.setValue(0.15 + 0.85 * sum)
8  │    broadcast(vertex)   ←────
9  end
```

Take per-vertex rank and distribute to all outbound edges (memory inefficient: replicates per-vertex rank to all edges)

Alternative model: assume vertex data can be kept in memory and redefine neighborRank() function
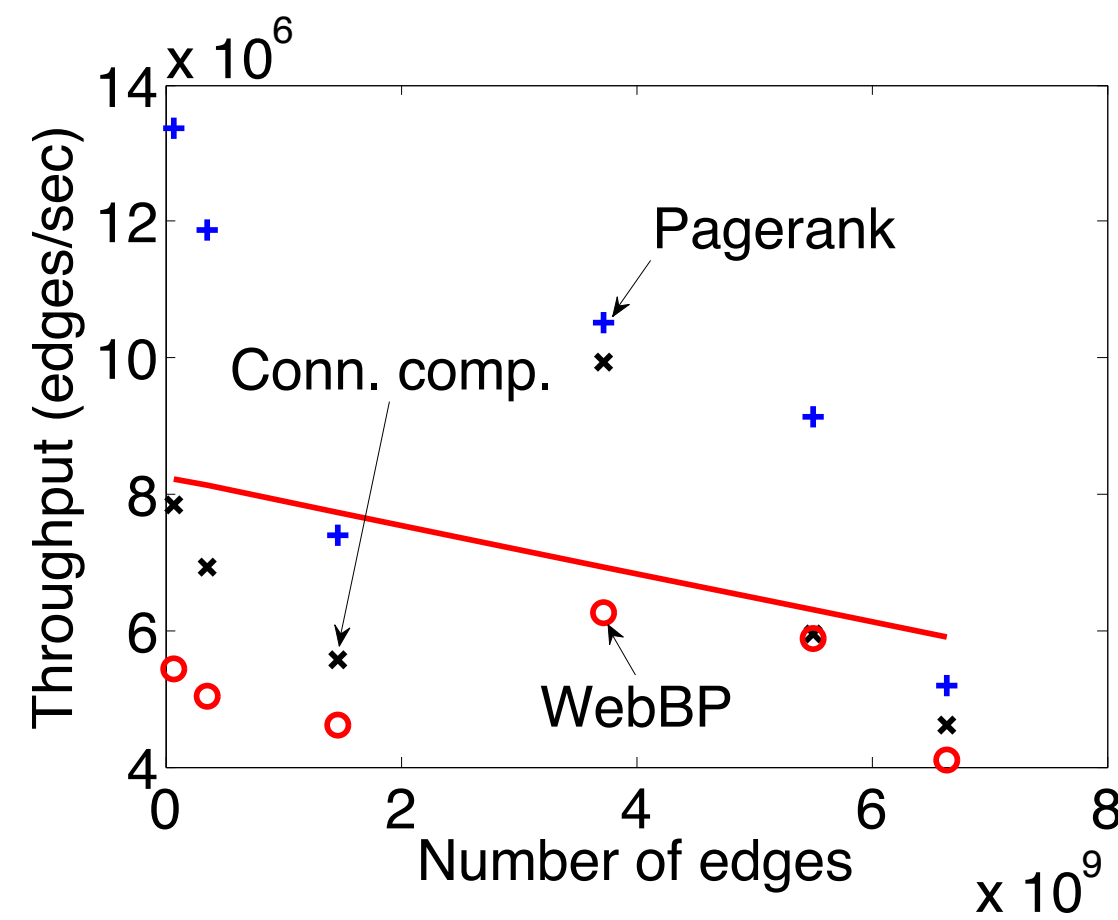
```
1  typedef: EdgeType { float weight; }
2  float[] in_mem_vert
3  neighborRank(edge)  begin
4  │    return edge.weight * in_mem_vert[edge.vertex_id]
5  end
```
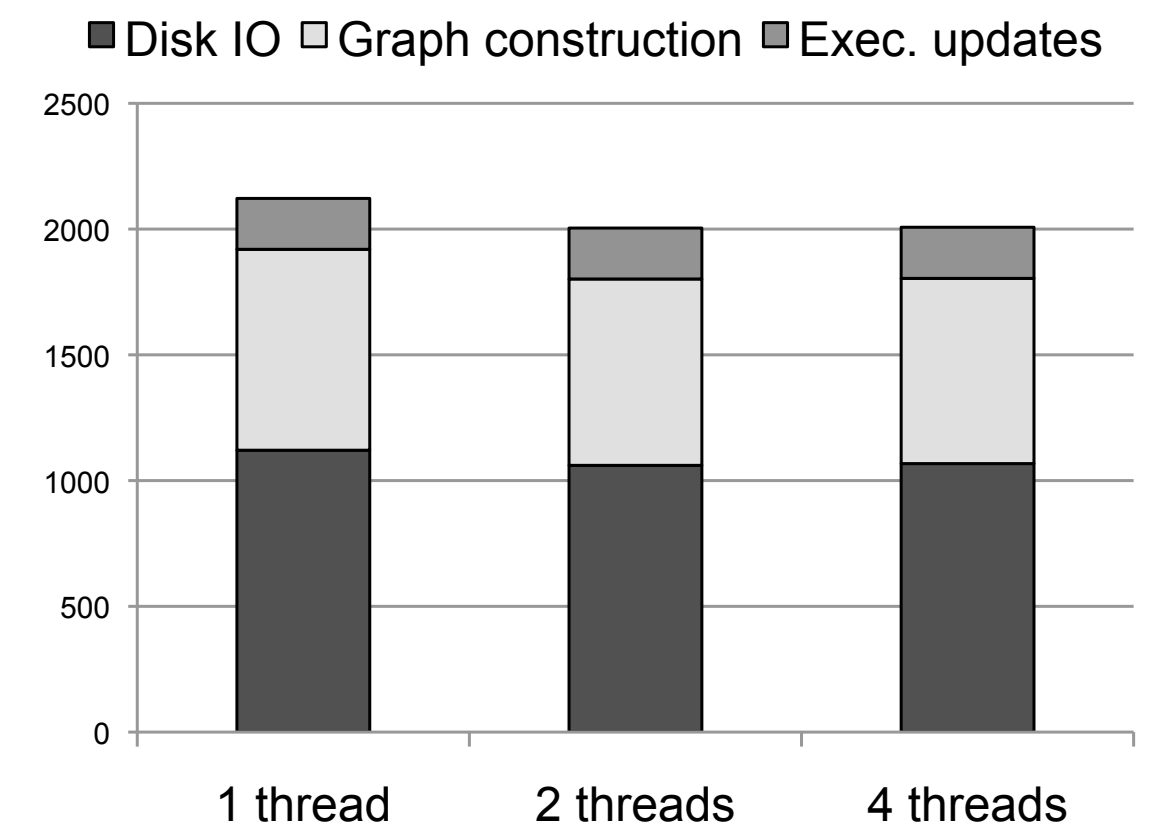
Performance on a Mac mini (8 GB RAM)
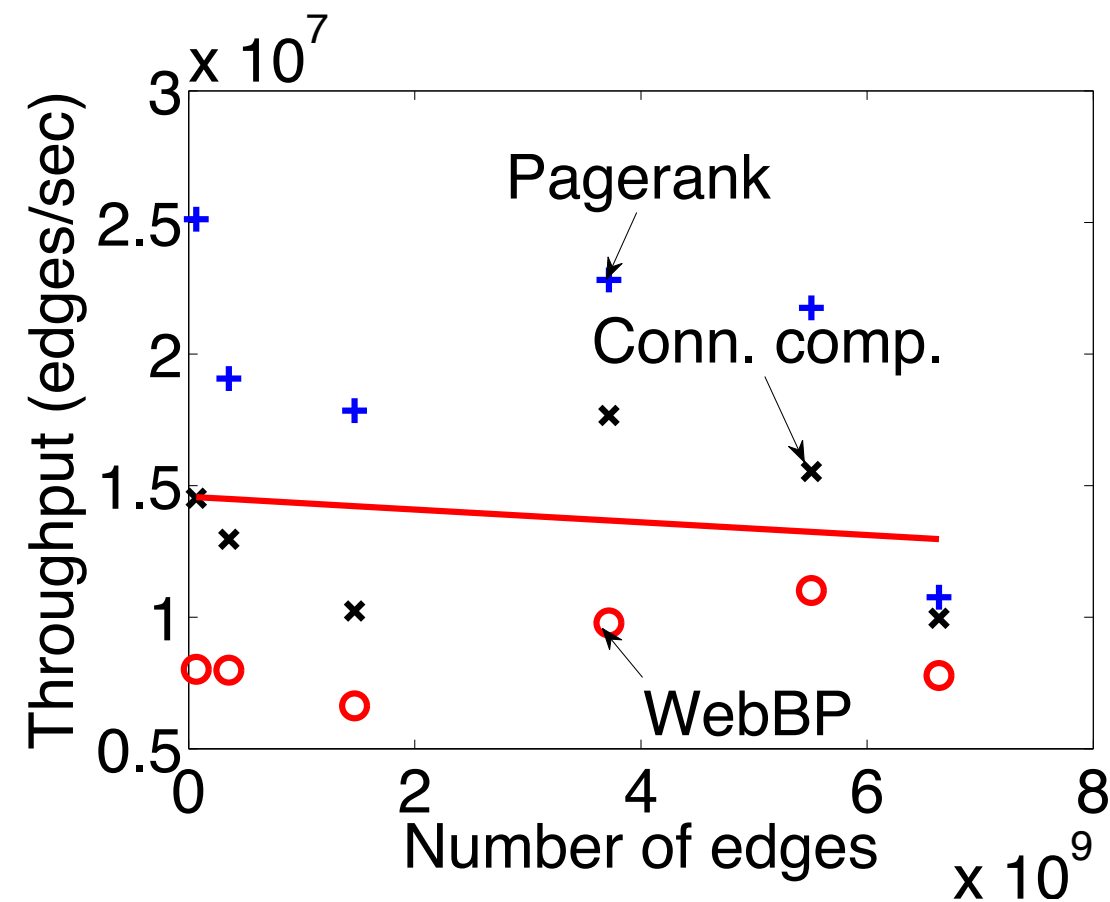
(a) Performance: SSD

(b) Performance : Hard drive

(c) Runtime breakdown

Throughput (edges/sec) remains stable as graph size is increased

- **Desirable property: through**

2023

Graph compression

- **Recall**: graph operations are often BW-bound

- **Implication**: using CPU instructions to reduce BW requirements can benefit overall performance (the processor is waiting on memory anyway!)

- **Idea**: **store graph compressed** in memory, **decompress on-the-fly** when operation wants to read data

Compressing an edge list

Vertex Id   32
Outgoing Edges   1001 10 5 30 6 1025 200000 1010 1024 100000 1030 275000

---

1. **Sort edges** for each vertex

    5 6 10 30 1001 1010 1024 1025 1030 100000 200000 275000

2. **Compute differences**

    5 6 10 30 1001 1010 1024 1025 1030 100000 200000 275000
    0 1   4 20   971   9   14   1   5   98070 100000   75000

3. **Group into sections** requiring same number of bytes

    relative to   5   6 10 30 1001 1010 1024 1025 1030 100000 200000 275000
    vertex index -27   1   4 20   971   9   14   1   5   98070 100000   75000
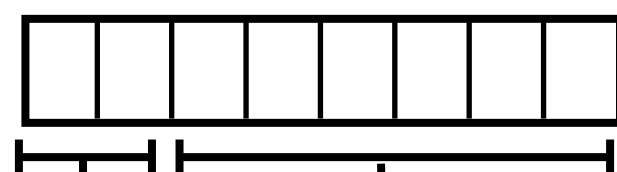
    1 byte   2 bytes   1 byte   4 bytes

4. **Encode deltas**

    Uncompressed encoding: 12 x 4 bytes = 48 bytes
    Compressed encoding: 26 bytes

    1-byte group header
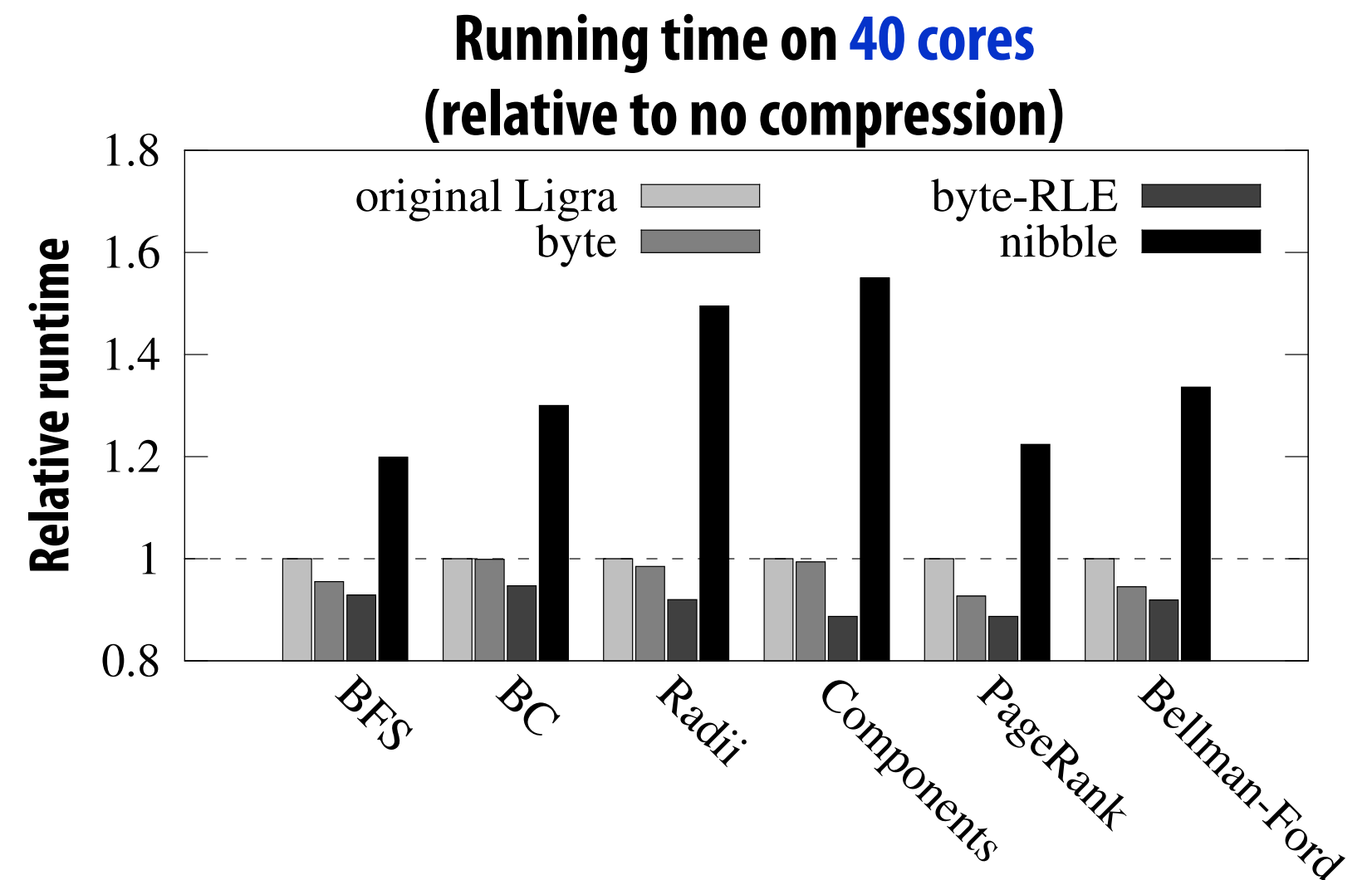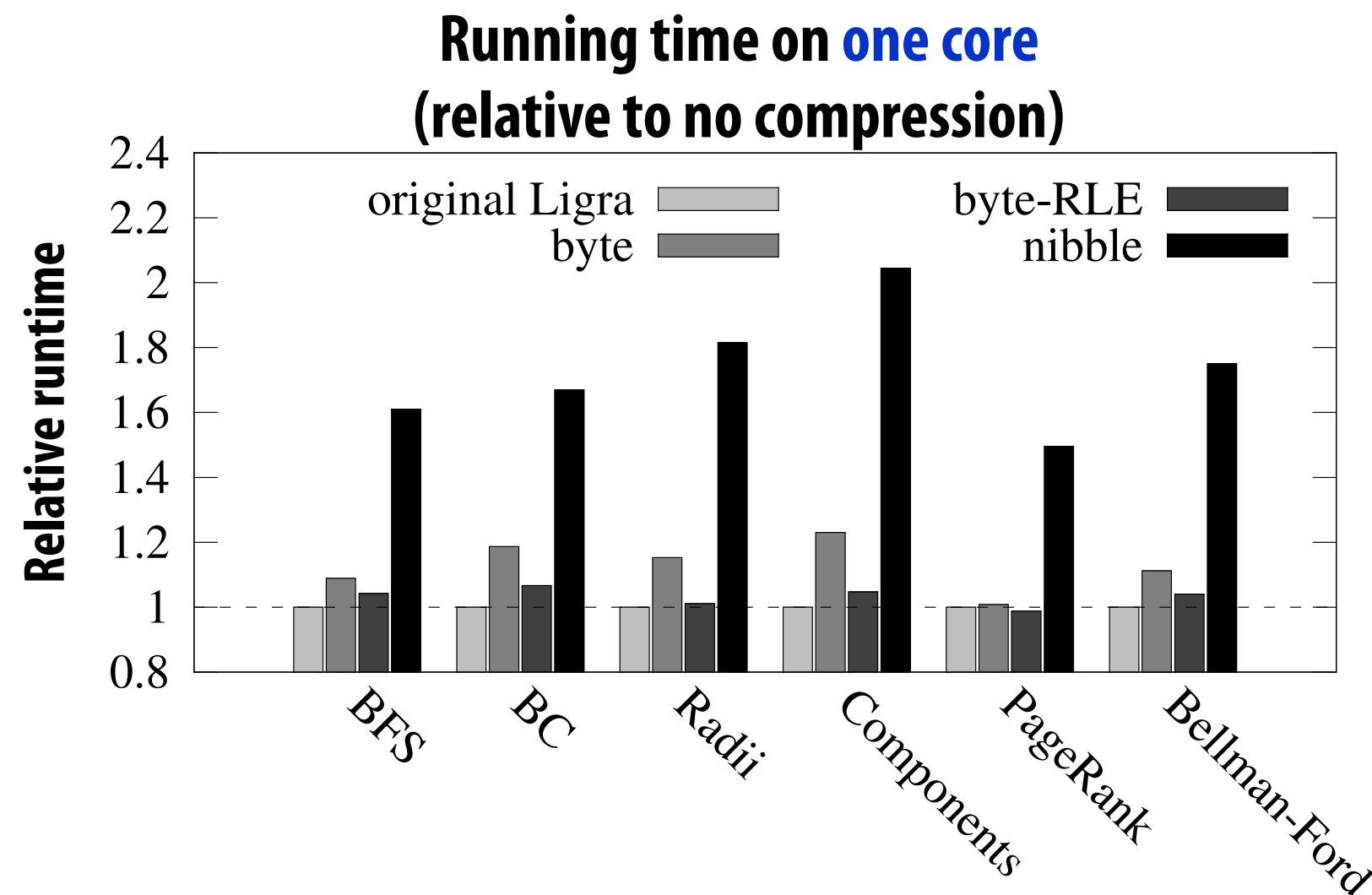
    6 bits: number of edges in group
    2 bits: encoding width (1, 2, 4 bytes)

    [ONE_BYTE, 4], -27, 1, 4, 20   (5 bytes)

    [TWO_BYTE, 1], 971   (3 bytes)

    [ONE_BYTE, 4], 9, 14, 1, 5   (5 bytes)

    [FOUR_BYTE, 3], 98070, 100000, 75000 (13 bytes)

Performance impact of graph compression

[Shun et al. DCC 2015]

Running time on one core
(relative to no compression)

Legend: original Ligra, byte, byte-RLE, nibble

Running time on 40 cores
(relative to no compression)

Legend: original Ligra, byte, byte-RLE, nibble

- ■ **Benefit of graph compression increases with higher core count**, since computation is increasingly bandwidth bound

- ■ **Performance improves even if graphs already fit in memory**
  - – Added benefit is that compression enables larger graphs to fit in memory

* Different data points on graphs are different compression schemes
(byte-RLE is the scheme on the previous slide)

Summary

- **Today there is significant interest in high performance computation on large graphs**

- **Graph processing frameworks abstract details of efficient graph processing from application developer**

  - **handle parallelism and synchronization for the application developer**

  - **handle graph distribution (across a cluster)**

  - **may also handle graph compression and efficient iteration order (e.g., to efficiently stream off slow storage)**

- **Great example of domain-specific programming frameworks**

  - **for more, see: GraphLab, GraphX, Pregel, Ligra/Ligra+**