

Lecture 20:

Domain-specific programming on graphs

**Parallel Computer Architecture and Programming
CMU 15-418/15-618, Fall 2024**

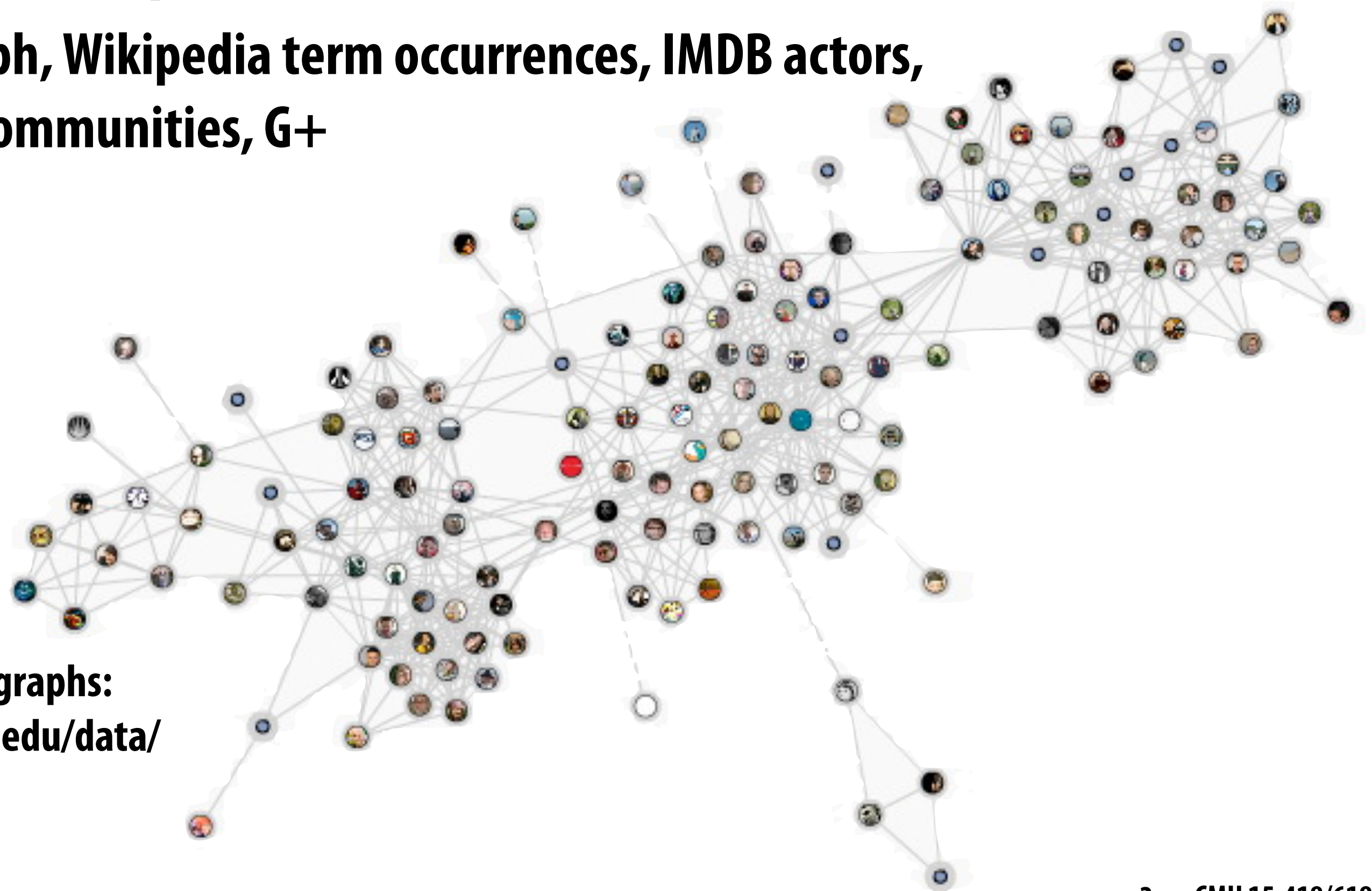
Today's topic: analyzing big graphs

- **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+

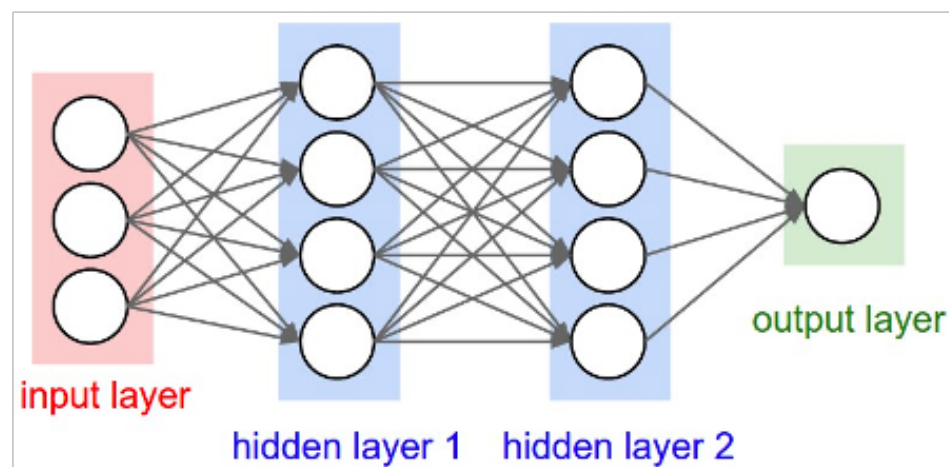


Good source of public graphs:
<https://snap.stanford.edu/data/>

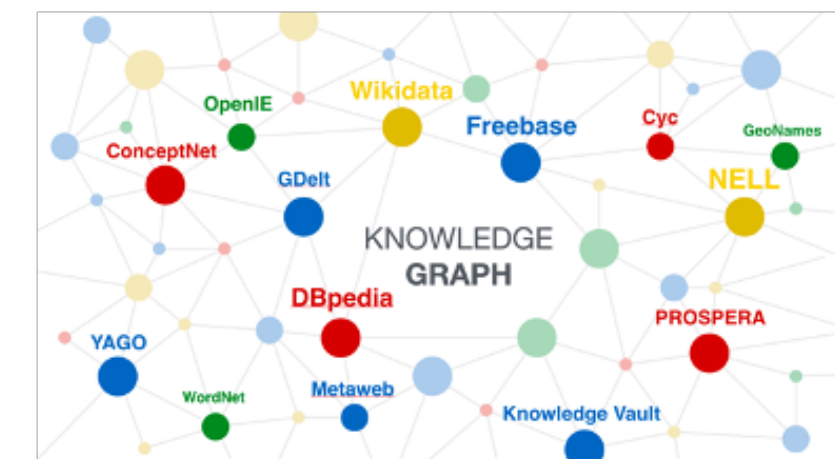
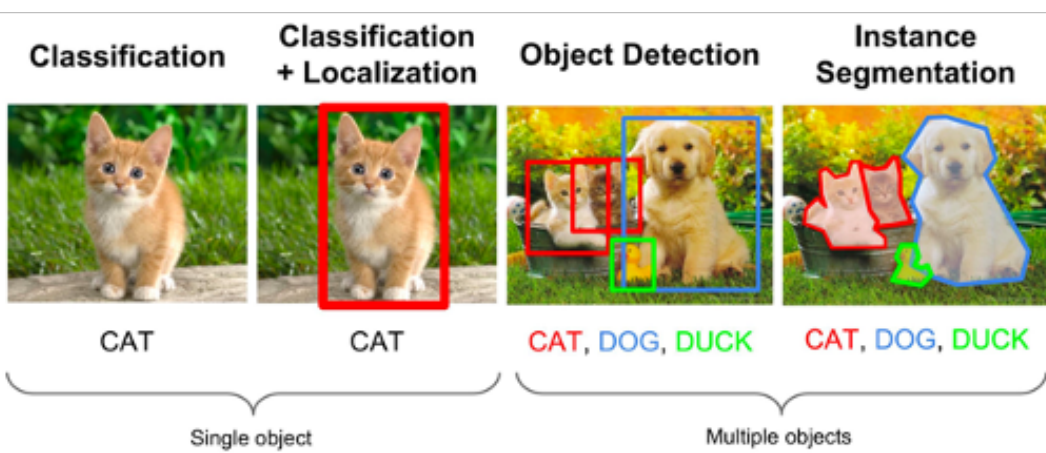
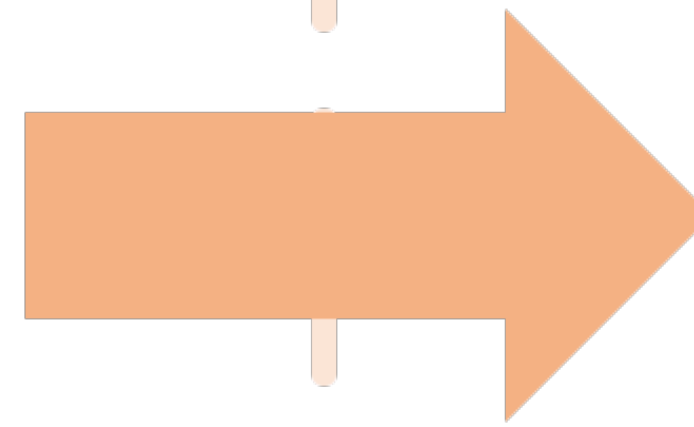
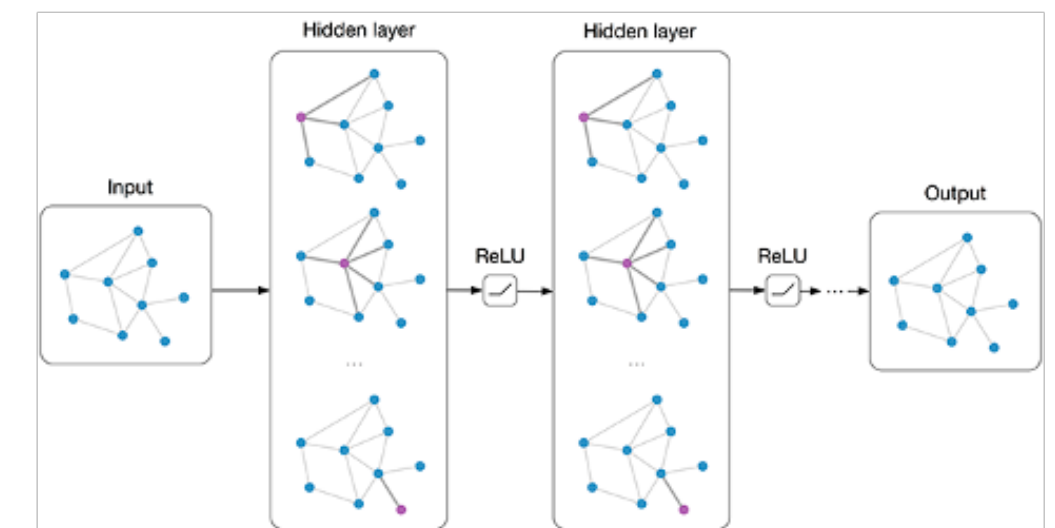
Today's topic: analyzing big graphs

Emerging interests in machine learning on graphs

Neural Networks



Graph Neural Networks



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)

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

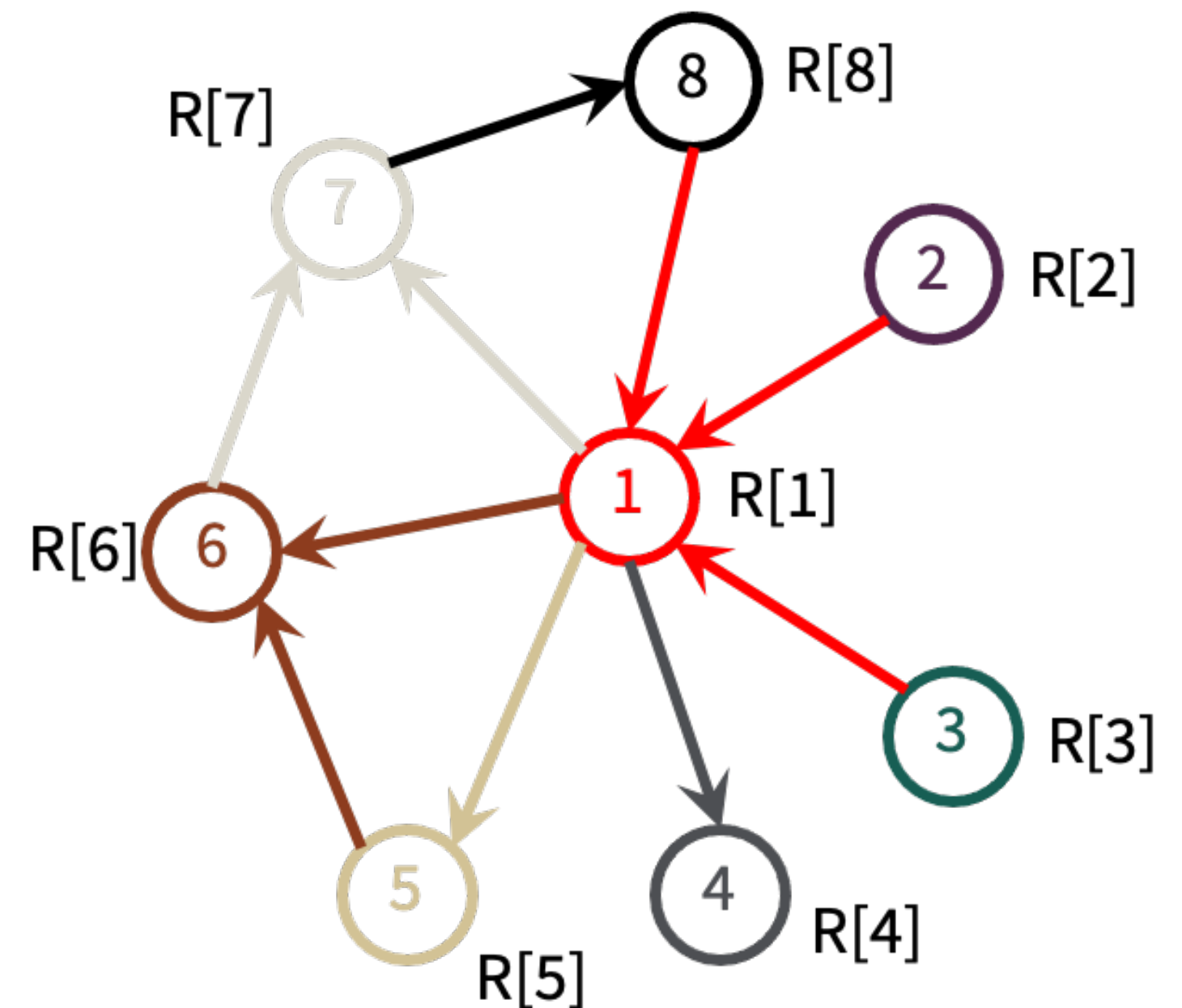
Graph edges = links between pages

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

Rank of page i

discount

Weighted combination of rank of pages that link to it



- A system for describing iterative 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** $u \rightarrow v$

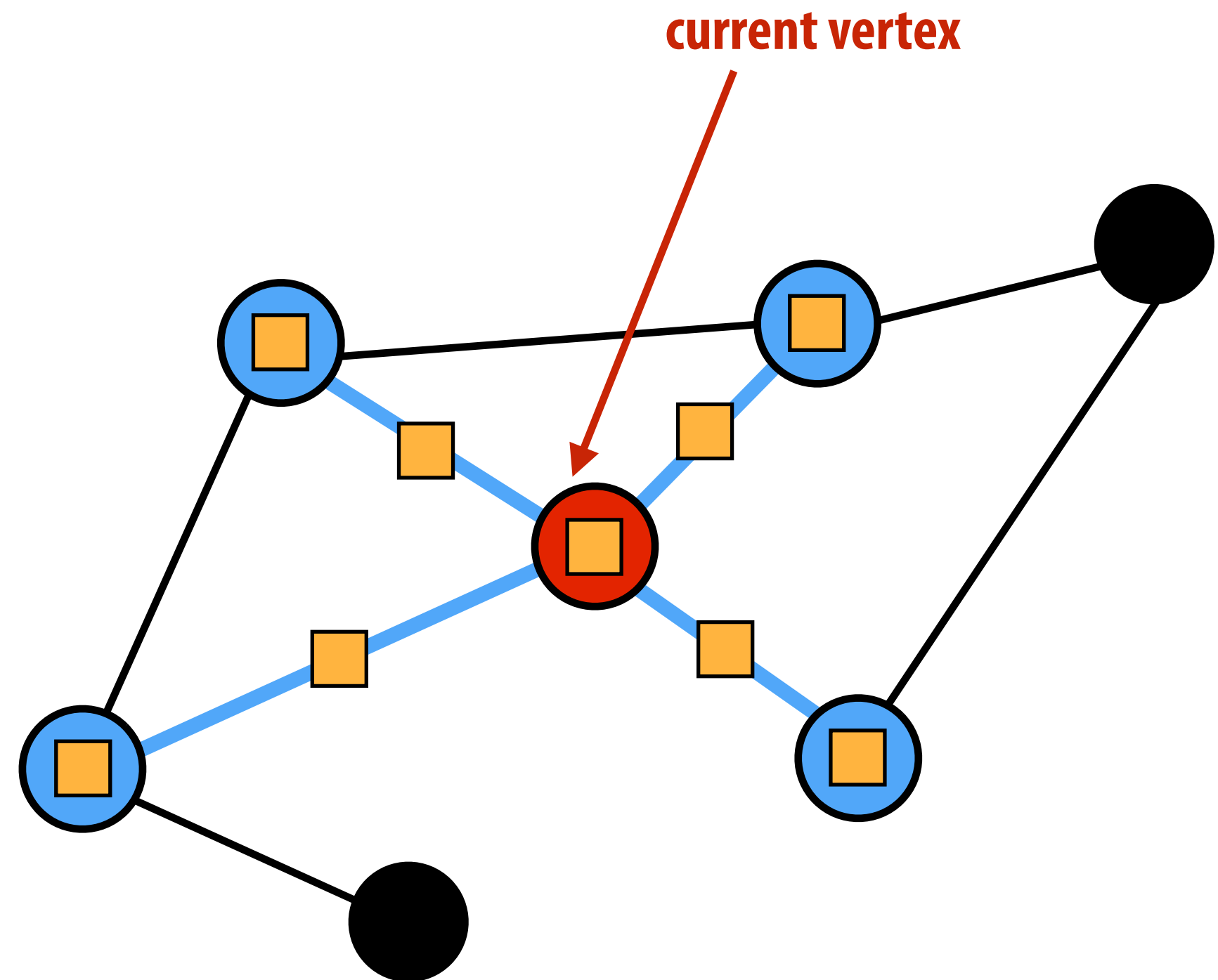
■ Read-only global data

- 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:

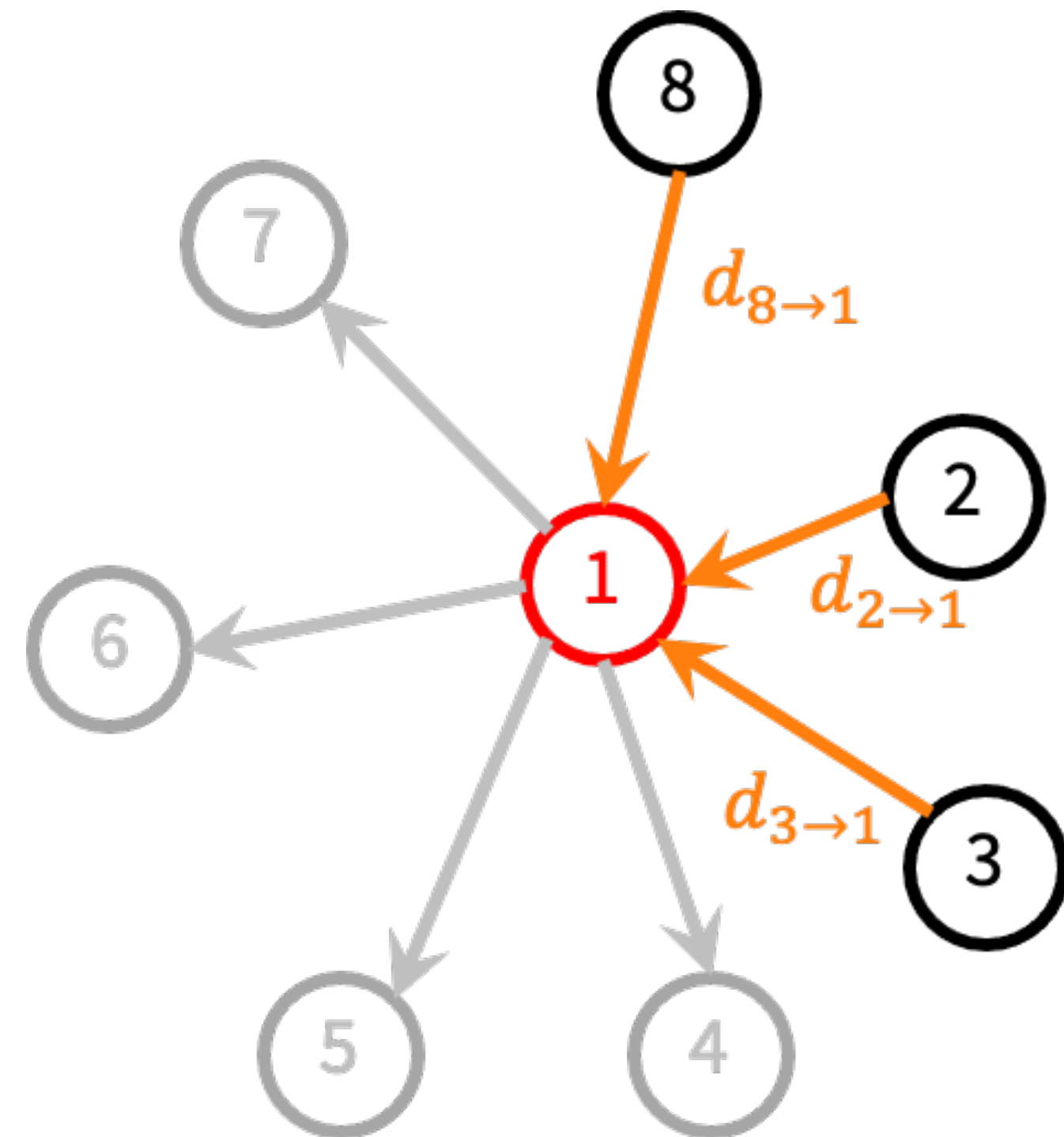
- The current vertex
- Adjacent edges
- Adjacent vertices



 = 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** $a_u = \sum_{v \in Nbrs} d_{v \rightarrow v}$

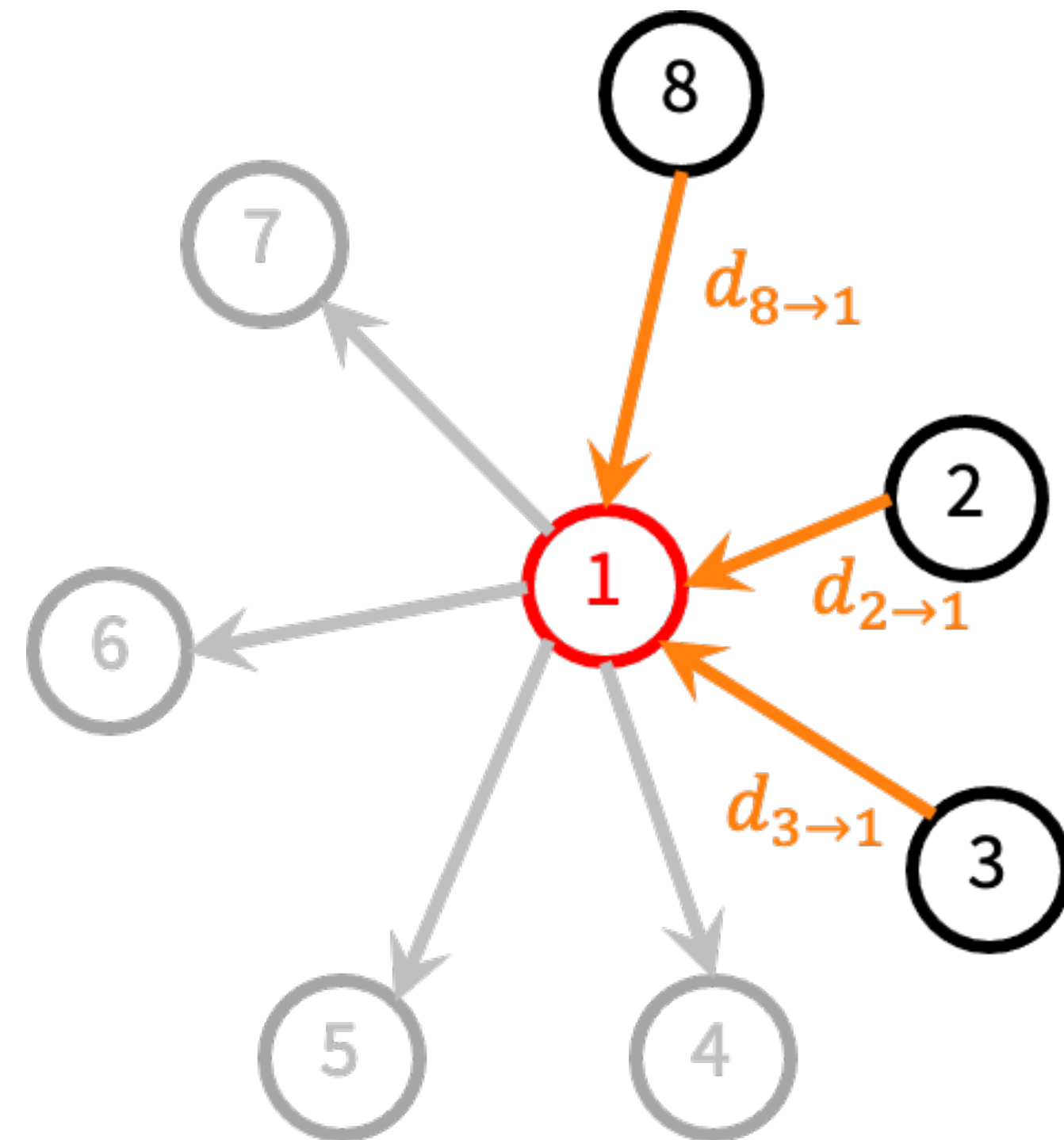


Gather-Apply Scatter (GAS)

- **Gather:** accumulate information from neighbors
- **Apply:** update the value of the central vertex

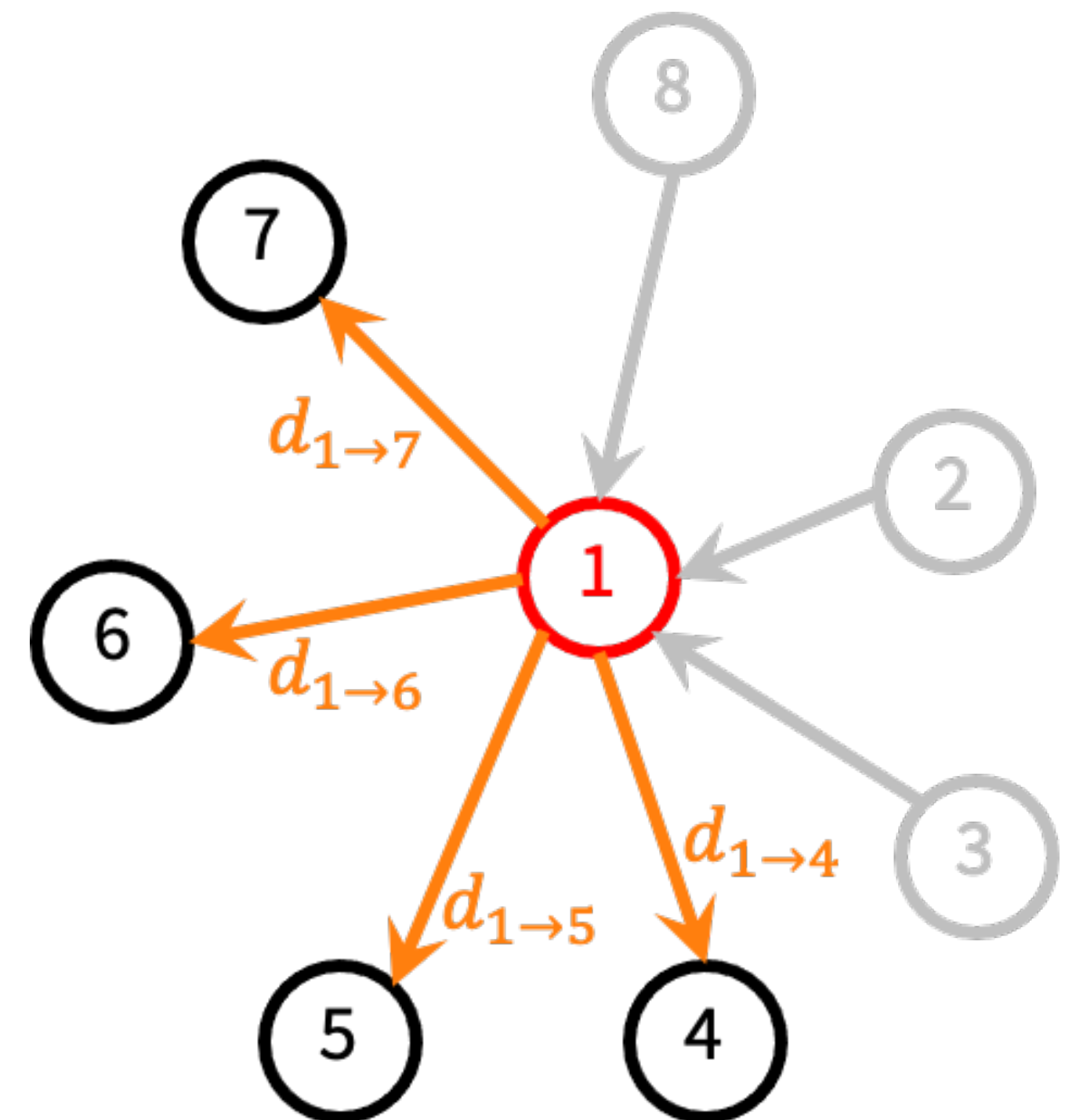
$$a_u = \sum_{v \in \text{Nbrs}} d_{v \rightarrow v}$$

$$d_u^{\text{new}} = \text{update}(d_u, a_u)$$



Gather-Apply Scatter (GAS)

- **Gather:** accumulate information from neighbors $a_u = \sum_{v \in Nbrs} d_{v \rightarrow v}$
- **Apply:** update the value of the central vertex $d_u^{new} = update(d_u, a_u)$
- **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)

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

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

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

```
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;  
}
```

Define edges to gather over in "gather phase"

```
// 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();  
}
```

Compute value to accumulate for each edge

```
// 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;  
}
```

Update vertex rank

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

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) { }
}
```

Per-vertex “counter”



```
// 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();
}
```

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**)

```
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

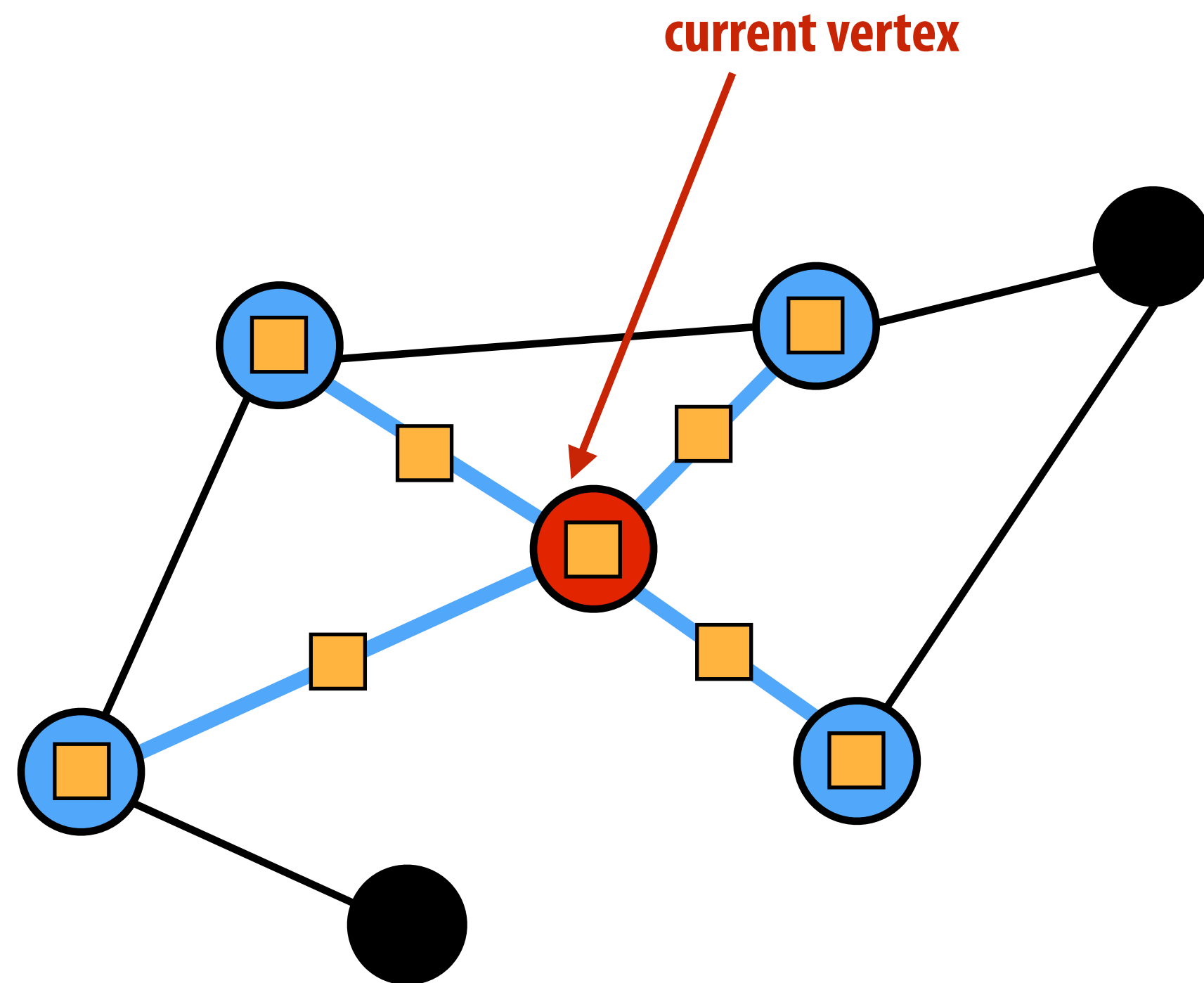
```
    // Scatter now needed if algorithm has not converged  
    edge_dir_type scatter_edges(icontext_type& context,  
                                const vertex_type& vertex) const {  
        if (perform_scatter) return graphlab::OUT_EDGES;  
        else return graphlab::NO_EDGES;  
    }
```

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

 Schedule update of
neighbor vertices

Synchronizing parallel execution

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



 = vertex or edge data in scope of red vertex

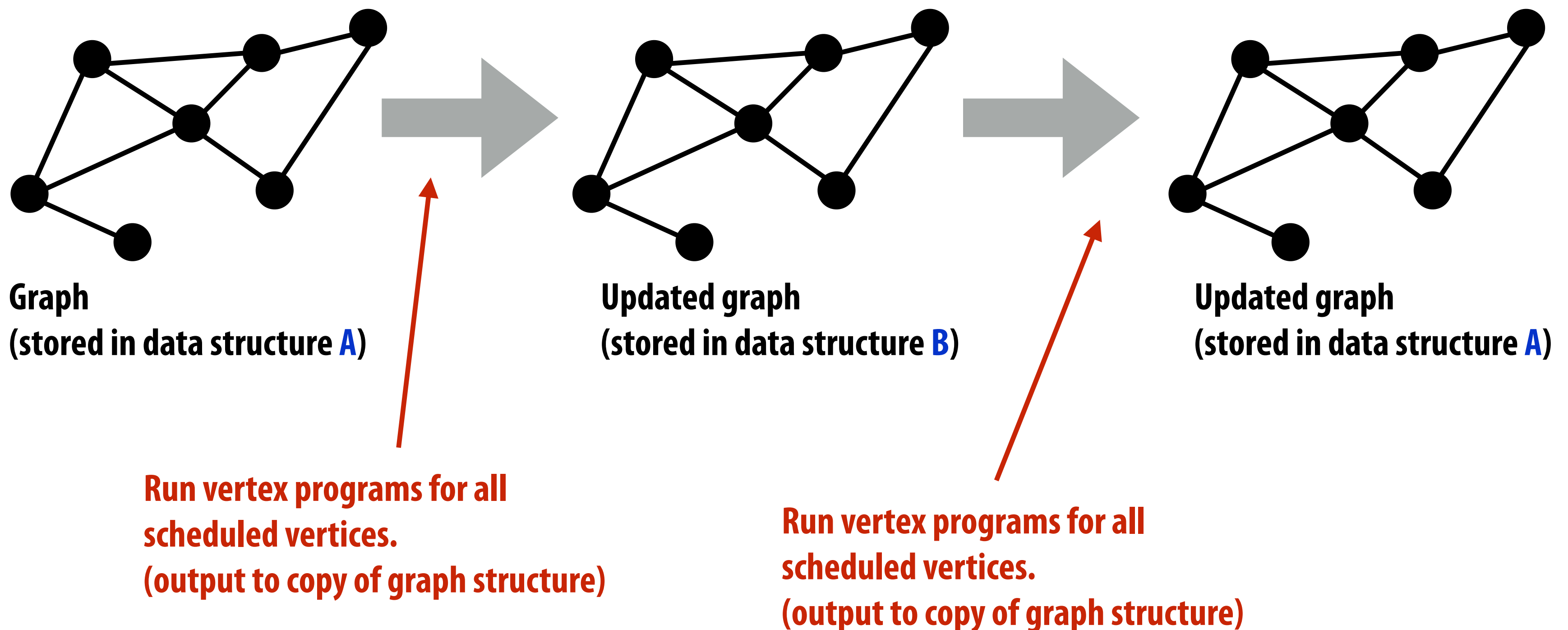
Programs specify what **granularity of atomicity** ("consistency") they want
GraphLab runtime to provide: this determines amount of available parallelism

- **"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”)



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**
 - **Implication**: 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

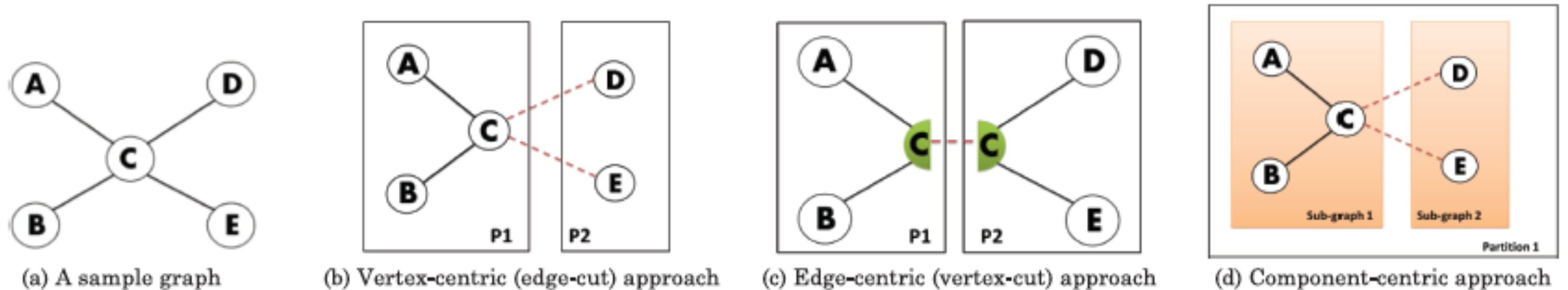


Figure: Safiollah Heidari, Yogesh Simmhan, Rodrigo N. Calheiros, and Rajkumar Buyya. 2018. Scalable Graph Processing Frameworks: A Taxonomy and Open Challenges. ACM Comput. Surv. 51, 3, Article 60 (June 2018).

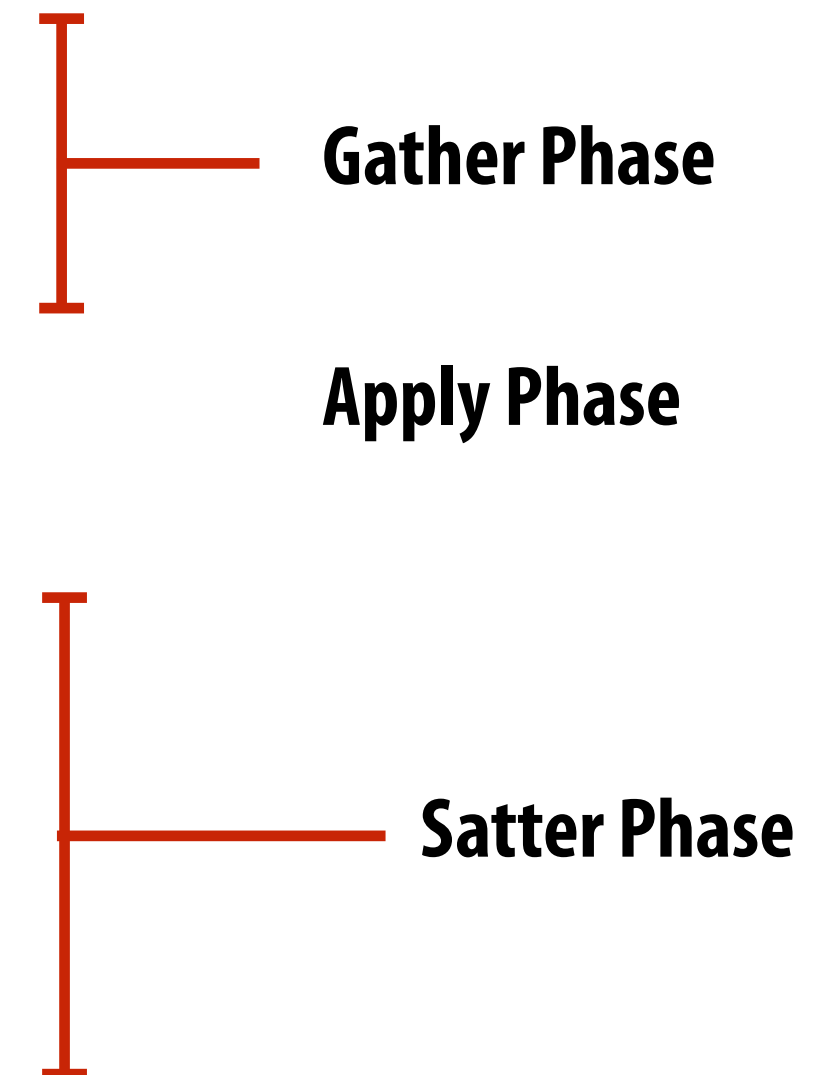
- **Vertex** centric: GraphLab, Pregel, GPS
- **Edge** centric: Chaos, X-Stream
- **Sub-graph** centric: Giraph++, GoFish

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

PageRank in Pregel

```
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();
    }
  }
};
```



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

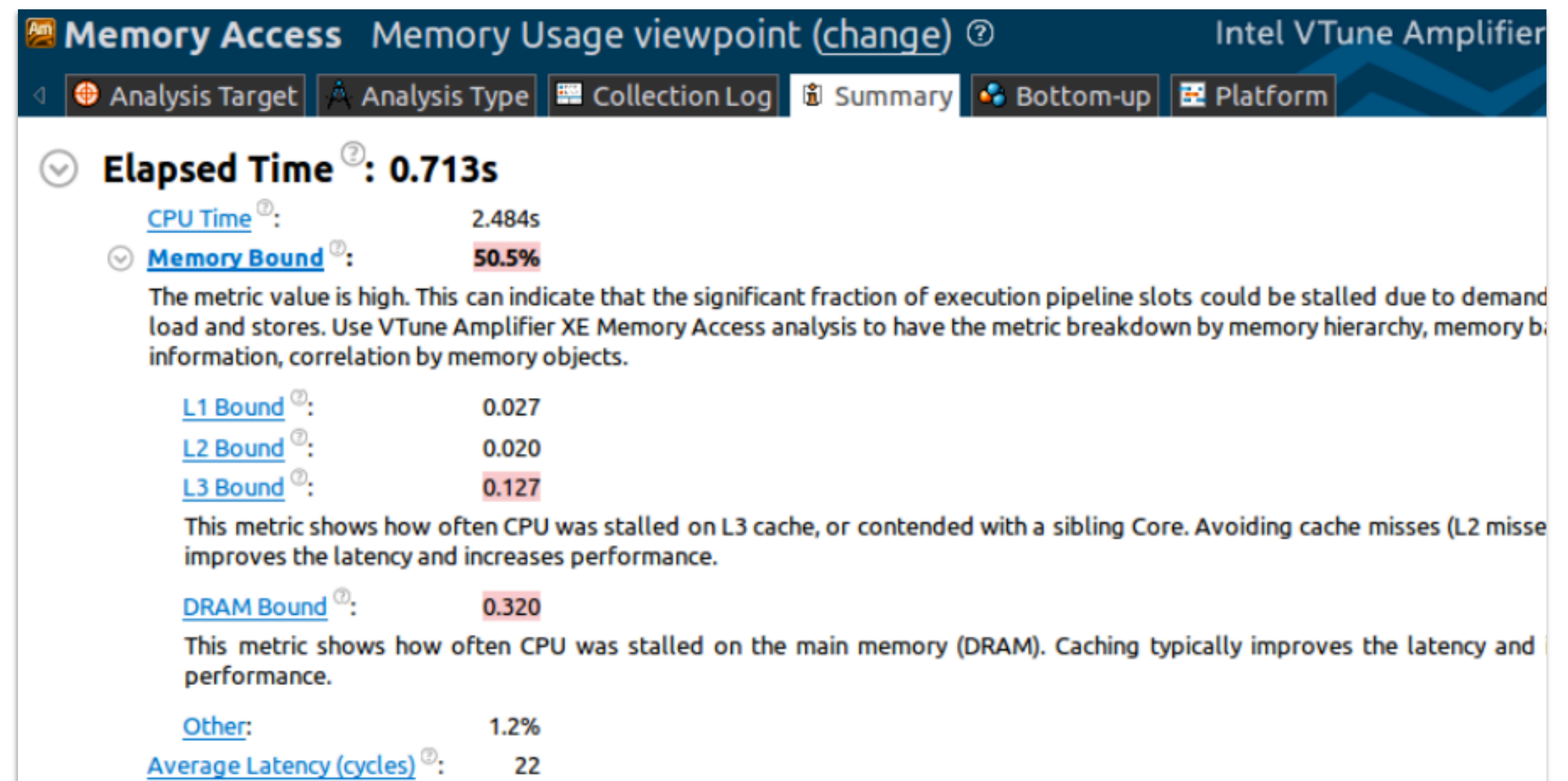
(now we are talking about implementation)

Wait a minute...

- So far in this lecture, we've discussed issues such as parallelism, synchronization ...
- But graph processing typically has **low arithmetic intensity**

Walking over edges accesses information from "random" graph vertices

VTune profiling results: Memory bandwidth bound!



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 *

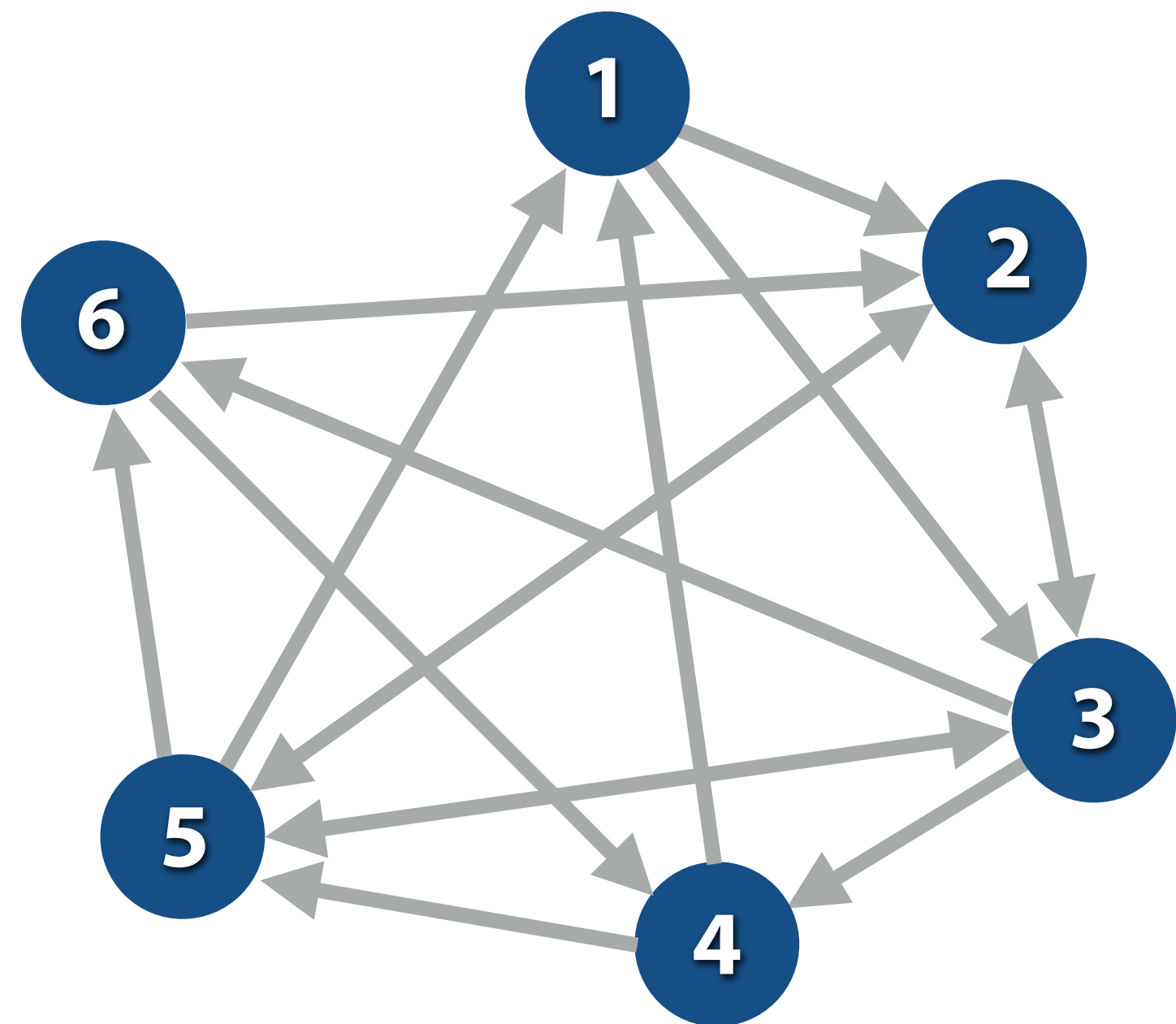
1. Reorganize graph structure to **increase locality**
2. **Compress** the graph

* 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

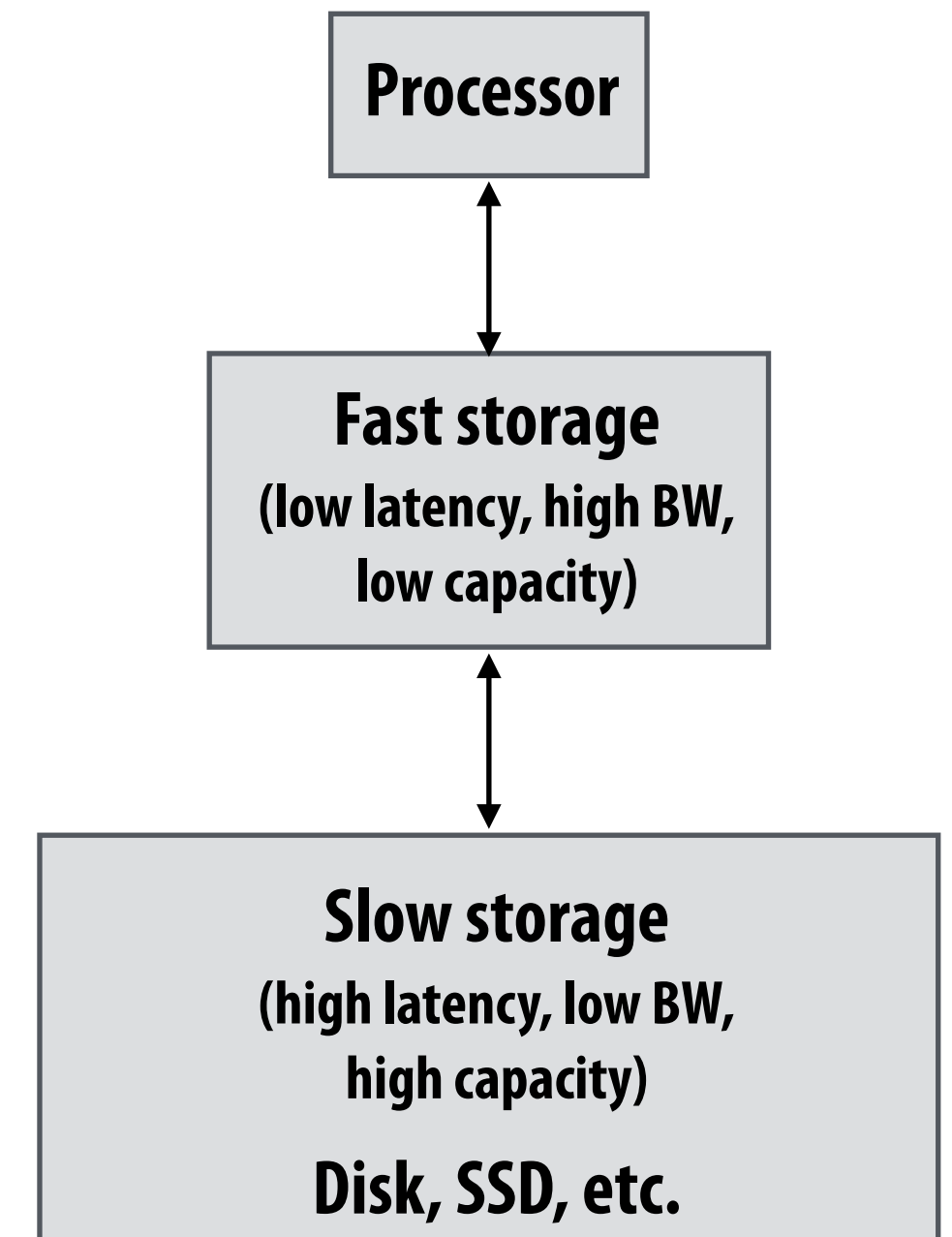
- **Challenge: cannot fit all edges in memory for large graphs (graph vertices may fit)**
 - From example graph representation:
 - Each edge represented twice in graph structure (as incoming/outgoing edge)
 - 8 bytes per edge to represent adjacency
 - May also need to store per-edge values (e.g., 4 bytes 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 be 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?**



* 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

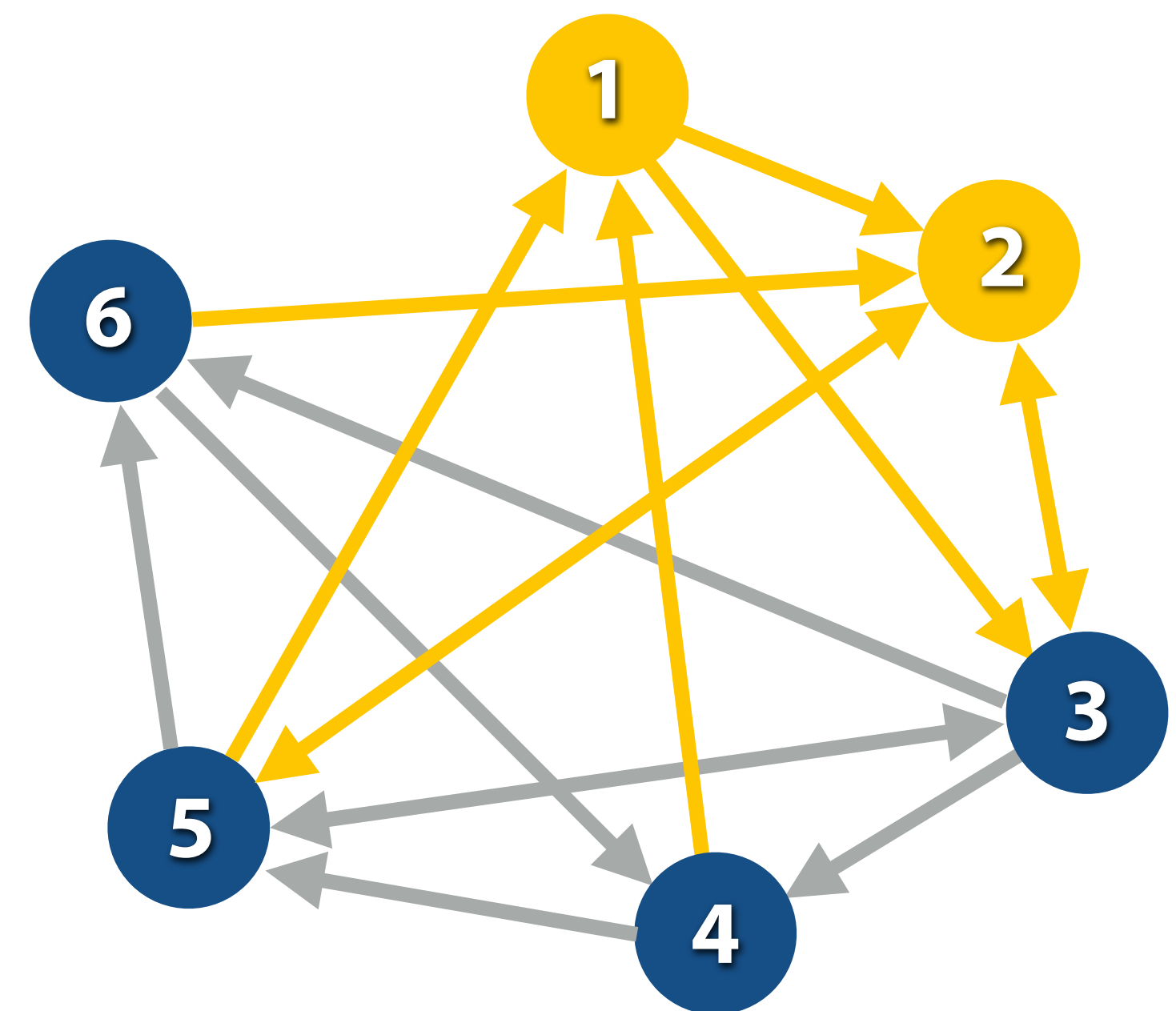
Sharded graph representation

GraphChi: Large-scale graph computation on just a PC
[Kryola et al. 2013]

- **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)			Shard 2: vertices (3-4)			Shard 3: vertices (5-6)		
src	dst	value	src	dst	value	src	dst	value
1	2	0.3	1	3	0.4	2	5	0.6
3	2	0.2	2	3	0.9	3	5	0.9
4	1	0.8	3	4	0.15	4	6	0.85
5	1	0.25	5	3	0.2	5	6	0.3
	2	0.6	6	4	0.9	6	5	0.2
6	2	0.1						

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

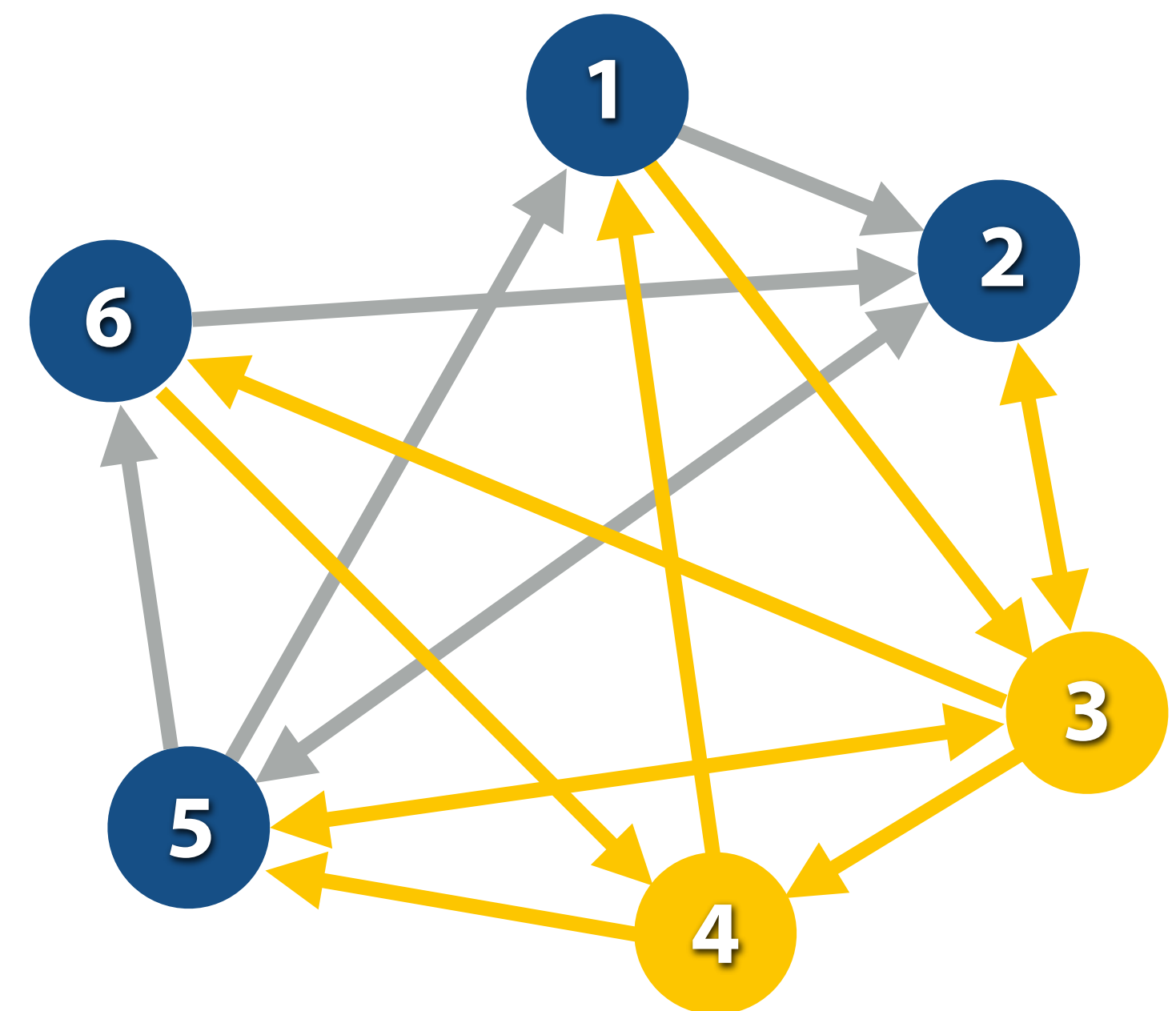
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- **Partition** graph vertices into intervals (sized so that subgraph for interval fits in memory)
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Shard 1: vertices (1-2)			Shard 2: vertices (3-4)			Shard 3: vertices (5-6)		
src	dst	value	src	dst	value	src	dst	value
1	2	0.3	1	3	0.4	2	5	0.6
3	2	0.2	2	3	0.9	3	5	0.9
4	1	0.8	3	4	0.15	6	6	0.85
5	1	0.25	5	3	0.2	4	5	0.3
	2	0.6	6	4	0.9	5	6	0.2
6	2	0.1						

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



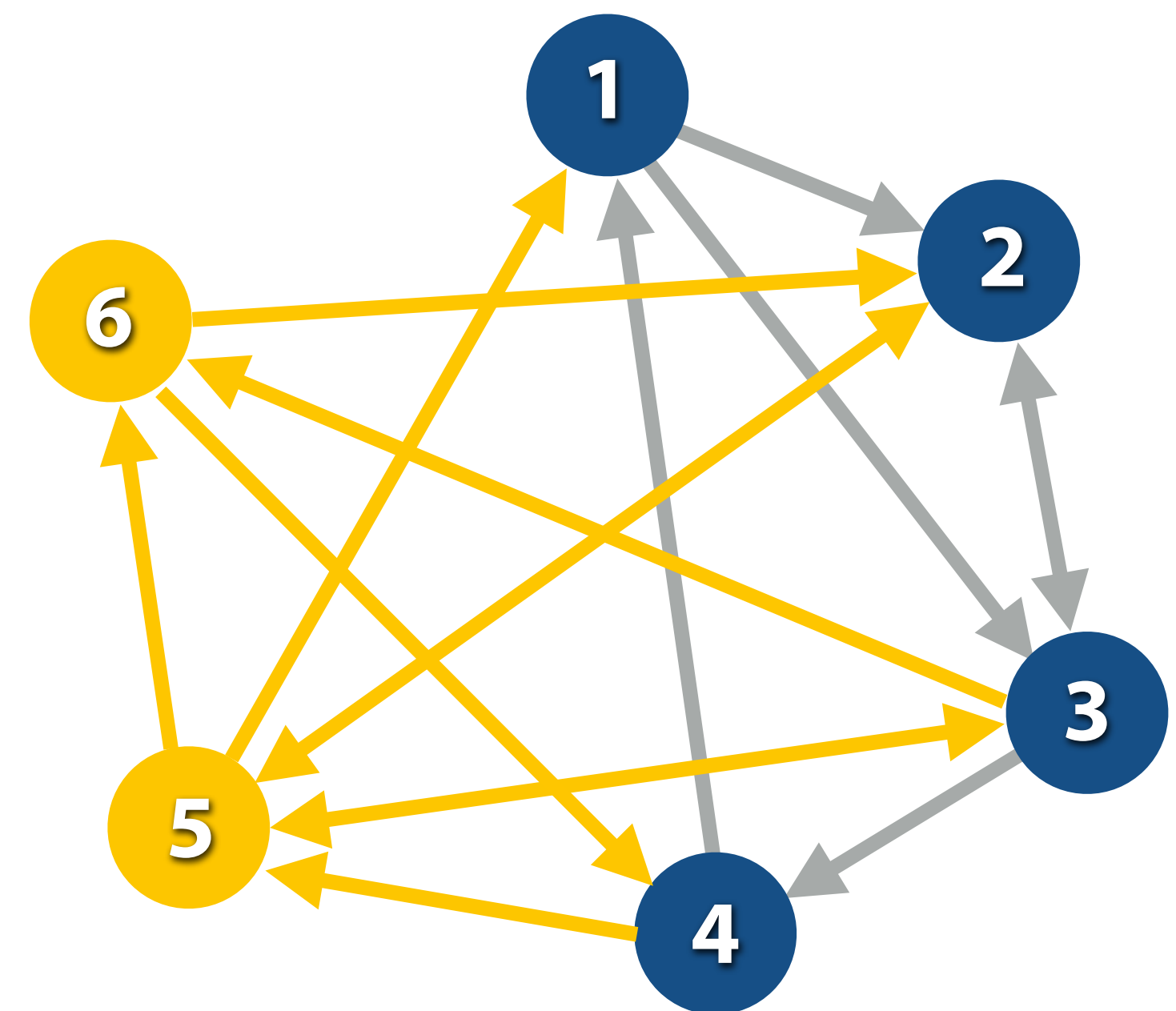
Sharded graph representation

GraphChi: Large-scale graph computation on just a PC [Kryola et al. 2013]

- **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)			Shard 2: vertices (3-4)			Shard 3: vertices (5-6)		
src	dst	value	src	dst	value	src	dst	value
1	2	0.3	1	3	0.4	2	5	0.6
3	2	0.2	2	3	0.9	3	5	0.9
4	1	0.8	3	4	0.15	6	0.85	
5	1	0.25	5	3	0.2	4	5	0.3
	2	0.6	6	4	0.9	5	6	0.2
6	2	0.1						

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:

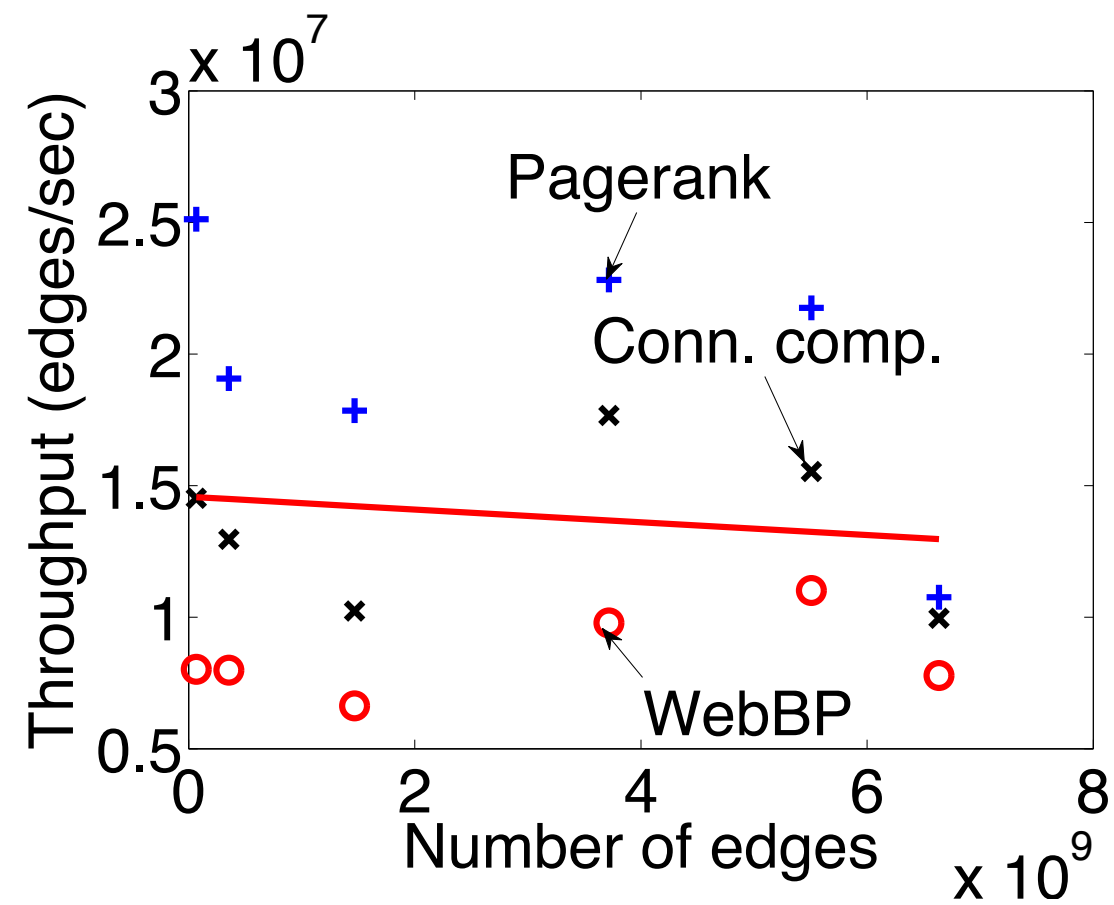
```
1 typedef: VertexType float
2 Update(vertex) begin
3   | var sum ← 0
4   | for e in vertex.inEdges() do
5   |   | sum += e.weight * neighborRank(e)
6   | end
7   | vertex.setValue(0.15 + 0.85 * sum)
8   | broadcast(vertex)
9 end
```

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

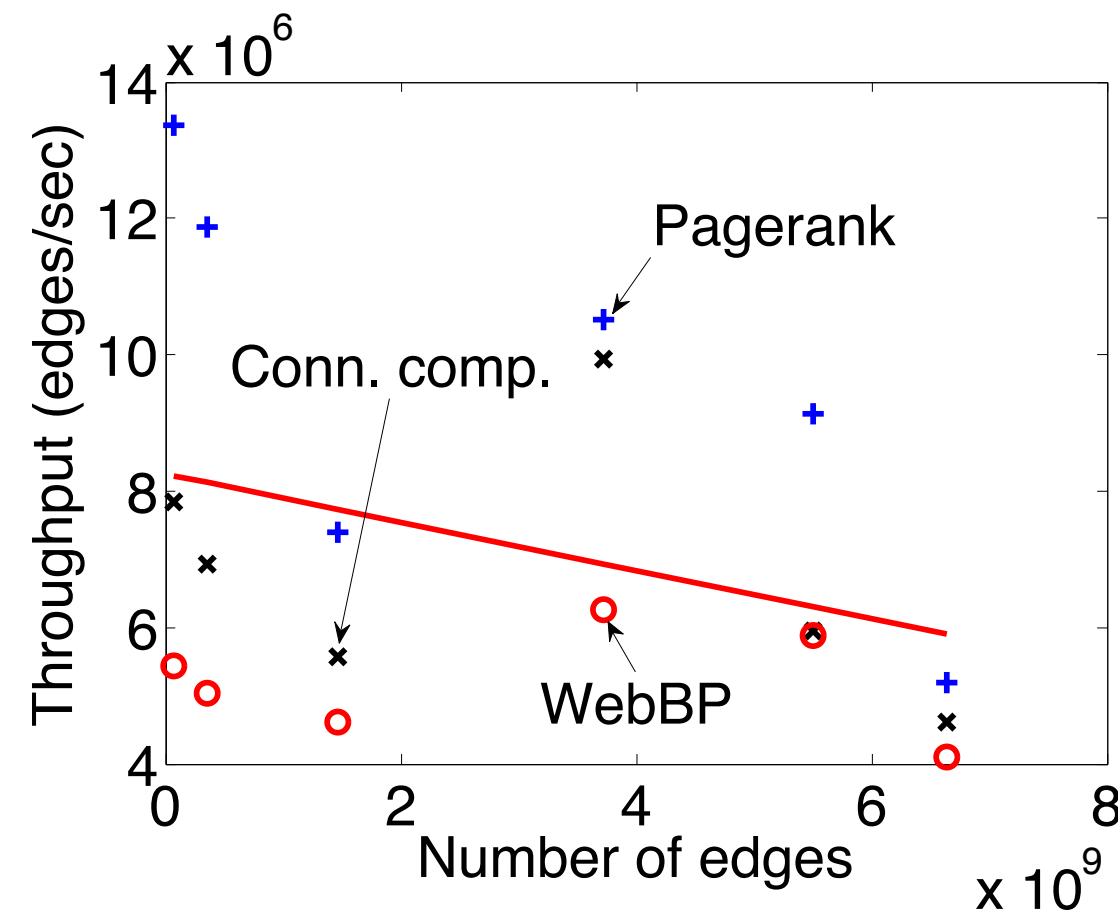
Alternative model: assume vertex data can be kept in memory and redefine neighborRank() function

```
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
```

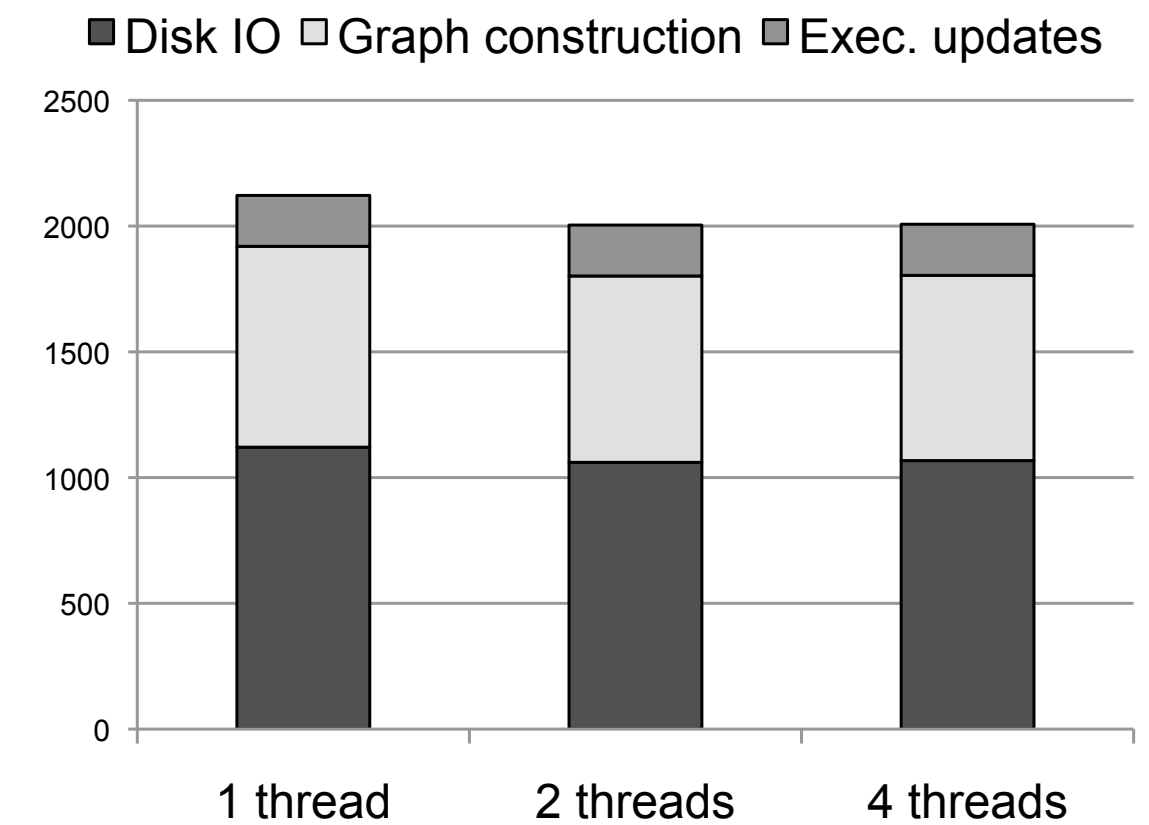
Performance on a Mac mini (8 GB RAM)



(a) Performance: SSD



(b) Performance : Hard drive



(c) Runtime breakdown

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

- **Desirable property: throughput largely invariant of dataset size**

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 vertex index

5 6 10 30 1001 1010 1024 1025 1030 100000 200000 275000
-27 1 4 20 971 9 14 1 5 98070 100000 75000

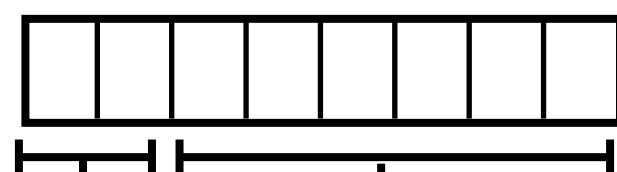
1 byte 2 bytes 1 byte 4 bytes

4. Encode deltas

Uncompressed encoding: 12 x 4 bytes = 48 bytes

Compressed encoding: 26 bytes

1-byte group header



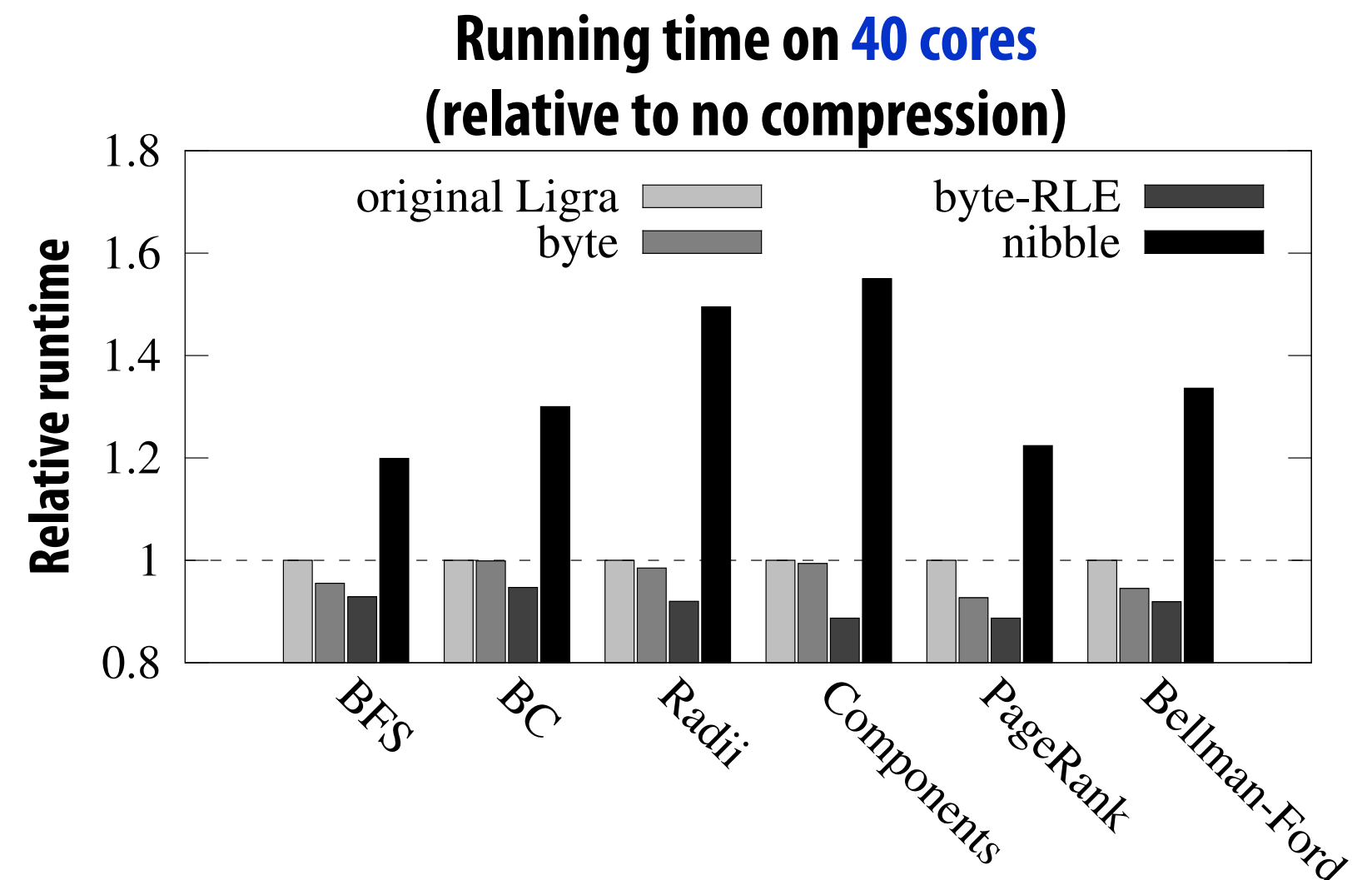
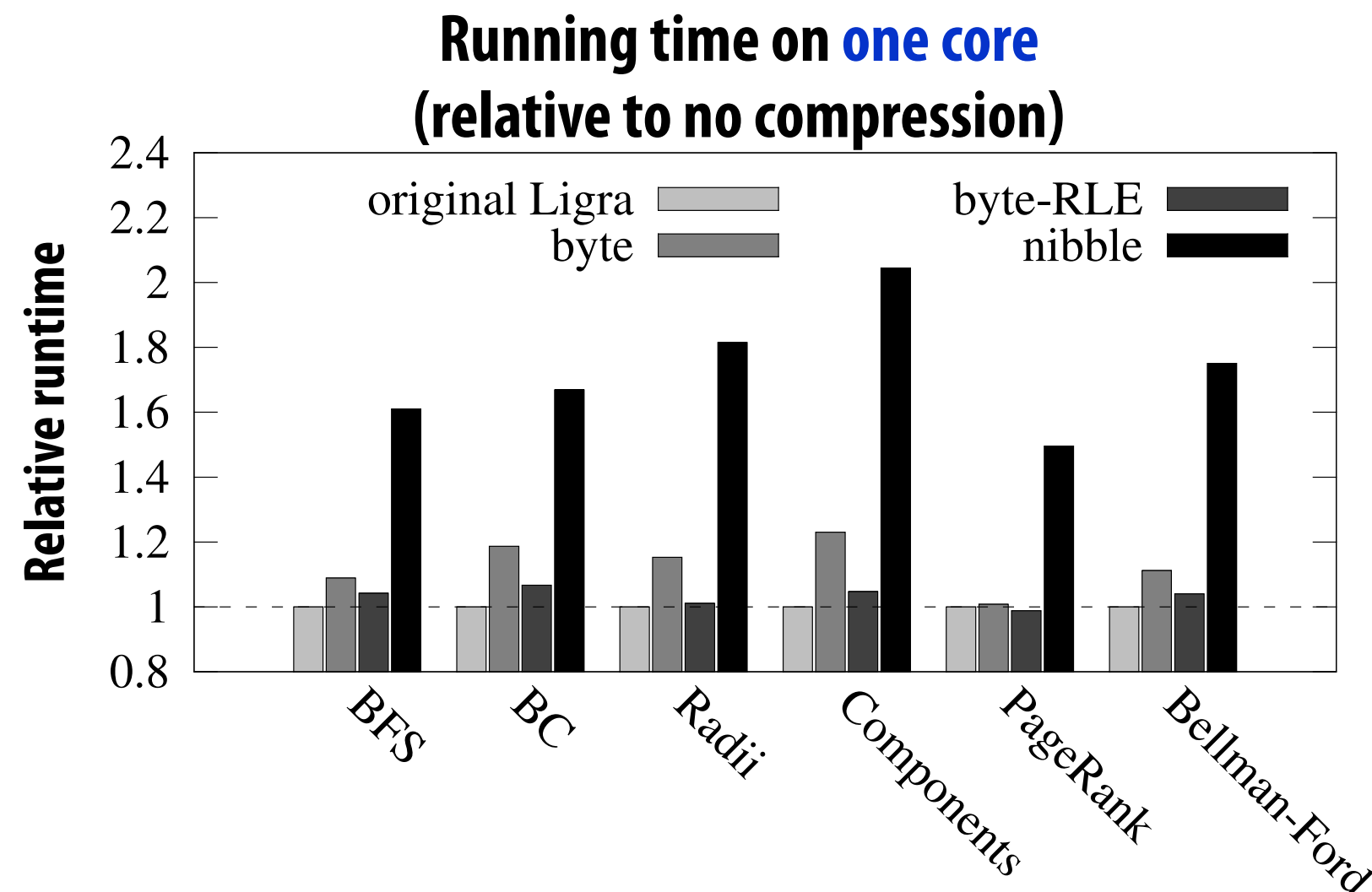
6 bits: number of edges in group

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]



- **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+**