GraphBLAS: concepts, algorithms, and applications

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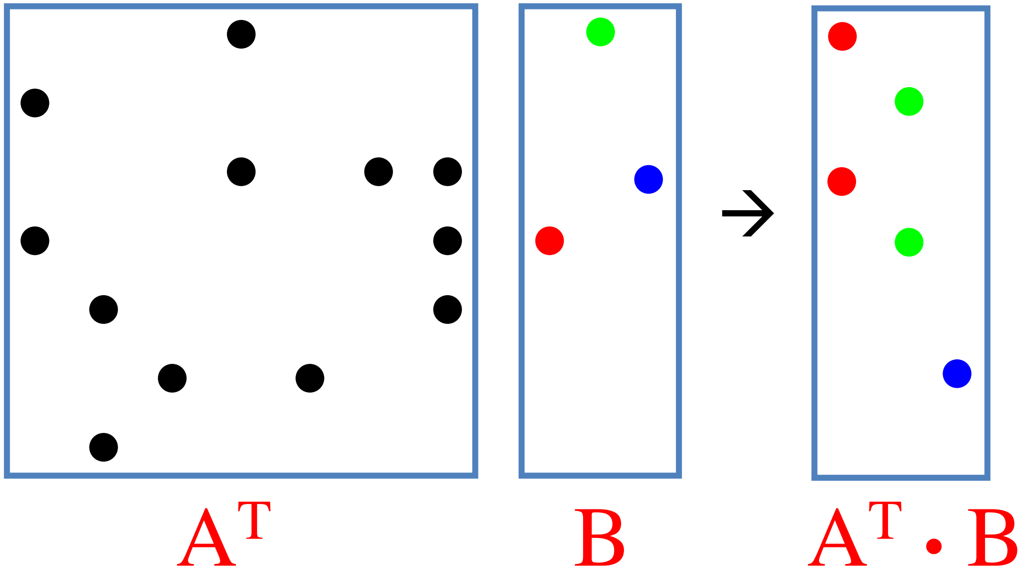
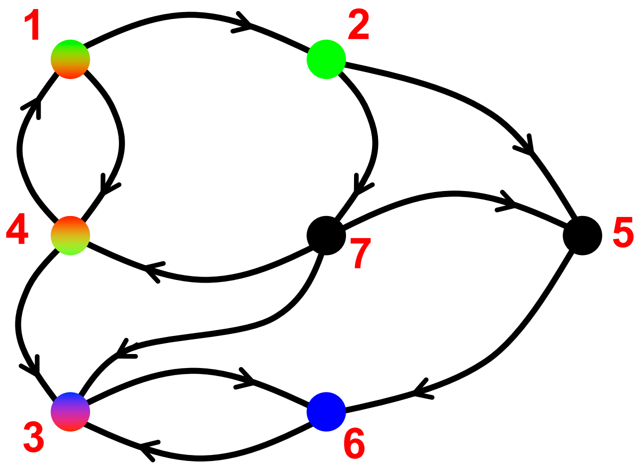
14th Scheduling Workshop
June 27, 2019. Bordeaux

Graphs in the language of matrices



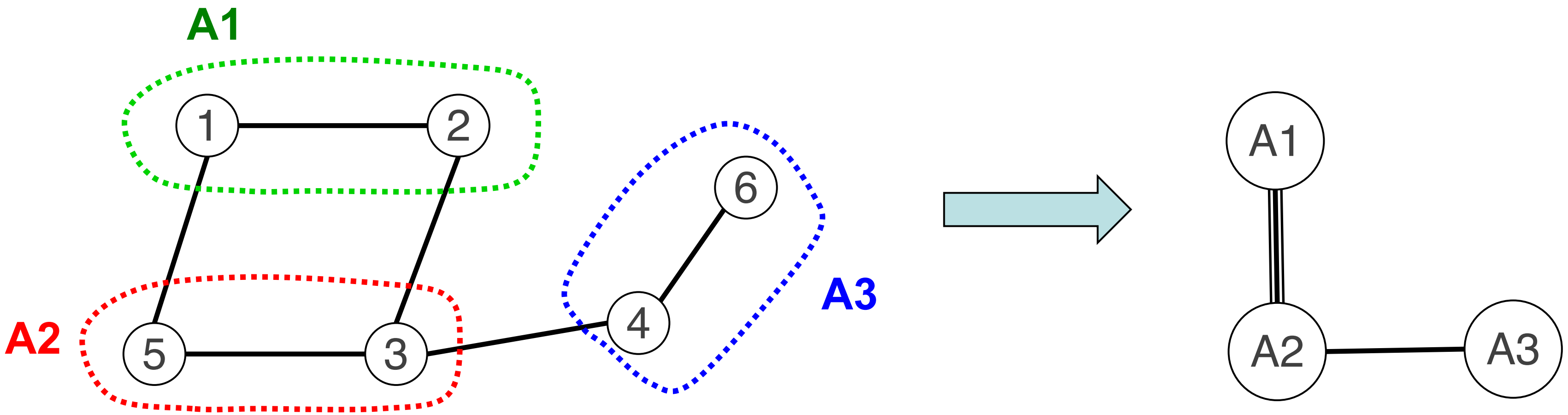


- Sparse array representation => space efficient
- Sparse matrix-matrix multiplication => work efficient
- Three possible levels of parallelism: searches, vertices, edges
- Highly-parallel implementation for Betweenness Centrality*

*: A measure of influence in graphs, based on shortest paths

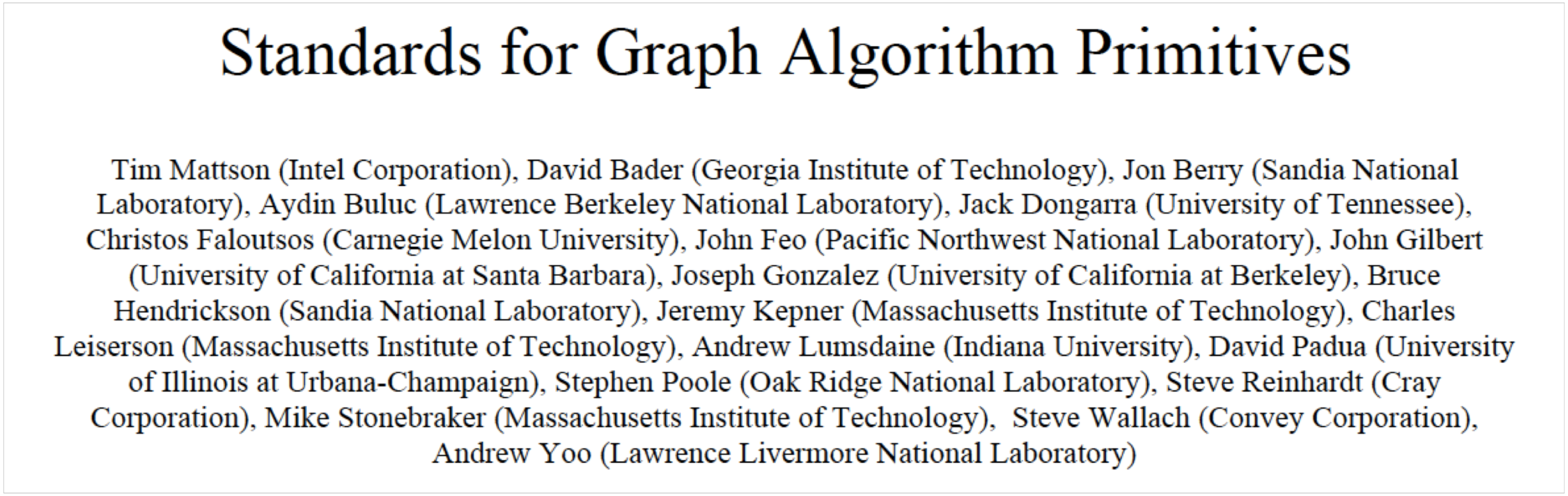
Coarsening via sparse matrix-matrix products

$$\begin{bmatrix} 1 & 1 & & & & \\ & & 1 & & 1 & \\ & & & 1 & & 1 \end{bmatrix} \times \begin{array}{c|cccccc} & 1 & 2 & 3 & 4 & 5 & 6 \\ \hline 1 & & \bullet & & & \bullet & \\ 2 & \bullet & & \bullet & & & \\ 3 & & \bullet & & \bullet & \bullet & \\ 4 & & & \bullet & & & \bullet \\ 5 & \bullet & & \bullet & & & \\ 6 & & & & \bullet & & \end{array} \times \begin{bmatrix} 1 & & \\ 1 & & \\ & 1 & \\ & & 1 \\ & 1 & \\ & & 1 \end{bmatrix} = \begin{bmatrix} & 2 & \\ 2 & & 1 \\ & 1 & \end{bmatrix}$$



Aydin Buluç and John R. Gilbert. Parallel sparse matrix-matrix multiplication and indexing: Implementation and experiments. *SIAM Journal of Scientific Computing (SISC), 2012*.

The GraphBLAS effort



Standards for Graph Algorithm Primitives

Tim Mattson (Intel Corporation), David Bader (Georgia Institute of Technology), Jon Berry (Sandia National Laboratory), Aydin Buluc (Lawrence Berkeley National Laboratory), Jack Dongarra (University of Tennessee), Christos Faloutsos (Carnegie Melon University), John Feo (Pacific Northwest National Laboratory), John Gilbert (University of California at Santa Barbara), Joseph Gonzalez (University of California at Berkeley), Bruce Hendrickson (Sandia National Laboratory), Jeremy Kepner (Massachusetts Institute of Technology), Charles Leiserson (Massachusetts Institute of Technology), Andrew Lumsdaine (Indiana University), David Padua (University of Illinois at Urbana-Champaign), Stephen Poole (Oak Ridge National Laboratory), Steve Reinhardt (Cray Corporation), Mike Stonebraker (Massachusetts Institute of Technology), Steve Wallach (Convey Corporation), Andrew Yoo (Lawrence Livermore National Laboratory)

Abstract-- It is our view that the state of the art in constructing a large collection of graph algorithms in terms of linear algebraic operations is mature enough to support the emergence of a standard set of primitive building blocks. This paper is a position paper defining the problem and announcing our intention to launch an open effort to define this standard.

- The GraphBLAS Forum: http://graphblas.org
- Graphs: Architectures, Programming, and Learning (GrAPL @IPDPS): http://hpc.pnl.gov/grapl/

GraphBLAS Status: C API 1.2 released <u>and</u> in use

- Implementations of the GraphBLAS C specification:
  - SuiteSparse http://faculty.cse.tamu.edu/davis/suitesparse.html
  - IBM https://github.com/IBM/ibmgraphblas
  - Test suite for validating an implementation of the C-spec from SEI/CMU

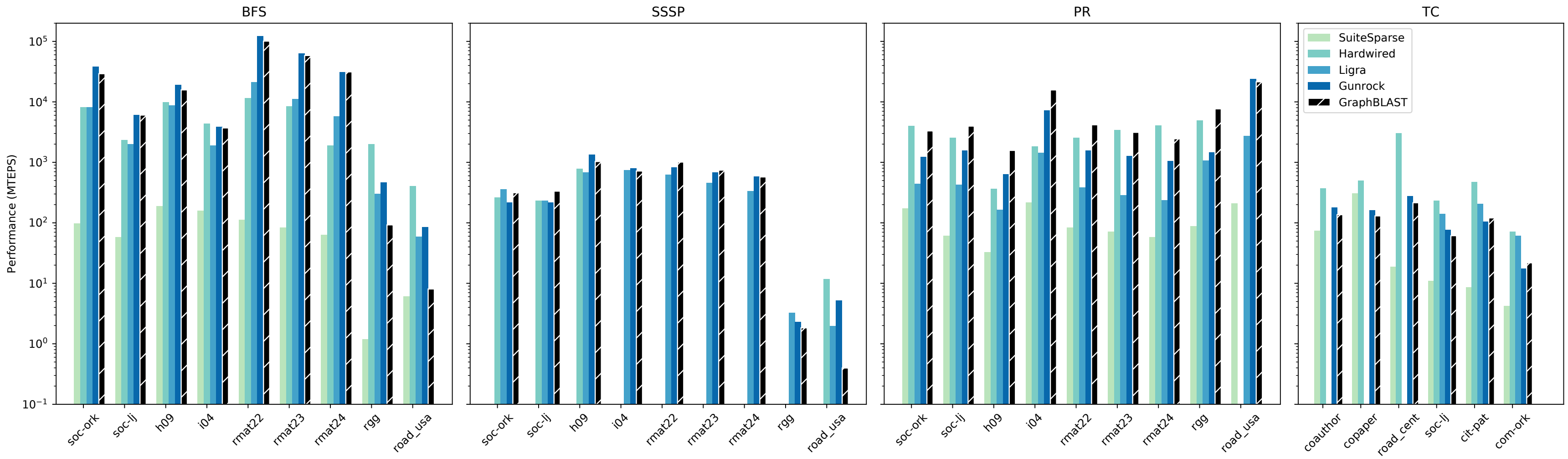
    … to be released “soon”

- Systems using the GraphBLAS
  - RedisGraph v1.0 preview release:
    - RedisGraph is a graph database architecture implemented as a Redis Module, using GraphBLAS sparse matrices for internal data representation and linear algebra for query execution.
    - https://redislabs.com/blog/release-redisgraph-v1-0-preview/
  - Lincoln Labs GraphProcessor designed around the GraphBLAS.

- C++ bindings to the GraphBLAS
  - GBTL from SEI/CMU: https://github.com/cmu-sei/gbtl
  - GraphBLAST for GPUs: http://github.com/gunrock/graphblast

GraphBLAST preliminary performance

[contact me for preprint]



Shown applications (more implemented)

- Breadth-first-search (BFS)
- Single-source shortest-path (SSSP)
- PageRank (PR)
- Triangle counting (TC)

Design principles:

1. Exploit input sparsity => direction-optimization
2. Exploit output sparsity => masking
3. Proper load-balancing => key for GPU implementations

GraphBLAS C API

- A binding of the GraphBLAS math to the C programming language.

- Requires C99 extended with function polymorphism based on static-types and number-of-parameters.
  - All modern C compilers in common use today support these extensions

- Basic include file with function prototypes, types, and constants
  - `#include <GraphBLAS.h>`

- Includes a few types and opaque objects (e.g. matrices and vectors) to give implementations maximum flexibility

  `GrB_Index` → An integer type used to set dimensions and index into arrays

  `GrB_Matrix` → A 2D sparse array, row indices, column indices and values

  `GrB_Vector` → A 1D sparse Array

  - … plus additional opaque objects we'll describe later (descriptors, semirings, binary operators, and unary operators)

GraphBLAS C API: Basic definitions

- **Opaque object**: An object manipulated strictly through the GraphBLAS API whose implementation is not defined by the GraphBLAS specification.

- **Transparent object**: an object whose structure is fully exposed to the programmer. E.g.: an array of tuples <i, j, value>

- **Method**: Any C function that manipulates a GraphBLAS opaque object.

- **Domain**: the set of available values used for the elements of matrices, the elements of vectors, and when defining operators.
  - Examples are `GrB_UINT64, GrB_INT32, GrB_BOOL, GrB_FP32`

- **Operation**: a method that corresponds to an operation defined in the GraphBLAS math spec. http://www.mit.edu/~kepner/GraphBLAS/GraphBLAS-Math-release.pdf
  - Examples: matrix multiply, matrix vector multiply, reduction, apply

Design principles of the GraphBLAS C API

- Object-oriented
  - **All objects are opaque, represented by handles**
  - Only GraphBLAS methods can manipulate those objects
- **Separation of data (matrices and vectors) and operations**
  - Only explicitly defined elements of a matrix or vector have values
  - The “structural zeros” are undefined
  - Any matrix/vector can be used with any semiring of compatible domain
  - Semantics are defined so that the “zero” value does not matter (most of the time)
- Blocking and nonblocking modes
  - **Blocking:** each method completes before returning
  - **Nonblocking:** methods may return early (must verify correctness of call)
  - Facilitated by opaqueness of objects
- Procedural specification
  - Semantics of each method is defined through process to compute output
  - Any implementation that produces the same output is conforming

GraphBLAS C API Spec (http://graphblas.org)

- **Goal:** A crucial piece of the GraphBLAS effort is to translate the mathematical specification to an actual Application Programming Interface (API) that
  i. is faithful to the mathematics as much as possible, and
  ii. enables efficient implementations on modern hardware.
- **Impact:** All graph and machine learning algorithms that can be expressed in the language of linear algebra
- **Innovation:** Function signatures (e.g. mxm, vxm, assign, extract), parallelism constructs (blocking v. non-blocking), fundamental objects (masks, matrices, vectors, descriptors), a hierarchy of algebras (functions, monoids, and semiring)

```
GrB_info GrB_mxm(GrB_Matrix                *C,      // destination
                 const GrB_Matrix           Mask,
                 const GrB_BinaryOp         accum,
                 const GrB_Semiring         op,
                 const GrB_Matrix           A,
                 const GrB_Matrix           B
              [, const Descriptor           desc]);
```

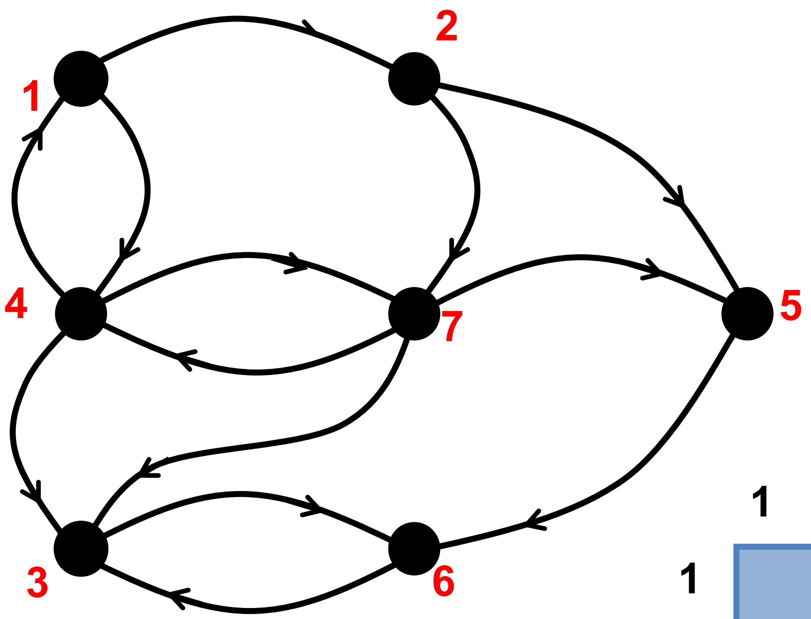
$$C(\neg M) \oplus= A^T \oplus.\otimes B^T$$

A.Buluç, T. Mattson, S. McMillan, J. Moreira, **C. Yang**. “The GraphBLAS C API Specification”, version 1.2.0

Examples of semirings in graph algorithms

Real field: **(R, +, x)**	Classical numerical linear algebra
Boolean algebra: **({0 1}, |, &)**	Graph connectivity
Tropical semiring: **(R U {∞}, min, +)**	Shortest paths
(S, select, select)	Select subgraph, or contract nodes to form quotient graph
(edge/vertex attributes, vertex data aggregation, edge data processing)	Schema for user-specified computation at vertices and edges
(R, max, +)	Graph matching &network alignment
(R, min, times)	Maximal independent set

- **Shortened semiring notation: (Set, Add, Multiply)**. Both identities omitted.
- **Add:** Traverses edges, **Multiply:** Combines edges/paths at a vertex
- Neither add nor multiply needs to have an inverse.
- Both **add** and **multiply** are **associative**, **multiply distributes** over **add**



Breadth-first search in the language of matrices

from

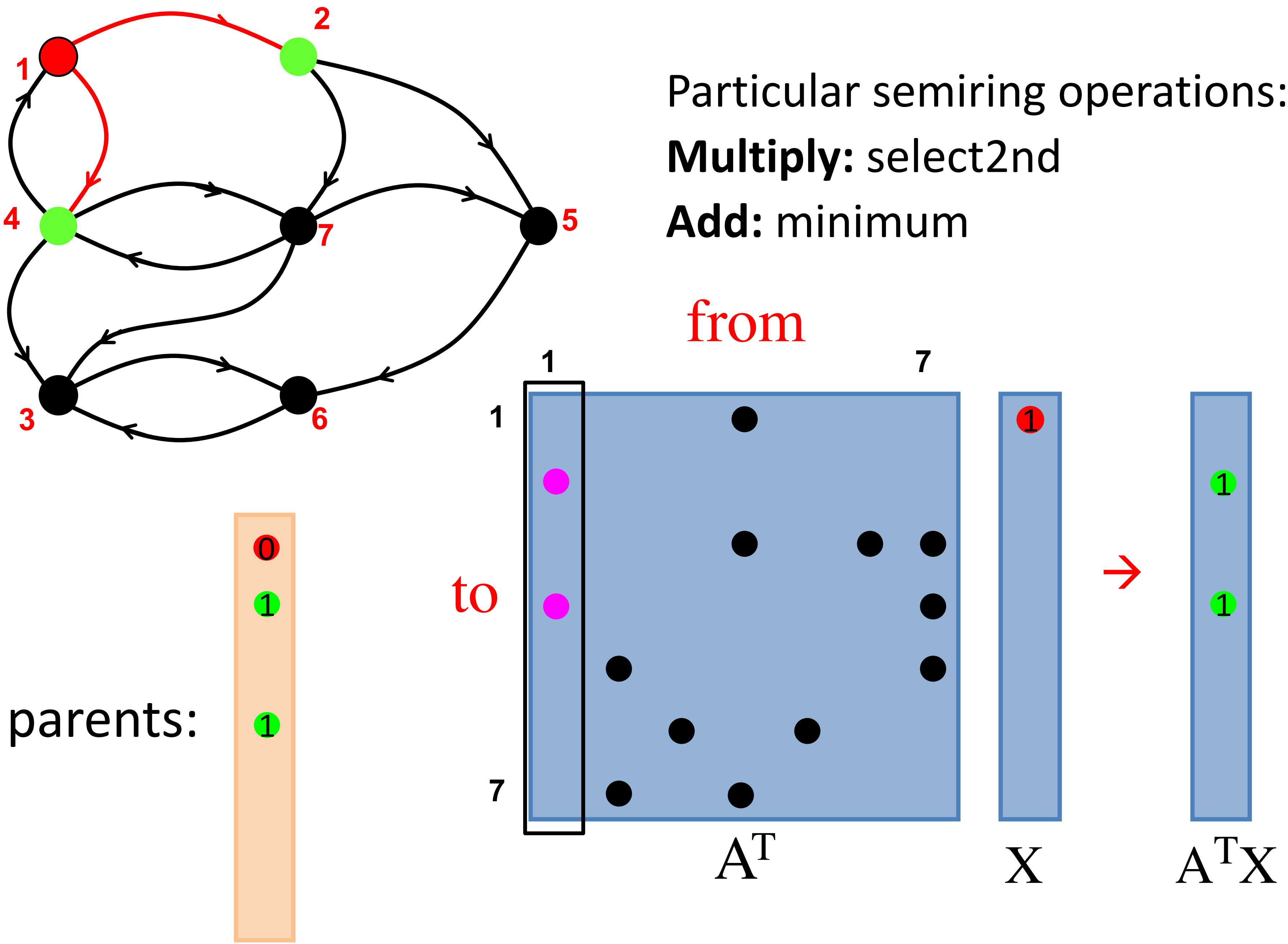
$$
\begin{array}{c|ccccccc}
 & 1 & & & & & & 7 \\
\hline
1 & & & & ● & & & \\
 & ● & & & & & & \\
 & & & & ● & & ● & ● \\
\text{to} & ● & & & & & & ● \\
 & & ● & & & & & ● \\
 & & & ● & & ● & & \\
7 & & ● & & ● & & & \\
\end{array}
$$

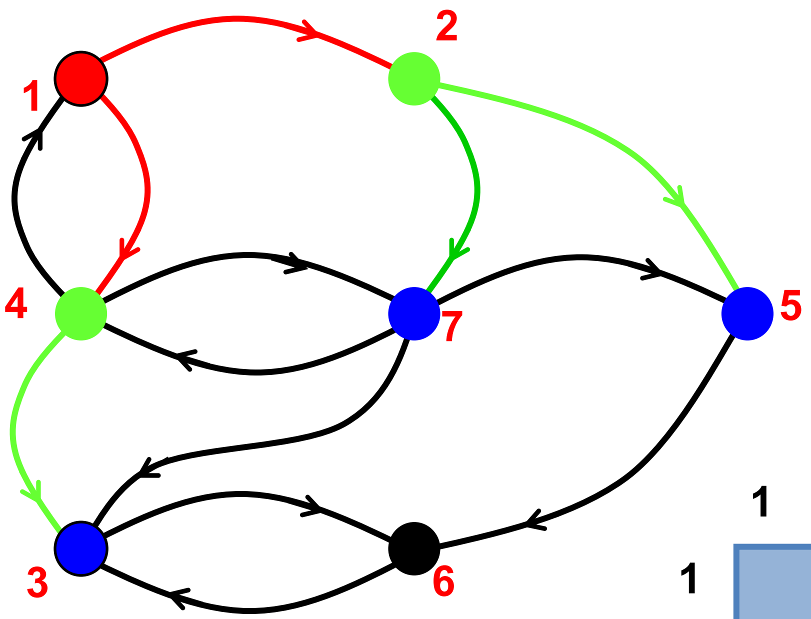
A^T

Particular semiring operations:

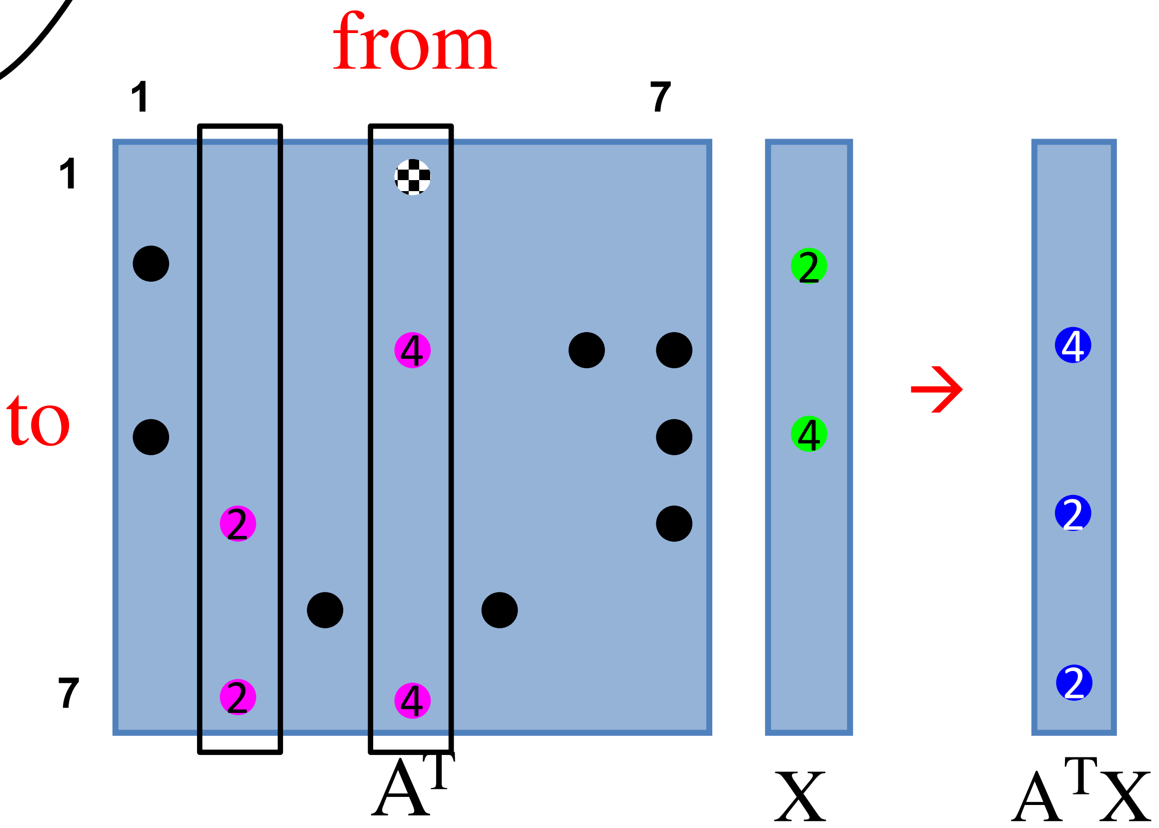
Multiply: select2nd

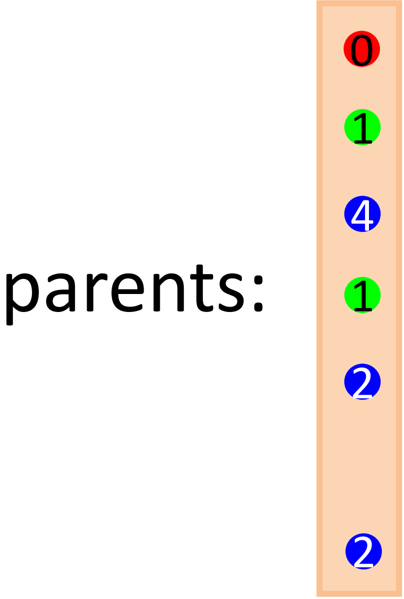
Add: minimum



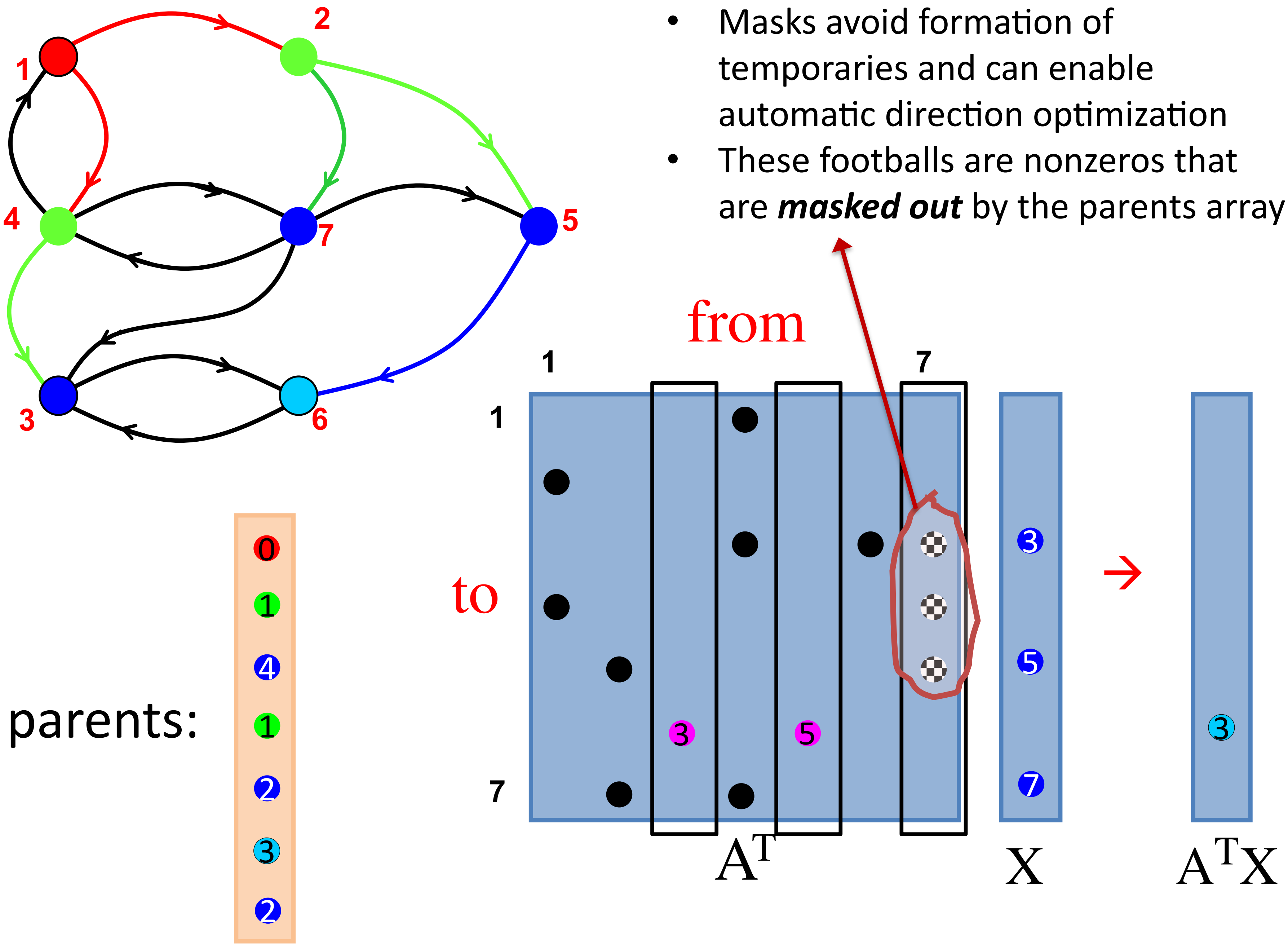


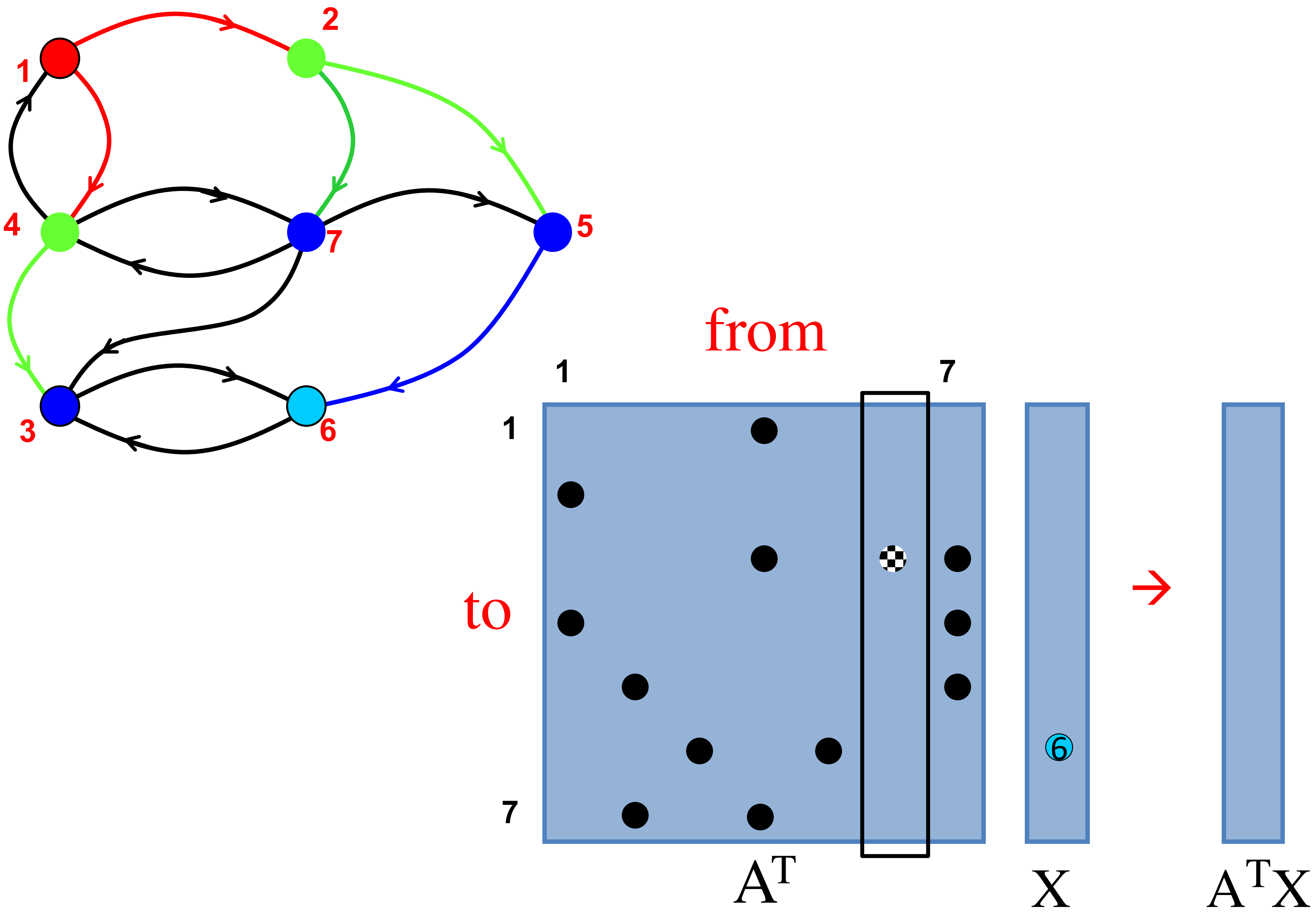
Select vertex with minimum label as parent





- Masks avoid formation of temporaries and can enable automatic direction optimization
- These footballs are nonzeros that are ***masked out*** by the parents array



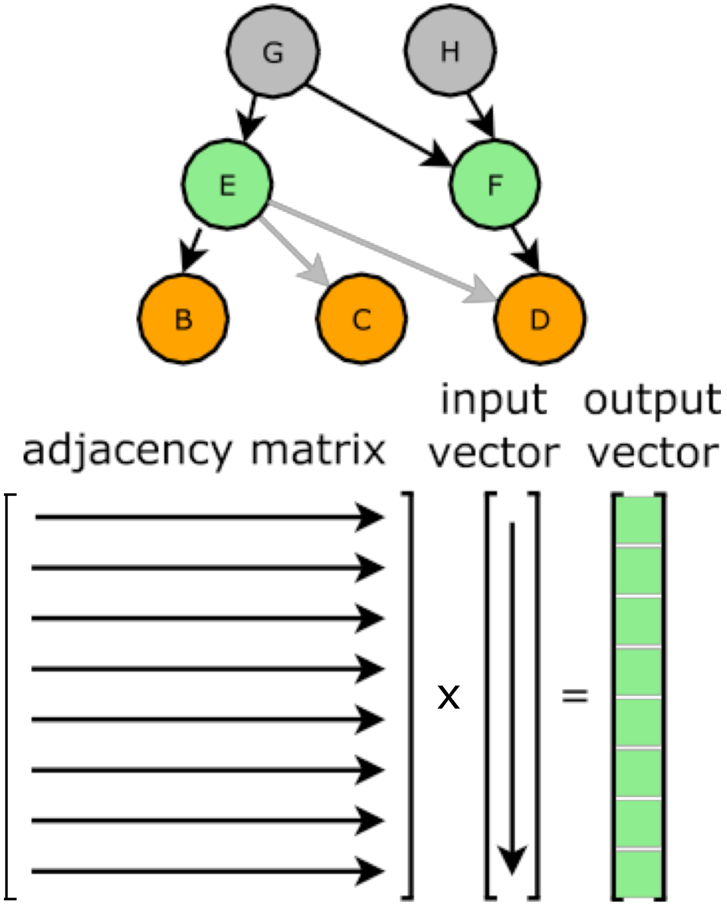

2
1
4
7
5
3
6
from
1
7
1
to
7
6
A^T
X
A^TX

BFS in GraphBLAS with Masks

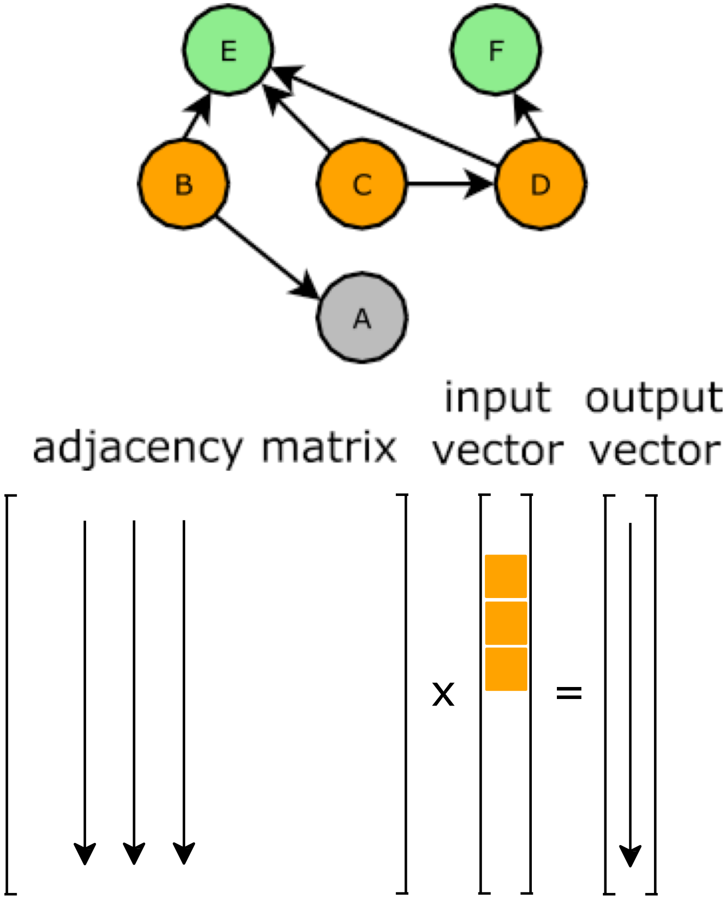
```
GrB_Vector q;                                   // vertices visited in each level
GrB_Vector_new(&q,GrB_BOOL,n);                  // Vector<bool> q(n) = false
GrB_Vector_setElement(q,(bool)true,s);          // q[s] = true, false everywhere else

GrB_Monoid Lor;                                 // Logical-or monoid
GrB_Monoid_new(&Lor,GrB_LOR,false);

GrB_Semiring Boolean;                           // Boolean semiring
GrB_Semiring_new(&Boolean,Lor,GrB_LAND);

GrB_Descriptor desc;                            // Descriptor for vxm
GrB_Descriptor_new(&desc);
GrB_Descriptor_set(desc,GrB_MASK,GrB_SCMP);     // invert the mask
GrB_Descriptor_set(desc,GrB_OUTP,GrB_REPLACE);// clear the output before assignment

GrB_UnaryOp apply_level;
GrB_UnaryOp_new(&apply_level,return_level,GrB_INT32,GrB_BOOL);

/*
 * BFS traversal and label the vertices.
 */
level = 0;
GrB_Index nvals;
do {
  ++level;                                      // next level (start with 1)
   GrB_apply(*v,GrB_NULL,GrB_PLUS_INT32,apply_level,q,GrB_NULL);   // v[q] = level
   GrB_vxm(q,*v,GrB_NULL,Boolean,q,A,desc);     // q[!v] = q ||.&& A ; finds all the
                                                // unvisited successors from current q
   GrB_Vector_nvals(&nvals, q);
} while (nvals);                                // if there is no successor in q, we are done.
```

Push-pull ≡ column-row matvec!

Pull

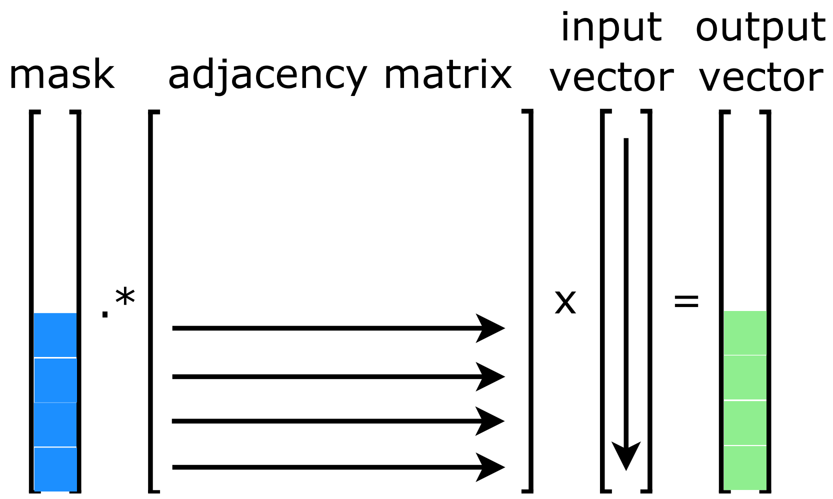


Push

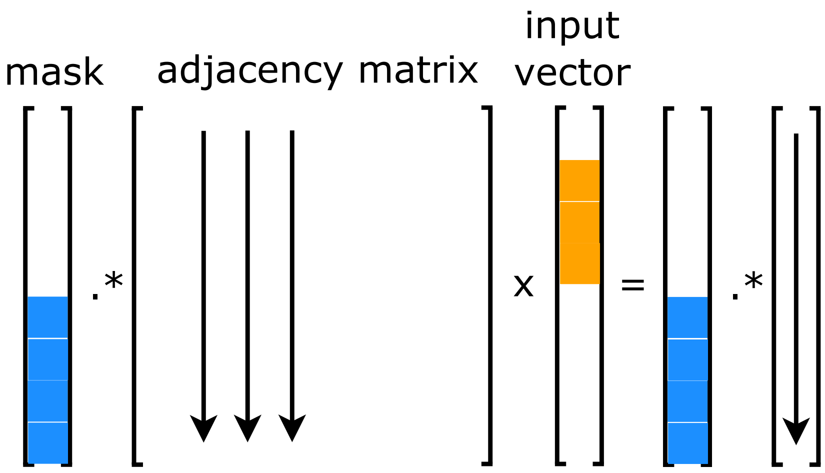


Yang, C., Buluc, A. and Owens, J.D., Implementing Push-Pull Efficiently in GraphBLAS. *ICPP'18*

Masks make “pull” implementable in GraphBLAS



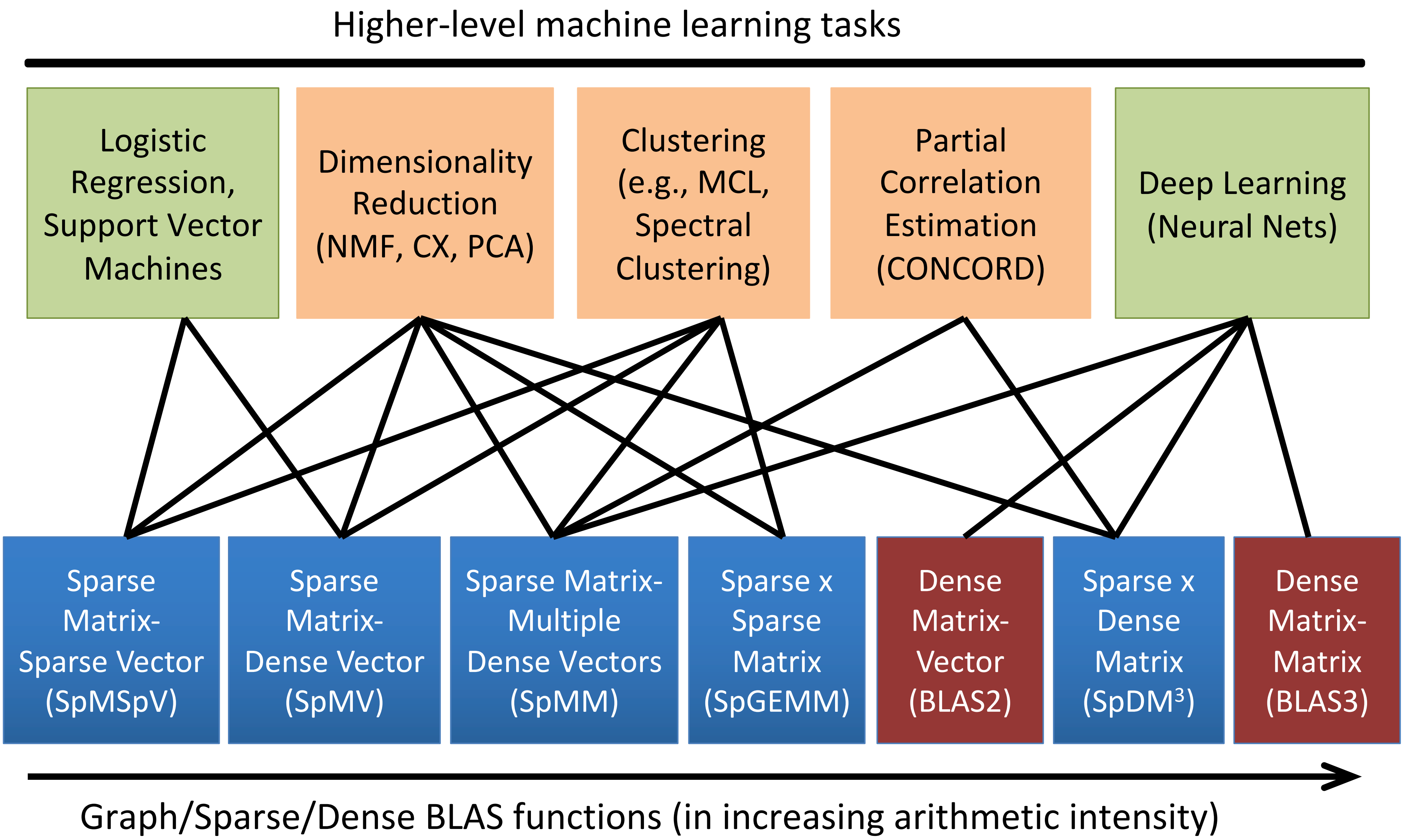
Row-based matvec w/ mask



Column-based matvec w/ mask

- **Pull** is better for sufficiently sparse masks; **push** otherwise
- **Claim**: “direction optimization” would have been discovered automatically by the GraphBLAS runtime if we designed the interface back half a decade ago.

Machine Learning relies a lot on Linear Algebra too



Higher-level machine learning tasks

Logistic Regression, Support Vector Machines

Dimensionality Reduction (NMF, CX, PCA)

Clustering (e.g., MCL, Spectral Clustering)

Partial Correlation Estimation (CONCORD)

Deep Learning (Neural Nets)

Sparse Matrix-Sparse Vector (SpMSpV)

Sparse Matrix-Dense Vector (SpMV)

Sparse Matrix-Multiple Dense Vectors (SpMM)

Sparse x Sparse Matrix (SpGEMM)

Dense Matrix-Vector (BLAS2)

Sparse x Dense Matrix (SpDM^3)

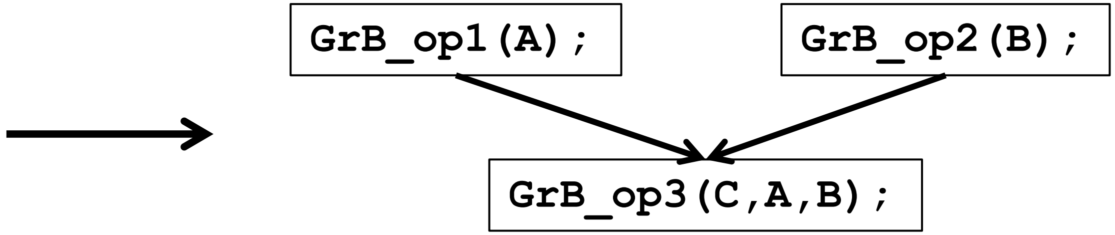
Dense Matrix-Matrix (BLAS3)

Graph/Sparse/Dense BLAS functions (in increasing arithmetic intensity)

Execution modes

- A GraphBLAS program defines a DAG of operations.
- Objects are defined by the sequence of GraphBLAS method calls, but the value of the object is not assured until a GraphBLAS method queries its state.
- This gives an implementation flexibility to optimize the execution (fusing methods, replacing method sequences by more efficient ones, etc.)

```
GrB_op1(A);
GrB_op2(B);
GrB_op3(C,A,B);
```



```
GrB_op1(A);
GrB_op2(B);
GrB_op3(C,A,B);
```

- An execution of a GraphBLAS program defines a context for the library.
- The execution runs in one of two modes:
  - **Blocking mode** … executes methods in program order with each method completing before the next is called
  - **Non-Blocking mode** … methods launched in order. Complete in any order consistent with the DAG. Objects do not exit in fully defined state until queried.
- Most implementations only support Blocking mode. SuiteSparse:GraphBLAS uses nonblocking for assign and setElement

Opportunities in non-blocking mode

- Suppose you are solving a linear system on the Kronecker product graph
- Actually happens when you are computing similarity between two graphs
- Using “graph kernels” enable machine learning on graph structures data, such as proteins and other molecules.

$$\mathbf{C} = \underset{N\,x\,M}{\mathbf{A}} \otimes \underset{K\,x\,L}{\mathbf{B}} \doteq \underset{N*K\;x\;M*L}{\begin{pmatrix} a_{1,1}\mathbf{B} & a_{1,2}\mathbf{B} & \dots & a_{1,m}\mathbf{B} \\ a_{2,1}\mathbf{B} & a_{2,2}\mathbf{B} & \dots & a_{2,m}\mathbf{B} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n,1}\mathbf{B} & a_{n,2}\mathbf{B} & \dots & a_{n,m}\mathbf{B} \end{pmatrix}}$$

- The Kronecker product itself has huge memory footprint and lots of redundancy (NK+ML dimension but NKML apparent values)

Opportunities in non-blocking mode

- The only way to write this in GraphBLAS or any other library we know of:

```
        GrB_kronecker(C, …, A, B, …); // C=A⊗B
        GrB_mxv(y, …, C, x, …); // y=C x
```

- What we would rather call:

```
        GrB_kronxv(y, …, A, B, x …); // y= (A⊗B) x
```

- But that would result in API bloat and would lead us to a rabbit hole.
- There are many other examples:
  - KFAC (optimization method for deep learning),
  - Triple matrix product (graph contraction and AMG restriction),
  - Triangle counting (who needs the list of triangles when all we need is the count)

- **Solution**: **A JIT that performs automatic operator fusion**

Status: GraphBLAS C API Specification v 1.3

New operations and methods

- Kronecker product (matrices)
- Apply w/ binary op. and scalar
- Edge (element) removal
- Resizing matrices/vectors

New built-in operators, descriptors, and other things

- Structure-only masks
- Bitwise binary ops for integers
- GrB_LXNOR boolean binary op
- GrB_ANY binary op/monoid
- Built-in descriptors
- Built-in monoids and semirings

Specification clarifications

- Language regarding “implied zero”
- Disclaimers against over-specification
- Relaxing reduction to scalar specification
- Clarifying distributive requirements
- Improving language about completions
- Removing language about annihilators
- Clarifying init() and finalize() errors
- Clarify aliasing requirements of user-defined operators
- Define value of all enums

New and updated examples

- …but more in LAGraph

Acknowledgments

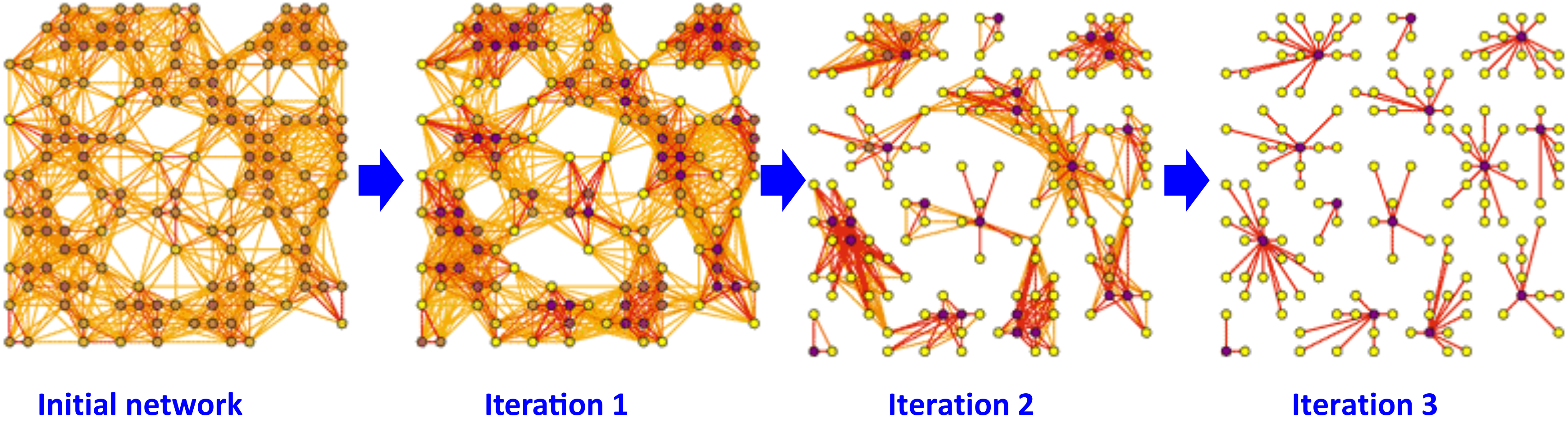
Ariful Azad, David Bader, Tim Davis, John Gilbert, Jeremy Kepner, Nikos Kyrpides, Tim Mattson, Scott McMillan, Jose Moreira, Lenny Oliker, John Owens, Christos Ouzounis, Georgios Pavlopoulos, Oguz Selvitopi, Yu-Hang Tang, Carl Yang, Kathy Yelick.

- The GraphBLAS Forum: http://graphblas.org
- My lab: http://passion.lbl.gov
- Graphs: Architectures, Programming, and Learning (GrAPL @IPDPS): http://hpc.pnl.gov/grapl/

[Extra] Some applications

Markov Cluster Algorithm (MCL)

Widely popular and successful algorithm for discovering clusters in protein interaction and protein similarity networks



Initial network

Iteration 1

Iteration 2

Iteration 3

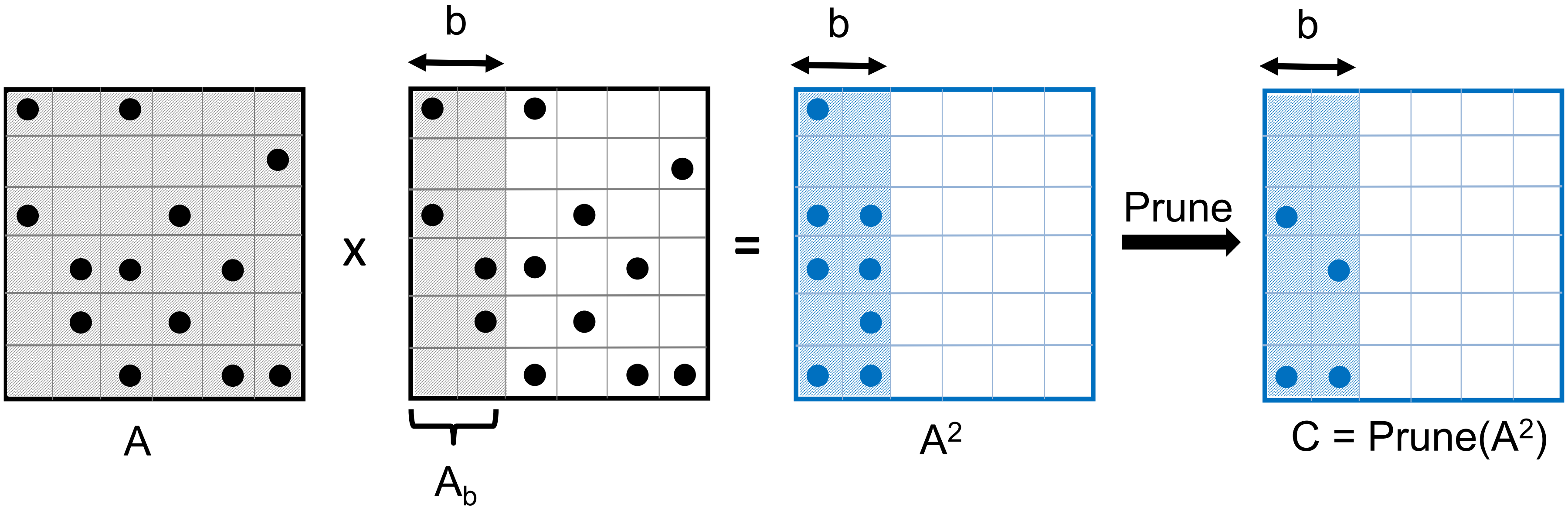
At each iteration:

Step 1 (Expansion): Squaring the matrix while
pruning (a) small entries, (b) denser columns

Naïve implementation: sparse matrix-matrix product (SpGEMM), followed by column-wise top-K selection and column-wise pruning

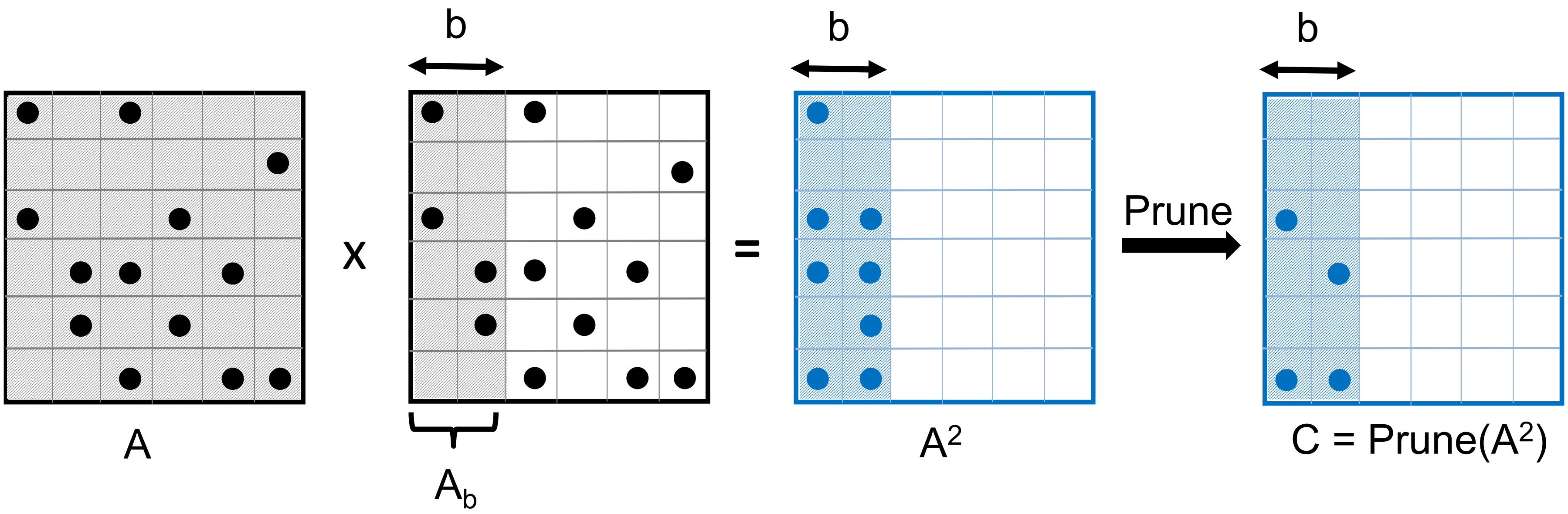
Step 2 (Inflation) : taking powers entry-wise

A combined expansion and pruning step



- ❑ b: number of columns in the output constructed at once
  - – Smaller b: less parallelism, memory efficient (b=1 is equivalent to sparse matrix-sparse vector multiplication used in MCL)
  - – Larger b: more parallelism, memory intensive

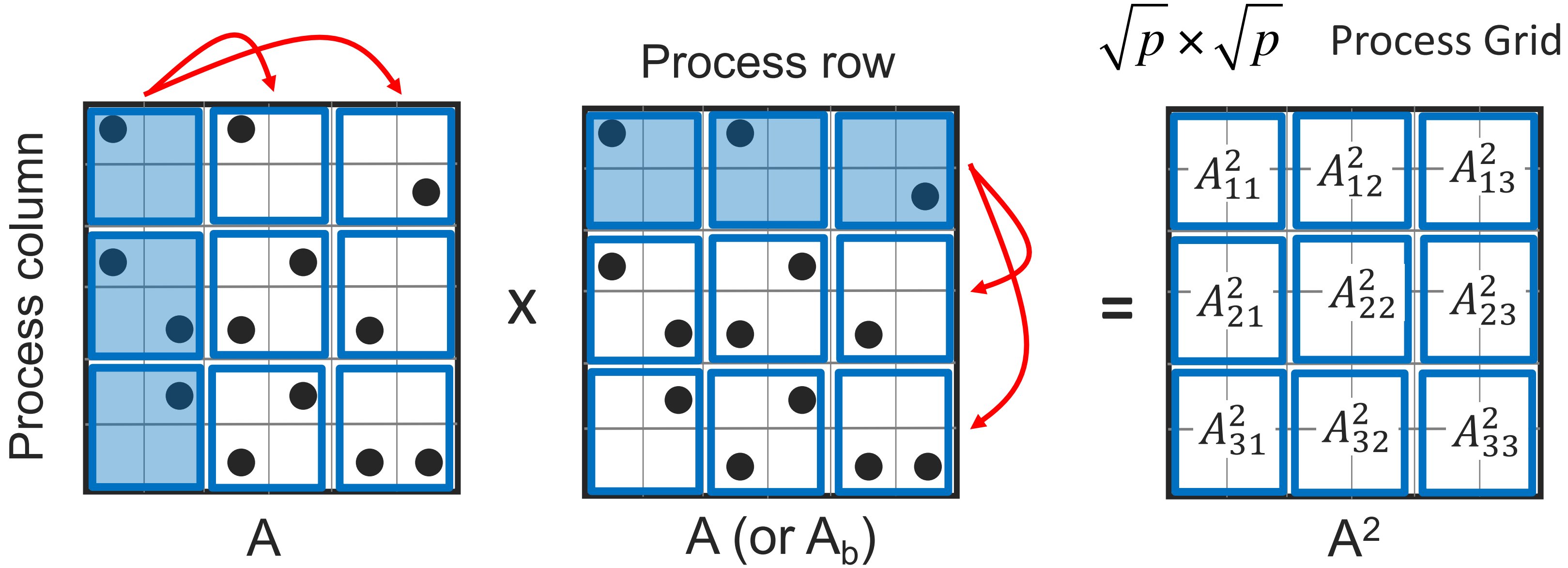
A combined expansion and pruning step



- ❑ b: number of columns in the output constructed at once
  - – HipMCL selects b dynamically as permitted by the available memory
  - – The algorithm works in h=N/b phases where N is the number of columns (vertices in the network) in the matrix

HipMCL: High-performance MCL

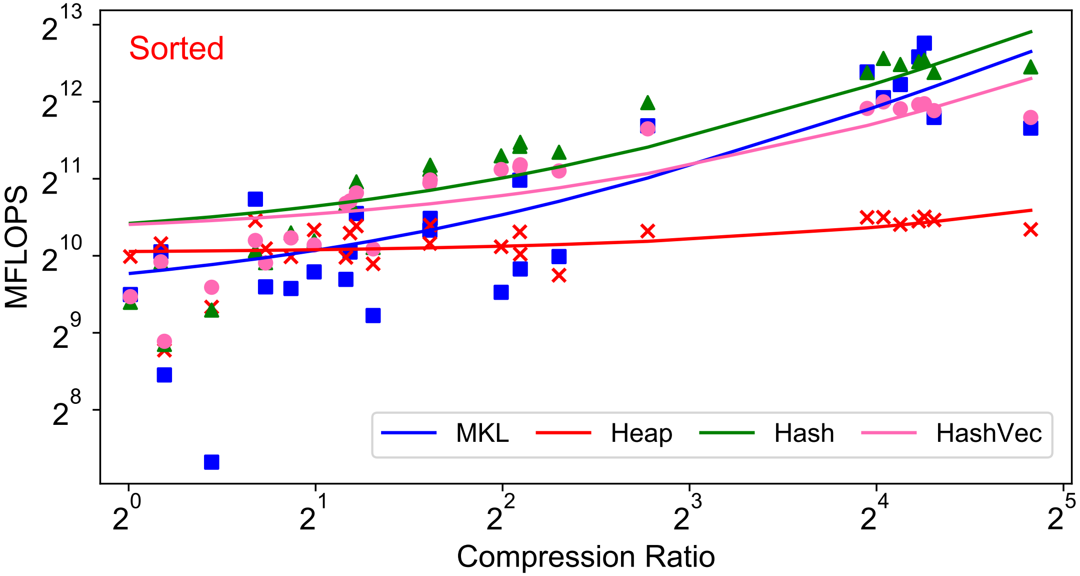
- MCL process is both **computationally expensive** and **memory hungry**, limiting the sizes of networks that can be clustered
- HipMCL overcomes such limitation via **sparse parallel algorithms**.
- **Up to 1000X times faster** than original MCL with same accuracy.

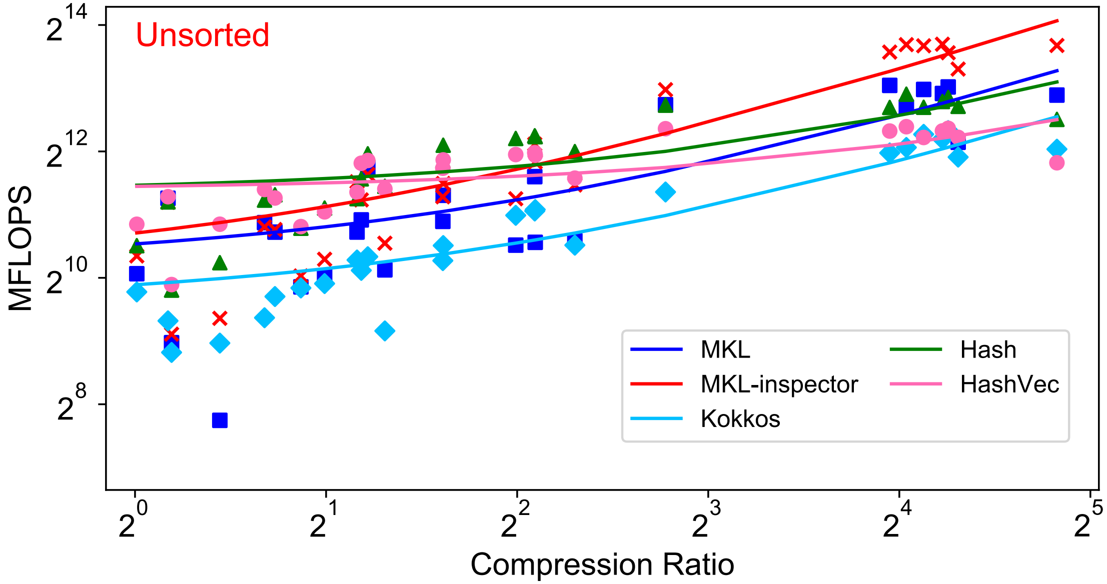


A. Azad, G. Pavlopoulos, C. Ouzounis, N. Kyrpides, A. Buluç; HipMCL: a high-performance parallel implementation of the Markov clustering algorithm for large-scale networks, *Nucleic Acids Research, 2018*

New shared-memory SpGEMM kernels

- Compression ratio (CR): flops/nnz(C)
- Combinatorial BLAS and HipMCL uses heap
- Stable performance but significant gap in high CR
- HipMCL inputs have high CR





- We will integrate hash algorithms to CombBLAS and HipMCL

Yusuke Nagasaka, Satoshi Matsuoka, Ariful Azad, and Aydin Buluc. High-performance sparse matrix-matrix products on intel KNL and multicore architectures. In ICPPW, 2018.

SpGEMM on GPUs: tested libraries

- **bhsparse** [1]
  - Hybrid method for result matrix pre-allocation
    - 3 strategies (heap-based,
  - Parallel insert operations via fast merging
  - Heuristic-based load balancing (bins)

- **rmerge2** [2]
  - Iterative row-merging
  - Aggregate duplicate column indices via warp shuffles (merge $W = 32$ rows)
  - Requires no shared memory but many registers
  - Grouping into cases for load balancing

- **nsparse** [3]
  - Linear probing shared-memory hash table
  - Row grouping based on number of nonzero elements or intermediate products (load balancing)
  - Warp shuffle and shared memory for accumulations
  - Concurrent kernel execution via streams
- Performance might differ depending on
  - Compression rate
  - Matrix structure
  - GPU microarchitecture

If these authors implemented the standard GrB_mxm, things would be much more portable. But we are still doing great compared to 5+ years ago when the SpGEMM primitive wasn't popular.

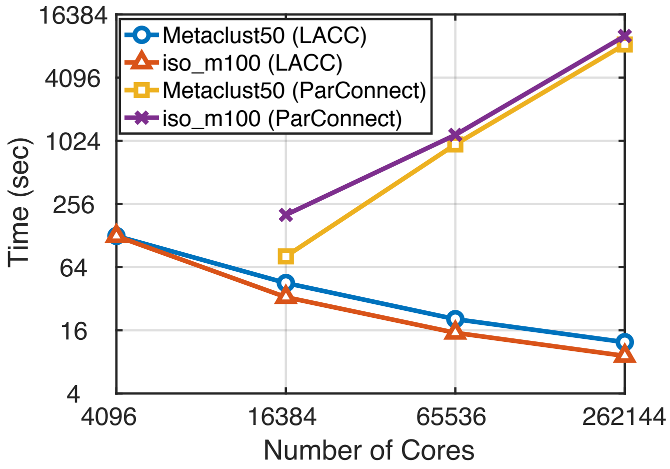
[1] Liu, Weifeng, and Brian Vinter. "An efficient GPU general sparse matrix-matrix multiplication for irregular data." In Parallel and Distributed Processing Symposium, 2014 IEEE 28th International, pp. 370-381. IEEE, 2014.

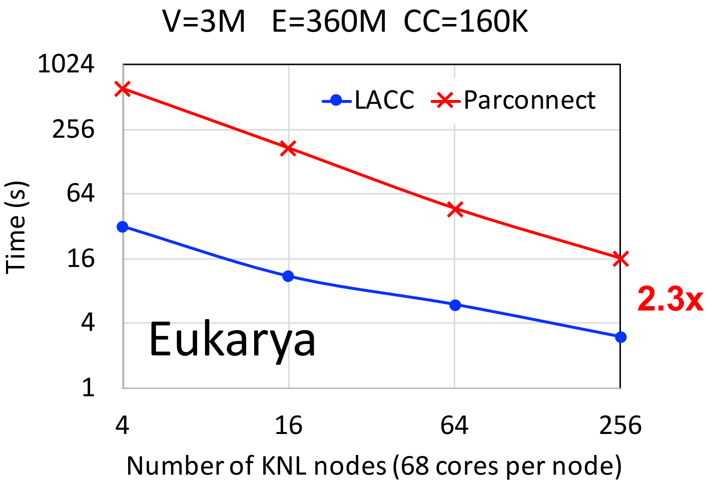
[2] Gremse, Felix, Kerstin Küpper, and Uwe Naumann. "Memory-Efficient Sparse Matrix-Matrix Multiplication by Row Merging on Many-Core Architectures." SIAM Journal on Scientific Computing 40, no. 4 (2018): C429-C449.

[3] Nagasaka, Yusuke, Akira Nukada, and Satoshi Matsuoka. "High-Performance and Memory-Saving Sparse General Matrix-Matrix Multiplication for NVIDIA Pascal GPU." In 2017 46th International Conference on Parallel Processing (ICPP), pp. 101-110. IEEE, 2017.

LACC: Parallel Connected Components

Parallel connected components for cluster identification (after MCL iterations converge): Awerbuch-Shiloach algorithm using SpMSpV and a few other GraphBLAS operations





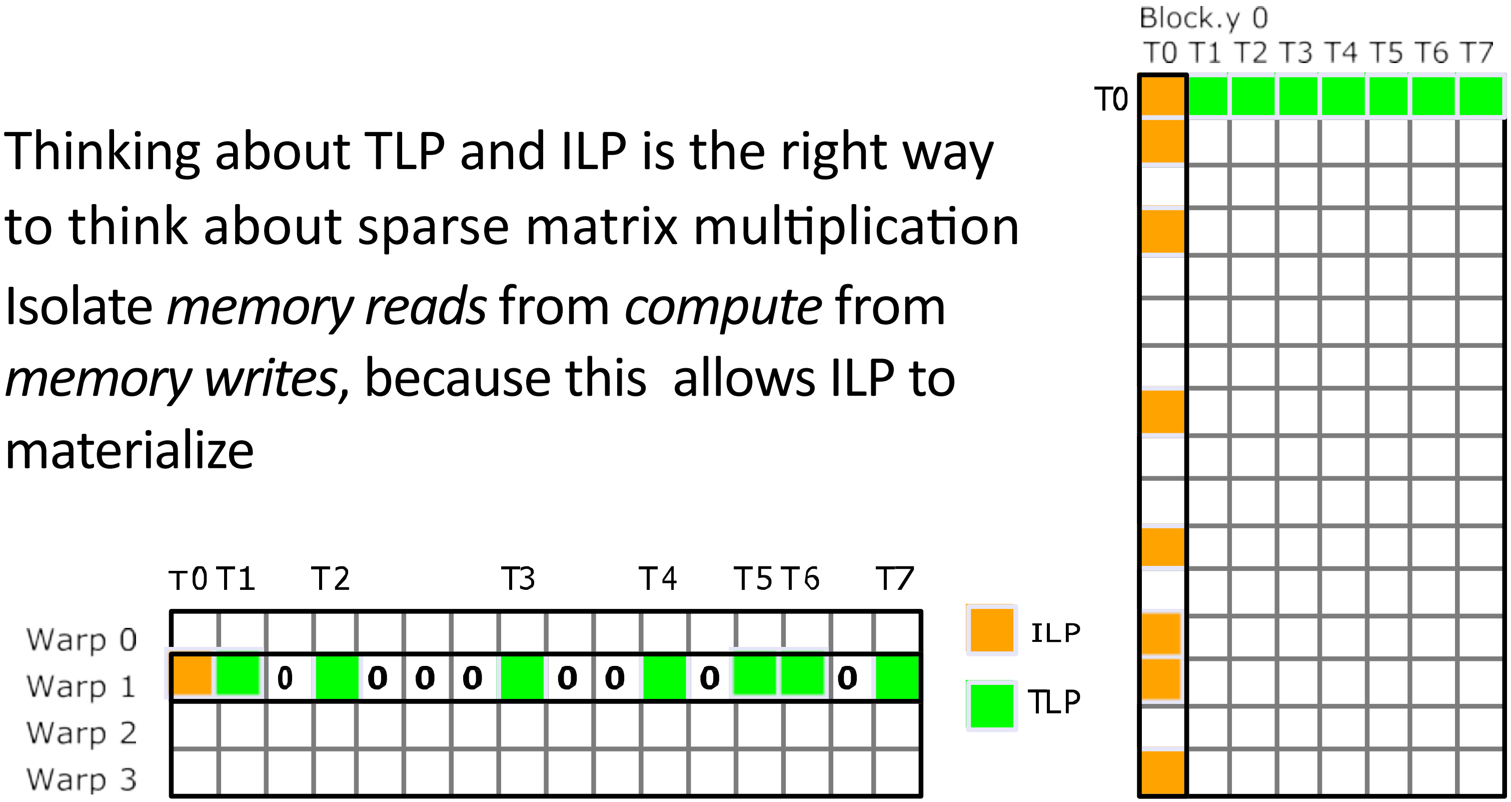
Impact: More than 2x faster connected component identification across different scales. Orders of magnitude faster at large concurrencies, enabling continued scaling of HipMCL by removing this potential Amdahl's bottleneck.

A. Azad, and A. Buluc, LACC: A Linear-Algebraic Algorithm for Finding Connected Components in Distributed Memory. IPDPS, 2019

[Extra] Some more kernels

Sparse Matrix – Multi Vector Multiplication (SpMM) on the GPU

- Thinking about TLP and ILP is the right way to think about sparse matrix multiplication
- Isolate *memory reads* from *compute* from *memory writes*, because this allows ILP to materialize



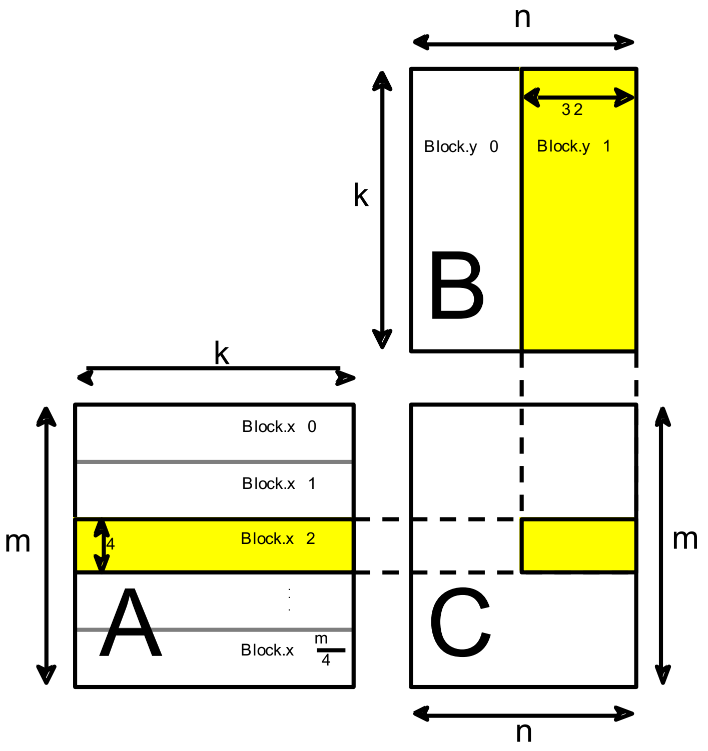
(a) Sparse matrix A

(b) Dense matrix B

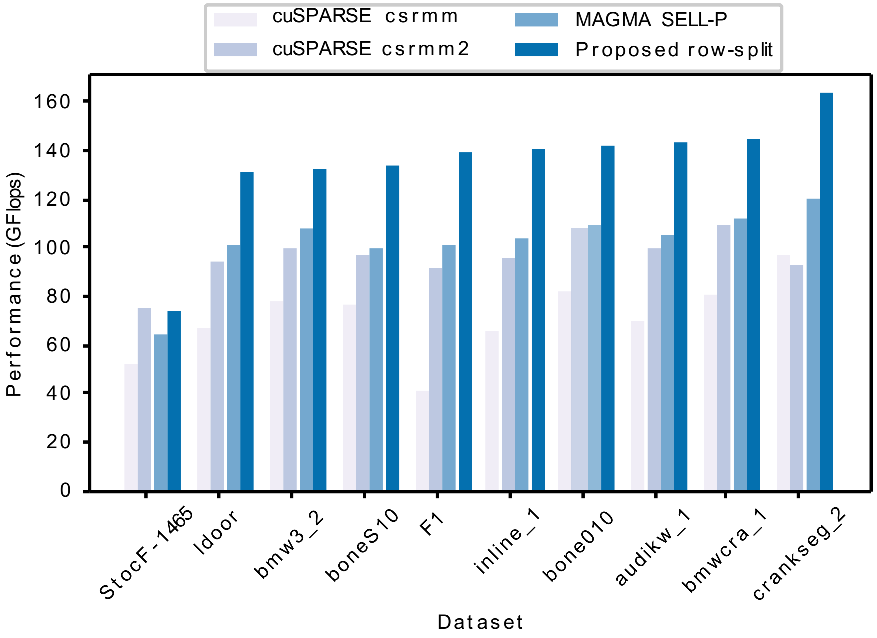
1. T0 broadcasts 0 to T1, T2, ..., T7
2. T0, T1, T2, ..., T7 do coalesced memory access for row 0

Carl Yang, Aydin Buluç, and John D Owens. Design principles for sparse matrix multiplication on the GPU. In Euro-Par, 2018. Distinguished Paper and Best Artifact Awards

Sparse Matrix – Multi Vector Multiplication (SpMM) on the GPU



A new data access pattern

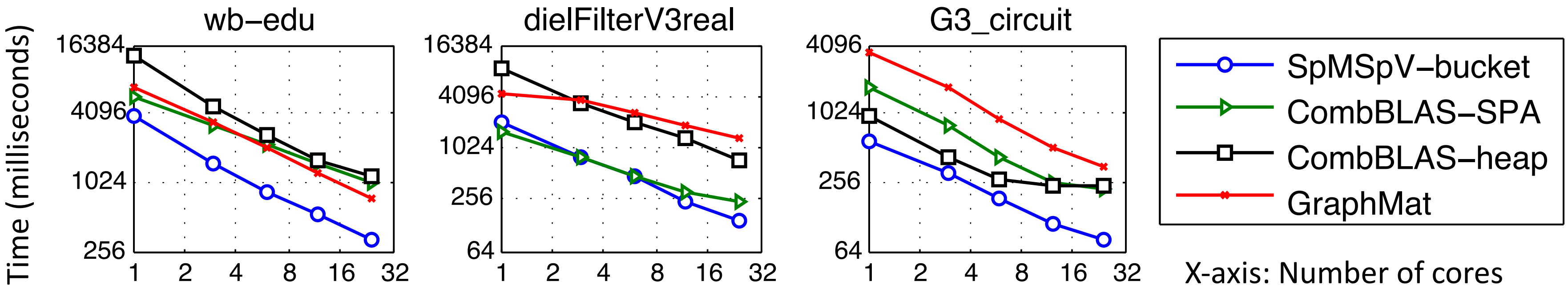


The paper also proposes a merge-based algorithm for sparser inputs

Carl Yang, Aydin Buluç, and John D Owens. Design principles for sparse matrix multiplication on the GPU. In Euro-Par, 2018. Distinguished Paper and Best Artifact Awards

A work-efficient parallel algorithm for sparse matrix-sparse vector multiplication (SpMSpV)

- **Goal:** A scalable SpMSpV algorithm without doing more work on higher concurrency
- **Application:** Breadth-first search, graph matching, support vector machines, etc.
- **Algorithmic innovation:**
  - Attains work-efficiency by arranging necessary columns of the matrix into buckets where each bucket is processed by a single thread
  - Avoids synchronization by row-wise partitioning of the matrix on the fly
- **Performance:**
  - First ever work-efficient algorithm for SpMSpV that attains up to 15x speedup on a 24-core Intel Ivy Bridge processor and up to 49x speedup on a 64-core KNL processor
  - Up to an order of magnitude faster than its competitors, especially for sparser vector



X-axis: Number of cores (Intel Ivy Bridge)

A.Azad, A. Buluç. A work-efficient parallel sparse matrix-sparse vector multiplication algorithm. IPDPS'17