# LAGraph: A Graph Algorithm and Network Analysis Library for GraphBLAS

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Abstract—IMHO, the motivation for this work can be summarized as follows (Gabor):

To ensure portability, the primitives of GraphBLAS are quite low-level.

Formulating efficient algorithms using these primitives requires expertise from the user.

To mitigate this challenge, the LAGraph library provides efficient implementations through a convenient API that can be used by users. Additionally, it demonstrates best practices for algorithm implementers.

design decisions, easy mode/expert mode, GAP algorithms, ... Index Terms—Graph Processing, Graph Algorithms, Graph Analytics, Linear Algebra, GraphBLAS

#### I. Introduction

LAGraph is a library of Graph Algorithms based on the GraphBLAS

Key contributions:

- document design decisions for LAGraph
- present a concise notation for GraphBLAS algorihms
- algorithms of the GAP benchmark suite [5] used in the IISWC benchmark paper [3]
- improve data ingestion performance, e.g. using SIMD techniques [18]

Recently, numerous graph processing systems have targeted GPUs such as the GraphBLAS Template Library (GBTL) [29], Gunrock [25] and GraphBLAST [28], as well as FPGAs [6].

However, in the near future we expect even more heterogeneous hardware architectures including graph-specific hardware based on the Programmable Integrated Unified Memory Architecture (PIUMA) [2]. Additionally, graph processing workloads can be offloaded to machine learning accelerators, e.g., Tensor Processing Units (TPUs) [16], systolic arrays using reconfigurable dataflow architecture [13], sparse linear algebrabased deep learning accelerators [20].

Previous GraphBLAS design papers: theory [21], C API [23], C++ API [8], distributed API [7], LAGraph [22]

Popular libraries: igraph [11], NetworkX [1], SNAP [19] offer very limited or no parallelism.

TODO: add two paragraphs with a high-level overview of LAGraph

```
// This is a minted code block inside a float region
int main() {
   return 0; // return zero
}
```

Listing 1: Example 2

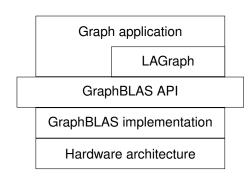


Fig. 1: Separation of concerns using the GraphBLAS API.

## II. DESIGN DECISIONS

## **TODO: Jim**

We investigate the following design questions:

- data structure for representing a graph
- basic/advanced mode
- algorithm calling conventions
- · error handling
- user-contributed algorithms
- ———
- how to work around typecasting being expensive in GraphBLAS
- terminology: properties (parameters? features?)
- multi-threadable

<sup>1</sup>A non peer-reviewed comparison of 6 popular graph algorithms libraries is available at https://www.timlrx.com/blog/benchmark-of-popular-graph-network-packages-v2.

```
typedef struct LAGraph_Graph_struct
2
      GrB_Matrix
                            // adjacency matrix of the graph
      LAGraph_Kind kind;
                            // kind of graph: directed, etc.
       // cached properties
      GrB_Matrix
                   AT;
                            // transpose of A
      GrB Vector
                    row dearee:
      GrB_Vector
                    col_degree;
      LAGraph_BooleanProperty A_pattern_is_symmetric;
      int64_t
                   ndiag; // -1 if unknown
11
12
    *LAGraph_Graph;
  typedef struct LAGraph_Graph_struct *LAGraph_Graph;
14
   // creating a graph
17
  GrB_Matrix M;
  // ...construction of M omitted
18
  LAGraph_Graph G;
20
  LAGraph_New(&G, &M, LAGRAPH_DIRECTED_ADJACENCY);
21
22
    operating on properties
  LAGraph_Property_AT(G, msg);
                                 // compute/cache
```

Listing 2: LAGraph\_Graph data structure and methods.

#### A. Core data structure

The primary data structure in LAGraph is the LAGraph\_Graph which consists of primary components and cached properties. The data structure is not opaque, providing the user with full access to access and modify all internal components, unlike the way GraphBLAS objects behave. This data structure is shown at the top of Listing 2 and defined ultimately on Line 14.

The primary components of this struct are a GraphBLAS matrix named A and an enumeration kind. The kind indicates how the matrix should be interpreted. Currently, the only kinds defined are LAGRAPH\_ADJACENCY\_UNDIRECTED and LAGRAPH\_ADJACENCY\_DIRECTED, but more options will be added in the future. Creating the Graph object is performed on Line 21 of Listing 2. Following this call, M will be NULL. The matrix previously pointed to by M now lives at G->A. This "move" constructor helps avoid memory freeing errors.

Cached properties include the transpose of A, the row degrees, column degrees, etc. They can be computed from the primary components, but doing so repeatedly for each algorithm utilizing A would be wasteful. Having them live inside the Graph object helps simplify algorithm call signatures. Utility functions exist to compute each cached property. For example, Line 24 of Listing 2 will compute the transpose of G->A and store it as G->AT. Following this call, any algorithm which is given G will have access to both A and its transpose.

Because the Graph object is opaque, any piece of code may set the transpose as well. For instance, if an algorithm computes the transpose as part of its normal logic, it could directly set G->AT. The expectation is that the Graph object will always remain consistent. If G->A is modified, all cached properties must be either be set as unknown or modified to reflect the change. Properties which are not known are set to

NULL or LAGRAPH\_BOOLEAN\_UNKNOWN in the case of Boolean properties. This expectation is a convention that all LAGraph algorithm implementers are expected to follow.

#### B. User modes

Algorithms in LAGraph target two types of user modes: Basic and Advanced. The Basic user mode is for those wanting things to "just work", are less concerned about performance, and may be less experienced with the library. The Advanced user mode is for those whose primary concern is performance and are willing to conform to stricter requirements to achieve that goal.

Algorithms targeting the Basic mode typically have limited options. Often, there will only be one function for a given algorithm. Under the hood, that single algorithm might take different paths depending on the shape or size of the input graph. The idea is that a basic user wants to compute PageRank or Betweenness Centrality, but doesn't want to have to understand the five different ways to compute them. They simply want the correct answer.

Algorithms targeting the Advanced mode are often highly specialized implementations of an algorithm. The Advanced mode user is expected to understand details such as push-pull and batch mode and why different techniques are better for each graph. Advanced mode algorithms are very strict in their input. If the input doesn't match the expected kind, an error will be raised.

Advanced mode algorithms will also raise an error if a cached property is needed by an algorithm, but is not currently available on the Graph object. While Basic mode algorithms are free to compute and cache properties on the Graph object, Advanced mode algorithms never will. The idea is to never surprise the user with unexpected additional computation. An Advanced mode user must opt-in to all computations.

Often, Basic mode algorithms will inspect the input, possibly compute properties or transform the data, and finally call one of the Advanced mode algorithms to do the actual work on the graph. Having these two user modes allows LAGraph to target a wider range of users who vary in their experience with graph algorithms.

#### C. Algorithm calling conventions

Algorithms in LAGraph follow a general calling convention.

```
int algorithm
  (
       // outputs:
       TYPE *out1,
       TYPE *out2,
       // input/output
       TYPE inout,
       // inputs
10
       TYPE input1,
11
       TYPE input2,
13
       // error message holder
14
       char *msg
15
```

The return value is always an int with the following meaning:

- =0 -> success
- <0 -> error
- >0 -> warning

The meaning of a given error or warning value is algorithmspecific and should be listed in the documentation for the algorithm.

Outputs appear first and are passed by reference. A pointer should be created by the caller, but memory will be allocated by the algorithm. If the output is not needed, a NULL is passed and the algorithm will not return that output.

Input/Output arguments are passed by value. The expectation is that the object will be modified. This supports things like batch mode in which a frontier is updated and returned to the caller. It also supports Basic mode algorithms which may modify a Graph object by adding cached properties.

Inputs are passed by value and should never be changed by the algorithm.

The final argument of any LAGraph algorithm is the error message holder. This must be char[] of size LAGRAPH\_MSG\_LEN. When the algorithm returns an error or a warning, a message may be placed in this array as additional information. Because the caller creates this array, the caller must free the memory or reuse it as appropriate. If the algorithm is successful, it should fill the message array with an empty string to clear any previous message.

#### D. Error handling

Because every algorithm in LAGraph can return an error, the return value of every call should be checked before proceeding. To make this less burdensome for a C-based library, LAGraph provides a convenience macro which works similar to try/catch in other languages.

```
#define LAGraph_TRY(LAGraph_method)
      int LAGraph_status = LAGraph_method;
      if (LAGraph_status < 0)</pre>
          LAGraph_CATCH (LAGraph_status);
 }
```

LAGraph\_CATCH can be defined before an algorithm and will be called in the event of an error. This allows for proper freeing of memory and other necessary tasks.

A similar macro, GrB\_TRY, will call GrB\_CATCH when making GraphBLAS calls which return a GrB\_Info value other than GrB\_SUCCESS or GrB\_NO\_VALUE.

LAGraph\_TRY and GrB\_TRY provide an easy to use and easy to read method for dealing with error checking while writing graph algorithms.

#### E. Contributing algorithms

The LAGraph project welcomes contributions from all graph practitioners who understand the GraphBLAS vision of using the language of linear algebra to express graph computations. However, as a matter of practical concern, many users want a

stable experience when using LAGraph for doing real work. To balance these, the LAGraph repository will have both a stable and an experimental folder.

New algorithms or modifications of existing algorithms will first be added to the experimental folder. The release schedule of experimental algorithms will generally be much faster than the stable release and there is no expectation of a bug-free experience. The goal is to generate lots of ideas and allow uninhibited contributions to push the boundary of what is possible with the GraphBLAS. The stable release will be fully tested and will move much slower, targeting the needs of those who want to use LAGraph as a complete, production-grade library rather than as a research project.

#### III. NOTATION

"guiding principles": understandable (biggest probability of first guess to be correct), similar to existing notations [9]

TODO: initial draft by Gabor

**TODO:** explain masks

TODO: explain replace/merge as per Scott's email

TODO: revise Scott, Tim D, and Tim M TODO: consider adding semiring table

what do masks mean?

the mask restricts the scope of the computation to the elements selected by the mask (m) or the complement of these elements  $(\neg \mathbf{m})$ 

there are variations based on (1) how the elements are selected (based on the values in the mask or the structure of the mask) (2) how the elements outside the selected ones are treated (they are replaced with implicit zeros or they are kept intact and *merged* with the results of the computation)

by default, masks should use merge semantics, i.e. the computation can only effect elements selected by the mask, elements outside the mask are unaffected  $\mathbf{w}\langle \mathbf{m} \rangle$  and  $\mathbf{w}\langle \neg \mathbf{m} \rangle$ 

replace semantics, i.e. they annihilate all elements outside the mask. this is denoted with  $\mathbf{w}\langle \mathbf{m}, \mathbf{r} \rangle$  and  $\mathbf{w}\langle \neg \mathbf{m}, \mathbf{r} \rangle$ 

by default, element values in the mask are checked and elements with zero value are not used to avoid this, we use structural masks  $\mathbf{w}\langle s(\mathbf{m})\rangle$  and  $\mathbf{w}\langle \neg s(\mathbf{m})\rangle$ 

Combining replace semantics and structural masks is possible:  $\mathbf{w}\langle s(\mathbf{m}), \mathbf{r} \rangle \mathbf{w}\langle \neg s(\mathbf{m}), \mathbf{r} \rangle$ 

Initializing scalars, vectors, and matrices (GraphBLAS methods):

- let:  $s \in \mathbb{Q}_{64}$
- let:  $\mathbf{w} \in \mathbb{Q}_{32}^n$
- let:  $\mathbf{A} \in \mathbb{N}_{16}^{m \times n}$  let:  $\mathbf{A} \in \mathbb{Z}_{64}^{k \times m}$ 
  - a) Transposition: separate operator + descriptor (1)

vectors can be interpreted as row/column vectors, we do not transpose them manually

extensions

conversion table

operation/method	description	notation	
mxm vxm mxv	matrix-matrix multiplication vector-matrix multiplication matrix-vector multiplication	$\begin{array}{c} \mathbf{C}\langle\mathbf{M}\rangle\odot=\mathbf{A}\oplus.\otimes\mathbf{B}\\ \mathbf{w}^{T}\langle\mathbf{m}^{T}\rangle\odot=\mathbf{u}^{T}\oplus.\otimes\mathbf{A}\\ \mathbf{w}\langle\mathbf{m}\rangle\odot=\mathbf{A}\oplus.\otimes\mathbf{u} \end{array}$	
eWiseAdd	element-wise addition using operator op on elements in the set union of structures of $\mathbf{A}/\mathbf{B}$ and $\mathbf{u}/\mathbf{v}$	$\mathbf{C}\langle\mathbf{M} angle\odot\mathbf{=}\mathbf{A}op_{\cup}\mathbf{B}\ \mathbf{w}\langle\mathbf{m} angle\odot\mathbf{=}\mathbf{u}op_{\cup}\mathbf{v}$	
eWiseMult	element-wise multiplication using operator op on elements in the set intersection of structures of $\mathbf{A}/\mathbf{B}$ and $\mathbf{u}/\mathbf{v}$	$\mathbf{C}\langle\mathbf{M} angle\odot=\mathbf{A}op_\cap\mathbf{B}\ \mathbf{w}\langle\mathbf{m} angle\odot=\mathbf{u}op_\cap\mathbf{v}$	
extract	extract submatrix from matrix $A$ using indices $i$ and indices $j$ extract the $i$ th row vector from matrix $A$ extract the $j$ th column vector from matrix $A$ extract subvector from $\mathbf{u}$ using indices $i$	$egin{aligned} \mathbf{C}\langle\mathbf{M} angle\odot&\mathbf{A}(i,j)\ \mathbf{w}\langle\mathbf{m} angle\odot&\mathbf{A}(i,:)\ \mathbf{w}\langle\mathbf{m} angle\odot&\mathbf{A}(:,j)\ \mathbf{w}\langle\mathbf{m} angle\odot&\mathbf{a}(:,j) \end{aligned}$	
assign	assign matrix to submatrix with mask for <b>C</b> assign scalar to submatrix with mask for <b>C</b> assign vector to subvector with mask for <b>w</b> assign scalar to subvector with mask for <b>w</b>	$\mathbf{C}\langle\mathbf{M}\rangle(i,j)\odot=\mathbf{A}$ $\mathbf{C}\langle\mathbf{M}\rangle(i,j)\odot=s$ $\mathbf{w}\langle\mathbf{m}\rangle(i)\odot=\mathbf{u}$ $\mathbf{w}\langle\mathbf{m}\rangle(i)\odot=s$	
subassign (GxB)	assign matrix to submatrix with submask for $\mathbf{C}(i,j)$ assign scalar to submatrix with submask for $\mathbf{C}(i,j)$ assign vector to subvector with submask for $\mathbf{w}(i)$ assign scalar to subvector with submask for $\mathbf{w}(i)$	$\begin{array}{l} \mathbf{C}(i,j)\langle\mathbf{M}\rangle\bigcirc=\mathbf{A}\\ \mathbf{C}(i,j)\langle\mathbf{M}\rangle\bigcirc=s\\ \mathbf{w}(i)\langle\mathbf{m}\rangle\bigcirc=\mathbf{u}\\ \mathbf{w}(i)\langle\mathbf{m}\rangle\bigcirc=s \end{array}$	
apply	apply unary operator $f$ with optional thunk $k$	$\mathbf{C}\langle\mathbf{M}\rangle\bigcirc=f(\mathbf{A},k)$ $\mathbf{w}\langle\mathbf{m}\rangle\bigcirc=f(\mathbf{u},k)$	
select	apply select operator $f$ with optional thunk $k$	$\mathbf{C}\langle\mathbf{M}\rangle\odot=\mathbf{A}\langle f(\mathbf{A},k)\rangle$ $\mathbf{w}\langle\mathbf{m}\rangle\odot=\mathbf{u}\langle f(\mathbf{u},k)\rangle$	
reduce	row-wise reduce matrix to column vector reduce matrix to scalar reduce vector to scalar	$\mathbf{w}\langle\mathbf{m}\rangle\odot=[\oplus_{j}\mathbf{A}(:,j)]\\s\odot=[\oplus_{i,j}\mathbf{A}(i,j)]\\s\odot=[\oplus_{i}\mathbf{u}(i)]$	
transpose	transpose	$\mathbf{C}\langle\mathbf{M}\rangle\odot=\mathbf{A}^T$	
kronecker	Kronecker multiplication using operator op	$\mathbf{C}\langle\mathbf{M}\rangle\odot=\mathrm{kron}(\mathbf{A},op,\mathbf{B})$	
dup	duplicate matrix duplicate vector	$\begin{matrix} \mathbf{C} \!$	
build	matrix from tuples vector from tuples	$\mathbf{C} \leftrightarrow \{i,j,x\}$ $\mathbf{w} \leftrightarrow \{i,x\}$	
extractTuples	extract index arrays $(i,j)$ and value arrays $(x)$	$\{i,j,x\} \leftarrow \mathbf{A}$ $\{i,x\} \leftarrow \mathbf{u}$	
extractElement	extract element to scalar	$egin{aligned} s &= \mathbf{A}(i,j) \ s &= \mathbf{u}(i) \end{aligned}$	
setElement	set element	$egin{aligned} \mathbf{C}(i,j) &= s \ \mathbf{w}(i) &= s \end{aligned}$	

TABLE I: GraphBLAS operations and methods based on [12]. *Notation:* Matrices and vectors are typeset in bold, starting with uppercase (**A**) and lowercase (**u**) letters, respectively. Scalars including indices are lowercase italic (k, i, j) while arrays are lowercase bold italic (k, k, k). k and k are the addition and multiplication operators forming a semiring and default to conventional arithmetic k and k operators. k is the accumulator operator. Operations can be modified via a descriptor; matrices can be transposed (k), the mask can be complemented, and the mask can be valued (shown above) or structural (k). A structural mask can also be complemented (k). The result can be cleared after using it as input to the mask/accumulator step (k). Not all methods are listed (creating new ops, monoids, and semirings, clearing a matrix/vector, etc.). For the assign operation, the dimensions of the masks are the same as the output's: k dim(k) = dim(k) and dim(k) = dim(k). For the subassign operation, the dimensions of the masks are the same as the submasks: k nrows(k) = k for vectors.

#### IV. ALGORITHMS

### A. Breadth-First Search (BFS)

The breadth-first search (BFS) builds on the observation that a vector-matrix multiplication  $\mathbf{f}^\mathsf{T}\mathbf{A}$  expresses the navigation from the nodes selected by vector  $\mathbf{f}$  in the graph represented by  $\mathbf{A}$ . The direction-optimizing push/pull BFS [4] is simple to express in GraphBLAS [27]. If  $\mathbf{A}$  is held by row, then  $\mathbf{f}^\mathsf{T}\mathbf{A}$  is a push step, while  $\mathbf{B}\mathbf{f}$  is a pull step, where  $\mathbf{B}=\mathbf{A}^\mathsf{T}$  is the explicit transpose of  $\mathbf{A}$ , also held by row. Other GraphBLAS libraries, e.g., GraphBLAST, store both directions and perform direction-optimization automatically [28]. The push-only BFS is shown in Alg. 1, while the push/pull BFS is Alg. 2.

The GraphBLAS BFS relies on the any secondi semiring to compute a single step,  $\mathbf{q}\langle\neg s(\mathbf{p})\rangle = \mathbf{q}^T\mathbf{A}$ , where  $\mathbf{q}$  is the current frontier (using  $\mathbf{q}$  as short for queue),  $\mathbf{p}$  is the parent vector, and  $\mathbf{A}$  is the adjacency matrix. This step assigns the parents of newly nodes, which do not yet have a parent, using the complemented structural mask  $\langle\neg s(\mathbf{p})\rangle$ .

Consider a matrix multiply for conventional linear algebra, where the  $\oplus$  monoid sums a set of t entries to obtain a single scalar for computing  $c_{ij} = \sum a_{ik}b_{kj}$  in the matrix multiply  $\mathbf{C} = \mathbf{AB}$ . The any monoid performs the reduction of t entries to a single number by merely selecting any one of the t entries as the result  $c_{ij}$ . The selection is done non-deterministically, allowing for a benign race condition. In the BFS, this corresponds to selecting any valid parent of a newly discovered node. Indeed, the creation of the any operator was inspired by Scott Beamer's bfs.cc method in the GAP benchmark, which has the same benign race condition. The any monoid translates the concept of this benign race condition to construct a valid BFS tree into a linear algebraic operation, suitable for implementation in GraphBLAS.

The secondi operator is the multiplicative operator in the any.secondi semiring, where the result of  $a_{ik}b_{kj}$  is simply the index k in the semiring for  $\mathbf{C} = \mathbf{AB}$ . This gives the id of the parent node for a newly discovered node in the next frontier. The any monoid then selects any valid parent k.

## Algorithm 1: Parents BFS.

```
Input: A, startVertex

1 Function ParentsBFS

2 \mathbf{p}(startVertex) = startVertex

3 \mathbf{q}(startVertex) = startVertex

4 \mathbf{for}\ level = 1\ \mathbf{to}\ nrows(\mathbf{A}) - 1\ \mathbf{do}

5 \mathbf{q}^{\mathsf{T}}\langle \neg s(\mathbf{p}^{\mathsf{T}}), \mathbf{r} \rangle = \mathbf{q}^{\mathsf{T}}\ any.secondi\ \mathbf{A}

6 \mathbf{p}\langle s(\mathbf{q}) \rangle = \mathbf{q}

1 \mathbf{for}\ nvals(\mathbf{q}) = 0\ \mathbf{for}

2 \mathbf{for}\ return
```

### B. Betweenness Centrality (BC)

The vertex betweenness-centrality metric is a weighted measure of the number of shorted paths that go through any

# Algorithm 2: Direction Optimizing Parent BFS.

```
Input: A, A^T, start Vertex
1 Function DirectionOptimizingBFS
            \mathbf{q}(startVertex) = 0
3
            for level = 1 to nrows(\mathbf{A}) - 1 do
                   if Push(\mathbf{A}, \mathbf{q}) then
 4
                    |\mathbf{q}^{\mathsf{T}}\langle \mathbf{g}(\mathbf{p}^{\mathsf{T}}), \mathbf{r} \rangle = \mathbf{q}^{\mathsf{T}} any secondi \mathbf{A}
 5
 6
                          \mathbf{q}\langle \neg s(\mathbf{p}), \mathbf{r} 
angle = \mathbf{A}^\mathsf{T} any secondi \mathbf{q}
 7
                   \mathbf{p}\langle s(\mathbf{q})\rangle = \mathbf{q}
 8
                   if nvals(\mathbf{q}) = 0 then
 9
                          return
10
```

given node,

$$\sum_{s \neq i \neq t} \frac{\sigma(s, t|i)}{\sigma s, t},$$

where  $\sigma(s,t)$  is the total number of shortest paths from node s to t, and  $\sigma(s,t|i)$  is the total number of shortest paths from node s to t that pass through node i. This is expensive to compute, so in practice, a subset of source nodes s are chosen at random (a batch).

Like the BFS, direction-optimization is incredibly simple to add to the LAGraph algorithm for batched betweenness-centrality (BC). It only requires a simple heuristic to determine which direction to use, followed by masked matrix-matrix multiplication with the matrix or its transpose:  $\mathbf{F}\langle \neg s(\mathbf{P})\rangle = \mathbf{F}\mathbf{B}^\mathsf{T}$  (the pull) or  $\mathbf{F}\langle \neg s(\mathbf{P})\rangle = \mathbf{F}\mathbf{A}$  (the push), where  $\mathbf{A}$  is the adjacency matrix of the graph and  $\mathbf{B} = \mathbf{A}^\mathsf{T}$  is its explicit transpose,  $\mathbf{F}$  is the frontier, and the complemented structural mask  $\neg s(\mathbf{P})$  is the set of unvisited nodes. The multiplication  $\mathbf{F}\mathbf{B}^\mathsf{T}$  relies on the descriptor to represent the transpose of  $\mathbf{B}$ , which is not explicitly transposed. In the backward phase, the pull step is  $\mathbf{W} = \mathbf{W}\mathbf{A}^\mathsf{T}$  while the push is  $\mathbf{W} = \mathbf{W}\mathbf{B}$ , where  $\mathbf{W}$  is the 4-by-n matrix in which centrality is accumulated.

To simplify the presentation of the entire BC algorithm, Alg. 3 does not show the direction-optimization. It is the same transformation as the pair of BFS algorithms, where the push-only step (line 5 of Alg. 1), is expanded to a push/pull hueristic (lines 4-7 of Alg. 2).

### C. PageRank (PR)

PageRank (PR) computes the importance of each node as a recursively-defined metric: a web page is important if important pages link to it. Alg. 4 shows the GraphBLAS implemenation of PR as specified in the GAP Benchmark. It uses the plus.second semiring, where  $\operatorname{second}(x,y)=y$ , so it can ignore any edge weights in the input matrix. The PR in GAP does not properly handle dangling vertices in the graph. The Graphalytics benchmark has a PageRank variant which avoids this problem [15]. We have included this version to compare its performance with the GAP benchmark algorithm pr.cc.

## Algorithm 3: Betweenness centrality.

```
1 Function BrandesBC
        // The NumSp structure holds the number of
            shortest paths for each node and starting
            vertex discovered so far.
        // Initialized to source vertices.
        NumSp \leftrightarrow \{s, [1, 1, ..., 1]\}
 2
        // The Frontier holds the number of shortest paths
            for each node and starting vertex discovered so
        Frontier \leftarrow \{s, [1, 1, \dots, 1]\}
3
        \mathbf{Frontier}\langle \neg s(\mathbf{NumSp}), \mathbf{r} \rangle = \mathbf{Frontierplus}. \mathsf{first} \mathbf{A}
 4
             // The Sigmas matrices store frontier
            information for each level of the BFS phase.
        // BFS phase (forward sweep)
        for d=0 to nrows(\mathbf{A}) do
5
             // Sigmas[d](:,s)=d^{th} level frontier from
                 source vertex s
             let: \mathbf{Sigmas}[d] \in \mathbb{B}^{n \times nsver}
 6
             \mathbf{Sigmas}[d](:,:) = \mathbf{Frontier} \hspace{0.2cm} \texttt{// Convert matrix}
 7
               to Boolean
             NumSp += Frontier
                                                    // Accumulate path
               counts
             Frontier\langle \neg s(\mathbf{NumSp}), \mathbf{r} \rangle =
 9
              Frontier plus.first A
                                                    // Update frontier
             if nvals(Frontier) = 0 then
10
                 break
11
        let: \mathbf{BCU} \in \mathbb{Q}_{32}^{n \times nsver}
12
        BCU(:) = 1.0
                                  // Make {f BCU} dense, initialize
13
          all elements to 1.0\,
        let: \mathbf{W} \in \mathbb{Q}_{32}^{n \times nsver}
14
        // Tally phase (backward sweep)
        for i = d - 1 downto 0 do
15
             \mathbf{W}\langle s(\mathbf{Sigmas}[i]), \mathbf{r}\rangle = \mathbf{BCU} \operatorname{\mathsf{div}}_{\cap} \mathbf{NumSp}
16
             \mathbf{W}\langle s(\mathbf{Sigmas}[i-1]), \mathbf{r}\rangle = \mathbf{W} plus.first \mathbf{A}^{\mathsf{T}}
17
               // Add contributions by successors and mask
               with that BFS level's frontier.
             \mathbf{BCU} += \mathbf{W} \times_{\cap} \mathbf{NumSp}
18
        // Row reduce {f BCU} and subtract nsver from every
            entry to account for 1 extra value per BCU
            row element
        \mathbf{delta}(:) = -nsver
19
        delta += [+_i BCU(:, j)]
20
```

## D. Single-Source Shortest-Paths (SSSP)

A Delta-Stepping Single-Source-Shortest-Path algorithm in GraphBLAS is shown in Alg. 5. It relies on the min.plus semiring. Since it is a fairly complex algorithm, refer to [24] for a description of the method.

## E. Triangle Counting (TC)

The triangle counting (TC) problem is to compute the number of unique cliques of size 3 in a graph. The TC algorithm is shown in Alg. 6, based on [26]. It starts with a heuristic that decides when to sort the input graph by ascending degree. Next, it constructs the lower and upper triangular part and computes a masked matrix multiply using the plus.pair

## Algorithm 4: PageRank (as specified in the GAPBS).

```
Data: \mathbf{A} \in \mathbb{B}^{n \times n}
                                                               // adjacency matrix
               damping
                                                                  // damping factor
               tol
                                                           // stopping tolerance
               itermax
                                           // maximum number of iterations
    Result: \mathbf{r} \in \mathbb{O}^n
 1 Function PageRank
          teleport = \frac{1-\alpha}{\pi}
 2
          \mathbf{r}(0:n-1) = \frac{1}{n}, \mathbf{t} = \mathbb{Q}^n
\mathbf{d_{out}} = [+_j \mathbf{A}(:,j)] // precomputed rowdegree
 3
 4
 5
          \mathbf{d} = \mathbf{d_{out}} \; \mathsf{div}_\cap \; damping // prescale with damping
          for k = 1 to numIterations do
 6
 7
                 swap t and r // t is now the prior rank
                 \mathbf{w} = \mathbf{t} \operatorname{\mathsf{div}}_{\cap} \mathbf{d}
 8
                \mathbf{r}(0:n-1) = teleport
 9
                \mathbf{r} += \mathbf{A}^\mathsf{T} plus.second \mathbf{w}
10
11
                 \mathbf{t} = abs(\mathbf{t})
12
                if [+_i \mathbf{t}(:)] < tol then
13
                     return
14
```

## **Algorithm 5:** SSSP (delta-stepping).

Data:

```
\mathbf{A}, \mathbf{A_H}, \mathbf{A_L} \in \mathbb{Q}^{|V| \times |V|}
              s, i \in \mathbb{N}
              \Delta \in \mathbb{Q}
             \mathbf{t}, \mathbf{t_{Req}} \in \mathbb{Q}^{|V|}
              \mathbf{t_{B_i}}, \mathbf{e} \in \mathbb{N}^{|V|}
 1 Function DeltaStepping
                 \mathbf{A_L} = \mathbf{A} \langle 0 < \mathbf{A} \le \Delta \rangle
 2
                 \mathbf{A_H} = \mathbf{A} \langle \Delta < \mathbf{A} \rangle
 3
                 \mathbf{t}(:) = \infty
 4
                 \mathbf{t}(s) = 0
 5
                 while \operatorname{nvals}(\mathbf{t}\langle i\Delta \leq \mathbf{t}\rangle) \neq 0 do
  6
  7
                            s = 0
                           \mathbf{t_{B_i}} = \mathbf{t} \langle i\Delta \leq \mathbf{t} < (i+1)\Delta \rangle
  8
                            while \mathbf{t_{B_i}} \neq 0 do
  9
                                     \mathbf{t_{Req}} = \mathbf{A_L^T} min.plus (\mathbf{t} \otimes \mathbf{t_{B_i}})
10
                                     \mathbf{e} = \mathbf{t} \langle 0 < \mathbf{e} \oplus \mathbf{t}_{\mathbf{B}_i} \rangle
11
                                     \mathbf{t_{B_i}} = \mathbf{t} \langle i\Delta \leq \mathbf{t_{Req}} <
12
                                       (i+1)\Delta
angle\otimes(\mathbf{t_{Req}}\ \mathsf{min}_{\cup}\ \mathbf{t})
13
                                     \mathbf{t} = \mathbf{t} \; \mathsf{min}_{\cup} \; \mathbf{t_{Req}}
                           \mathbf{t_{Req}} = \mathbf{A_H^T} \text{ min.plus } (\mathbf{t} \otimes \mathbf{e})
14
                           \mathbf{t} = \mathbf{t} \; \mathsf{min}_{\cup} \; \mathbf{t_{Req}}
15
                            i = i + 1
16
```

semiring. Internally, a dot product method is used in SS:GrB, because U is transposed via the descriptor. The pair is the simple function pair(x,y)=1. When used in a semiring, it acts like the times operator of the conventional semiring, except that it can ignore the values of its inputs and treat them both

## Algorithm 6: Triangle counting

```
Data: \mathbf{A} \in \mathbb{B}^{n \times n}
   Result: t \in \mathbb{N}
1 Function TriangleCount
          sample the mean and median degree of A
2
3
          if mean > 4 \times median then
                \mathbf{p} = permutation to sort degree, ascending order
4
               \mathbf{A} = \mathbf{A}(\mathbf{p}, \mathbf{p})
5
          \mathbf{L} = \operatorname{tril}(\mathbf{A})
6
          \mathbf{U} = \mathrm{triu}(\mathbf{A})
7
          \mathbf{C}\langle s(\mathbf{L})\rangle = \mathbf{L} plus.pair \mathbf{U}^\mathsf{T}
8
          t = [+_{ij} \mathbf{C}(i,j)]
```

as 1. This semiring is useful for structural computations, such as triangle counting, when the edge weights of a graph may be present but should be ignored in a particular algorithm.

## F. Connected Components

The connected components algorithm in LAGraph (Alg. 7) is written by Zhang, Azad, and Buluç [30], [31]. The method maintains a forest of trees represented by a parent vector, and interatively merges trees until no more merging is possible. The method as shown in Alg. 7 is a simplified variant that it operates on the entire graph. In the LAGraph version, a subgraph is constructed first, and the method finds the connected components of the subgraph, and then operates on the entire graph.

**Algorithm 7:** Connected components (FastSV).

```
1 Function FastSV
 2
          n = nrows(\mathbf{A})
          gf = f
 3
          dup = gf
          mngf = gf
 5
          \{i,x\} \leftarrow \mathbf{f}
 6
          repeat
 7
               // Step 1: Stochastic hooking
               \mathbf{mngf} = \mathbf{mngf} \, \mathsf{min} \, \mathbf{A}
 8
               \mathbf{mngf} = \mathbf{mngf} second.min \mathbf{gf}
               f(x) = f \min mngf
10
                // Step 2: Aggressive hooking
               \mathbf{f} = \mathbf{f} \; \mathsf{min} \; \mathbf{mngf}
11
               // Step 3: Shortcutting
               \mathbf{f} = \mathbf{f} \; \mathsf{min} \; \mathbf{gf}
12
               // Step 4: Calculate grandparents
13
                \{i,x\} \leftarrow \mathbf{f}
                \mathbf{gf} = \mathbf{f}(x)
14
                // Step 5: Check termination
                \mathbf{diff} = \mathbf{dup} \neq \mathbf{gf}
15
                sum = [\bigoplus_i \mathbf{diff}(i)]
16
                dup = gf
17
          until sum == 0
18
```

#### V. UTILITY FUCTIONS

LAGraph includes a set of utility functions that operate on a graph. All function names are prefixed with LAGraph\_ so we exclude that prefix in the names below, for brevity.

- Graph Properties: An LAGraph\_Graph includes cached properties which can be assigned by Basic methods, or which are required by Advanced methods.

  DeleteProperties clear all properies, Property\_AT computes the transpose of the adjacency matrix G->A, Property\_RowDegree computes the row degrees of G->A, Property\_ColDegree computes the column degrees of G->A, and Property\_ASymmetricPattern determines if the pattern of G->A is symmetric or unsymmetric.
- **Display and debug:** CheckGraph checks the validity of a graph. Since the graph is not opaque, a user application is able to change a graph arbitrarily and thus might make it an invalid object. **DisplayGraph** displays a graph and its properties.
- Memory management: Wrappers for malloc, calloc, realloc, and free, allowing a user application to select the memory manager to be used. These default to the ANSI C11 library functions.
- Graph I/O: BinRead and BinWrite read/write a GrB\_Matrix in binary form. MMRead and MMWrite read-/write a GrB\_Matrix in Matrix Market form.
- Matrix operations: Pattern returns a boolean matrix containing the pattern of a matrix. IsEqual determines if two matrices are equal. It selects the appropriate GrB\_EQ\_T operator that matches the matrix type, and then calls IsAll. IsAll compares two matrices and returns false if the pattern of the two matrices differ. It then uses a given comparator operator to compare all pairs of entries, and returns true if all comparisons return true.
- Degree operations: SortByDegree returns a permutation that sorts a graph by its row/column degrees, and SampleDegree computes a quick estimate of the mean and median row/column degrees.
- Error handling: LAGraph\_TRY and GrB\_TRY are helper macros for a simple try/catch mechanism. They require the user application to define LAGraph\_CATCH and GrB\_CATCH.
- Other: TypeName returns a string with the name of a GrB\_Type. KindName returns a string with of graph kind (directed or undirected). Tic and Toc provide a portable timer. Sort1, Sort2, and Sort3 sort 1, 2, or 3 integer arrays.

#### VI. EVALUATION

The performance of LAGraph can only be considered in context of an implementation of the underlying GraphBLAS library. This is discussed in Section VI-A, followed by performance results of the new LAGraph API on the 6 algorithms in the GAP Benchmark [4].

## A. SuiteSparse Extensions

In a prior paper ([3]), an early draft of Suite-Sparse:GraphBLAS v4.0.0 (Aug 2020) was compared with the GAP benchmark [4] and four other graph libraries. This prior version of SS:GrB included two primary data structures for its sparse matrices: compressed sparse vector, and a hypersparse variant [10], both held by row or by column. It included a draft implementation of a bitmap data structure that could only be used in a prototype breadth-first search. Since then, SuiteSparse:GraphBLAS v4.0.3 has been released, with full support for bitmap and full matrices for all its operations. In an *m*-by-*n* bitmap matrix, the values are held in a full array of size mn, and another int8\_t array of size mn holds the sparsity pattern of the matrix. A full matrix is a simple dense array of size mn.

The bitmap format is particularly important for the "pull" phase of an algorithm, as used in direction-optimizing breadth-first-search [4], [27]. The GAP benchmark suite uses this method by holding its frontier as a bitmap in the pull step and as a list in the push step. The GAP BFS was shown to be typically the fastest BFS amongst the 6 graph libraries compared in [3] (for 4 of the 5 benchmark graphs). With the addition of the bitmap format to SS:GrB, LAGraph+SS:GrB is able to come within a factor of 2 or so of the performance of the highly-tuned BFS GAP benchmark (see the results in the next section), for those 4 graphs. At the same time, however, the BFS is very easily expressed in LAGraph as an easy-to-read and easy-to-write code. This enables non-experts to obtain a reasonably high level of performance with modest programming effort when writing their own graph algorithms.

Additional optimizations added to SS:GrB in the past year include a lazy sort. Normally, SS:GrB keeps its vectors sorted (row vectors in a CSR matrix, or column vectors if the matrix is held by column), with entries sorted in ascending order of column or row index, respectively. This simplifies the many algorithms that operate on a GrB\_Matrix. However, some algorithms naturally produce a jumbled result (matrix multiply in particular), while many algorithms are tolerant of jumbled input matrices. We thus allow the sort to be left pending. The lazy sort joins two other kinds of pending work in SS:GrB: pending tuples and zombies [12]. A pending tuple is an entry that is held inside a matrix in an unsorted list, awaiting insertion into the CSR/CSC format of a GrB\_Matrix. A zombie is the opposite: it is an entry in the CSR/CSC format that has been marked for deletion, but has not yet been deleted from the matrix. With the lazy sort, the sort is postponed until another algorithm requires sorted input matrices. If the sort is lazy enough, it might never occur, which is the case for the LAGraph BFS and BC.

Another useful addition to SS:GrB is the new positional binary operators, such as the any secondi used in the BFS.

#### B. Performance Results

Our benchmark environment is an NVIDIA DGX Station (donated to Texas A&M by NVIDIA in support of this research). It includes a 20-core Intel(R) Xeon(R) CPU E5-2698 v4 @

Algorithm:	gı	aph, with	run time	in seconds	
package	Kron	Urand	Twitter	Web	Road
BC : GAP	31.52	46.36	10.82	3.01	1.50
BC : SS	24.52	30.69	9.11	8.43	34.06
BFS : GAP	.31	.58	.22	.34	.25
BFS: SS	.52	1.22	.33	.66	3.32
PR : GAP	19.81	25.29	15.16	5.13	1.01
PR:SS	22.17	27.71	17.21	9.30	1.34
CC : GAP	.53	1.66	.23	.22	.05
CC : SS	3.36	4.47	1.47	1.97	.98
SSSP : GAP	4.91	7.23	2.02	.81	.21
SSSP : SS	17.37	25.54	8.54	9.61	46.79
TC : GAP	374.08	21.83	79.58	22.18	.03
TC: SS	917.99	34.01	239.58	34.65	.23

TABLE II: Run time of GAP and LAGraph+SS:GrB

graph	nodes	entries in A	graph kind
Kron	134,217,726	4,223,264,644	undirected
Urand	134,217,728	4,294,966,740	undirected
Twitter	61,578,415	1,468,364,884	directed
Web	50,636,151	1,930,292,948	directed
Road	23,947,347	57,708,624	directed

TABLE III: Benchmark matrices (https://sparse.tamu.edu/GAP)

2.20GHz, with 40 threads. All codes were compiled with gcc 5.4.0 (-O3). All default settings were used, which means that hyperthreading was enabled. The system has 256GB of RAM in a single socket (no NUMA effects). LAGraph (Feb 7, 2021) and SuiteSparse:GraphBLAS 4.0.4-draft (Feb 7, 2021) were used. The NVIDIA DGX Station includes four P100 GPUs, but no GPUs were used by this experiment (a GPU-accelerated SS:GrB is in progress). Table II lists the run time (in seconds) for the GAP benchmark and LAGraph+SS:GrB for the 6 algorithms on the 5 benchmark matrices. The benchmark matrices are listed in Table III.

With the simple addition of the bitmap (needed for the pull step), the push/pull optimization in BC resulted in a nearly 2x performance gain in the GraphBLAS method for the largest matrices, as compared to the SS:GrB version used for the results presented in [3].

With this change the BC method in LAGraph+SS:GrB is not only expressible in a simple, elegant code, but it is also faster than the highly-tuned GAP benchmark method, bc.cc, for the three largest matrices (1.3x for Kron, 1.5x for Urand, and 1.2x for Twitter).

With the addition of bitmap format (which makes push/pull optimization very simple to express, and very fast) and the any.secondi semiring, the BFS of a directed or undirected graph is easily expressed in GraphBLAS, and has a performance that is only about 1.5x to 2x slower than the GAP benchmark. We expect the remaining performance gap arises from two issues:

1) The GAP assumes that the graph has fewer than 2<sup>32</sup> nodes and edges, and thus uses 32-bit integers throughout. GraphBLAS is written for larger problems, and thus relies solely on 64-bit integers. This cannot be easily changed in GraphBLAS, but rather than "fixing" GraphBLAS to use smaller integers, it is the GAP algorithms that would need to be updated for larger graphs in the future. In the

- current GAP benchmark graphs, two graphs are chosen with almost exactly 4 billion edges. Graphs of current interest in large data science can easily exceed  $2^{32}$  nodes and edges [17].
- 2) In GraphBLAS, the BFS must be expressed as two calls. The first computes  $\mathbf{q}\langle \neg \mathbf{p} \rangle = \mathbf{q}^{\mathsf{T}} \mathbf{A}$ , and the second updates the parent vector,  $\mathbf{p}\langle s(\mathbf{q}) \rangle = \mathbf{q}$ :

GrB\_vxm (q, p, NULL, semiring, q, A, GrB\_DESC\_RSC);
GrB\_assign (p, q, NULL, q, GrB\_ALL, n, GrB\_DESC\_S);

In Scott Beamer's bfs.cc, these two steps are fused, and the matrix-vector multiplication can write its result directly into the parent vector p. This could be implemented in a future GraphBLAS library, since the GraphBLAS API allows for a non-blocking mode where work is queued and done later, thus enabling a fusion of these two steps. SS:GrB exploits the non-blocking mode (for its lazy sort, pending tuples, and zombies) but does not *yet* exploit the fusion of GrB\_vxm and GrB\_assign. We intend to exploit this in the future.

Note that for the Road graph, LAGraph+SS:GrB is quite slow for all but PageRank (PR). The primary reason for this is the high diameter of the Road graph (about 6980). This requires 6980 iterations of GraphBLAS in the BFS, each with a tiny amount of work. Each call to GraphBLAS does several malloc and frees, and in some cases the workspace must be initialized. A future version of SS:GrB is planned that will eliminate this work entirely, by implementing an internal memory pool. There may be other overheads, but we hope that a memory pool, fusion to fully exploit non-blocking mode, and other optimization will address this large performance gap for the Road graph for these algorithms.

LAGraph+SS:GrB is also up to 3x slower than the GAP for the triangle counting problem (for all but the Road graph, where it is even slower). This performance gap can be eliminated entirely in the future, if the GrB\_mxm and GrB\_reduce are combined in a single fused step, by a full exploitation of the GraphBLAS non-blocking mode. The current method computes  $\mathbf{C}\langle s(\mathbf{L})\rangle = \mathbf{L}\mathbf{U}^\mathsf{T}$ , followed by the reduction of  $\mathbf{C}$  to a single scalar. The matrix  $\mathbf{C}$  is then discarded. All that GraphBLAS needs is a fused kernel that does not explicitly instantiate the temporary matrix  $\mathbf{C}$ . This is permitted by the GraphBLAS  $\mathbf{C}$  API Specification, but not yet implemented in SS:GrB.

#### VII. CONCLUSION

Future work - ideas:

- Create a Python wrapper for LAGraph
- Implement the LDBC Graphalytics benchmark [14]
- Improve data ingestion performance using e.g., SIMD instructions [18]

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## TODO: add acks

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