LAGraph: A Community Effort to Collect Graph Algorithms built on top of the GraphBLAS

Tim Mattson[‡], Tim Davis[⋄], Manoj Kumar[¶], Aydın Buluç[†], Scott McMillan[§], José Moreira[¶], Carl Yang^{*,†}

[†]Intel Corporation [†]Computational Research Division, Lawrence Berkeley National Laboratory

[†]Texas A&M University ¶IBM Corporation §Software Engineering Institute, Carnegie Mellon University

*Electrical and Computer Engineering Department, University of California, Davis

Abstract—In 2013, we released a position paper to launch a community effort to define a common set of building blocks for constructing graph algorithms in the language of Linear Algebra. This led to the GraphBLAS. We released a specification for the C programming language binding to the GraphBLAS in 2017. Since that release, multiple libraries that conform to the GraphBLAS C specification have been produced.

In this position paper, we launch the next phase of this ongoing community effort; a project to assemble a set of high level graph algorithms built on top of the GraphBLAS. While many of these algorithms are well-known with high quality implementations available, they have not been assembled in one place and integrated with the GraphBLAS. We call this project the *LAGraph graph algorithm project* and with this position paper, put out a call for collaborators to join us. While the initial goal is to just assemble these algorithms into a single framework, the long term goal is a library of production-worthy code; with the LAGraph library serving as an open source repository of verified graph algorithms that use the GraphBLAS.

Index Terms—Graph Algorithms, Linear Algebra, Graph-BLAS

I. INTRODUCTION

Graphs are an essential abstraction for a wide range of problems. There are many ways to represent algorithms over graphs. One class of methods defines graphs in terms of matrices. For example, we can define a graph in terms of an adjacency matrix where the rows and columns are labeled by the vertices and the non-zero elements of the matrix are the edges between vertices.

Expressing graph algorithms in the "language of linear algebra" [1] is a mature subject. Multiple high performance graph libraries based on sparse linear algebra [2], [3], [4], [5], [6] have been developed. With this "Graphs as Linear Algebra" approach established, a community of researchers came together to define common building blocks for graphs expressed in the language of linear algebra. They launched this effort with a position paper [7] in 2013 and formed the GraphBLAS Forum [8]. After almost three years of steady work, the GraphBLAS forum completed the mathematical formalizations of the GraphBLAS [9]. With another one and a half years of work, the group completed the C language binding to the GraphBLAS [10].

Currently there are multiple implementations of the Graph-BLAS C specification. We have learned a great deal about how to define the operations within the GraphBLAS and

how to implement them efficiently. We are now ready to launch the next phase of the project: to produce a library of high level graph algorithms implemented on top of the GraphBLAS. We call this library of algorithms *LAGraph*. Just as we launched the GraphBLAS project with a position paper, we are launching this next phase of the project with a position paper.

The goals of the LAGraph effort is first and foremost to bring together the full range of known graph algorithms that can be constructed with the GraphBLAS. From this collection we will be able to systematically assess the coverage of graph algorithms based on Linear Algebra. This will also serve as raw material in ongoing studies of the fundamental design patterns exploited by linear algebra based graph algorithms.

The basic outline of the LAGraph project is summarized in Figure 1. The library of algorithms is the single box towards the middle of the figure. These algorithms use the GraphBLAS C API which exists as a separate implementation for a wide range of hardware targets at the bottom of the figure. To motivate our work and stay aligned with the way data scientists work with graph algorithms, we need to appreciate that people will use a wide range of languages to access the graph algorithms. A good library must be able to work whether called directly from C or indirectly through a wrapper in Python. Furthermore, the developers of the graph algorithm libraries will need a test harness to validate the algorithms, I/O utilities, and a build system. All of these components must be addressed as part of the LAGraph project.

Initially, LAGraph is not intended to be a production-worthy library of high level graph algorithms. We expect over time, however, that from the LAGraph effort, we will produce such a library. Anticipating that goal, we are constructing the library "as if" it was to be used by data analytics end-users; i.e. by people who need the results from graph algorithms with little concern for how they are implemented. This requirement of building a library for *end-users* as opposed to a library for *graph algorithm researchers* has far reaching implications for the design of this software.

We start the paper with a brief summary of the objects and operations defined in the C specification of the GraphBLAS. We then summarize some of the early libraries that implement the GraphBLAS C specification. Next, we describe the repository where we will build LAGraph. This is important

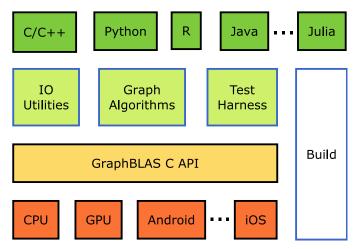


Fig. 1: **LAGraph Project Overview.** The project consists of a library of graph algorithms, assorted components to support algorithm development and validation (a test harness and I/O utilities) and it must interface to a wide range of languages. underneath these components is a build system, implementations of the GraphBLAS, and a variety of hardware targets.

since the purpose of a position paper is to attract a community of researchers to join the effort which means we want people to understand how to work with and perhaps contribute algorithms to the repository. We then discuss the challenges we faced in writing the early version LAGraph and what it suggests about future developments needed in the GraphBLAS themselves. We close with concluding remarks.

II. THE GRAPHBLAS

Consider a graph represented as an n-by-n adjacency matrix \mathbf{A} , where A_{ij} is the weight of the edge from vertex i to vertex j, and a second k-by-n matrix \mathbf{B} representing a subset (of size k) of the vertices in the graph, such that B_{ji} is 1 if the jth element of the subset is vertex i (and all other elements of \mathbf{B} are 0). The traditional matrix product $\mathbf{B} \times \mathbf{A}$ over real arithmetic of these two matrices returns the cost based on the edge weights of reaching the set of vertices adjacent to the vertices in \mathbf{B} . This fundamental operation can be used to construct a wide range of graph algorithms.

We extend the range of graph operations by keeping the basic pattern of a matrix-matrix multiplication, but varying the operators and the interpretation of the values in the matrices (the *domain*). By carefully choosing operators and the domain, we control the relation between matrix operations familiar in linear algebra and graph operations, thereby enabling composable graph algorithms.

In addition to matrix multiplication, the GraphBLAS math specification defines a range of additional operations over matrices and vectors. These are summarized in Table I.

In mapping the GraphBLAS as a set of mathematical operators onto the C programming language we made a number of fundamental choices [10]. First, the core data structures TABLE I: A mathematical overview of the fundamental GraphBLAS operations supported in this specification. A, B, and C are GraphBLAS matrices; \mathbf{u} , \mathbf{v} , and \mathbf{w} are GraphBLAS vectors; i and j are single indices; \mathbf{i} and \mathbf{j} are arrays of indices; \oplus and \otimes are arbitrary element-wise operators; the element-wise \odot operator is used for the optional accumulation with the output GraphBLAS object where $x\odot=y$ implies $x=x\odot y$; and $F_u()$ is a unary function. Although not shown here, the input matrices \mathbf{A} and \mathbf{B} may be selected for transposition prior to the operation, and masks can be used to control which values are written to the output GraphBLAS object.

Operation name	Mathematical description		
mxm	$\mathbf{C} \odot = \mathbf{A} \oplus . \otimes \mathbf{B}$		
mxv	$\mathbf{w} \odot = \mathbf{A} \oplus . \otimes \mathbf{v}$		
vxm	$\mathbf{w}^T \odot = \mathbf{v}^T \oplus . \otimes \mathbf{A}$		
eWiseMult	$\mathbf{C} \odot = \mathbf{A} \otimes \mathbf{B}$		
	$\mathbf{w} \odot = \mathbf{u} \otimes \mathbf{v}$		
eWiseAdd	$\mathbf{C} \odot = \mathbf{A} \oplus \mathbf{B}$		
	$\mathbf{w} \odot = \mathbf{u} \oplus \mathbf{v}$		
reduce (row)	$\mathbf{w} \odot = \bigoplus_{j} \mathbf{A}(:,j)$		
apply	$\mathbf{C} \odot = F_u(\mathbf{A})$		
	$\mathbf{w} \odot = F_u(\mathbf{u})$		
transpose	$\mathbf{C} \odot = \mathbf{A}^T$		
extract	$\mathbf{C} \odot = \mathbf{A}(\mathbf{i}, \mathbf{j})$		
	$\mathbf{w} \odot = \mathbf{u}(\mathbf{i})$		
assign	$\mathbf{C}(\mathbf{i},\mathbf{j}) \odot = \mathbf{A}$		
-	$\mathbf{w}(\mathbf{i})$ $\odot = \mathbf{u}$		

required to represent the objects defined by the GraphBLAS are opaque. The GraphBLAS API defines a contract with the programmer for how these objects will be used, but the implementations and underlying data structures are left to the implementation. This opaqueness is critical if the API is to serve diverse hardware ranging from CPUs to GPUs to specialized graph hardware. Second, we defined a non-blocking execution model that allows lazy evaluation. Ultimately, to optimize sparse linear algebra software we need to aggressively fuse operations and even restructure algorithms. This requirement meant that we had to carefully define when results from a sequence of GraphBLAS operations must be materialized.

Since the release of the GraphBLAS specification, several implementations of the GraphBLAS have been developed.

A. SuiteSparse:GraphBLAS

SuiteSparse:GraphBLAS is the first full implementation of the GraphBLAS standard, first released in November of 2017. It is available at http://suitesparse.com [11].

The design of a GraphBLAS library is flexible, because its data structures are opaque to the user. SuiteSparse:GraphBLAS uses a compressed-sparse vector data structure, in four different forms. A matrix can be stored in row-major order (CSR), or column-major order (CSC). Each sparse vector consists of a sorted list of indices, and the corresponding numerical values. The sparse vectors are packed together into two arrays, and another "pointer array" (of size equal to the dimension of the matrix, say n) keeps track of where each row (or column) starts. The memory taken is O(n+e) for a CSR

matrix with n rows or a CSC matrix with n columns, and with e entries. Most graphs have e = O(n) entries, but some graphs (and in particular, subgraphs) can be hypersparse [12], with e << n. In the hypersparse form, the pointer array itself becomes sparse, and empty vectors take no space at all. The space is reduced to O(e), so that matrices with enormous dimensions can be created, as long as e << n. SuiteSparse:GraphBLAS exploits hypersparsity automatically, and all methods can operate on all four matrix formats in any combination.

The ability to incrementally modify a graph is critical in many applications. GraphBLAS includes two operations that can make small incremental changes to a graph/matrix: namely GrB setElement and GrB assign. It would be exceedingly slow to insert or delete a single entry in a CSR or CSC format, taking O(n+e) time **per entry** inserted or deleted. Instead, the non-blocking aspect of GraphBLAS is exploited. Fast deletion of entries is handled by creating zombies, which are entries tagged for later deletion. Fast insertion is handled with *pending tuples*, which is a separate unordered list of (i, j, a_{ij}) for each new entry. When a matrix operation occurs (such as matrix multiply), all zombies are killed and all pending tuples are assembled, in a single $O(n+e+p\log p)$ step (for p pending tuples), or $O(e + p \log p)$ in the hypersparse case. As a result, it is just as fast to use a sequence of e GrB setElement operations to build a matrix, as it is to create an array of e tuples and use GrB build. Internally, SuiteSparse:GraphBLAS is building the list itself, for the user, and then does a GrB build when the matrix needs to be completed.

To enable high-performance matrix-matrix multiply, a code generation mechanism is used to build functions for each semiring that can be created with built-in operators. The functions can rely on Gustavson's method [13], a dot product method, and a heap-based method [14], all with masked variants. A current prototype of the package adds an early exit mechanism for the MIN, MAX, OR, and AND monoids, where a dot product can terminate as soon as a terminal value is found in the result (true for OR, for example). This will enable a fast direction-optimizing BFS [15] to be written in GraphBLAS. The "pull" is a dot product, and the "push" a saxpy-based operation (Gustavson's or the heap method).

Since its creation was commissioned as the GraphBLAS reference implementation, testing is a vital component to the package. In SuiteSparse:GraphBLAS, each GraphBLAS operation was written twice: once in high-performance algorithms in C, and again in a very simple and short MATLAB script, using dense matrices with the required type. The pattern in the MATLAB version is held as a separate Boolean matrix. For example, GrB_assign requires about 3,908 lines of C (not counting comments), but only 161 lines in MATLAB. Of those 161 lines, 33 are for error-checking that do not need to be considered when determining conformance to the spec. The MATLAB functions are not intended to be fast. Instead, they exactly mimic the GraphBLAS API Specification, line by line, so they can be visually inspected for conformance

to the spec. For example, matrix multiply is written with a brute-force triply-nested for loop. Then, to test the package, each computation is done both in SuiteSparse:GraphBLAS (via a MATLAB interface) and in the MATLAB mimic. The tests pass only if the results are identical in both value and pattern (even with identical floating-point roundoff error, in most cases).

The current release is single-threaded, but an OpenMP implementation is in progress. SuiteSparse:GraphBLAS appears in Debian and Ubuntu Linux distros, and has been released as part of the RedisGraph database module of the Redis database systems, by RedisLabs, Inc. [16].

B. IBM GraphBLAS

TODO: Manoj and Jose: Describe the IBM GraphBLAS implementation [17]

C. GBTL: GraphBLAS Template Library

The first version of the GraphBLAS Template Library (GBTL) was written in C++ when the GraphBLAS C API project was just beginning. It was used, in part, to study early ideas under discussion in the specification process and was released as a proof of concept prior to the finalization of the GraphBLAS API Specification [18], [19]. With the release of the GraphBLAS C API Specification [10] in 2017, GBTL was updated to conform to the mathematical behavior defined by the specification and released as version 2.0 [20]. Unlike the C API Specification, GBTL is written in C++ and makes judicious use of templates to make the generic aspects of the GraphBLAS specification easier to implement and more natural for the C++ programming language. When the GraphBLAS language committee starts its work on the C++ language binding to the GraphBLAS, GBTL will be submitted as a proposed starting point for the discussion.

As illustrated in Figure 2, central to GBTL's design is the concept of a separation of concerns between implementation of algorithms written in terms of the GraphBLAS primitives and the implementation of those primitives on a targeted hardware platform. Today the separation of concerns is defined by the GraphBLAS API Specification. Above this API, GBTL has developed and includes a collection of graph algorithms written against its C++ API and has already been shown to be easily translated to the C API. Below the separation/API, different implementations of the GraphBLAS library can be supported for different hardware architectures (referred to as "backends"). In this way we verify that algorithms written once against the API can run on different targeted hardware. In terms of backend implementations, a mathematically correct reference implementation (not optimized) for single threaded CPU is provided with Version 2.0 of GBTL (version 1.0 also had a GPU implementation). Other backend implementations are currently under development to target specialized computer architectures.

Another development effort closely related to GBTL is a DSL in Python called pyGB [21]. The goal for pyGB is to closely resemble the GraphBLAS mathematical notation found

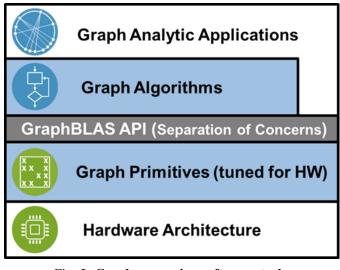


Fig. 2: Graph processing software stack.

Fig. 3: Depth-BFS function in pyGB.

in the GraphBLAS math spec [9]. PyGB is a framework is designed and implemented to dispatch dynamically generated and compiled templated classes that make calls into native GBTL code. It demonstrates how Python's syntax and dynamic execution provides a high-level abstraction with minimal performance penalty. While we leave a detailed discussion of pyGB to elsewhere [21] we provide a depth-BFS function using pyGB in Figure 3. Notice how the meaning of the code is straightforward since the DSL closely tracks the notation from the GraphBLAS math spec. We believe in the long run, the future of graph algorithms will depend heavily on such DSLs.

D. GraphBLAST GraphBLAS

GraphBLAST [22] is the first high-performance GPU (graphics processing unit) implementation of GraphBLAS. Inspired by the design of GBTL, the architecture of GraphBLAST is also C++ based and maintains a separation of concerns between a top-level interface defined by the GraphBLAS C API specification and the low-level backend.

One novel aspect about GraphBLAST is that it supports performance-oriented optimizations such as direction-optimization (also known as push-pull traversal), which was discovered by Beamer, Asanovic and Patterson [15] and generalized by Shun [23] to other graph algorithms. Yang, Buluç and Owens [24] show that this optimization is key for a GraphBLAS implementation to meet the performance of state-of-the-art graph frameworks on the GPU like Gunrock [25].

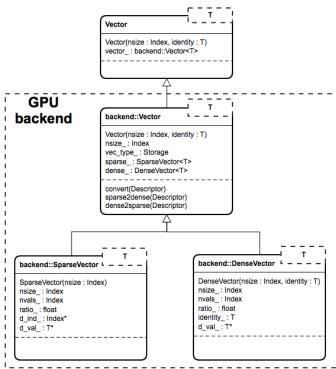


Fig. 4: GraphBLAST Vector UML diagram.

In each iteration of an GrB_mxv , the GraphBLAST backend checks whether the vector sparsity was has crossed a threshold k. If it has gone above the threshold, then the traversal will switch from push to pull. If it has gone below the threshold, then the traversal will switch from pull to push. If neither outcome has occurred, then it will use the traversal it used in a previous iteration.

To support direction-optimization, the GraphBLAST backend maintains a SparseVector and DenseVector object as shown in Figure 4. The push traversal is performed using Gustavson's method as a sparse-matrix sparse-vector multiply (SpMSpV) between the SparseVector and the adjacency matrix transpose in CSC format. The pull traversal is performed in a dot-product manner as a sparse-matrix dense-vector multiply (SpMV) between the DenseVector and the adjacency matrix in CSR format. This raises the issue of having to keep around two copies of each GrB_Matrix object when it is not symmetric. An environmental variable is used to control whether the user wants this performance-oriented storage, or whether they want a more memory-inexpensive storage of only CSR or only CSC in which case the direction-optimization feature is disabled.

Direction-optimization is a good example where the power of abstracting away implementation details shines through, and the linear algebraic approach to graph analytics is at its most powerful. The end user has two conflicting desires:

 They want to communicate their request abstractly enough that they do not have to decide whether the matrix-vector multiply is implemented as push, pull or any of the myriad possible ways.

Algorithm	Ligra [23]	GraphIt [26]	GraphBLAS
Breadth-first-search	29	22	25
Single-source shortest-path	55	25	25
Local graph clustering	84	N/A	45

TABLE II: Comparison of lines of C++ application code counted by 'cloc' except for numbers of GraphIt, which come from the paper [26]. N/A means not implemented. The specific GraphBLAS implementation for this comparison is GraphBLAST [22].

2) They want their computation to be described *specifically* enough that the computer can optimize for the best approach for doing the computation.

This desire is met by GrB_mxv, which is at the same time *abstract* enough to not limit the computer in choosing push traversal when it should be choosing pull traversal, yet *specific* enough that the computer has enough information to cut corners and pick the best algorithm.

Table II shows a comparison of how many lines of code it takes an implementation of GraphBLAS to express a given algorithm in C++. It is compared with two state-of-the-art graph frameworks in shared memory, the aforementioned Ligra [23] and GraphIt [26], which is a DSL (domain specific language) designed for expressing graph algorithms.

III. LAGRAPH REPOSITORY

The hypothesis underlying the GraphBLAS is that algorithm designers can focus on expressing their algorithms in terms of the high level linear algebra operations defined in the GraphBLAS while leaving low level optimizations to any particular hardware platform to the implementor of the GraphBLAS. Ultimately, we want hardware vendors to be responsible for creating highly tuned versions of the GraphBLAS specialized to the features of their systems.

Algorithm designers will naturally wonder how much performance is lost due to the use of a high level API such as the GraphBLAS. We believe the GraphBLAS bring inherent efficiency advantages to a graph algorithms due to the more structures access to data afforded by the sparse linear algebra formats. This is an untested hypothesis, however, since until now, we have not had multiple implementations of a high level API tuned to the features of a range of platforms.

Testing this hypothesis of the performance potential afforded by the GraphBLAS is a major outcome we anticipate from the LAGraph project. By collecting high level graph algorithms and validating them across an engaged community, we will produce the library of algorithms needed to evaluate the effectiveness of the GraphBLAS approach.

Before we can conduct such experiments, however, we need to collect graph algorithms implemented on top of the GraphBLAS. We have created a git hub repository at https://github.com/GraphBLAS/LAGraph for members of the LAGraph community to use to contribute GraphBLAS algorithms. The basic elements of the repository include:

- A Build System for creating the LAGraph library and the test routines.
- A library of utilities including loading matrices from disk in Matrix Market format [27], evaluating results, and creating random test matrices.
- A directory of graph algorithms.
- A directory holding a test harness for each algorithm.

We will write documentation, a programmer's reference guide and define procedures for how people can add new algorithms.

IV. DISCUSSION

We are early in the LAGraph project. At this point, we've defined the basic structure of the repository and the overall goals of the project. We have built an early framework for testing and core utility routines to support software development. Finally, we assembled a few algorithms which we are using to test the basic structure of the software system.

Even at this early phase of the project, we have learned a great deal about how the GraphBLAS will interact with end-users. The objects manipulated by the GraphBLAS are opaque. An implementation needs complete freedom in how data structures underlying the GraphBLAS are implemented. A graph algorithm, however, is used as part of a processing pipeline. For example, data may exist in data frames. A subset of the data is collected and filtered to produce relationships represented by a graph. Properties of the graph are computed and based on the result a new branch in the processing pipeline may be accessed.

The key here is that graphs inside the GraphBLAS are opaque, but externally they are anything but opaque. This suggests that we need to define functions to import and export data in standard sparse array formats into LAGraph. The initial thinking was that this import functionality would be part of LAGraph and not the GraphBLAS. The only way to do that, however, is if we repacked the input sparse format into separate arrays for column indices, row indices, and values and then use <code>GrB_build_matrix</code> to construct the GraphBLAS matrix object. This would extremely inefficient. We need a way to directly import arrays in standard sparse formats into the GraphBLAS and since the GraphBLAS data types are opaque, this can only be done as a GraphBLAS routine.

Graph algorithms do not occur in isolation. The LAGraph library, therefore, needs to return a handle to an opaque GraphBLAS object so it can be used without incurring copy overhead in subsequent graph operations. Given the nonblocking execution model, this raises interesting design questions about how memory consistency between the library and the application is managed.

Graphs can be quite large. Hence, we do not believe the default mode should be that sparse arrays input to LAGraph are copied into a separate memory region to hold the opaque GraphBLAS object. We believe it is important that the memory for the input array be used to hold the GraphBLAS object. This means the input array is "destroyed" (from the perspective of LAGraph, another external library, or the user application) and

replaced with the GraphBLAS opaque object. Since during a computation it is common that elements of a matrix fill-in, the GraphBLAS routines will in some cases need to allocate additional memory during a calculation. This may require deallocating memory and reallocating a larger block of memory. This means we will likely encounter situations where a region of memory allocated in an application is deallocated inside a library routine. This violates the separation of concerns between application and library code expected in well engineered software. There is also the question of communicating to the library routine how the input sparse array was allocated in the first place so the right deallocator can be used.

A draft of SuiteSparse:GraphBLAS includes a working and fully-tested implementation of the import/export feature, using a strategy much like the "move constructor" of C++. For the export of a CSC matrix, for example, three arrays are removed from the GraphBLAS matrix A: a pointer array Ap of size n+1, an index array Ai of size e, and a values array Ax. The row indices of the jth column of the matrix appear as the list Ai [Ap[j]...Ap[j+1]], and the values are in the same locations in Ax. This format is identical to the simple CSC sparse matrix data structure in CSparse [28], except that GraphBLAS allows for many built-in types and arbitrary user-defined types.

The remains of the GraphBLAS object A are then deleted, but all of its content is now "owned" by the external library (LAGraph, say), which is then responsible for freeing these three arrays. Assuming that the opaque GraphBLAS object A is already in the CSC format, the export takes just O(1) time, and no new memory is allocated. The external library (LAGraph, in particular) now has access to the graph. If the GraphBLAS implementation does not support the CSC format in its internal opaque data structure, it can allocate these arrays, populate them, and then free A. The effect is the same; only the performance differs. Opacity is maintained, while at the same time reducing time required for the export from $\Omega(e)$ (for GrB_extractTuples) to as little as O(1).

The import is symmetric with the export: LAGraph (or any other external library) passes in the three arrays Ap, Ai, and Ax, which are then either incorporated as-is into the GrB_Matrix A (taking O(1) time), or copied and freed (taking O(e) time and memory). Either way, the three arrays are now owned by GraphBLAS, not the external library, and would be freed at some point no later than GrB_free(&A). Since the matrix A is opaque, the GraphBLAS library can select whatever method it chooses to take ownership of Ap, Ai, and Ax: a copy (in O(e) time, or a move construction in O(1) time. It may choose later to realloc these arrays if the number of entries needs to grow.

After an export of \mathbb{A} , and then an import of the same arrays, the GraphBLAS matrix \mathbb{A} is perfectly reconstructed, ideally in a total of O(1) time. SuiteSparse:GraphBLAS supports the import/export of all four of its formats: CSR, CSC, and their hypersparse variants.

A malloc of these Ap, Ai, and Ax arrays by an exter-

nal library followed by a freeing of the same space inside GraphBLAS with GrB_free(&A) requires both libraries to agree on using the same malloc/free routines. To do this, the GraphBLAS API would need to be augmented to allow an external library to select which malloc/free routines should be used.

The point of these issues is that in designing an effective library, there are a host of complicated issues to resolve. A major part of the research contribution of this project will be how we solve these issues.

V. CONCLUSION

The GraphBLAS forum started its work on standard building blocks for graphs in the language of linear algebra in 2013 [7]. We now have a C specification for the GraphBLAS [10] and multiple implementations [11], [20], [29]. The next step in this journey is to define a library of high level graph algorithms that are based on the GraphBLAS.

The GraphBLAS was a community effort launched by a position paper. This is a position paper to launch LAGraph, our community effort to collect and validate a set of high quality graph algorithms that run on top of the GraphBLAS. We urge readers interested in joining us as we work on LAGraph to contact any of the authors of this position paper.

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TODO: Aydın Buluç Carl Yang and maybe Scott will need to acknowledge someone.

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