GraphBLAS: Building a C++ Matrix API for Graph Algorithms

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October 24-29

About Us





Ben, PhD Candidate at UC Berkeley

Data structures and algorithms for **parallel** programs. Working on C++ library of distributed data structures. Please hire me!

Scott, Principal Engineer at CMU SEI

Graph/ML/Al algorithms for large- and smallscale parallel systems. Working on **GBTL**, a linear algebra-based C++ library for graph analytics.

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DM21-0916



This Talk

Background: How and why to use **matrix algebra** for **graphs**?

What are the important **data structures** and **concepts**?

Prior work in the **GraphBLAS community**, C API

Overview of our draft C++ API







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How might this interoperate with standard C++, graph library proposal?

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What are the important **data structures** and **concepts**?

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What This Talk Is Not

A C++ standards proposal

- A complete evaluation of graph programming models





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Graphs: Understanding relationships between items

Graph: A visual representation of a set of vertices and the connections between them (edges).



Graph is a pair (V, E):

- -V is a set of vertices
- -E is a set of paired vertices (edges)

$$V = \{0, 1, 2, 3, 4, 5, 6\}$$

 $E = \{(0,1), (0,3), (1,4), (1,6), (2,5), (3,0), \}$ (3.2), (4.5), (5.2), (6.2), (6,3), (6,4)

Ordered pairs results in directed graphs (shown)

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Graph Analysis is Important and Pervasive



Graphs as Adjacency Matrices

Graphs are represented as adjacency matrices that usually have sparse and irregular structure.





 $\mathbf{A}_{ij} = \begin{cases} \bullet & (v_i, v_j) \in E \\ \emptyset & (v_i, v_j) \notin E \end{cases}$

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GraphBLAS Timeline

Book – Papers – GraphBLAS standards – SuiteSparse:GraphBLAS releases



Graph Algorithms in the Language of Linear Algebra

Standards for graph algorithm primitives, **HPEC**

Seven good reasons. ICCS

Mathematical C API. foundations. **GABB**@ **HPEC IPDPS**

LAGraph, **GrAPL***^(a)* **IPDPS**



The GraphBLAS "standard"

Goal: separate the concerns of the hardware/library/application designers. 1979: BLAS Basic Linear Algebra Subprograms (BLAS 2 '88, BLAS 3 '90)







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The GraphBLAS "standard"

Goal: separate the concerns of the hardware/library/application designers.

- 1979: BLAS Basic Linear Algebra Subprograms (BLAS 2 '88, BLAS 3 '90)
- 2001: Sparse BLAS an extension to BLAS (little uptake)
 - an effort to define standard building blocks for graph algorithms in the language of linear algebra



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2013: GraphBLAS





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Graphs as Adjacency Matrices





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Graph Operations as Matrix Operations





• Matrix-vector multiply \rightarrow find neighbors

- In-neighbors: use A
- Out-neighbors: use AT

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Graph Operations as Matrix Operations

Finding out-neighbors is used many graph algorithms.





- Matrix-vector multiply \rightarrow find neighbors
 - In-neighbors: use A
 - Out-neighbors: use A^T

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Graph Operations as Matrix Operations

Another way to look at matrix-vector multiply...





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(0)

 (\mathbb{I})

2

B

4





What is $\oplus . \otimes ??$





Matrix multiplication

Conventional matrix multiplication uses arithmetic plus (+) and times (x):

$$\mathbf{y} = \mathbf{A} \mathbf{x}$$
$$\mathbf{y}(i) = \sum_{k} \mathbf{A}(i,k) \cdot \mathbf{x}(k)$$

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Matrix multiplication on semirings

Conventional matrix multiplication uses arithmetic plus (+) and times (x):

$$\mathbf{y} = \mathbf{A} \mathbf{x}$$
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The generalized form uses "arbitrary" operators "plus" (\oplus) and "times" (\otimes):

$$\mathbf{y} = \mathbf{A} \bigoplus \mathbf{N} \otimes \mathbf{x}$$
$$\mathbf{y}(i) = \bigoplus_{k} \mathbf{A}(i,k) \otimes \mathbf{x}(k)$$

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A cornerstone of GraphBLAS: Supports arbitrary semirings that override the addition and multiplication operators $(\oplus \otimes)$.









GraphBLAS semirings \oplus . \otimes

- \oplus is commutative binary operator with an identity, **0** (called a monoid)
- \otimes is a binary operator.
- The identity of \oplus , is the annihilator of \otimes^*

• $a = a \oplus \mathbf{0} = \mathbf{0} \oplus a$

• $\mathbf{0} = a \otimes \mathbf{0} = \mathbf{0} \otimes a$

Semiring	Valid values	\oplus	\otimes	0	Graph semantics
integer arithmetic	$a \in \mathbb{N}$	+	•	0	number of paths
real arithmetic	$a \in \mathbb{R}$	+	·	0	strength of all paths
boolean	$a \in \{ false, true \}$	V	Λ	false	connectivity
min-plus (tropical)	$a \in \mathbb{R} \cup \{+\infty\}$	min	+	+∞	shortest path
max-plus	$a \in \mathbb{R} \cup \{-\infty\}$	max	+	$-\infty$	longest path

*In GraphBLAS this is not enforced nor required

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GraphBLAS Primitives

- Basic objects (opaque types)
 - Matrices (sparse or dense), vectors (sparse or dense), algebraic operators (semirings)
- Fundamental operations over these objects



...plus reduction, transpose, Kronecker product, filtering, transform, etc.

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•	•			
		•	•	



One more thing... write masks: $\langle m \rangle$

Often not interested in some nodes...





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One more thing... write masks: (m)



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Example: Breadth-First Search (levels) f(*src*) = •







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Example: Breadth-First Search (levels)

 $level = \mathbf{0}$ $\mathbf{v} += level * \mathbf{f}$





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 (\mathbb{I})

2

3

4

5

6





Example: Breadth-First Search (levels)

level = 0 $\mathbf{v} += level * \mathbf{f} // Use \mathbf{v} as a mask, \langle \overline{\mathbf{v}} \rangle.$





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(1)

2

3

4

(5)





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level = 0 $\mathbf{v} += level * \mathbf{f}$ $\mathbf{f}'\langle \mathbf{\bar{v}} \rangle = \mathbf{A}^{\mathsf{T}} \oplus \otimes \mathbf{f}$ $\mathbf{f} = \mathbf{f}'$



A^T 0 1 2 3 4 5 6 \bigcirc \bigcirc 2 3 4 (5) (6)

2

3

4

5

6

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PV

level = 1 $\mathbf{v} += level * \mathbf{f}$ $\mathbf{f}'\langle \bar{\mathbf{v}} \rangle = \mathbf{A}^{\mathsf{T}} \oplus . \otimes \mathbf{f}$ $\mathbf{f} = \mathbf{f}'$





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level = 2 $\mathbf{v} += level * \mathbf{f}$ $\mathbf{f}'\langle \bar{\mathbf{v}} \rangle = \mathbf{A}^{\mathsf{T}} \oplus . \otimes \mathbf{f}$ $\mathbf{f} = \mathbf{f}'$



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level = 3 $\mathbf{v} += level * \mathbf{f}$ $\mathbf{f}'\langle \bar{\mathbf{v}} \rangle = \mathbf{A}^{\mathsf{T}} \oplus . \otimes \mathbf{f}$ $\mathbf{f} = \mathbf{f}'$ if **f**.empty() return v





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- Input: adjacency matrix A (Boolean), source vertex src (integer)
- Output: visited vertices vector, v (integer)
- Workspace: frontier vector f (Boolean)
- 1. $\mathbf{f}(src) = true$
- 2. level = 0
- 3. while ! **f**.empty()
- 4. $\mathbf{v} += level * \mathbf{f}$
- 5. $\mathbf{f} \langle \bar{\mathbf{v}} \rangle = \mathbf{A}^{\mathsf{T}} \oplus . \otimes \mathbf{f}$
- 6. ++level

// using the Boolean semiring (OR.AND)

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Prior work: GraphBLAS C API and Onwards





Provides uniform API for graph algorithms in the language of linear algebra



- Revolve around sparse matrix and vector operations which can use **arbitrary semirings** instead of classical (+, *)
- Current version of C API spec. is 1.3 (2.0 arriving imminently!)
- C offers great portability (Python, bindings, etc.), but has some disadvantages...

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The Problem with Types...

- If you're familiar with the
 (C)BLAS, there is a function for
 each scalar type
- GraphBLAS supports a wide variety of scalar types and binary operators
- Combinatorial explosion

```
float* a_ptr = get_matrix(...);
cblas_sgemm(..., m, n, k, 1.0f, a_ptr, ...);
```

```
double* a_ptr = get_matrix(...);
cblas_dgemm(..., m, n, k, 1.0, a_ptr, ...);
```

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```

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- For each predefined GraphBLAS operator, the C API requires a separate C function for each of 11 predefined types:

GrB_PLUS_BOOL, GrB_PLUS_INT8, GrB_PLUS_UINT8, GrB_PLUS_INT16, GrB_PLUS_UINT16, GrB_PLUS_INT32, GrB_PLUS_UINT32, GrB_PLUS_INT64, GrB_PLUS_UINT64, GrB_PLUS_FP32, GrB_PLUS_FP64.

- There are over 1000 combinations of predefined operators and types.
- Creates a large burden on implementers, who mostly resort to automatic code generation



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\$, GrB_PLUS_UINT16, GrB_PLUS_INT32,



• User-defined types must be trivially copyable types (i.e. memcpy-able).

```
struct MyComplex {
  int ireal; int iimag;
};
```

• This simplifies API and improves performance, but **limits expressiveness**.

```
GrB Type complex type;
GrB_Type_new(&complex_type,
             sizeof(MvComplex));
GrB Matrix A;
GrB Matrix new(&A, complex type, 100, 100);
```

 Users have already run into cases where they wish to use more complex types.



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C API: Issues with Types

C API users pass **function pointers** to custom operators

```
void scale 2(void *out, const void *in) {
 *(int*)out = 2 * (*(int*)in);
}
```

```
GrB UnaryOp my scale 2;
GrB UnaryOp new(&my scale 2, scale 2,
                GrB INT32, GrB INT32);
```

Required for any operator on user-defined types, but also allows for **operators on** built-in types left out of the spec Function pointers (e.g. scale_2) then used in **performance-critical** inner loops:

```
GrB apply(C, ..., my scale 2, A, desc);
```



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Drafting a GraphBLAS C++ API





C++ Has a Rich Type System

- User-defined types are first-class types
- They simply need be copy constructible, etc.
- Things like **views** can simplify APIs





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- User-defined types are first-class types
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- Things like **views** can simplify APIs





Disclaimer: API in Progress

- The GraphBLAS C++ API is still in draft process
- Specific names and APIs may change
- There are currently two draft implementations, <u>GBTL</u> and <u>RGRI</u>
- Some slide contents may be in RGRI, but not necessarily in C++ spec (yet)



Algorithms



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Algorithms



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Algorithms



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Algorithms



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- A matrix is a collection of stored values
- It has a **shape** (number of rows, cols)
- It has a size (number of stored values)
- Can access individual locations
- Can iterate over values







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GraphBLAS Matrix

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Matrix





GraphBLAS Matrix

- A matrix is a collection of stored values
- It has a **shape** (number of rows, cols)
- It has a size (number of stored values)
- Not included: implicit zero value! - Can access
- Can iterate over values

Matrix





- Distinct set of keys
- Each key associated with a value
- Individual lookup/insertion by key
- Iteration over unordered range of values





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Sparse Matrix - *Differences* from std::unordered_map

- key_type is pair-like type filled with
 integral values
- Matrix shape restricts valid key values [{2, 3}]
- Implementation will use highly [{4,
 specialized sparse matrix formats [{7,
- Indices and value may not be materialized in memory





Sparse Matrix - * Differences* from std::unordered map

- **key_type** is **pair-like type** filled with integral values
- Matrix shape restricts valid key values -
- Implementation will use highly specialized sparse matrix formats
 - [{7, 0}]

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Sparse Matrix - * Differences* from std::unordered_map

```
using key type = std::pair<int, int>;
using map type = int;
```

```
unordered_map<key_type, map_type> x = ...;
```

```
auto iter = x.begin();
```

[blank] value = *iter;

 $[\{0, 1\}] \longrightarrow 120$ $[{2, 3}] \longrightarrow 122$ [{4, 3}] [{7, 0}]







Sparse Matrix - *Differences* from std::unordered_map



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using key_type = std::pair<int, int>;
using map type = int;
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```

```
auto iter = x.begin();
```

using value type = std::pair<const key type,</pre> map type>;

```
value type& value = *iter;
```

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- Need to enable a variety of different sparse matrix formats
- Most formats separate values and indices, may not store some indices
- This means we need to use a custom reference type for indices

Storage Format

Row Pointers

0	2	3	3	3	6	6	
С	Column Indices						
0	2	2	2	3	4	3	

Sparse Matrix Representation

Compressed Sparse Row (CSR)



	8		2	
			5	
		7	1	2
,				
			1	





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- Need to enable a variety of different sparse matrix formats
- Most formats **separate values** and **indices**, may not store some indices
- This means we need to use a **custom** reference type for indices

Sparse Matrix Representation

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Compressed Sparse Row (CSR) Storage Format

8		2	
		5	
	7	1	2
		1	





- Need to enable **a variety** of different sparse matrix formats

Storage Format

Row Pointers

0	2	3	3	3	6	e
Co	Column Indices					
0	2	2	2	3	4	

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Compressed Sparse Row (CSR)



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Sparse Matrix Representation

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Compressed Sparse Row (CSR)



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- Need to enable **a variety** of different **Row Pointers** 3 3 66 0 sparse matrix formats **Column Indices** 2 2 3 4 3 indices, may Custom reference type, like vector<bool>::reference - Most formats separate va - This means we need to use a custom **reference type** for indices **Sparse Matrix** Representation

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Compressed Sparse Row (CSR) Storage Format



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			5	
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,				
			1	





Matrix Data Structure





Matrix Data Structure





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Matrix Data Structure: Attributes

Attributes

Shape Dimensions of matrix (Graph: number of vertices) Size Number of stored values (Graph: number of edges)

grb::matrix<float> x({1024, 1024});
size_t m = x.shape()[0];
size_t n = x.shape()[1];
size_t nnz = x.size();





Matrix Data Structure: Element Access

Element Access

Direct access to stored values

operator[] Find or insert value by index

find

Find value by index

grb::matrix<float, int> m({1024, 1024}); $m[{0, 0}] = 12;$ $m[{1, 1}] = 12;$ $m[{2, 2}] = 12;$ $m[{3, 3}] = 12;$ if (m.find({3, 3}) != m.end()) { // Should run, just set elem 3, 3 to 12. } if (m.find({4, 4}) != m.end()) { // Will not run, have not yet set elem 4, 4 }

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Matrix Data Structure: Iteration

Iteration

Iteration over stored values

Can read: row, column, value

Can write: value only

Iteration allows support for standard C++ algorithms.

```
grb::matrix<float, int> m = ...;
for (auto iter = m.begin(); iter != m.end();
     ++iter) {
  float x = *iter;
}
for (auto&& [i, j, v] : m) {
  v = 12:
  printf("Elem. %d, %d set to %f\n", i, j, v);
}
std::reduce(m.begin(), m.end(), float(0));
```

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- Many potential **sparse** matrix formats
- Each format has different iteration patterns
- Inefficient to enforce a particular iteration order



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* Diagrams by Matt Eding at https://matteding.github.io/2019/04/25/sparse-matrices/

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Offset $\rightarrow +$









Matrix Data Structure





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Matrix Data Structure: Iteration

- Unordered iteration over stored values
- Range of **size()** matrix entry<T, I> elements
- **Tuple-like type** with access to indices and T& reference to value

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GraphBLAS Concepts

Algorithms



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Matrix





Binary Operators

Functors that operate on two inputs, producing a single output

 $T \times U \rightarrow V$

Rule: types **T**, **U**, and **V** are determined by matrices. Op. must accept T, U, V.

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```
grb::ewise_add(c, ..., a, b,
auto my_op = [](auto a, auto b) {
               return a*b + 2;
             };
grb::ewise_mult(c, ..., a, b, my_op);
```

std::plus<int>());



- Monoids are **mathematical objects**, consisting of:
- A commutative binary operator
- A type **T**
- A mathematical identity





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- Given a **binary operator fn** and a **type T**, we can ask:

Does binary op. **fn** form a monoid on type T?

- Depends on whether monoid_traits specialization exists

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using grb;

bool test = is monoid v<std::plus<>, int>;

// Prints "1" for true std::cout << test << std::endl;</pre>

int identity = monoid traits<std::plus<>, int>::identity();

// Prints "0", since identity for std::plus<> // on type `int` is `0` std::cout << identity << std::endl;</pre>



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- Use pre-defined binary ops such as grb::plus, grb::multiplies
- Define a **specialization** of grb::monoid traits
- Add **identity() method** to op
- Use make monoid helper function

```
using grb;
```

```
// Using a pre-defined binary op
grb::plus<> fn;
std::plus<> fn_stl;
```

```
bool g = is_monoid<grb::plus<>, int>::value;
bool s = is_monoid<std::plus<>, int>::value;
```

```
std::cout << g << " " << s << std::endl;</pre>
```

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```
struct my_plus {
  float operator()(float a, float b) {
    return a + b;
  float identity() {
    return 0.0f;
};
. . .
int i =
     grb::monoid_traits<my_plus, int>::identity();
```



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```
auto my_op = [](auto a, auto b) {
               return a * b:
             };
```

auto my_monoid = make_monoid(my_op, 1);

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Semirings combine a binary op b and a **monoid m**, where **b** distributes over **m**

1) **Pre-define** a number of semirings

2) Users can **build semirings** with make semiring

```
auto semiring =
           grb::plus multiplies semiring();
auto my_times = [](auto a, auto b) {
                  return a*b;
                };
auto my_plus = [](auto a, auto b) {
                 return a+b;
              };
auto m_plus = grb::make_monoid(my_plus, 0);
auto my_semiring =
```

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- grb::make_semiring(m_plus, my_times);



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GraphBLAS Concepts

Algorithms



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Matrix





Views

Views provide a (typically **transformed**) view of a matrix

We can create views representing transpose, structure, complement, etc.

This simplifies API, removes some of need for **descriptors**.

```
grb::matrix<float> a = ...;
```

auto a t = grb::transpose(a);

auto b = grb::multiply(a, a t);

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Provide a **const view of a matrix** with each stored value transformed

- Can be used to create structure-only view

```
grb::matrix<float> a = ...;
auto t =
   [](grb::matrix_entry<float> e) {
     return true;
   };
auto a_t = grb::transform_view(a, t);
for (auto&& [i, j, v] : a_t) {
  printf("Elem (%d, %d): %f\n",
         i, j, v);
}
```



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	true	
rue	true	true
	true	
- +) (



- Range of matrix elements
- **Element-wise** access methods



- Shape
- Stored values convertible to bool







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GraphBLAS Concepts



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Matrix





Algorithms

The primary algorithms of interest are:

1) Generalized matrix multiplication -- using mask and arbitrary semiring

2) Elementwise operations





Accepts matrices, mask, semiring, accumulator, and flag to control merge behavior

Input matrices could be grb::matrix or views

Similar to C API

using grb;

```
matrix<float> a = get_matrix(...);
matrix<float> b = get_matrix(...);
```

matrix<float> c({a.shape()[0], b.shape()[1]});

mxm(c, plus<>{}, a, b, no_mask{}, plus_multiplies_semiring{});

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MatrixRange - an output range of matrix elements, plus element access and shape

ConstMatrixRange - an input range of matrix elements, plus const element access and shape

MaskMatrixRange - ConstMatrixRange with values convertible to bool

template < typename CMatrixType,</pre> typename Accumulator, typename AMatrixType, typename BMatrixType, typename MaskType, **typename** Semiring> **void** mxm(CMatrixType&& c, Accumulator&& acc, AMatrixType&& a, BMatrixType&& b, MaskType&& mask, Semiring&& s);



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template <MatrixRange C,</pre> typename Accumulator, ConstMatrixRange A, **ConstMatrixRange** B, typename MaskType, typename Semiring> void mxm(C&& c, Accumulator&& acc, A&& a, A&& b, MaskType&& mask, Semiring&& s);





MatrixRange - an output range of matrix elements, plus element access and shape

ConstMatrixRange - an input range of matrix elements, plus **const** element access and shape

MaskMatrixRange - ConstMatrixRange with values convertible to bool

template <MatrixRange C,</pre> typename Accumulator, ConstMatrixRange A, ConstMatrixRange B, MaskMatrixRange M, **typename** Semiring> **void** mxm(C&& c, Accumulator&& acc, A&& a, B&& b, M&& mask, Semiring&& s);







Matrix Times Matrix

```
grb::matrix<float> c = ...;
grb::matrix<float> a = ...;
```

```
auto a_t = grb::transpose(a);
auto mask = grb::structure(c);
```

```
grb::mxm(c, mask,
         grb::plus{},
         grb::plus times semiring{},
         a, a t);
```

Matrix Times Matrix (mxm)

```
Very similar to C API
```

Accepts matrices, mask, accumulator, semiring, and flag to control merge behavior

Input matrices could be grb::matrix or views

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Interoperability with C++ Algorithms

- C++ GraphBLAS matrices are ranges, which allows us to use C++ standard algorithms
- Area for exploration: implementing GraphBLAS operations with standard C++ algorithms
- One dimensional iteration somewhat limited, but 2D iteration concepts are coming (next slide)

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Interoperability with C++ Graph Library

- C++ graph library proposal^[P1709] provides standard concepts for iterating over graphs, graph algorithms
- We aren't currently using multidimensional iteration
- We should closely examine **opportunities** for **interoperability**
 - Implement mxm using graph library concepts
 - Build adapters for graph library concepts to fulfill GrB concepts, vice-versa





We can use matrix algebra to implement graph algorithms

Can support a variety of different sparse matrix formats

Provide high-level interfaces for algorithms



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