## Introduction to GraphBLAS

A linear algebraic approach for concise, portable, and high-performance graph algorithms

> Gábor Szárnyas 2020/12/12

#### Motivation

## GRAPHBLAS

- Graph algorithms are challenging to program

   o irregular access patterns → poor locality
   o caching and parallelization are difficult
- Optimizations often limit portability
- The GraphBLAS introduces an abstraction layer using the language of linear algebra
   o graph = sparse matrix

 $\circ$  traversal step  $\equiv$  vector-matrix multiplication



## GRAPHBLAS

- Graph algorithms are challenging to program

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- Optimizations often limit portability
- The GraphBLAS introduces an abstraction layer using the language of linear algebra

   graph = sparse matrix
   traversal step = vector-matrix multiplication



#### What makes graph computations difficult?

## **GRAPH PROCESSING CHALLENGES**

connectedness the "curse of connectedness"

computer architectures contemporary computer architectures are good at processing linear and hierarchical data structures, such as *lists*, *stacks*, or *trees* 

caching and parallelization

a massive amount of random data access is required, CPU has frequent cache misses, and implementing parallelism is difficult



B. Shao, Y. Li, H. Wang, H. Xia (Microsoft Research), *Trinity Graph Engine and its Applications,* IEEE Data Engineering Bulleting 2017

## **GRAPH PROCESSING CHALLENGES**

Graph algorithm have a *high communication-to-computation ratio*.

Speedup with a CPU that has better arithmetic performance:

- machine learning  $\rightarrow$  **a lot**
- relational queries  $\rightarrow$  **some**
- graph processing → **very little**

Standard latency hiding techniques break down, e.g. pre-fetching and branch prediction provide little benefit.

Use a data representation and computation model which are expressive, machine-friendly, and portable.

## LINEAR ALGEBRA-BASED GRAPH PROCESSING

- Graphs are encoded as sparse adjacency matrices.
- Use vector/matrix operations to express graph algorithms.



## The GraphBLAS standard

# THE GRAPHBLAS STANDARD

**Goal:** separate the concerns of the hardware, library, and application designers.

- 1979: BLAS Basic Linear Algebra Subprograms
- 2001: Sparse BLAS an extension to BLAS (little uptake)
- 2013: GraphBLAS an effort to define standard building blocks for graph algorithms in the language of linear algebra





S. McMillan @ SEI Research Review (Carnegie Mellon University, 2015): *Graph algorithms on future architectures* 

#### **GRAPHBLAS TIMELINE**

**Book — Papers — GraphBLAS standards — SuiteSparse:GraphBLAS releases** 



# **GRAPH ALGORITHMS IN LINEAR ALGEBRA**

**Notation:** n = |V|, m = |E|. The complexity cells contain asymptotic bounds. **Takeaway:** The majority of common graph algorithms can be expressed efficiently in LA.

problem	algorithm	canonical complexity $\Theta$	LA-based complexity $\Theta$
breadth-first search		m	m
single source shortest paths	Dijkstra	$m + n \log n$	$n^2$
single-source shortest paths	Bellman-Ford	mn	mn
all-pairs shortest paths	Floyd-Warshall	$n^3$	$n^3$
minimum channing trop	Prim	$m + n \log n$	$n^2$
minimum spanning tree	Borůvka	$m \log n$	$m \log n$
maximum flow	Edmonds-Karp	$m^2n$	$m^2n$
greedy greedy		$m + n \log n$	$mn + n^2$
maximal independent set	Luby	$m + n \log n$	$m \log n$



Based on the table in J. Kepner: *Analytic Theory of Power Law Graphs,* SIAM Workshop for HPC on Large Graphs, 2008

See also L. Dhulipala, G.E. Blelloch, J. Shun: *Theoretically Efficient Parallel Graph Algorithms Can Be Fast and Scalable,* SPAA 2018

# **KEY FEATURES OF GRAPHBLAS**

- Portable: supports x86; GPUs (WIP), Arm (planned)
- Efficient: within one order-of-magnitude compared to hand-tuned code
- Concise: most textbook algorithms can be expressed with a few operations
- Composable: the output of an algorithm can be used as an input of a subsequent algorithm

 Flexible: can express algorithms on typed graphs and property graphs

#### Theoretical foundations of the GraphBLAS

## DENSE MATRIX MULTIPLICATION

Definition:  $\mathbf{C} = \mathbf{AB}$   $\mathbf{C}(i,j) = \sum_{k} \mathbf{A}(i,k) \times \mathbf{B}(k,j)$ 

Example:

$$C(2,3) = A(2,1) \times B(1,3) + A(2,2) \times B(2,3) + A(2,3) \times B(3,3) = 2 \times 5 + 3 \times 0 + 6 \times 4 = 34$$



# SPARSE MATRIX MULTIPLICATION

Definition:  $\mathbf{C} = \mathbf{A}\mathbf{B} = \mathbf{A} \bigoplus \mathbf{B}$   $\mathbf{C}(i,j) = \bigoplus_{\substack{k \in \text{ind}(\mathbf{A}(i,:)) \cap \text{ind}(\mathbf{B}(:,j))}} \mathbf{A}(i,k) \otimes \mathbf{B}(k,j)$ 

Sparse matrix multiplication only evaluates the multiplication operator  $\otimes$  for positions where there is a non-zero element in both  $\mathbf{A}(i,k)$  and  $\mathbf{B}(k,j)$ .

Example:

$$C(2,3) = A(2,1) \times B(1,3) + A(2,3) \times B(3,3)$$
  
= 2 × 5 + 6 × 4 = 34

(2)3 В 2×5 = 10 (1) $\bigcirc$ 5 6×4 = 24<sup>2</sup> 3 2 3 A (1)(1)10 + 24 34 6 3  $\bigcirc$  $C = A \oplus \otimes B$ 

# MATRIX MULTIPLICATION $C = A \oplus . \otimes B$

#### Multiplication on dense matrices

 $\mathbf{C}(i,j) = \bigoplus_{i} \mathbf{A}(i,k) \otimes \mathbf{B}(k,j)$ 

<u>Multiplication on sparse matrices</u>

$$\mathbf{C}(i,j) = \bigoplus_{k \in \mathrm{ind}(\mathbf{A}(i,:)) \cap \mathrm{ind}(\mathbf{B}(:,j))} \mathbf{A}(i,k) \otimes \mathbf{B}(k,j)$$

#### Example: $\mathbf{C} = \mathbf{A} \oplus . \otimes \mathbf{B}$



**ADJACENCY MATRIX** 

$$\mathbf{A}_{ij} = \begin{cases} 1 & \text{if } (v_i, v_j) \in E \\ 0 & \text{if } (v_i, v_j) \notin E \end{cases}$$





**ADJACENCY MATRIX** 

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#### ADJACENCY MATRIX TRANSPOSED

$$\mathbf{A}_{ij}^{\mathsf{T}} = \begin{cases} 1 & \text{if } (v_j, v_i) \in E \\ 0 & \text{if } (v_j, v_i) \notin E \end{cases}$$





#### ADJACENCY MATRIX TRANSPOSED

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#### **GRAPH TRAVERSAL WITH MATRIX MULTIPLICATION**



#### **GRAPH TRAVERSAL WITH MATRIX MULTIPLICATION**



## **GRAPHBLAS SEMIRINGS\***

The  $(D, \bigoplus, \otimes, 0)$  algebraic structure is a GraphBLAS semiring if

•  $\langle D, \bigoplus, 0 \rangle$  is a commutative monoid using the addition operation  $\bigoplus: D \times D \to D$ , where  $\forall a, b, c \in D$ , if the following hold:

 $\circ$  Commutative  $a \oplus b = b \oplus a$ 

 $\circ$  Associative  $(a \oplus b) \oplus c = a \oplus (b \oplus c)$ 

 $\circ$  Identity  $a \oplus 0 = a$ 

• The multiplication operator is a closed binary operator  $\otimes: D \times D \to D$ .

The mathematical definition of a semiring requires that  $\otimes$  is a monoid and distributes over  $\oplus$ . GraphBLAS omits these requirements.

## SEMIRINGS

semiring	domain	$\oplus$	$\otimes$	0	graph semantics
any-pair	{T, F}	any	pair	F	traversal step
integer arithmetic	$\mathbb{N}$	+	×	0	number of paths
min-plus	$\mathbb{R} \cup \{+\infty\}$	min	+	$+\infty$	shortest path

The default semiring is the conventional one:

- $\otimes$  defaults to the arithmetic multiplication operator.
- $\oplus$  defaults to the arithmetic addition operator.

## MATRIX-VECTOR MULTIPLICATION SEMANTICS



## MATRIX-VECTOR MULTIPLICATION SEMANTICS

6 7

1

1

**f** (+)



### MATRIX-VECTOR MULTIPLICATION SEMANTICS



#### ELEMENT-WISE MULTIPLICATION: $A \otimes B$

 $(\mathbb{T})$ 









(5)

3





















6





#### **ELEMENT-WISE ADDITION:** $A \oplus B$

 $(\mathbb{T})$ 









 




 $\mathbf{A} \bigoplus \mathbf{B}$  ① (5) 6 7



## TURNING A GRAPH INTO UNDIRECTED: $\mathbf{A} \oplus \mathbf{A}^{\mathsf{T}}$

 $\oplus$ 











 $\mathbf{A} \bigoplus \mathbf{A}^{\mathsf{T}} \ \underline{0} \ \underline{2} \ \underline{3} \ \underline{4} \ \underline{5} \ \underline{6} \ \underline{7}$ 



# MASKING

Prevent redundant computations by reducing the scope of an operation Operations can be executed

- without a mask
- with a regular mask
- with a complemented mask



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# **NOTATION\***

Symbols:
A, B, C, M – matrices
u, v, w, m – vectors
s – scalar
i, j – indices
(M), (m) – masks

- Operators:
  - $\circ \oplus$  addition
  - $\circ \otimes$  multiplication
  - $\circ$   $\oslash$  division
  - $\circ$  <sup>T</sup> transpose

symbol	operation	notation
⊕.⊗	matrix-matrix multiplication	$\mathbf{C}\langle \mathbf{M} \rangle = \mathbf{A} \oplus . \otimes \mathbf{B}$
	vector-matrix multiplication	$\mathbf{w}\langle \mathbf{m} \rangle = \mathbf{v} \oplus . \otimes \mathbf{A}$
	matrix-vector multiplication	$\mathbf{w}\langle \mathbf{m} \rangle = \mathbf{A} \oplus . \otimes \mathbf{v}$
$\otimes$	element-wise multiplication	$\mathbf{C}\langle \mathbf{M} \rangle = \mathbf{A} \otimes \mathbf{B}$
	(set intersection of patterns)	$\mathbf{w}\langle \mathbf{m}  angle = \mathbf{u} \otimes \mathbf{v}$
$\oplus$	element-wise addition	$C\langle M \rangle = A \oplus B$
	(set union of patterns)	$\mathbf{w}\langle \mathbf{m}  angle = \mathbf{u} \oplus \mathbf{v}$
f	applyupany operator	$\mathbf{C}\langle \mathbf{M}\rangle = f(\mathbf{A})$
	apply unary operator	$\mathbf{w} \langle \mathbf{m} \rangle = f(\mathbf{v})$
[⊕…]	reduce to vector	$\mathbf{w} \langle \mathbf{m} \rangle = \left[ \bigoplus_{j} \mathbf{A}(:,j) \right]$
	reduce to scalar	$s = \left[ \bigoplus_{ij} \mathbf{A}(i,j) \right]$
$\mathbf{A}^{T}$	transpose matrix	$\mathbf{C}\langle \mathbf{M} \rangle = \mathbf{A}^{\top}$

Vectors can act as both column and row vectors.

(Notation omitted for accumulator, selection, extraction, assignment...)
## LINEAR ALGEBRAIC PRIMITIVES FOR GRAPHS #1

#### **Element-wise addition:** union of non-zero elements



Sparse matrix times sparse vector: process incoming edges



**Element-wise multiplication:** intersection of non-zero elements





Sparse vector times sparse matrix: process outgoing edges





## LINEAR ALGEBRAIC PRIMITIVES FOR GRAPHS #2

**Sparse matrix times sparse matrix:** process connecting outgoing edges



**Reduction:** aggregate values in each row



Matrix transpose: reverse edges

0		0		0	
	0			0	
0	0			0	
		0	0		

**Apply:** apply unary operator on all values





1		4		9
9	4			
			1	

#### Breadth-first search

## **BFS: BREADTH-FIRST SEARCH**

#### Algorithm:

 $_{\rm O}$  Start from a given vertex

 "Explore all neighbour vertices at the present level prior to moving on to the vertices at the next level" [Wikipedia]

#### Variants:

- Levels compute traversal level for each vertex
- **Parents** compute parent for each vertex
- **MSBFS** start traversal from multiple source vertices

#### Breadth-first search / Levels









## **BFS – LEVELS: ALGORITHM**

- Ô
- Input: adjacency matrix A, source vertex s, #vertices n
- Output: vector of visited vertices v (integer)
- Workspace: frontier vector **f** (Boolean)
- 1. f(s) = T
- 2. for *level* = 1 to n 1 \*terminate earlier if **f** is empty
- 3.  $\mathbf{s}\langle \mathbf{f} \rangle = level$  assign the level value to the vertices in the frontier
- 4. clear(f) clear the frontier **f**
- 5.  $\mathbf{f}\langle \neg \mathbf{s} \rangle = \mathbf{f}$  any pair **A** advance the frontier

### Breadth-first search / Parents









## **BFS – PARENTS: ALGORITHM**

- Q
- Input: adjacency matrix A, source vertex s, #vertices n
- Output: parent vertices vector p (integer)
- Workspace: vertex index vector idx (integer), frontier vector
  f (integer)
- 1.  $idx = [1 2 \dots n]$  we assume 1-based indexing here
- 2. f(s) = s
- 3. p(s) = 0
- 4. for l = 1 to n 1 \*terminate earlier if the frontier is empty
- 5.  $f\langle \neg p \rangle = f \min . \text{ first } A$  advance the frontier
- 6.  $\mathbf{p}\langle \mathbf{f} \rangle = \mathbf{f}$
- 7.  $\mathbf{f} \langle \mathbf{f} \rangle = \mathbf{i} \mathbf{d} \mathbf{x}$

assign parent ids to the frontier's vertices assign vertex ids  $\mathbf{f}(i) = i$ 

## **BFS – PARENTS: OPTIMIZATIONS**

- If getting deterministic results is not a requirement (i.e. any parent vertex can be returned), instead of min.sel1st, one can use the any.first semiring.
- This optimization is allowed by the GAP Benchmark Suite.
- Direction-optimizing traversal (push/pull) can be exploited.
- The secondi (note the "i") semiring can be used to express the BFS Parent algorithm. When using this semiring, one does not even have to look at the values in either A of f.



This algorithm is described in:

Evaluation of Graph Analytics Frameworks Using the GAP Benchmark Suite, IISWC 2020

#### Multi-source BFS

## **MULTI-SOURCE BFS – LEVELS**



## **MULTI-SOURCE BFS – PARENTS**



## **BFS – PERFORMANCE**

- Naïve BFS impls can be slow on real graphs with skewed distributions – further optimizations are needed.
- Direction-optimizing BFS was published in 2012.
  - $\circ$  Switches between push (vA) and pull (A<sup>T</sup>v) during execution:
    - Use the push direction when the frontier is small
    - Use the pull direction when the frontier becomes large
  - $_{\odot}$  Adopted to GraphBLAS in 2018 (Yang et al.'s ICPP paper)



S. Beamer, K. Asanovic, D. Patterson: *Direction-Optimizing Breadth-First Search,* SC 2012



C. Yang: *High-performance linear algebra-based graph framework on the GPU,* PhD thesis, UC Davis, 2019



C. Yang, A. Buluç, J.D. Owens: *Implementing Push-Pull Efficiently in GraphBLAS,* ICPP 2018

A. Buluç: *GraphBLAS: Concepts, algorithms, and applications,* Scheduling Workshop, 2019

### Single-source shortest paths

## SSSP – SINGLE-SOURCE SHORTEST PATHS

#### Problem:

 From a given start vertex s, find the shortest paths to every other (reachable) vertex in the graph

#### Bellman-Ford algorithm:

• Relaxes all edges in each step • Guaranteed to find the shortest path using at most n - 1 steps

#### Observation:

 The relaxation step can be captured using a VM multiplication
 Unlike in BFS, there is no masking here, as revisiting edges that have been visited previously can be useful.













**Input:** adjacency matrix **A**, source vertex *s*, #vertices *n* 

$$\mathbf{A}_{ij} = \begin{cases} 0 & \text{if } i = j \\ w(e_{ij}) & \text{if } e_{ij} \in E \\ \infty & \text{if } e_{ij} \notin E \end{cases}$$

#### **Output:** distance vector **d** (real)

- 1.  $\mathbf{d} = [\infty \infty \dots \infty]$
- 2. d(s) = 0
- 3. for k = 1 to n 1 \*terminate earlier if we reach a fixed point
- 4.  $\mathbf{d} = \mathbf{d} \min \mathbf{A}$

Optimizations for BFS (push/pull) also work here.

### Triangle count / Definition

## **TRIANGLE COUNT**

- IEEE GraphChallenge: an annual competition at the HPEC conference
- The task of the 2017 GraphChallenge was triangle count: given a graph G, count the number of triangles.
- Triangle = "set of three mutually adjacent vertices in a graph"
- Many solutions employed a linear algebraic computation model





Number of unique triangles:

30



GraphChallenge.org: Raising the Bar on Graph Analytic Performance, HPEC 2018

## Triangle count / Naïve algorithm

# TC EXAMPLE: NAÏVE APPROACH



### Triangle count / Masked algorithm

## TC EXAMPLE: ELEMENT-WISE MULTIPLICATION



## TC EXAMPLE: ELEMENT-WISE MULTIPLICATION


#### The importance of masking

# THE IMPORTANCE OF MASKING

- **Q:** Is masking absolutely necessary?
- **A:** Yes, it can reduce the complexity of some algorithms. We demonstrate this with two examples.



A simple corner case is the star graph: there are  $(n-1)^2$  wedges but none of them close into triangles.

We do quadratic work while it's clear that there are no triangles in the graph (it's a tree).

 $A \oplus \otimes A \oplus \otimes A$  $A \oplus . \otimes A$ 



A full bipartite graph  $K_{2,3}$ with the vertices in the top partition connected.

A bipartite graph only has cycles of even length, so it's easy to see that all triangles will contain the two vertices in the top partition. Still,  $A \oplus . \otimes A$ enumerates all wedges starting and ending in the bottom partition, thus performing a lot of unnecessary work.

 $A \oplus \otimes A \oplus \otimes A$  $A \oplus \otimes A$ 



Masking avoids the materialization of large interim data sets by ensuring that we only enumerate wedges whose endpoints are already connected.

(5)



#### Triangle count / Cohen's algorithm

# **COHEN'S ALGORITHM: PSEUDOCODE**

**Input:** adjacency matrix **A** 

- **Output:** triangle count *t*
- Workspace: matrices L, U, B, C
- 1.  $\mathbf{L} = tril(\mathbf{A})$
- 2.  $\mathbf{U} = triu(\mathbf{A})$
- 3.  $\mathbf{B} = \mathbf{L} \oplus . \otimes \mathbf{U}$
- 4.  $\mathbf{C} = \mathbf{B} \otimes \mathbf{A}$
- 5.  $t = \sum C/2$  sum the values in C and divide by 2

J. Cohen: Graph Twiddling in a MapReduce World, Comput. Sci. Eng. 2009

extract the lower triangle from A extract the upper triangle from A



### **COHEN'S ALGORITHM**



### **COHEN'S ALGORITHM: MASKING**



			1	1
			1	1
	1			
1			1	2
				1
	1			
	2	1		

$$\mathbf{C}\langle \mathbf{A} 
angle = \mathbf{L} \oplus . \otimes \mathbf{U}$$
  
 $t = \sum \mathbf{C} / \mathbf{2}$ 

#### Triangle count / Sandia algorithm

# SANDIA ALGORITHM

Input: adjacency matrix A Output: triangle count *t* Workspace: matrices L, U, B, C

- 1.  $\mathbf{L} = tril(\mathbf{A})$
- 2.  $C\langle L \rangle = L \oplus . \otimes L$
- 3.  $t = \sum C$

extract the lower triangle from A multiply matrices L and L using mask L sum the values in C



M.M. Wolf et al. (Sandia National Laboratories): Fast linear algebra-based triangle counting with KokkosKernels, HPEC 2017



### SANDIA ALGORITHM



	1					
	1	1	1			
		1				
			1	1	1	
		1	1	1	1	
	1					
			1			
1		2	1			

$$C\langle \mathbf{L} \rangle = \mathbf{L} \bigoplus . \bigotimes \mathbf{L}$$
  
 $t = \sum \mathbf{C}$ 

#### Triangle count / CMU algorithm

# CMU ALGORITHM

• Iterates on the vertices of the graph, extracts corresponding submatrices and computes  $t = t + a_{10}^{\mathsf{T}} \bigoplus \otimes A_{20} \bigoplus \otimes a_{12}$ 

Tradeoffs:

 $_{\odot}$  does not require mxm, only vxm and mxv  $_{\odot}$  slower than mxm-based algorithms



• The formula is derived using the matrix trace  $tr(\mathbf{A}) = \sum_{i=0}^{n-1} \mathbf{A}_{ii}$  and its invariant property under cyclic permutation, e.g.  $tr(\mathbf{ABC}) = tr(\mathbf{BCA}) = tr(\mathbf{CAB})$ . See the paper for details.

T.M. Low et al. (Carnegie Mellon University): *First look: linear algebra-based triangle counting without matrix multiplication,* HPEC 2017

# CMU ALGORITHM: PSEUDOCODE

Input: adjacency matrix A

**Output:** triangle count *t* 

Workspace: matrices  $\mathbf{A}_{20}$ ,  $\mathbf{C}$ , vectors  $\mathbf{a}_{10}$ ,  $\mathbf{a}_{12}^{\mathsf{T}}$ 

1. for 
$$i = 2$$
 to  $n - 1$ 

2. 
$$\mathbf{A}_{20} = \mathbf{A}[i+1:n,0:i-1]$$

3. 
$$\mathbf{a}_{10} = \mathbf{A}[0:i-1,i]$$

4. 
$$\mathbf{a}_{12} = \mathbf{A}[i, i+1:n]$$

5. 
$$t = t + a_{10}^{\mathsf{T}} \bigoplus \otimes A_{20} \bigoplus \otimes a_{12}$$





T.M. Low et al. (Carnegie Mellon University):

First look: linear algebra-based triangle counting without matrix multiplication, HPEC 2017



# PROVABLY CORRECT ALGORITHMS

The "CMU algorithm" belongs to a family of algorithms which can be derived using the "FLAME approach".

There are 8 similar algorithms in total, the one presented here is Algorithm 2.

Algorithm: $\tilde{\Delta} := \frac{1}{6} \Gamma(\hat{A}^3)$				
$ \begin{array}{c c c} A \to \begin{pmatrix} A_{TL} & A_{TR} \\ \hline A_{TR}^T & A_{BR} \end{pmatrix} \\ \text{where}  A_{TL} \text{ is a } 0 \times 0 \text{ m} \\ \text{while } m(A_{TL}) < m(A) \text{ d} 0 \end{array} $	natrix o			
$\begin{pmatrix} A_{TL} & A_{TR} \\ \hline A_{TR}^T & A_{BR} \end{pmatrix} \rightarrow \begin{pmatrix} - & - & - \\ - & - & - \\ \hline & & \\ & & $	$ \begin{array}{c c c} A_{00} & a_{01} & A_{02} \\ \hline a_{01}^T & \alpha_{11} & a_{12}^T \\ \hline A_{02}^T & a_{12} & A_{22} \end{array} \right) \\ \text{natrix} $			
Algorithm 1	Algorithm 2			
$\Delta:=\Delta+rac{1}{2}a_{01}^TA_{00}a_{01}$	$\Delta := \Delta + a_{01}^T A_{02} a_{21}$			
Algorithm 3	Algorithm 4			
$egin{aligned} \Delta &:= \Delta + rac{1}{2}a_{01}^TA_{00}a_{01}\ \Delta &:= \Delta + rac{1}{2}a_{12}^TA_{22}a_{12}\ \Delta &:= \Delta - a_{01}^TA_{02}a_{21} \end{aligned}$	$\Delta := \Delta + rac{1}{2}a_{12}^TA_{22}a_{12}$			
$\begin{pmatrix} A_{TL} & A_{TR} \\ \hline A_{TR}^T & A_{BR} \end{pmatrix} \leftarrow \begin{pmatrix} - \\ - \\ - \\ - \\ \text{endwhile} \end{pmatrix}$	$ \begin{array}{c c c} A_{00} & a_{01} & A_{02} \\ \hline a_{01}^T & \alpha_{11} & a_{12}^T \\ \hline A_{02}^T & a_{12} & A_{22} \end{array} \right) $			

Algorithm: $\tilde{t} := \frac{1}{6}\Gamma(A^3)$					
$A \rightarrow \begin{pmatrix} A_{TL} & A_{TR} \\ \hline & & & \end{pmatrix}$					
$\begin{pmatrix} A_{TR}^{I} \mid A_{BR} \end{pmatrix}$					
where $A_{BR}$ is a $0 \times 0$ f while $m(A_{TL}) < m(A)$ d					
while $m(ATL) < m(A)$	while $m(A_{TL}) < m(A)$ do				
$\begin{pmatrix} A_{TL} & A_{TR} \\ \hline a_{01} & a_{01} & a_{11} & a_{12}^T \end{pmatrix} \rightarrow \begin{pmatrix} A_{01} & A_{01} & A_{02} \\ \hline a_{01} & a_{11} & a_{12}^T \end{pmatrix}$					
$\begin{pmatrix} A_{TR}^{I} \mid A_{BR} \end{pmatrix} \begin{pmatrix} G_{1} \mid I_{12} \mid I_{22} \end{pmatrix}$					
where $\alpha_{11}$ is a 1 × 1 matrix					
Algorithm 5	Algorithm 6				
$\Delta:=\Delta+rac{1}{2}a_{01}^TA_{00}a_{01}$	$\Delta:=\Delta+a_{01}^TA_{02}a_{21}$				
Algorithm 7	Algorithm 8				
$egin{array}{lll} \Delta := \Delta + rac{1}{2}a_{01}^TA_{00}a_{01}\ \Delta := \Delta + rac{1}{2}a_{12}^TA_{22}a_{12} \end{array}$	$\Delta:=\Delta+rac{1}{2}a_{12}^TA_{22}a_{12}$				
$\Delta := \Delta - a_{01}^T A_{02} a_{21}$					
$\begin{pmatrix} A_{TL} & A_{TR} \\ \hline A_{TR}^T & A_{BR} \end{pmatrix} \leftarrow \begin{pmatrix} - & - & - \\ - & - & - \\ - & - & - \\ \text{endwhile} \end{pmatrix}$	$ \begin{array}{c c c} A_{00} & a_{01} & A_{02} \\ \hline a_{01}^T & \alpha_{11} & a_{21}^T \\ \hline A_{02}^T & a_{21} & A_{22} \end{array} \right) $				



M. Lee, T.M. Low (Carnegie Mellon University): A family of provably correct algorithms for exact triangle counting, CORRECTNESS @ SC 2017



### Vertex-wise triangle count

## **VERTEX-WISE TRIANGLE COUNT**

Triangle: a set of three mutually adjacent vertices.



- Usages:
- Global clustering coefficient
- Local clustering coefficient
- Finding communities





GraphChallenge.org: Raising the Bar on Graph Analytic Performance, HPEC 2018

### **TC: ELEMENT-WISE MULTIPLICATION**



## **TC: ELEMENT-WISE MULTIPLICATION**



# TC: ALGORITHM



Input: adjacency matrix A Output: vector tri Workspace: matrix TRI

- 1. **TRI** $\langle A \rangle = A \oplus \otimes A$  compute the triangle count matrix
- 2. **tri** =  $[\bigoplus_j \mathbf{TRI}(:, j)]/2$  compute the triangle count vector

#### Optimization: use L, the lower triangular part of A to avoid duplicates. $TRI(A) = A \oplus O \otimes L$

**Worst-case optimal joins:** There are deep theoretical connections between masked matrix multiplication and relational joins. It has been proven in 2013 that for the triangle query, binary joins always provide suboptimal runtime, which gave rise to new research on the family of worst-case optimal multi-way joins algorithms.

### Local clustering coefficient

## LCC: LOCAL CLUSTERING COEFFICIENT

 $LCC(v) = \frac{\text{#edges between neighbours of } v}{\text{#possible edges between neighbours of } v}$ 

$$|\mathsf{I}|N(v)| \le 1, \, \mathsf{LCC}(v) = 0$$

Important metric in social network analysis.

The numerator is the number of *triangles* in v, tri(v). The denominator is the number of *wedges* in v, wed(v).  $LCC(v) = \frac{tri(v)}{wed(v)}$ 

The difficult part is tri(v).

#### LCC: NUMBER OF WEDGES IN EACH VERTEX

$$LCC(v) = \frac{tri(v)}{wed(v)}$$

For wed(v), we determine the #wedges for each vertex as the 2-combination of its degree:

$$\operatorname{comb2}(x) = \frac{x \cdot (x-1)}{2}$$

• Given the degrees  $deg = [\bigoplus_j A(:, j)]$ , we compute wed by applying a unary function on the elements of the vector:

$$wed = comb2(deg)$$

LCC EXAMPLE: NUMBER OF WEDGES



(1)

 $\overline{(7)}$ 



### LCC EXAMPLE: COMPLETE ALGORITHM



# LCC: ALGORITHM

- Input: adjacency matrix A
- Output: vector lcc
- Workspace: matrix TRI, vectors tri, deg, wed, and lcc
- 1. **TRI** $\langle A \rangle = A \oplus \otimes A$  compute triangle count matrix
- 2. **tri** =  $[\bigoplus_j \mathbf{TRI}(:,j)]/2$  reduce to triangle count vector
- 3.  $deg = [\bigoplus_j A(:, j)]$  reduce to vertex degree vector
- 4. wed = comb2(deg)
- 5.  $lcc = tri \oslash wed$  LCC vector



M. Aznaveh, J. Chen, T.A. Davis, B. Hegyi, S.P. Kolodziej, T.G. Mattson, G. Szárnyas: *Parallel GraphBLAS with OpenMP,* Workshop on Combinatorial Scientific Computing 2020

apply comb2 to get wedge count vector

## LCC: FURTHER OPTIMIZATIONS

Further optimization: use L, the lower triangular part of A.

#### $\mathbf{TRI}\langle \mathbf{A}\rangle = \mathbf{A} \oplus . \otimes \mathbf{L}$

The number of wedges is now the 2-combination of **deg**.  $comb2(x) = \frac{x \cdot (x - 1)}{2}$ 

Permuting the adjacency matrix allows further optimizations.

### LCC EXAMPLE: LOWER TRIANGULAR PART OF MX.



PageRank

### PAGERANK – DEFINITION (LDBC GRAPHALYTICS)



 $\alpha$ : damping factor

*dng*: dangling vertices,  $dng = \{w \in V : |N_{out}(w)| = 0\}$ 

There are dozens of PR definitions, some treat dangling vertices differently.

### PAGERANK – IN LINEAR ALGEBRA

Initially:

$$\mathbf{pr}_0 = [1 \ 1 \ \dots \ 1] \oslash n, \quad \mathbf{outd} = [\bigoplus_j \mathbf{A}(:, j)]$$

In each iteration:

$$PR_{k}(v) = \frac{1-\alpha}{n} + \alpha \cdot \sum_{u \in N_{in}(v)} \frac{PR_{k-1}(u)}{|N_{out}(u)|} + \frac{\alpha}{n} \cdot \sum_{w \in dng} PR_{k-1}(w)$$

$$\mathbf{pr}_{k} = \frac{1 - \alpha}{n} \oplus \alpha \otimes \left(\frac{\mathbf{pr}_{k-1}}{\mathbf{outd}}\right) \oplus \otimes \mathbf{A} \oplus \frac{\alpha}{n} \otimes \left[\bigoplus_{i} \left(\mathbf{pr}_{k} \otimes \overline{\mathbf{outd}}\right)(i)\right]$$
constant
SpMV
element-wise sparse vector-dense vector multiplication

# PAGERANK – ALGORITHM



**Input:** adjacency matrix **A**, damping factor  $\alpha$ , #iterations *t*, #vertices *n* 

- Output: PageRank vector pr (real); Workspace: vectors (real)
- 1. **pr** =  $[1 \ 1 \ ... \ 1] \oslash n$
- 2. **outdegrees** =  $\left[\bigoplus_{j} \mathbf{A}(:,j)\right]$
- 3. for k = 1 to t
- 4. **importance** =  $\alpha \otimes (\mathbf{pr} \oslash \mathbf{outdegrees}) \oplus \otimes \mathbf{A}$
- 5. **danglingVertexRanks** $\langle \neg outdegrees \rangle = pr(:)$
- 6.  $totalDanglingRank = \frac{\alpha}{n} \otimes [\bigoplus_i \text{danglingVertexRanks}(i)]$

7. 
$$\mathbf{pr} = \frac{1-\alpha}{n} \oplus totalDanglingRank \oplus \mathbf{importance}$$

*k*-truss

### **K-TRUSS**

Definition: the k-truss is a subset of the graph with the same number of vertices, where each edge appears in at least k – 2 triangles in the original graph.

# **K-TRUSS ALGORITHM**

- Input: adjacency matrix A, scalar k
- Output: k-truss adjacency matrix C
- Helper:  $f(x, support) = x \ge support$
- 1. **C** = **A**
- 2. for i = 1 to n 1
- 3.  $C(C) = C \oplus A C$  use the "plus-and" semiring
- 4.  $\mathbf{C} = f(\mathbf{C}, k 2)$  drop entries in **C** less than k 2
- 5. terminate if the number of non-zero values in **C** did not change



T.A. Davis: Graph algorithms via SuiteSparse:GraphBLAS: triangle counting and k-truss, HPEC 2018
#### Graph algorithms in GraphBLAS

## Community detection using label propagation

#### CDLP: COMMUNITY DETECTION USING LABEL PROPAGATION

**Goal:** assign a label to each vertex representing the community it belongs to. The algorithm (originally published in network science) is slightly altered to ensure deterministic execution. Initially:

$$L_0(v) = v$$

In the  $k^{\text{th}}$  iteration:  $L_k(v) = \min(\arg \max_l |\{u \in N(v) : L_{k-1}(u) = l\}|),$ where N(v) is the set of neighbours of v.

Run for *t* iterations or until reaching a fixed point.



U.N. Raghavan, R. Albert, S. Kumara: *Near linear time algorithm to detect community structures in large-scale networks*, Phys. Rev. E, 2007

## IDEA: CAPTURE CDLP IN PURE GRAPHBLAS

- Define a semiring that operates over occurrence vectors
- Operator: combines two occurrence vectors

 $\circ \{6 \rightarrow 1, 9 \rightarrow 1\} \bigoplus \{6 \rightarrow 1, 7 \rightarrow 2\} = \{6 \rightarrow 2, 7 \rightarrow 2, 9 \rightarrow 1\}$ 

- Convert each element in a row to an occurrence vector  $\circ \{6 \rightarrow 1\}, \{6 \rightarrow 1\}, \{7 \rightarrow 1\}, \{7 \rightarrow 1\}, \{9 \rightarrow 1\}$
- Reduce each row into a single occurrence vector:  $\circ \{6 \rightarrow 2, 7 \rightarrow 2, 9 \rightarrow 1\}$
- Select the min. mode element from the occurrence vector: 6
- Works on paper, but occurrence vectors need dynamic memory allocation, which leads to poor performance with the current GraphBLAS API

## CDLP IN LINEAR ALGEBRA: FASTER ALGORITHM

Extract each row from F

 $_{\odot}$  Easy if the matrix is stored in CSR format

- Select the minimum mode value in each row

   Sort elements using parallel merge sort
   Pick the min value that has the longest run (done in a single pass)
- Sort each row r
- Use the sorted list to compute mode(r)
- The matrix multiplications are always performed with a diagonal matrix as the second operand so we never need the addition operator. Therefore, we set it to ⊕ ≡ any.



(4)

(5)

6

 $\overline{7}$ 

- Initially, lab = [1 2 ... n]
- Propagate labels to create a "frequency matrix":  $\mathbf{F} = \mathbf{A}$  any . sel2nd diag(lab)











# CDLP: ALGORITHM

**Input:** adjacency matrix **A**, #vertices *n*, #iterations *t* **Output:** vector **lab Workspace:** matrix **F**, vector **r** 

- 1. lab = [1 2 ... n]
- 2. for k = 1 to t
- 3.  $\mathbf{F} = \mathbf{A}$  any sel2nd diag(lab)
- 4. for i = 1 to n
- 5. r = F(i,:)
- 6. sort(**r**)
- 7.  $lab(i) = select_min_mode(\mathbf{r})$

Can be batched and parallelized

# CDLP: ALGORITHM



**Input:** adjacency matrix **A**, #vertices *n*, #iterations *t* 

- Output: vector lab
- Workspace: matrix F, vector r, array of row indices I, array of values X
- 1. lab = [1 2 ... n]
- 2. for k = 1 to t
- 3.  $\mathbf{F} = \mathbf{A}$  any sel2nd diag(**lab**)
- 4.  $\langle \mathbf{I}, \underline{}, \mathbf{X} \rangle = \text{extract\_tuples}(\mathbf{F})$
- 5. merge\_sort\_pairs((**I**, **X**))
- 6. **lab** = for each row in **I**, select min mode value from **X**

## CDLP ON DIRECTED GRAPHS

For directed graphs, we compute the labels  $L_k(v)$  as:

 $\min(\arg \max_{l} \left[ \left| \{ u \in N_{in}(v) : L_{k-1}(u) = l \} \right| + \left| \{ u \in N_{out}(v) : L_{k-1}(u) = l \} \right| \right] \right)$ 

- In linear algebra, this can be expressed with two matrices:
  - $\circ$  **F**<sub>in</sub> = **A** any. sel2nd diag(**lab**)
  - $o \mathbf{F}_{out} = \mathbf{A}^{\mathsf{T}}$  any. sel2nd diag(**lab**)
- Simultaneously iterate over rows  $\mathbf{r}_{in}$  of  $\mathbf{F}_{in}$  and  $\mathbf{r}_{out}$  of  $\mathbf{F}_{out}$
- For each row pair, sort  $\mathbf{r}_{in} \cup \mathbf{r}_{out}$  and select the minimum mode value
- Batching also works:

 $\left( \langle \mathbf{I}_{in}, \underline{,}, \mathbf{X}_{in} \rangle = \text{extract\_tuples}(\mathbf{F}_{in}) \\ \circ \langle \mathbf{I}_{out}, \underline{,}, \mathbf{X}_{out} \rangle = \text{extract\_tuples}(\mathbf{F}_{out}) \right\} \text{merge\_sort\_pairs}(\langle \mathbf{I}_{in} \cup \mathbf{I}_{out}, \mathbf{X}_{in} \cup \mathbf{X}_{out} \rangle)$ 

#### Graph algorithms in GraphBLAS

#### Graph algorithms & GraphBLAS primitives

## **GRAPH ALGORITHMS & GRAPHBLAS PRIMITIVES**



GraphBLAS primitives in increasing cost



Based on the figure in A. Buluç:

Graph algorithms, computational motifs, and GraphBLAS, ECP Meeting 2018

#### GraphBLAS and SuiteSparse internals

## **GRAPHBLAS C API**

 "A crucial piece of the GraphBLAS effort is to translate the mathematical specification to an API that

o is faithful to the mathematics as much as possible, and
 o enables efficient implementations on modern hardware."



mxm(Matrix \*C, Matrix M, BinaryOp accum, Semiring op, Matrix A, Matrix B, Descriptor desc)

A. Buluç et al.: *Design of the GraphBLAS C API,* GABB@IPDPS 2017

## **GRAPHBLAS OBJECTS**

- GraphBLAS objects are opaque: the matrix representation can be adjusted to suit the data distribution, hardware, etc.
- The typical representations compressed formats are:

   CSR: Compressed Sparse Row
   CSC: Compressed Sparse Column (also known as CCS)



CSR representation of A:



## SUITESPARSE: GRAPHBLAS INTERNALS

- Authored by Prof. Tim Davis at Texas A&M University, based on his SuiteSparse library (used in MATLAB).
- Design decisions, algorithms and data structures are discussed in the TOMS paper and in the User Guide.
- Extensions: methods and types prefixed with GxB.
- Sophisticated load balancer for multi-threaded execution.
- A GPU implementation is work-in-progress.



T.A. Davis: Algorithm 1000: SuiteSparse:GraphBLAS: graph algorithms in the language of sparse linear algebra, ACM TOMS, 2019

SuiteSparse:GraphBLAS: graph algorithms via sparse matrix operations on semirings The only Tax Act formary Sept 2017 Spars Days 2017 et CERFACS

T.A. Davis: *SuiteSparse:GraphBLAS: graph algorithms via sparse matrix operations on semirings,* Sparse Days 2017

#### Further reading and libraries

## RESOURCES

#### Presentations and tutorials for learning GraphBLAS:



J.R. Gilbert:

*GraphBLAS: Graph Algorithms in the Language of Linear Algebra,* Seminar talk since 2014



S. McMillan and T.G. Mattson:

A Hands-On Introduction to the GraphBLAS, Tutorial at HPEC since 2018



A. Buluç:

GraphBLAS: Concepts, algorithms, and applications, Scheduling Workshop, 2019



M. Kumar, J.E. Moreira, P. Pattnaik: *GraphBLAS: Handling performance concerns in large graph analytics,* Computing Frontiers 2018



List of GraphBLAS-related books, papers, presentations, posters, software, etc. <u>szarnyasg/graphblas-pointers</u>

# THE LAGRAPH LIBRARY

- Similar to the LAPACK library for BLAS
- Uses SuiteSparse:GraphBLAS
- Implementations of common algorithms
   o BFS, SSSP, LCC, PageRank, Boruvka
  - Triangle count, k-truss
  - CDLP (community detection using label propagation)
  - Weakly connected components, Strongly Connected Components
  - $\circ$  Betweenness centrality
  - $\circ$  Deep neural network



T.G. Mattson et al.: *LAGraph: A Community Effort to Collect Graph Algorithms Built on Top of the GraphBLAS,* GrAPL@IPDPS 2019



## **REQUIREMENTS BY GRAPH COMPUTATIONS**

Libraries for linear-algebra based graph processing support the following features (prioritized):

- 1. Sparse matrices For reasonable performance
- 2. Arbitrary semirings For expressive power
- 3. Masking A big reduction in complexity for some algos
- 4. Parallel execution Constant speedup, ideally by #threads

Most libraries **only satisfy requirement #1:** Intel MKL, Eigen, Boost uBLAS, MTL4, Armadillo, NIST Sparse BLAS, GMM++, CUSP, Numpy

Exceptions are the Efficient Java Matrix Library (EJML) and Julia's SparseArrays library, where arbitrary semirings can be used.

## **GRAPHBLAS PAPERS AND BOOKS**

Standards for Graph Algorithm Primitives
$_{\odot}$ Position paper by 19 authors @ IEEE HPEC 2013

- Novel Algebras for Advanced Analytics in Julia
   Technical paper on semirings in Julia @ IEEE HPEC 2013
- Mathematical Foundations of the GraphBLAS
   Theory paper by 16 authors @ IEEE HPEC 2016
- Design of the GraphBLAS C API
   Design decisions and overview of the C API @ GABB@IPDPS 2017
- Algorithm 1000: SuiteSparse:GraphBLAS: graph algorithms in the language of sparse linear algebra
   Algorithms in the SuiteSparse implementation @ ACM TOMS 2019

### BOOKS



Graph Algorithms in the Language of Linear Algebra

 Edited by J. Kepner and J.R. Gilbert, published by SIAM in 2011
 Algorithms for connected components, shortest paths, max-flow, betwenness centrality, spanning tree, graph generation, etc.
 Algorithms and data structure for fast matrix multiplication
 Predates GraphBLAS: preliminary notation, no API usage



#### Mathematics of Big Data

Authored by Jananthan & Kepner, published by MIT Press in 2018
 Generalizes the semiring-based approach for associative arrays
 Contains important papers, including the HPEC'16 paper above
 Discusses D4M (Dynamic Distributed Dimensional Data Model)

## **GRAPHBLAS COMMUNITY**

Wiki: graphblas.org | Communication: primarily mailing list Annual events:

- May: IEEE IPDPS conference
  - o GrAPL workshop (Graphs, Architectures, Programming and Learning), a merger of
    - GABB (Graph Algorithms Building Blocks)
    - GraML (Graph Algorithms and Machine Learning)
  - See graphanalysis.org for previous editions
- Sep: IEEE HPEC conference

GraphBLAS BoF meeting

- Nov: IEEE/ACM Supercomputing conference
  - GraphBLAS Working Group
  - IA<sup>3</sup> workshop (Workshop on Irregular Applications: Architectures and Algorithms)

Blog: <u>AldenMath</u> by Timothy Alden Davis

## REDISGRAPH

- Graph database built on top of Redis with partial (but extending) support for the Cypher language
- Uses SuiteSparse:GraphBLAS for graph operations
- Preliminary benchmark results show good performance on traversal-heavy workloads



redisconf 19

R. Lipman, T.A. Davis: *Graph Algebra – Graph operations in the language of linear algebra* RedisConf 2018

R. Lipman: *RedisGraph internals* RedisConf 2019

## **GRAPHBLAS IMPLEMENTATIONS**

- SuiteSparse:GraphBLAS

   v1.0.0: Nov 2017 sequential
   v3.0.1: July 2019 parallel
   v4.0.1draft: Dec 2020 many optimizations, incl. bitmap format
- IBM GraphBLAS

Complete implementation in C++, released in May 2018
 Concise but sequential

- GBTL (GraphBLAS Template Library): C++
   v1.0: parallel but no longer maintained
   v2.0, v3.0: sequential
- GraphBLAST: GPU implementation, based on GBTL

## GRAPHULO

- Build on top of the Accumulo distributed key-value store
- Written in Java
- Focus on scalability



V. Gadepally et al.: *Graphulo: Linear Algebra Graph Kernels for NoSQL Databases,* GABB@IPDPS 2015



# **COMBBLAS: COMBINATORIAL BLAS**

- "an extensible distributed memory parallel graph library offering a small but powerful set of linear algebra primitives"
- Not a GraphBLAS implementation but serves as an incubator for new ideas that may later find their way into GraphBLAS
- Scales to 250k+ CPU cores
- Used on supercomputers such as Cray



A. Buluç, J.R. Gilbert: *The Combinatorial BLAS: design, implementation, and application,* International Journal of High Performance Computing Applications, 2011

## **PYGRAPHBLAS: PYTHON WRAPPER**

- Goal: Pythonic
   GraphBLAS wrapper,
   close to pseudo-code
- See example code for SSSP and triangle count
- Comes with Jupyter notebooks

```
def sssp(matrix, start):
```

```
v = Vector.from_type(matrix.gb_type, matrix.nrows)
v[start] = 0
```

```
with min_plus, Accum(min_int64):
    for _ in range(matrix.nrows):
        w = Vector.dup(v)
        v @= matrix
        if w == v:
            break
    return v
```

```
def sandia(A, L):
    return L.mxm(L, mask=L).reduce_int()
sandia(M, M.tril())
```



# **GRBLAS: PYTHON WRAPPER**

Goal: wrapper with an almost 1-to-1 mapping to the GrB API

 Comes with a Conda package
 Compiles user-defined functions to C
 Supports visualization

M(mask,	accum)	<< A.mxm(B, semiring)	#	m×m
w(mask,	accum)	<< A.mxv(v, semiring)	#	mxv
w(mask,	accum)	<< v.vxm(B, semiring)	#	VXM
M(mask,	accum)	<< A.ewise_add(B, binaryop)	#	eWiseAdd
M(mask,	accum)	<< A.ewise_mult(B, binaryop)	#	eWiseMult
M(mask,	accum)	<< A.kronecker(B, binaryop)	#	kronecker
M(mask,	accum)	<< A.T	#	transpose



#### Parallelism in GraphBLAS



#### THE CASE FOR LINEAR ALGEBRA-BASED GRAPH ALGORITHMS

Many irregular applications contain coarse-grained parallelism that can be exploited by abstractions at the proper level.

Traditional graph computation	Graphs in the language of linear algebra
Data-driven, unpredictable communication	Fixed communication patterns
Irregular and unstructured, poor	Operations on matrix blocks
locality of reference	exploit memory hierarchy
Fine-grained data accesses,	Coarse-grained parallelism,
dominated by latency	bandwidth-limited



D. Bader et al., *The GraphBLAS effort and its implications for Exascale,* SIAM Workshop on Exascale Applied Mathematics Challenges and Opportunities, 2014



## SUMMARY

- Linear algebra is a powerful abstraction

   Good expressive power
   Concise formulation of most graph algorithms
   Good performance
   Still lots of ongoing research
- Trade-offs:

Learning curve (maths, C programming, GraphBLAS API)
 Some algorithms are difficult to formulate in linear algebra
 Only a few GraphBLAS implementations (yet)

 Overall: GraphBLAS is a good abstraction layer for graph algorithms in the age of heterogeneous hardware
# *"Nuances"* – Some important adjustments to the definitions

## **GRAPHBLAS SEMIRINGS\***

The GraphBLAS specification defines semirings as follows:  $(D_{out}, D_{in_1}, D_{in_2}, \bigoplus, \otimes, 0)$  structure is a *GraphBLAS semiring* defined by

- $D_{\text{out}}$ ,  $D_{\text{in}_1}$ , and  $D_{\text{in}_2}$  three domains
- $\oplus: D_{\text{out}} \times D_{\text{out}} \to D_{\text{out}}$
- $\bigotimes: D_{\text{in}_1} \times D_{\text{in}_2} \to D_{\text{out}}$
- $0 \in D_{out}$

- an associative and commutative addition operation a multiplicative operation an identity element for  $\oplus$
- $A = \langle D_{out}, \bigoplus, 0 \rangle$  is a commutative monoid.  $F = \langle D_{out}, D_{in_1}, D_{in_2}, \otimes \rangle$  is a closed binary operator.

"It is expected that implementations will utilize IEEE-754 floating point arithmetic, which is not strictly associative." (C API specification)

# **NOTATION\***

- Symbols:
  - A, B, C, M matrices
  - $\circ$  **u**, **v**, **w**, **m** vectors
  - $\circ$  *s*, *k* scalar
  - $\circ$  *i*, *j* indices
  - $\circ \langle m \rangle$ ,  $\langle M \rangle$  masks
- Operators:
  - $\circ \oplus$  addition
  - $\circ$   $\otimes$  multiplication,  $\oslash$  division
  - $\circ ^{\top} transpose$ Not included in the  $\circ \odot - accumulator \rightarrow simplified table$

This table contains all GrB and GxB (SuiteSparse-specific) operations.

	symbol	operation	notation
	⊕.⊗	matrix-matrix multiplication	$C\langle M \rangle \bigcirc = A \oplus \otimes B$
		vector-matrix multiplication	$w\langle m \rangle \bigcirc = v \oplus . \otimes A$
		matrix-vector multiplication	$\mathbf{w}\langle \mathbf{m} \rangle \bigcirc = \mathbf{A} \oplus \otimes \mathbf{v}$
	$\otimes$	element-wise multiplication (set intersection of patterns)	$C\langle M \rangle \odot = A \otimes B$
			$w\langle m \rangle \odot = u \otimes v$
	Ð	element-wise addition (set union of patterns)	$C\langle M \rangle \odot = A \oplus B$
			$w\langle m \rangle \odot = u \oplus v$
	f	apply unary operator	$\mathbf{C}\langle \mathbf{M}\rangle \bigcirc = f(\mathbf{A})$
			$\mathbf{w}\langle \mathbf{m}\rangle \bigcirc = f(\mathbf{v})$
	[⊕…]	reduce to vector	$\mathbf{w}\langle \mathbf{m}\rangle \bigcirc = \left[\bigoplus_{j} \mathbf{A}(:,j)\right]$
		reduce to scalar	$s \bigcirc = \left[ \bigoplus_{ij} \mathbf{A}(i,j) \right]$
	$\mathbf{A}^{T}$	transpose matrix	$C\langleM\rangle\odot=A^{T}$
	_	extract submatrix	$C\langle M \rangle \bigcirc = A(i,j)$
			$w\langle m \rangle \odot = v(i)$
	_	assign submatrix with submask for <b>C(I, J</b> )	$C\langle M \rangle(i,j) \odot = A$
			$w\langle m \rangle(i) \odot = v$
	_	assign submatrix with mask for <b>C</b>	$C(i,j)\langle M\rangle \odot = A$
			$w(i)\langle m \rangle \odot = v$
	-	apply select operator (GxB)	$\mathbf{C}\langle \mathbf{M}\rangle \bigcirc = f(\mathbf{A},k)$
			$\mathbf{w}\langle \mathbf{m}\rangle \bigcirc = f(\mathbf{v},k)$
L	-	Kronecker product	$C\langle M \rangle \bigcirc = \operatorname{kron}(A, B)$

## LINEAR ALGEBRAIC PRIMITIVES FOR GRAPHS #3\*

#### Sparse matrix extraction: induced subgraph



#### Sparse matrix selection: filtering edges









**Kronecker product:** graph generation







## **MATRIX-VECTOR MULTIPLICATION\***

The operation  $\mathbf{v} \oplus \otimes \mathbf{A}$  gives the vertices reachable from the ones in  $\mathbf{v}$ . However, GraphBLAS publications and implementations often use  $\mathbf{A}^{\mathsf{T}} \oplus \otimes \mathbf{v}$  instead. The difference between these is that the former produces a row vector, while the latter produces a column vector:  $\mathbf{v} \oplus \otimes \mathbf{A} \equiv (\mathbf{A}^{\mathsf{T}} \oplus \otimes \mathbf{v}^{\mathsf{T}})^{\mathsf{T}}$ 

The GraphBLAS does not distinguish row/column vectors, therefore the notations are (formally) equivalent:

 $\mathbf{v} \oplus . \otimes \mathbf{A} \equiv \mathbf{A}^{\mathsf{T}} \oplus . \otimes \mathbf{v}$ 

## **ELEMENT-WISE SUBTRACTION**

*Element-wise subtraction* can be defined as an *element-wise addition* on the INT64\_MINUS monoid. It has the following semantics  $C = A \ominus B$  is computed on the union of the patterns of the input matrices **A** and **B**.

For cells where only one input matrix has a non-zero value but the other does not (e.g. B[0,0] = 1 but A[0,0] is empty), the result is the non-zero value: C[0,0] = 1.



This might come across as counter-intuitive first but it confirms the specification:

<sup>3070</sup> The intermediate matrix  $\widetilde{\mathbf{T}} = \langle \mathbf{D}_{out}(\mathsf{op}), \mathbf{nrows}(\widetilde{\mathbf{A}}), \mathbf{ncols}(\widetilde{\mathbf{A}}), \{(i, j, T_{ij}) : \mathbf{ind}(\widetilde{\mathbf{A}}) \cap \mathbf{ind}(\widetilde{\mathbf{B}}) \neq \emptyset \} \rangle$ <sup>3071</sup> is created. The value of each of its elements is computed by

3072 
$$T_{ij} = (\widetilde{\mathbf{A}}(i,j) \oplus \widetilde{\mathbf{B}}(i,j)), \forall (i,j) \in \mathbf{ind}(\widetilde{\mathbf{A}}) \cap \mathbf{ind}(\widetilde{\mathbf{B}})$$

- $T_{ij} = \widetilde{\mathbf{A}}(i,j), \forall (i,j) \in (\mathbf{ind}(\widetilde{\mathbf{A}}) (\mathbf{ind}(\widetilde{\mathbf{B}}) \cap \mathbf{ind}(\widetilde{\mathbf{A}})))$
- $T_{ij} = \widetilde{\mathbf{B}}(i.j), \forall (i,j) \in (\mathbf{ind}(\widetilde{\mathbf{B}}) (\mathbf{ind}(\widetilde{\mathbf{B}}) \cap \mathbf{ind}(\widetilde{\mathbf{A}})))$

<sup>3077</sup> where the difference operator in the previous expressions refers to set difference.

## More semirings



Semantics: reachability





6 7

1

1

f⊕









## Case study: SIGMOD 2014 Contest

#### Overview

## SIGMOD 2014 PROGRAMMING CONTEST

#### <u>Annual contest</u>

- Teams compete on database-related programming tasks
- Highly-optimized C++ implementations

#### <u>2014 event</u>

Tasks on the LDBC social network graph

 Benchmark data set for property graphs
 People, forums, comments, hashtags, etc.

## 4 queries

 $_{\odot}$  Mix of filtering operations and graph algorithms

## QUERY TEMPLATE

Compute an induced subgraph over Person-knows-Person
 Run the graph algorithm on the subgraph





## OVERVIEW OF QUERIES 1, 2, 3



## **GRAPHBLAS SOLUTION OF THE QUERIES**

- Loading includes relabelling UINT64 vertex IDs to a contiguous sequence 0 ... N 1.
- Filtering the induced subgraph from the property graph is mostly straightforward and composable with the algorithms.
- The algorithms can be concisely expressed in GraphBLAS:
   Connected components ✓ → FastSV [Zhang et al., PPSC'20]
   BFS ✓
  - Bidirectional BFS
  - $_{\odot}$  All-source BFS + bitwise optimization
  - $\circ$  Multi-source bidirectional BFS

## Case study: SIGMOD 2014 Contest



## **BFS: BREADTH-FIRST SEARCH**



## **BFS: BREADTH-FIRST SEARCH**



## **BFS: BREADTH-FIRST SEARCH**



### Case study: SIGMOD 2014 Contest

#### All-source BFS

## Q4: CLOSENESS CENTRALITY VALUES

Q4 computes the top-*k* Person vertices based on their exact *closeness centrality values*:

$$CCV(p) = \frac{(C(p) - 1)^2}{(n - 1) \cdot s(p)}$$

where

- C(p) is the size of the connected component of vertex p,
- *n* is the number of vertices in the induced graph,
- s(p) is the sum of geodesic distances to all other reachable persons from p.

s(p) is challenging: needs unweighted all-pairs shortest paths.



Next⟨¬Seen⟩ = A any . pair Frontier Seen' = Seen any Next

## **BOOLEAN ALL-SOURCE BFS ALGORITHM**



A any . pair Frontier

#### Case study: SIGMOD 2014 Contest

#### Bitwise all-source BFS

## BITWISE ALL-SOURCE BFS ALGORITHM

- For large graphs, the all-source BFS algorithm might need to run 500k+ traversals
- Two top-ranking teams used bitwise operations to process traversals in batches of 64 [<u>Then et al., VLDB'15</u>]
- This idea can be adopted in the GraphBLAS algorithm by o using UINT64 values
  - o performing the multiplication on the bor second semiring, where bor is "bitwise or" and second(x, y) = y

5-10x speedup compared to the Boolean all-source BFS

## **BITWISE ALL-SOURCE BFS ALGORITHM**



A bor . second Frontier

Seen bor Next

## **BITWISE ALL-SOURCE BFS ALGORITHM**



A bor . second Frontier

Seen bor Next

#### Case study: SIGMOD 2014 Contest

#### **Bidirectional BFS**

## **BIDIRECTIONAL BFS**

Advance frontiers alternately and intersect them



<u>Length = 1</u>  $\times$ next1 land frontier2  $\bigcirc$ =Λ  $\bigcirc$  $\bigcirc$  $\bigcirc$ Λ =<u>Length = 2</u>  $\checkmark$ 

next1 land next2

#### Case study: SIGMOD 2014 Contest

#### **Bidirectional MSBFS**

## **BIDIRECTIONAL MSBFS ALGORITHM**

- Pairwise reachability problem:
   From a given set of k vertices, which pairs of vertices are reachable from each other with at most h hops?
- Naïve solution:

Run a *k*-source MSBFS for *h* steps and check reachability. The frontiers get large as they grow exponentially.

Better solution:

Advance all frontiers simultaneously for  $\lceil h/2 \rceil$  iterations.









To get paths of at most 4 hops, we compute

**Seen**[2] any.pair **Seen**[2]<sup> $\top$ </sup>

Here, we found paths between all pairs:

- from 1 to 5,
- from 1 to 6,
- from (5) to (6).


### Case study: SIGMOD 2014 Contest

### Results

## **BENCHMARK RESULTS**

- The top solution of AWFY vs. SuiteSparse:GraphBLAS v3.3.3
- AWFY's solution uses SIMD instructions  $\rightarrow$  difficult to port
- GraphBLAS load times are slow (see details in paper)



# SUMMARY

- An interesting case study, see <u>technical report</u>
- GraphBLAS can capture mixed workloads

   Induced subgraph computations are simple to express
   Algorithms are concise, bitwise optimizations can be adopted
   Performance is *sometimes* on par with specialized solutions
- Future optimizations
  - $_{\odot}$  Q1: filter the induced subgraph on-the-fly
  - o Q4: use more sophisticated unweighted shortest path algorithms



M. Elekes et al., *A GraphBLAS solution to the SIGMOD 2014 Programming Contest using multi-source BFS,* HPEC 2020

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# **ABOUT THIS PRESENTATION**

- This presentation is intended to serve as an introduction to semiring-based graph processing and the GraphBLAS.
- Common graph algorithms (BFS, shortest path, PageRank, etc.) are used to demonstrate the features of GraphBLAS. Many of the algorithms presented are part of the LAGraph library.
- The presentation complements existing technical talks on GraphBLAS and can form a basis of anything from a short 20min overview to 2×90min lectures on the GraphBLAS.
- The slides contain numerous references to papers and talks.
- There are detailed textual explanations on some slides to make them usable as a learning material.

# **TECHNICAL DETAILS**

- The slides were created with PowerPoint 2016 using the Open Sans and DejaVu Sans Mono font families (embedded in the presentation).
- The mathematical expressions are typeset with PowerPoint's built-in Equation Editor.
- The circled numbers (denoting graph vertices) are rendered using the standard Wingdings font.
- The text is written in Oxford English.
- The icons for referenced papers and talks are clickable and will lead to an open-access / preprint / author's copy version of the referred work (if such copy exists). The icons depict the first page of the cited document.