GraphBLAS: A linear algebraic approach for high-performance graph algorithms

Gábor Szárnyas
szarnyas@mit.bme.hu
WHAT MAKES GRAPH PROCESSING DIFFICULT?

- the “curse of connectedness”
- contemporary computer architectures are good at processing linear and hierarchical data structures, such as Lists, Stacks, or Trees
- 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 Bulletin 2017
Graph processing in linear algebra
ADJACENCY MATRIX

\[ A_{ij} = \begin{cases} 
1 & \text{if } (v_i, v_j) \in E \\
0 & \text{if } (v_i, v_j) \notin E 
\end{cases} \]
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Most cells are zero: sparse matrix

source 7

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Most cells are zero: sparse matrix
Use vector/matrix operations to express graph algorithms: $vA^k$ means $k$ hops in the graph.
Use vector/matrix operations to express graph algorithms:

$vA^k$ means $k$ hops in the graph.
BOOKS ON LINEAR ALGEBRA FOR GRAPH PROCESSING

  - *The Design and Analysis of Computer Algorithms*

- 1990: Cormen-Leiserson-Rivest book
  - *Introduction to Algorithms*

  - *Graph Algorithms in the Language of Linear Algebra*

A lot of literature but few practical implementations and particularly few easy-to-use libraries.
THE GRAPHBLAS STANDARD

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

- 1979: BLAS  Basic Linear Algebra Subprograms (dense)
- 2001: Sparse BLAS  an extension to BLAS (insufficient for graphs, little uptake)
- 2013: GraphBLAS  standard building blocks for graph algorithms in LA
Semiring-based graph computations
**Definition:**

\[ \mathbf{C} = \mathbf{A} \mathbf{B} \]

\[ C(i,j) = \sum_k A(i,k) \cdot B(k,j) \]

**Example:**

\[ C(2,3) = A(2,1) \cdot B(1,3) + A(2,2) \cdot B(2,3) \]

\[ = 2 \cdot 5 + 3 \cdot 4 = 22 \]
MATRIX MULTIPLICATION ON SEMIRINGS

- Using the conventional semiring

\[ C = AB \]
\[ C(i, j) = \sum_k A(i, k) \cdot B(k, j) \]

- Use arbitrary semirings that override the \( \oplus \) addition and \( \otimes \) multiplication operators. Generalized formula (simplified)

\[ C = A \oplus \otimes B \]
\[ C(i, j) = \bigoplus_k A(i, k) \otimes B(k, j) \]
The \( \langle D, \oplus, \otimes, 0 \rangle \) algebraic structure is a GraphBLAS semiring if

- \( \langle D, \oplus, 0 \rangle \) is a commutative monoid over domain \( D \) with an addition operator \( \oplus \) and identity \( 0 \), where \( \forall a, b, c \in D \):
  - Commutative \( a \oplus b = b \oplus a \)
  - Associative \( (a \oplus b) \oplus c = a \oplus (b \oplus c) \)
  - Identity \( a \oplus 0 = a \)

- The multiplication operator is a closed binary operator \( \otimes : D \times D \rightarrow D \).

This is less strict than the standard mathematical definition which requires that \( \otimes \) is a monoid and distributes over \( \oplus \).
## COMMON SEMIRINGS

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**Notation:** \( \mathbf{A} \oplus \otimes \mathbf{B} \) is a matrix multiplication using addition \( \oplus \) and multiplication \( \otimes \), e.g. \( \mathbf{A} \lor \land \mathbf{B} \). The default is \( \mathbf{A} + \cdot \mathbf{B} \).
Semantics: number of paths

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\[ \begin{pmatrix}
  1 & 2 & 3 & 4 & 5 & 6 & 7 \\
  1 & 1 & 1 & 1 & 1 & 1 & 1 \\
  1 & 1 & 1 & 1 & 1 & 1 & 1 \\
  1 & 1 & 1 & 1 & 1 & 1 & 1 \\
  1 & 1 & 1 & 1 & 1 & 1 & 1 \\
  1 & 1 & 1 & 1 & 1 & 1 & 1 \\
  1 & 1 & 1 & 1 & 1 & 1 & 1 \\
\end{pmatrix} \]

\[ \begin{pmatrix}
  0 & 0 & 0 & 1 & 0 & 1 & 0 \\
\end{pmatrix} \]
**Semantics:** reachability

### Semiring and Domain

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$a \in \{F, T\}$

### Identity Element

- Identity element: $F$
- $T \land T = T$
- $T \lor T = T$
- $v \lor T = T$
- $v \land A$
Matrix Multiplication Semantics

Semiring: $\min$-plus
Domain: $a \in \mathbb{R} \cup \{\infty\}$

Semantics: shortest path

\[
\begin{align*}
0.5 + 0.4 &= 0.9 \\
0.6 + 0.5 &= 1.1
\end{align*}
\]

\[
\begin{align*}
\min(0.9, 1.1) &= 0.9 \\
v \min . + A
\end{align*}
\]
Graph algorithms in GraphBLAS

Single-source shortest path
SSSP – SINGLE-SOURCE SHORTEST PATHS

Problem:
- From a given start node $s$, find the shortest paths to every other (reachable) node in the graph

Bellman-Ford algorithm:
- Relaxes all edges in each step
- Guaranteed to find the shortest paths using at most $n - 1$ steps

Observation:
- The relaxation step can be captured using a VM multiplication
SSSP – ALGEBRAIC BELLMAN-FORD

We use the \textbf{min-plus} semiring with identity $\infty$.

\[
A_{ij} = \begin{cases} 
0 & \text{if } i = j \\
w(e_{ij}) & \text{if } e_{ij} \in E \\ \infty & \text{if } e_{ij} \notin E
\end{cases}
\]

\[
d = [\infty \infty \ldots \infty]
\]

\[
d(s) = 0
\]

\[
d\]
SSSP – ALGEBRAIC BELLMAN-FORD

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$\delta_{min}^+$

$\mathbb{A}$

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SSSP – ALGEBRAIC BELLMAN-FORD

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| min-plus     | $a \in \mathbb{R} \cup \{\infty\}$ | min | + | $\infty$

**Graph:**

- **Nodes:** 1, 2, 3, 4, 5, 6, 7
- **Edges:**
  - 1 to 2: 0.3
  - 2 to 4: 0.8
  - 4 to 7: 0.5
  - 7 to 5: 0.8
  - 5 to 6: 0.1
  - 6 to 3: 0.5
  - 3 to 1: 0.4

**Matrix A:**

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**Matrix d min. + A:**

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**Notes:**
- The semiring is min-plus, with the set $a \in \mathbb{R} \cup \{\infty\}$, and the operations are min for $\oplus$, plus for $\otimes$, and $\infty$ for 0.
- The graph shows directed edges with weights.
- The matrix A represents the adjacency matrix of the graph.
- The matrix d represents the distance matrix, where $d_{ij}$ is the shortest path from node i to node j.
- The matrix d min. + A combines the distance matrix with the adjacency matrix to find the shortest path distances considering the min-plus semiring operations.
SSSP – ALGEBRAIC BELLMAN-FORD

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<td>( a \in \mathbb{R} \cup {\infty} )</td>
<td>min</td>
<td>+</td>
<td>( \infty )</td>
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\[
\begin{align*}
\mathbf{A} & = \begin{bmatrix}
0 & .3 & .8 \\
0 & .1 & .7 \\
0 & .5 & .2 \\
.2 & .4 & 0 \\
0 & .1 & 0 \\
.5 & 0 & .1 \\
.1 & .5 & .9 \\
.3 & 1 & .2 & 1 & 1 & 1 & 1 & 1 \\
\end{bmatrix} \\
\mathbf{d} & = \begin{bmatrix}
0 & .3 & \infty & .8 & \infty & \infty & \infty & \infty \\
0 & .1 & .7 & \infty & .5 & .2 & .4 & 0 \\
0 & .5 & .2 & .4 & 0 & .1 & .5 & .9 \\
0 & .3 & 1 & .2 & 1 & 1 & 1 & 1 & 1 \\
\end{bmatrix}
\end{align*}
\]

\[\mathbf{d} \text{ min.} + \mathbf{A}\]
SSSP – ALGEBRAIC BELLMAN-FORD

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\[
\mathbf{d} \begin{bmatrix}
0.3 & 0.8 & 0.7 & 0.8 & 0.4 & \infty & 1 \\
0.1 & 0.1 & 0.5 & 0.2 & 0 & 0.1 & 0.1 \\
0.5 & 0.1 & 0.5 & 0.1 & 0.5 & 0.9 & 0 \\
0.4 & 0.8 & 0.7 & 0.1 & 0.5 & 0 & 0 \\
\end{bmatrix}
\]

\[
\mathbf{d} \text{ min.} + \mathbf{A} = \begin{bmatrix}
0.3 & 1.1 & 1.8 & 0.4 & 0.5 & 1 \\
\end{bmatrix}
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SSSP – ALGEBRAIC BELLMAN-FORD

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<td>+</td>
<td>$\infty$</td>
</tr>
</tbody>
</table>

$$d_0 = 0.3, 1.1, .8, .4, .5, 1$$

$$A = \begin{pmatrix}
0 & .3 & .8 \\
0 & 0 & .1 & .7 \\
0 & 0 & 0 & .5 \\
.2 & .4 & 0 & 0 & .1 \\
.5 & 0 & 0 & 0 & .9 \\
.1 & .5 & .9 & 0 & 0 \\
\end{pmatrix}$$

$$d_{min.+A} = 0.3, 1, 1.8, .4, .5, 1$$
SSSP – ALGEBRAIC BELLMAN-FORD

<table>
<thead>
<tr>
<th>semiring</th>
<th>set</th>
<th>⊕</th>
<th>⊗</th>
<th>0</th>
</tr>
</thead>
<tbody>
<tr>
<td>min-plus</td>
<td>$a \in \mathbb{R} \cup {\infty}$</td>
<td>min</td>
<td>+</td>
<td>$\infty$</td>
</tr>
</tbody>
</table>

![Graph and matrix](image)

\[
\begin{matrix}
0 & 0.3 & 0.8 \\
0 & 0 & 0.1 & 0.7 \\
0 & 0 & 0 & 0.5 \\
0.2 & 0.4 & 0 & 0.1 \\
0.5 & 0 & 0 & 0 \\
0.5 & 1.5 & 0.9 & 0 \\
0.1 & 0.5 & 0 & 0 \\
\end{matrix}
\]

\[
\begin{matrix}
0.3 & 1 & 0.8 & 0.4 & 0.5 & 1 \\
0.3 & 1 & 0.8 & 0.4 & 0.5 & 1 \\
\end{matrix}
\]

\[d \text{ min.} + A\]
SSSP – ALGEBRAIC BELLMAN-FORD ALGO.  

**Input:** adjacency matrix $A$, source node $s$, #nodes $n$

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

**Output:** distance vector $d \in (\mathbb{R} \cup \{\infty\})^n$

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

Optimization: switch between $d \min.+ A$ and $A^\top \min.+ d$ (push/pull).
Graph algorithms in GraphBLAS

Node-wise triangle count
NODE-WISE TRIANGLE COUNT

Triangle – Def 1: a set of three mutually adjacent nodes.

\[ \begin{align*} &v \end{align*} \]

Def 2: a three-length closed path.

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

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

\[
\text{tri} = \text{diag}^{-1}(A \oplus \otimes A \oplus \otimes A)
\]
**TC: OPTIMIZATION**

**Observation:** Matrix $\mathbf{A} \oplus \otimes \mathbf{A} \oplus \otimes \mathbf{A}$ is no longer sparse.

**Optimization:** Use element-wise multiplication $\otimes$ to close wedges into triangles:

$$\text{TRI} = \mathbf{A} \oplus \otimes \mathbf{A} \otimes \mathbf{A}$$

Then, perform a row-wise summation to get the number of triangles in each row:

$$\text{tri} = [\oplus_j \text{TRI}(:,j)]$$
TC: ELEMENT-WISE MULTIPLICATION

\[
\text{TRI} = A \oplus \bigotimes A \otimes A
\]

\[
\text{tri} = [\oplus_j \text{TRI}(:,j)]
\]

\(A \oplus \bigotimes A\) is still very dense.
**TC: ELEMENT-WISE MULTIPLICATION**

Masking limits where the operation is computed. Here, we use \( A \) as a mask for \( A \oplus \otimes A \).

\[
\text{TRI}(A) = A \oplus \otimes A
\]

\[
\text{tri} = [\oplus_j \text{TRI}(::j)]
\]
TC: ALGORITHM

Input: adjacency matrix $A$
Output: vector $\text{tri}$
Workspace: matrix $\text{TRI}$

1. $\text{TRI}(A) = A \oplus \otimes A$  
   compute the triangle count matrix
2. $\text{tri} = \left[ \oplus_j \text{TRI}(\cdot,j) \right]$  
   compute the triangle count vector

Optimization: use $L$, the lower triangular part of $A$ to avoid duplicates.

$$\text{TRI}(A) = A \oplus \otimes L$$

Worst-case optimal joins: There are deep theoretical connections between masked matrix multiplication and relational join's. 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.
Graph algorithms in GraphBLAS

Other algorithms
# GRAPH ALGORITHMS IN GRAPHBLAS

**Notation:** $n = |V|, m = |E|$. The complexity cells contain asymptotic bounds.

**Takeaway:** The majority of common graph algorithms can be expressed efficiently in LA.

<table>
<thead>
<tr>
<th>problem category</th>
<th>algorithm</th>
<th>canonical complexity $\Theta$</th>
<th>LA-based complexity $\Theta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>breadth-first search</td>
<td>Dijkstra</td>
<td>$m + n \log n$</td>
<td>$n^2$</td>
</tr>
<tr>
<td></td>
<td>Bellman-Ford</td>
<td>$mn$</td>
<td>$mn$</td>
</tr>
<tr>
<td>single-source shortest paths</td>
<td>Floyd-Warshall</td>
<td>$n^3$</td>
<td>$n^3$</td>
</tr>
<tr>
<td>minimum spanning tree</td>
<td>Prim</td>
<td>$m + n \log n$</td>
<td>$n^2$</td>
</tr>
<tr>
<td></td>
<td>Borůvka</td>
<td>$m \log n$</td>
<td>$m \log n$</td>
</tr>
<tr>
<td>maximum flow</td>
<td>Edmonds-Karp</td>
<td>$m^2n$</td>
<td>$m^2n$</td>
</tr>
<tr>
<td>maximal independent set</td>
<td>greedy</td>
<td>$m + n \log n$</td>
<td>$mn + n^2$</td>
</tr>
<tr>
<td></td>
<td>Luby</td>
<td>$m + n \log n$</td>
<td>$m \log n$</td>
</tr>
</tbody>
</table>


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

- “A crucial piece of the GraphBLAS effort is to translate the mathematical specification to an API that
  - is faithful to the mathematics as much as possible, and
  - enables efficient implementations on modern hardware.”

\[
\mathbf{C} \leftarrow \mathbf{M} \odot = \oplus \odot (\mathbf{A}^T, \mathbf{B}^T)
\]

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

- Authored by Prof. Tim Davis at Texas A&M University, based on his SuiteSparse library (used in MATLAB).
- Additional extension operations for efficiency.
- Sophisticated load balancer for multi-threaded execution.
- CPU-based, single machine implementation.
- Powers the RedisGraph graph database.

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

R. Lipman: *RedisGraph internals*, RedisConf 2019

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

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

Two libraries, both offer:

- Concise GraphBLAS operations
- Wrapping SuiteSparse:GrB
- Jupyter support

**Difference:** pygraphblas is more Pythonic, grblas strives to stay close to the C API.

```python
def sssp(A, s):
    d = Vector.from_type(A.type, A.nrows)
    d[s] = 0

    with min_plus_int64, Accum(min_int64):
        for _ in range(A.nrows):
            dn = Vector.dup(d)
            d @= A
            if dn == d:
                break
        return dn

def tricount(A):
    return A.mxm(A, mask=A).reduce_vector()
```
Benchmark results
SUITESPARSE:GRAPHBLAS / LDBC GRAPHALYTICS

**Twitter**
- 50M nodes, 2B edges

**d-8.8-zf**
- 168M nodes, 413M edges

**d-8.6-fb**
- 6M nodes, 422M edges

Ubuntu Server, 512 GB RAM, 64 CPU cores, 128 threads

Results from late 2019, new version is even faster
THE GAP BENCHMARK SUITE

- Part of the *Berkeley Graph Algorithm Platform* project
- Algorithms:
  - BFS, SSSP, PageRank, connected components
  - Betweenness centrality, triangle count
- Very efficient baseline implementation in C++
- Comparing executions of implementations that were carefully optimized and fine-tuned by research groups
- Ongoing benchmark effort, paper to be submitted in Q2


gap.cs.berkeley.edu/benchmark.html
Further reading and summary
RESOURCES

- List of GraphBLAS-related books, papers, presentations, posters, and software: [szarnyasg/graphblas-pointers](https://szarnyasg/graphblas-pointers)
- Library of GraphBLAS algorithms: [GraphBLAS/LAGraph](https://graphblas/lagraph)

Extended version of this talk: 200+ slides

- Theoretical foundations
- BFS variants, PageRank
- Clustering coefficient, $k$-truss and triangle count variants
- Community detection using label propagation
- Luby’s maximal independent set algorithm
- Computing connected components on an overlay graph
- Connections to relational algebra
SUMMARY

- Linear algebra is a powerful abstraction
  - Good expressive power
  - Concise formulation of most graph algorithms
  - Very good performance
  - Still lots of ongoing research

- Trade-offs:
  - Learning curve (theory and GraphBLAS API)
  - Some algorithms are difficult to formulate in linear algebra
  - Only a few GraphBLAS implementations (yet)

- Overall: a very promising programming model for graph algorithms suited to the age of heterogeneous hardware
ACKNOWLEDGEMENTS

- Tim Davis and Tim Mattson for helpful discussions, members of GraphBLAS mailing list for their detailed feedback.
- The LDBC Graphalytics task force for creating the benchmark and assisting in the measurements.
- Master’s students at BME for developing GraphBLAS-based algorithms: Bálint Hegyi, Márton Elekes, Petra Várhegyi, Lehel Boér