Graphs (GraphBLAS) and storage (TileDB) as Sparse Linear algebra

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• This is a speculative, academic style talk ... I am not describing or even suggesting ANYTHING about future products from Intel!!!

I work in Intel’s research labs. I don’t build products. Instead, I get to poke into dark corners and think silly thoughts... just to make sure we don’t miss any great ideas.

I have a really GREAT Job!!!!
A graph as a matrix

- Adjacency Matrix: A square matrix (usually sparse) where rows and columns are labeled by vertices and non-empty values are edges from a row vertex to a column vertex.

By using a matrix, I can turn graph algorithms into linear algebra.
GraphBLAS Math is a lot of fun, but without a software ecosystem the impact from all this cool math is negligible.
• Open-Source C library (Apache 2.0) conforms to the v2.0 C GraphBLAS specification.
• High performance, internal parallelism (OpenMP) for easy-to-code, fast Graph Algorithms
• Support from NSF, MIT Lincoln Labs, Intel, Nvidia, IBM, MathWorks, Redis Labs, and Julia Computing

https://people.engr.tamu.edu/davis/GraphBLAS.html
GraphBLAS Implementations

SuiteSparse library (Texas A&M): First fully conforming GraphBLAS release
  •  http://faculty.cse.tamu.edu/davis/suitesparse.html

GraphBLAS C (IBM): the second fully conforming release
  •  https://github.com/IBM/ibmgraphblas

GBTL: GraphBLAS Template Library (CMU/SEI/1U/PNNL): GraphBLAS C++ implementation
  •  https://github.com/cmu-sei/gbtl

GraphBLAST: A C++ implementation for GraphBLAS for GPUs (UC Davis)
  •  https://github.com/gunrock/graphblast

Python bindings:
  •  PyGB: A python wrapper around GBTL (UW/PNNL/CMU)
    •  https://github.com/jessecoleman/gbtl-python-binding
  •  pygraphblas: A python wrapper around SuiteSparse GraphBLAS
    •  https://github.com/michelp/pygraphblas
  •  Python-graphblas: Anaconda’s python wrapper around SuiteSparse GraphBLAS
    •  https://github.com/python-graphblas/python-graphblas

pggraphblas: A PostgreSQL wrapper around SuiteSparse GraphBLAS
  •  https://github.com/michelp/pggraphblas

Julia wrapper around SuiteSparse
  •  SuiteSparseGraphBLAS.jl

Matlab and Julia wrappers around SuiteSparse GraphBLAS
  •  https://aldenmath.com

Implementations in progress:
•  Intel and SEI/CMU are working on a C++ implementation. We will have a preliminary release running on clusters of CPUs, GPUs, and multiple CPUs
•  And soon Intel will have a Go implementation (wrapping SuiteSparse)

Third Party names are the property of their owners
Multilanguage support by wrapping SuiteSparse GraphBLAS

The GraphBLAS in Julia and Python: the PageRank and Triangle Centralities (HPEC’21)

Michel Pelletier  Will Kimmerer  Timothy A. Davis  Timothy G. Mattson

\[ c = \frac{(3A - 2\bar{T} + I)T1}{1^T T1} \]

- \( \bar{T} \) matrix of triangles of A
- \( T \) all zero, but 1 where T is non-zero
- 1 Matrix of all ones     I identity matrix

The math

**Julia**

```julia
function triangle_centrality1(A)
    T = mul(A, A', mask=A, desc=S)
    y = reduce(+, T, dims=2)
    k = reduce(+, y)
    return (3.*mul(A,y)-2.*mul(one.(T),y)+y) ./ k
end
```

**pygraphblas**

```python
def triangle_centrality1(A):
    T = A.mxm(A, mask=A, desc=ST1)
    y = T.reduce_vector()
    k = y.reduce_float()
    return (3 * (A@y) - 2 * (T.one()@y) + y) / k
```
Multilanguage support by wrapping SuiteSparse GraphBLAS

The GraphBLAS in Julia and Python: the PageRank and Triangle Centralities (HPEC'21)

Michel Pelletier      Will Kimmerer      Timothy A. Davis      Timothy G. Mattson

The math

\[ c = \frac{(3A - 2\bar{T} + I)T1}{1^T T1} \]

- \( T \): matrix of triangles of \( A \)
- \( \bar{T} \): all zero, but 1 where \( T \) is non-zero
- \( 1 \): Matrix of all ones

Expressivity/productivity in programming languages should be measured by how clear "the math" maps onto code.

These interfaces are highly productive by that measure

Julia

```julia
function triangle_centrality1(A)
    T = mul(A, A', mask=A, desc=S)
    y = reduce(+, T, dims=2)
    k = reduce(+, y)
    return (3.*mul(A,y)-2.*mul(one.(T),y)+y) ./ k
end
```

pygraphblas

```python
def triangle_centrality1(A):
    T = A.mxm(A, mask=A, desc=ST1)
    y = T.reduce_vector()
    k = y.reduce_float()
    return (3 * (A*y) - 2 * (T.one(@y) + y) / k
```
LAGraph: A curated collection of high level Graph Algorithms

Graph Algorithms built on top of the GraphBLAS.

LAGraph: A Community Effort to Collect Graph Algorithms Built on Top of the GraphBLAS

Tim Mattson\textsuperscript{1}, Timothy A. Davis\textsuperscript{2}, Manoj Kumar\textsuperscript{3}, Aydn Buluç\textsuperscript{4}, Scott McMillan\textsuperscript{5}, José Moreira\textsuperscript{6}, Carl Yang\textsuperscript{7,1

\textsuperscript{1}Intel Corporation \textsuperscript{2}Computational Research Division, Lawrence Berkeley National Laboratory
\textsuperscript{3}Texas A&M University \textsuperscript{4}IBM Corporation \textsuperscript{5}Software Engineering Institute, Carnegie Mellon University
\textsuperscript{6}Electrical and Computer Engineering Department, University of California, Davis

GrAPL 2019

Official release of LAGraph library v1.0 late 2021

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Integration of GraphBLAS with NetworkX
Jim Kitchen (Anaconda) and Erik Welch (Nvidia)

Integration of GraphBLAS with NetworkX
Jim Kitchen (Anaconda) and Erik Welch (Nvidia)

import networkx as nx
G = nx.erdos_renyi_graph(8000, 0.02)
k = nx.k_truss(G, 5)

8000 nodes, ~ 640,000 edges
This takes 10.7 seconds

The k-truss is the maximal induced subgraph of G with each edge belonging to at least k-2 triangles.

import networkx as nx
import graphblas_algorithms as ga
G = nx.erdos_renyi_graph(8000, 0.02)
G2 = ga.Graph.from_networkx(G)
k = nx.k_truss(G2, 5)

conda install -c conda-forge graphblas-algorithms
-or-
pip install graphblas-algorithms (Linux Only)

This takes 0.5 seconds
This takes 0.28 seconds
## Hardware
- **CPU**: Dual 20 Core Intel Xeon E5-2698 v4 2.2GHz
- **RAM**: 512 GB 2133 MHz DDR4 RDIMM
- **GPU**: NVIDIA DGX-1

## Benchmarks: GraphBLAS vs NetworkX

### Speed-up

<table>
<thead>
<tr>
<th></th>
<th>amazon</th>
<th>google</th>
<th>pokec</th>
<th>enron</th>
<th>preferentialAttachment</th>
<th>caidaRouterLevel</th>
<th>dblp</th>
<th>citationCiteseer</th>
<th>coAuthorsDBLP</th>
<th>as-Skitter</th>
<th>coPapersCiteseer</th>
<th>coPapersDBLP</th>
</tr>
</thead>
<tbody>
<tr>
<td># of vertices</td>
<td>262,111</td>
<td>916,428</td>
<td>1,632,804</td>
<td>36,692</td>
<td>100,000</td>
<td>192,244</td>
<td>326,186</td>
<td>268,495</td>
<td>299,067</td>
<td>1,696,415</td>
<td>434,102</td>
<td>5,404,486</td>
</tr>
<tr>
<td># of edges</td>
<td>1,234,877</td>
<td>5,105,039</td>
<td>30,622,564</td>
<td>367,662</td>
<td>999,970</td>
<td>1,218,132</td>
<td>1,615,400</td>
<td>2,313,294</td>
<td>1,955,352</td>
<td>22,190,596</td>
<td>32,071,440</td>
<td>30,491,458</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Measure</th>
<th>NetworkX run times</th>
</tr>
</thead>
<tbody>
<tr>
<td>degree centrality</td>
<td>0.25-1 s</td>
</tr>
<tr>
<td>reciprocity</td>
<td>3-5 min</td>
</tr>
<tr>
<td>generalized degree</td>
<td>10-30 min</td>
</tr>
<tr>
<td>k-truss(k=5)</td>
<td>30-100 min</td>
</tr>
<tr>
<td>pagerank</td>
<td>1 min</td>
</tr>
<tr>
<td>eigenvector centrality</td>
<td>30-100 min</td>
</tr>
<tr>
<td>katz centrality</td>
<td>hours-days</td>
</tr>
<tr>
<td>clustering</td>
<td>10-30 min</td>
</tr>
<tr>
<td>transitivity</td>
<td>10-30 min</td>
</tr>
<tr>
<td>square clustering</td>
<td>days-weeks?</td>
</tr>
<tr>
<td>pagerank (scipy)</td>
<td>0.25-1 s</td>
</tr>
</tbody>
</table>

*Note: NetworkX run times are approximate and may vary depending on the specific graph and configuration.*

### Benchmarks GraphBLAS vs NetworkX

<table>
<thead>
<tr>
<th>Benchmark</th>
<th>GraphBLAS</th>
<th>NetworkX</th>
</tr>
</thead>
<tbody>
<tr>
<td>speed-up amazon</td>
<td>32</td>
<td>48</td>
</tr>
<tr>
<td>speed-up google</td>
<td>29</td>
<td>60</td>
</tr>
<tr>
<td>speed-up pokec</td>
<td>31</td>
<td>140</td>
</tr>
<tr>
<td>speed-up enron</td>
<td>29</td>
<td>65</td>
</tr>
<tr>
<td>speed-up preferentialAttachment</td>
<td>180</td>
<td>200</td>
</tr>
<tr>
<td>speed-up caidaRouterLevel</td>
<td>140</td>
<td>150</td>
</tr>
<tr>
<td>speed-up dblp</td>
<td>140</td>
<td>150</td>
</tr>
<tr>
<td>speed-up citationCiteseer</td>
<td>180</td>
<td>200</td>
</tr>
<tr>
<td>speed-up coAuthorsDBLP</td>
<td>53</td>
<td>170</td>
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<tr>
<td>speed-up as-Skitter</td>
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<td>170</td>
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<tr>
<td>speed-up coPapersCiteseer</td>
<td>80</td>
<td>170</td>
</tr>
<tr>
<td>speed-up coPapersDBLP</td>
<td>80</td>
<td>170</td>
</tr>
</tbody>
</table>

*Note: Speed-up values represent the ratio of NetworkX run times compared to GraphBLAS.*
Moving Beyond Simple Graphs
Different Types of Graphs

• Simple Graphs: an edge connects one source to one destination.

• Hypergraphs: at least one edge from one source to multiple destinations.

• Multigraphs: Includes edges that share end points.
All these graph types can be handled with the GraphBLAS

Two Incidence Matrices can represent a wide range of graphs

Hypergraph:
Multiple Outputs from edge 12

Multigraph:
Multiple edges that share end points

Graph/Array source: Jananthan, Dibert, Kepner, Constructing Adjacency Arrays from Incidence Arrays, GABB'2017
Adjacency matrices from incidence matrices

Adjacency can be **projected** from two Incidence Matrices with Matrix Multiplication: $I^T O = IO$

```python
# with PLUS_SECOND:
IO = I.T @ O
```

Graph/Array source: Jananthan, Dibert, Kepner, Constructing Adjacency Arrays from Incidence Arrays, GABB'2017
Print edges that match “bob” “manages” ”jane“:

```python
>>> p(G(source='bob', property='manages', destination='jane'))
[manages(((bob, alice), (jane), (True))]
```
Speaking of property graphs …

- A graph database built on top of GrapghBLAS … one of our major, commercial success stories for the GraphBLAS

- Supports a subset of the Cypher query language … mapping elements of the language onto linear algebra operations.

RedisGraph

A Graph database built on Redis

RedisGraph is a graph database built on Redis. This graph database uses GraphBlas under the hood for its sparse adjacency matrix graph representation.

Primary features

- Based on the property graph model
- Nodes can have any number of labels
- Relationships have a relationship type
- Graphs represented as sparse adjacency matrices
- Cypher as the query language
- Cypher queries translate into linear algebra expressions

https://redis.io/docs/stack/graph/
The lesson from Edgar Codd so long ago was the power of an algebra to unify disparate approaches to a problem.

Relational algebras are great at data management, but they suck at computation. It would be stupid to build a PDE solver around a relational algebra.

So if we want ”one algebra to rule them all”, what should be our algebra?
Linear Algebra: One Algebra to rule them all

• Computational physics is basically applied linear algebra
  – We create differential equations from the physics, discretize domains to replace derivatives with differences, and solve resulting algebraic equations.
  – Since the differential operators are replaced by modest sized stencils, the arrays in physics problems are sparse (with a small number of exceptions such as in ab initio quantum chemistry).

• Graphs are linear algebra, databases map onto linear algebra, science and engineering is linear algebra … if you go deep enough, in almost any field, you end up doing linear algebra.

• All we need is a good library for Sparse Linear Algebra.
... to address data management, we need a storage engine to work with GraphBLAS
SuiteSparse to the rescue: SuiteSparse versus the Intel MKL sparse library

<table>
<thead>
<tr>
<th>computation</th>
<th>format</th>
<th>MKL method</th>
<th>MKL time (sec)</th>
<th>SuiteSparse time (sec)</th>
<th>speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>1st</td>
<td>2nd</td>
<td></td>
</tr>
<tr>
<td>y+=S*x</td>
<td>S by row</td>
<td>mkl_sparse_d_mv</td>
<td>2.54</td>
<td>1.27</td>
<td>2.10</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1.05</td>
</tr>
<tr>
<td>y+=S*x</td>
<td>S by col</td>
<td>mkl_sparse_d_mv</td>
<td>7.22</td>
<td>7.22</td>
<td>3.65</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>3.65</td>
</tr>
<tr>
<td>C+=S*F</td>
<td>S by row, F by row</td>
<td>mkl_sparse_d_mm</td>
<td>2.95</td>
<td>1.90</td>
<td>1.49</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>.96</td>
</tr>
<tr>
<td>C+=S*F</td>
<td>S by row, F by col</td>
<td>mkl_sparse_d_mm</td>
<td>6.12</td>
<td>4.99</td>
<td>4.13</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>3.37</td>
</tr>
<tr>
<td>C+=S*F</td>
<td>S by col, F by row</td>
<td>mkl_sparse_d_mm</td>
<td>28.82</td>
<td>28.82</td>
<td>2.09</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>2.09</td>
</tr>
<tr>
<td>C+=S*F</td>
<td>S by col, F by col</td>
<td>mkl_sparse_d_mm</td>
<td>78.82</td>
<td>5.17</td>
<td>8.40</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>.55</td>
</tr>
<tr>
<td>C=S+B</td>
<td>S by row</td>
<td>mkl_sparse_d_add</td>
<td>30.77</td>
<td>30.77</td>
<td>21.37</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>21.37</td>
</tr>
<tr>
<td>C=S' +B</td>
<td>S by row</td>
<td>mkl_sparse_d_add</td>
<td>102.09</td>
<td>27.30</td>
<td>6.26</td>
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<tr>
<td></td>
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<td></td>
<td></td>
<td></td>
<td>1.67</td>
</tr>
<tr>
<td>C=S'</td>
<td>S by row</td>
<td>mkl_sparse_convert_csr</td>
<td>77.27</td>
<td>77.27</td>
<td>5.22</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>5.22</td>
</tr>
</tbody>
</table>

Table 4. SuiteSparse vs MKL 2022 with the GAP-Twitter matrix

SuiteSparse GraphBLAS traditional sparse linear algebra as well as graphs.

All we need is a good storage engine for an end-to-end solution
TileDB an data storage manager: Optimized for Sparse Arrays

Logical representation

attribute values
\( (a_1, a_2, \ldots, a_m) \)
cell
empty cell
dimensions

Physical representation

coordinates
Files

\( (x, y) \)
tile
cell

\( a_1, a_2, \ldots, a_m \)

Tile: Atomic unit of processing

Manage array storage as tiles of different shape/size in the index space, but with \( \sim \)equal number of non-empty cells

TileDB Inc website: https://tiledb.io

The TileDB Array Data Storage Manager, Stavros Papadopoulos, Kushal Datta, Samuel Madden, Tim Mattson, VLDB 2017

Third Party names are the property of their owners
Conclusion

- SuiteSparse GraphBLAS + TileDB as a storage engine is the foundation of an end-to-end framework for data analytics.

- All that’s missing is a query engine supporting GQL that maps onto GraphBLAS

- I am looking for collaborators to implement the above (interface GraphBLAS to TileDB and combine with a GQL query engine). This would be fun and impactful. Let me know if you want to get involved.