

# GraphBLAS: Graph Algorithms in the Language of Linear Algebra

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## Multiple-source breadth-first search



- Sparse array representation => space efficient
- Sparse matrix-matrix multiplication => work efficient
- Three possible levels of parallelism: searches, vertices, edges



## **Coarsening via sparse matrix-matrix products**



A. Buluç, JG. Parallel sparse matrix-matrix multiplication and indexing: Implementation and experiments. *SIAM J. Scientific Computing, 2012*.

## Counting triangles (clustering coefficient)



#### <u>Clustering coefficient:</u>

- Pr (wedge i-j-k makes a triangle with edge i-k)
- 3 \* # triangles / # wedges
- 3 \* 4 / 19 = 0.63 in example
- may want to compute for each vertex j

Low-hinge algorithm to count triangles:

- hi hi
- Count triangles by lowest-degree vertex.
- hi hi
  - Enumerate "low-hinged" wedges.



- Keep wedges that close.

J. Cohen. Graph twiddling in a MapReduce world. IEEE CS&E, 2009.



## Counting triangles (clustering coefficient)



A = L + U	(hi->lo + lo->hi)
$L \times U = B$	(wedge, low hinge)
$A \wedge B = C$	(closed wedge)
sum(C)/2 =	4 triangles







A. Azad, A. Buluc, JG. Parallel triangle counting and enumeration using matrix algebra. *GABB*, 2015.



UCSB

## Counting triangles (clustering coefficient)



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$A \wedge B = C$	(closed wedge)
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<u>Spoiler</u>:  $(L \times L) \wedge L$  works better in practice [Wolf et al. 2017]

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## Graph algorithms in the language of linear algebra

- Kepner et al. study [2006]: fundamental graph algorithms including min spanning tree, shortest paths, independent set, max flow, clustering, ...
- SSCA#2 / centrality [2008]
- Basic breadth-first search / Graph500 [2010]
- Combinatorial BLAS [2010]



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But why do it this way in practice?

Picking the right level of abstraction: High enough to optimize, Low enough to be broadly useful

Vertex/edge graph	Graphs in the language of
computations	linear algebra
Unpredictable, data-driven communication patterns	Fixed communication patterns
Irregular data accesses,	Matrix block operations exploit
with poor locality	memory hierarchy
Fine grained data accesses, dominated by latency	Coarse grained parallelism, limited by bandwidth not latency

The (original) BLAS: Separation of concerns

#### The Basic Linear Algebra Subroutines had a revolutionary impact on computational linear algebra.

BLAS 1	vector ops	Lawson, Hanson, Kincaid, Krogh, 1979	LINPACK
BLAS 2	matrix-vector ops	Dongarra, Du Croz, Hammarling, Hanson, 1988	LINPACK on vector machines
BLAS 3	matrix-matrix ops	Dongarra, Du Croz, Duff, Hammarling, 1990	LAPACK on cache based machines

- Experts in mapping algorithms to hardware tuned BLAS for specific platforms.
- Experts in numerical linear algebra built software on top of the BLAS to get high performance "for free."

Today every computer, phone, etc. comes with /usr/lib/libblas



## Combinatorial BLAS (2010)

[Azad, Buluc, JG, Lugowski, ...]



An extensible distributed-memory library offering a small but powerful set of linear algebraic operations specifically targeting graph analytics.

- Aimed at graph algorithm designers/programmers who are not expert in mapping algorithms to parallel hardware.
- Flexible templated C++ interface.
- Scalable performance from laptop to 100,000-processor HPC.
- Open source software: <a href="mailto:people.eecs.berkeley.edu/~aydin/CombBLAS/html/">people.eecs.berkeley.edu/~aydin/CombBLAS/html/</a>
- Version 1.6.2 released April 2018.

A. Buluç, JG. The Combinatorial BLAS: Design, implementation, and applications. Int. J. HPC Appl. 2011.

## Launching the GraphBLAS effort

### • Manifesto, HPEC 2013:

### Standards for Graph Algorithm Primitives

Tim Mattson (Intel Corporation), David Bader (Georgia Institute of Technology), Jon Berry (Sandia National Laboratory), Aydin Buluc (Lawrence Berkeley National Laboratory), Jack Dongarra (University of Tennessee), Christos Faloutsos (Carnegie Melon University), John Feo (Pacific Northwest National Laboratory), John Gilbert (University of California at Santa Barbara), Joseph Gonzalez (University of California at Berkeley), Bruce Hendrickson (Sandia National Laboratory), Jeremy Kepner (Massachusetts Institute of Technology), Charles Leiserson (Massachusetts Institute of Technology), Andrew Lumsdaine (Indiana University), David Padua (University of Illinois at Urbana-Champaign), Stephen Poole (Oak Ridge National Laboratory), Steve Reinhardt (Cray Corporation), Mike Stonebraker (Massachusetts Institute of Technology), Steve Wallach (Convey Corporation), Andrew Yoo (Lawrence Livermore National Laboratory)

"It is our view that the state of the art in constructing a large collection of graph algorithms in terms of linear algebraic operations is mature enough to support the emergence of a standard set of primitive building blocks. This paper is a position paper defining the problem and announcing our intention to launch an open effort to define this standard."

- GraphBLAS Forum: <u>www.graphblas.org</u>
- Workshops at HPEC, IPDPS, SC
- Working group telecons and meetings



## The GraphBLAS are born

www.graphblas.org

#### • First the math, HPEC 2016:

### Mathematical Foundations of the GraphBLAS

Jeremy Kepner (MIT Lincoln Laboratory Supercomputing Center), Peter Aaltonen (Indiana University), David Bader (Georgia Institute of Technology), Aydın Buluç (Lawrence Berkeley National Laboratory), Franz Franchetti (Carnegie Mellon University), John Gilbert (University of California, Santa Barbara), Dylan Hutchison (University of Washington), Manoj Kumar (IBM), Andrew Lumsdaine (Indiana University), Henning Meyerhenke (Karlsruhe Institute of Technology), Scott McMillan (CMU Software Engineering Institute), Jose Moreira (IBM), John D. Owens (University of California, Davis), Carl Yang (University of California, Davis), Marcin Zalewski (Indiana University), Timothy Mattson (Intel)

### • Then the language bindings, GABB 2017:

### Design of the GraphBLAS API for C

Aydın Buluç<sup>†</sup>, Tim Mattson<sup>‡</sup>, Scott McMillan<sup>§</sup>, José Moreira<sup>¶</sup>, Carl Yang<sup>\*,†</sup>

<sup>†</sup>Computational Research Division, Lawrence Berkeley National Laboratory <sup>‡</sup>Intel Corporation §Software Engineering Institute, Carnegie Mellon University ¶IBM Corporation \*Electrical and Computer Engineering Department, University of California, Davis, USA



## **GraphBLAS:** Building blocks for graphs as linear algebra

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

• Operators:  $\bigoplus$ ,  $\bigotimes$  : semiring "add" and "multiply",  $\bigcirc$  : "accumulate"

• Objects: matrix, vector, monoid, semiring, ...

## Examples of semirings in graph algorithms

Real field: (R, +, ×)	Numerical linear algebra	
Boolean algebra: ({0 1}, or, and)	Connectivity & traversal	
Tropical semiring: (ℝ ∪ {∞}, min, +)	Shortest paths	
(S, select, select)	Select subgraph, or contract nodes to form quotient graph	
(ℝ, max, +)	Graph matching & network alignment	
(ℝ, max, ×)	Maximal independent set	
"values": edge/vertex attributes, "add": vertex data aggregation, "multiply": edge data processing	General schema for user-specified computation at vertices and edges	S I

## GraphBLAS C API

- #include <GraphBLAS.h>
- Example:

```
C(\neg M) \bigoplus = A^{\mathsf{T}} \bigoplus . \bigotimes B^{\mathsf{T}}
```

GrB_info GrB_mxm(GrB_Matrix	*C,
const GrB_Matrix	mask,
const GrB_BinaryOp	accum,
const GrB_Semiring	op,
const GrB_Matrix	A,
const GrB_Matrix	В
[, const GrB_Descriptor	<pre>desc]);</pre>

- Opaque objects, e.g.:
  - $GrB_Type \rightarrow Scalar type for semiring$
  - $GrB_BinaryOp \rightarrow Binary operation$
  - **GrB\_Semiring**  $\rightarrow$  Packages components of a semiring
  - **GrB\_Vector**  $\rightarrow$  1D (implicitly sparse) array

#### **GrB\_Matrix** $\rightarrow$ 2D sparse array, with row indices, column indices, and values

A. Buluç, T. Mattson, S. McMillan, J. Moreira, C. Yang. The GraphBLAS C API specification, version 1.2.0.

## Notes on the C API

- Objects are opaque
  - Only GraphBLAS methods can manipulate them
- Data (matrices and vectors) are separate from operations
  - Only explicitly defined elements of a sparse matrix or vector have values
  - The "structural zeros" are undefined; semantics are defined so that the "implicit zero" value does not matter (most of the time)
- Blocking and non-blocking modes
  - Blocking: methods must complete before returning
  - Non-blocking: methods may return early
  - Facilitates operation fusion and efficient add/delete ops
- Most operations allow a "mask" parameter
  - Specifies that only a subset of output values are required
  - Avoids computation and materialization of intermediate objects
  - Turns out to be surprisingly useful











## **BFS in GraphBLAS with masks**

```
1 Input: graph, frontier, levels

2 depth \leftarrow 0
```

```
3 while nvals(frontier) > 0:
```

```
4 depth \leftarrow depth + 1
```

```
5 levels[frontier] ← depth
```

```
6 frontier<\neglevels,replace> \leftarrow graph<sup>T</sup> \oplus.\otimes frontier
```

```
where \oplus . \otimes = \bigoplus . \otimes (\text{LogicalSemiring})
```

(a) Pseudocode

## **BFS in GraphBLAS with masks: C code**

```
GrB_Info bfs
                           // BFS of a graph (using vector assign & reduce)
(
    GrB_Vector *v_output, // v [i] is the BFS level of node i in the graph
    const GrB_Matrix A, // input graph, treated as if boolean in semiring
                   // starting node of the BFS
    GrB_Index s
)
{
   GrB Index n :
                                       // # of nodes in the graph
   GrB_Vector q = NULL;
                                       // nodes visited at each level
   GrB_Vector v = NULL;
                                       // result vector
                                      // Descriptor for vxm
   GrB_Descriptor desc = NULL ;
   GrB_Matrix_nrows (&n, A) ;
                                     // n = # of rows of A
   GrB_Vector_new (&v, GrB_INT32, n) ; // Vector<int32_t> v(n) = 0
   GrB_Vector_new (&q, GrB_BOOL, n) ; // Vector<bool> q(n) = false
   GrB_Vector_setElement (q, true, s) ; // q[s] = true, false elsewhere
   GrB_Descriptor_new (&desc) ;
    GrB_Descriptor_set (desc, GrB_MASK, GrB_SCMP) ; // invert the mask
    GrB_Descriptor_set (desc, GrB_OUTP, GrB_REPLACE) ; // clear q first
   bool successor = true ; // true when some successor found
   for (int32_t level = 1 ; successor && level <= n ; level++)</pre>
    {
       // v<q> = level, using vector assign with q as the mask
       GrB_assign (v, q, NULL, level, GrB_ALL, n, NULL);
       // q <!v > = q ||.& A ; finds all the unvisited
       // successors from current q, using !v as the mask
       GrB_vxm (q, v, NULL, GrB_LOR_LAND_BOOL, q, A, desc) ;
       // successor = ||(q)
       GrB_reduce (&successor, NULL, GrB_LOR_BOOL_MONOID, q, NULL) ;
    }
                    // return result
   *v_output = v;
                                                                      T. Davis. Algorithm 9xx:
   GrB_free (&q) ;
                                                                      SuiteSparse:GraphBLAS. ACM
   GrB_free (&desc) ;
                                                                      Trans. Math. Software, to appear.
    return (GrB_SUCCESS) ;
```

## **BFS in GraphBLAS with masks: Python & C++**

```
1 def bfs(graph, frontier, levels):
2 depth = 0
3 while frontier.nvals > 0:
4 depth += 1
5 levels[frontier][:] = depth
6 with gb.LogicalSemiring, gb.Replace:
```

```
frontier[~levels] = graph.T @ frontier
```

(b) PyGB



T. Mattson, T. Davis, M. Kumar, A. Buluc, S. McMillan, J. Moreira, C. Yang. LAGraph: A community effort to collect graph algorithms built on top of the GraphBLAS. *IPDPS 2019.* 

# SuiteSparse:GraphBLAS

- From Tim Davis (Texas A&M)
- First conforming implementation of C API
- Features:



- 960 semirings built in; also user-defined semirings
- Fast incremental updates using non-blocking mode and "zombies"
- Several sparse data structures & polyalgorithms under the hood
- Currently single-threaded
  - OpenMP near release, CUDA planned, MPI contemplated
- Performance on graph benchmarks (e.g. triangles, k-truss) comparable to highly-tuned custom C code
- Included in Debian and Ubuntu Linux distributions
- Used as computational engine in commercial RedisGraph product

T. Davis. Algorithm 9xx: SuiteSparse:GraphBLAS. ACM Trans. Math. Software, to appear.

## **Other GraphBLAS implementations**

#### • IBM GraphBLAS (IBM)

- Second fully conforming release of the GraphBLAS C API
- Descendant of IBM Graph Programming Interface
- GraphBLAS Template Library (SEI/CMU, PNNL, Indiana U)
  - C++ implementation of GraphBLAS math spec
  - With a C interface conforming to the GraphBLAS C API
- GraphBLAST (UC Davis)
  - GraphBLAS for GPU's, from the Gunrock graph library group
- PyGB (UW, PNNL, SEI/CMU)
  - Python DSL using the C++ GraphBLAS Template Library

### Friends of GraphBLAS: Linear-algebra-based graph libraries

- Combinatorial BLAS (LBNL, UCSB): C++ with MPI and OpenMP
- Graphulo (MIT): Java/Accumulo
- D4M (MIT): Matlab/Octave
- Graph Programming Interface (IBM): C
- GraphPad (Intel): C++, OpenMP, MPI

# Industrial impact: RedisGraph graph database

- From Redis Labs, enterprise / cloud database vendor.
- Emphasis on:
  - Query speed for large graphs
  - Mass insertion efficiency
  - Scaling Redis beyond singlenode memory
- SuiteSparse:GraphBLAS under the hood.
- Benchmarks: Query time dramatically better than competing graph databases.





P. Cailliau, T. Davis, V. Gadepally, J. Kepner, R. Lipman, J. Lovitz, K. Ouaknine. RedisGraph GraphBLAS enabled database. *GrAPL 2019.* 

### Machine Learning relies a lot on Linear Algebra too





Graph/Sparse/Dense BLAS functions (increasing arithmetic intensity)

## Sparse deep neural networks with GraphBLAS

### • From MIT-LL & IBM:

- DNN inference oscillates between two semirings: (+, ×) and (max, +)
- Sparsity is at the frontier of DNN research
- MIT/IEEE/Amazon
   Graph Challenge:
   Enable Large Sparse
   Deep Neural Networks
- Entries not limited to GraphBLAS solutions!
- Details at graphchallenge.org



# $\mathbf{Y}_{l+1} = \mathbf{h}(\mathbf{Y}_l \mathbf{W}_l + \mathbf{b}_l)$

Kepner, Kumar, Moreira, Pattnaik, Serrano, Tufo. Enabling massive deep neural networks with the GraphBLAS, *HPEC 2017*.

### Markov clustering algorithm

Popular and successful algorithm for discovering clusters in protein interaction and protein similarity networks



### At each iteration:

- **Step 1** (Expansion): Square the matrix
- **Step 2** (Pruning): Remove small entries and dense columns
- **Step 3** (Inflation): Take powers entry-wise

**Naïve implementation:** sparse matrix-matrix product (SpGEMM), followed by column-wise top-k selection and column-wise pruning

### **HipMCL: High-performance Markov clustering**

- MCL is both **computationally expensive** and **memory hungry**, limiting the sizes of networks that can be clustered.
- HipMCL overcomes these limitations via sparse parallel algorithms, with a combined expansion and pruning step.
- Up to 1000X times faster than original MCL with same accuracy.



A. Azad, G. Pavlopoulos, C. Ouzounis, N. Kyrpides, A. Buluç. HipMCL: A high-performance parallel implementation of the Markov clustering algorithm for large-scale networks. *Nucleic Acids Research, 2018* 

### LACC: Parallel Connected Components

#### **Scientific Achievement**

- LACC: Linear-Algebraic Connected Components
- New distributed-memory parallel connected component discovery algorithm using GraphBLAS primitives

#### Significance and Impact

- Finding connected components is a fundamental primitive for computing on graphs.
- More than 2x faster connected component identification across different scales.
- Orders of magnitude faster at large concurrencies.

#### **Research Details**

- Based on Awerbuch-Shiloach PRAM algorithm
- Used with the Exascale Application HipMCL
- Proper sparsity exploitation is the key to high performance



A. Azad and A. Buluc. LACC: A Linear-Algebraic Algorithm for Finding Connected Components in Distributed Memory. IPDPS, 2019





## Linear-algebra-based Kokkos graph infrastructure



- From Sandia Labs & Georgia Tech
- Sparse matrix-matrix multiplication (SpGEMM) kernel in Kokkos Kernels shared memory library
- Performance portable across architectures and parallel language infrastructures
- Benchmark: Counting triangles / clustering coefficient
- 2-time champion (2017, 2018) of IEEE HPEC Graph Challenge

A. Yasary, S.Rajamanickam, M. Wolf, J. Berry, U. Catalyurek. Fast triangle counting using Cilk. *IEEE HPEC, 2018*.

### Push-pull, or direction optimization in search [C. Yang PhD thesis, UC Davis]

Top-down BFS is worst-case optimal, but *pessimistic* for low-diameter graphs because when the frontier is at its peak, almost all edge examinations fail to claim a child.



for all *v* in frontier attempt to parent **all** neighbors(*v*)

#### Bottom-Up (Pull)



for all *v* in unvisited find *any* parent (neighbor(*v*) in frontier)



### **Beamer's direction-optimizing BFS**

- Switch from top-down/push to bottom-up/pull
- When the majority of the vertices have been reached.
- For 5+ years, thought to be impossible (efficiently) in the language of linear algebra

### Efficient push-pull in GraphBLAS [C. Yang PhD thesis, UC Davis]

- Push vs. pull corresponds to matvec multiplication by columns vs. rows.
- Row matvec is better for dense vector, column is better for sparse.
- Key insight: *Masking* changes the complexity!
- Three key optimizations:
  - Choose push or pull
  - Efficient use of masking •
  - Early exit from  $(\Lambda, \vee)$ • vector dot product



early-exit) cannot early-exit Performance (GTEPS) Speed-up Optimization Baseline 0.874 Structure only 1.411  $1.62 \times$ Change of direction 1.527  $1.08 \times$ Masking 3.932  $2.58\times$ Early exit 15.83  $4.02 \times$ Operand reuse 42.44  $2.68 \times$ 

=

Impact: Up to 100 MTEPS on 1 Xeon 4-core CPU plus 1 Tesla GPU.

C. Yang, A. Buluc, J. Owens. Implementing push-pull efficiently in GraphBLAS. ICPP 2018

### Matrix-based graph processor design at MIT-LL [Song, Kepner, et al. 2010]

#### **3-D Graph Processor**

William S. Song, Jeremy Kepner, Huy T. Nguyen, Joshua I. Kramer, Vitaliy Gleyzer, James R. Mann, Albert H. Horst, Larry L. Retherford, Robert A. Bond, Nadya T. Bliss, Eric I. Robinson, Sanjeev Mohindra, Julie Mullen Lincoln Laboratory, Massachusetts Institute Technology, Lexington, MA 02420



Figure 1: Computational Throughput Differences between Conventional and Graph Processing.



## **International impact of GraphBLAS**

- KAUST, Saudi Arabia [Jamour et al., EuroSys 2019] :
  - Matrix algebra for RDF triple stores
  - Demonstrated scaling to 512B triples on 2048 nodes
- CMU-Qatar / Qatar U [Ahmad et al., VLDB 2018] :
  - Automatic translation of vertex-edge programs to matrix ops
  - Demonstrated high performance on clouds and clusters
- Budapest U [Szarnyas, FOSDEM 2019] :
  - Multiplex graph metrics with GraphBLAS and other matrix libs
  - Interesting connections to complexity theory for database joins
- Huawei :
  - GraphBLAS in the cloud and on the mobile phone

# What's next for the GraphBLAS?

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

 $Tim \; Mattson^{\ddagger}, \; Timothy \; A. \; Davis^{\diamond}, \; Manoj \; Kumar^{\P}, \; Aydın \; Buluç^{\dagger}, \; Scott \; McMillan^{\$}, \; José \; Moreira^{\P}, \; Carl \; Yang^{*,\dagger}$ 

https://github.com/GraphBLAS/LAGraph

[GrAPL 2019]

# Motivation: Separation of Concerns



# **Algorithms in LAGraph today**

File Name	Algorithm
LACC_GraphBLAS	Connected components
LAGraph_BF_basic	Bellman-Ford single source shortest paths
LAGraph_BF_full	Bellman-Ford single source shortest paths, with tree
LAGraph_allktruss	All k-trusses of a graph
LAGraph_bfs_pushpull	Direction optimizing breadth-first search
LAGraph_bfs_simple	Conventional breadth-first search
LAGraph_dnn.c	Sparse deep neural network
LAGraph_ktruss	k-truss of a graph
LAGraph_lcc	Local clustering coefficient
LAGraph_pagerank	PageRank
LAGraph_tricount	Count triangles in a graph

LAGraph is open source, and solicits:

- More algorithms and implementations
- Use cases and requests for algorithms!

## Directions & challenges: LAGraph

- Additional practical use cases and uptake!
- Add algorithms with known linear algebraic formulations
   Centrality, clustering, subgraph counting, ...
- Investigate important graph algorithms that haven't yet been implemented in linear algebraic form

   A\* search, branch & bound, supervised learning, ...
- Integration with numerical linear algebra libraries
  - Spectral methods, Laplacian paradigm for graph algorithms, linear equation solvers, optimization
- Statistical perspective: distributions, stochastic graphs, ...
- Moving data in and out of opaque GraphBLAS objects
  - Data science workflows are often not opaque data: pandas frames, numpy arrays, CSR matrices



## **Directions & challenges: GraphBLAS**

- Moving data in and out of GraphBLAS
  - Probably want import/export functions within GraphBLAS (SuiteSparse has prototypes of this)
  - Also want finer-grained operations, e.g. iterators over edges, adjacencies, etc.
- Exploit and extend nonblocking mode for method fusion, matrix triple product optimization, etc.
- Robust multithreading support

   Current spec hides threads inside individual GraphBlas methods
- Robust support for distributed memory
   MPI, PGAS, other models?
- Finalizing more API specs
  - Extensions to C API spec for iterators, distributed execution, ...
  - In progress: Language bindings for Python, C++, ...



Ariful Azad, David Bader, Jon Berry, Aydin Buluc, Tim Davis, Kevin Deweese, Joe Eaton, Jeremy Kepner, Manoj Kumar, Adam Lugowski, Andrew Lumsdaine, Tim Mattson, Scott McMillan, Henning Meyerhenke, Jose Moreira, Veronika Neeley, John Owens, Steve Reinhardt, Viral Shah, Bill Song, Michael Wolf, Carl Yang



... and Intel, Microsoft, NSF, DOE Office of Science