UCSB

Graphs in the Language of Linear Algebra: Applications, Software, and Challenges

John R. Gilbert
University of California, Santa Barbara

Graph Algorithm Building Blocks
May 19, 2014

Support: Intel, Microsoft, DOE Office of Science, NSF

Thanks …

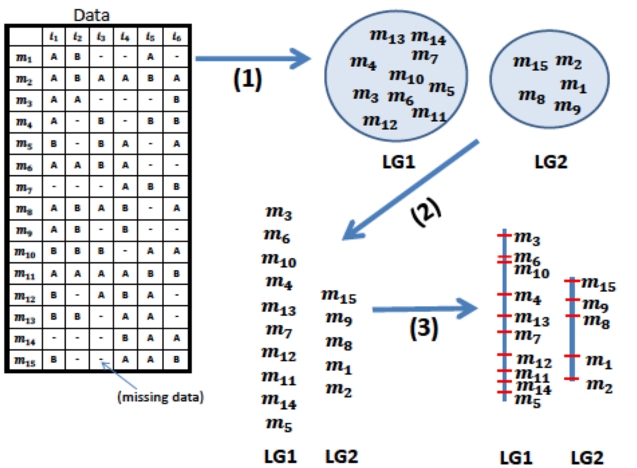
Lucas Bang (UCSB), Jon Berry (Sandia), Eric Boman (Sandia), Aydin Buluc (LBL), John Conroy (CCS), Kevin Deweese (UCSB), Erika Duriakova (Dublin), Armando Fox (UCB), Shoaib Kamil (MIT), Jeremy Kepner (MIT), Tristan Konolige (UCSB), Adam Lugowski (UCSB), Tim Mattson (Intel), Brad McRae (TNC), Dave Mizell (YarcData), Lenny Oliker (LBL), Carey Priebe (JHU), Steve Reinhardt (YarcData), Lijie Ren (Google), Eric Robinson (Lincoln), Viral Shah (UIDAI), Veronika Strnadova (UCSB), Yun Teng (UCSB), Joshua Vogelstein (Duke), Drew Waranis (UCSB), Sam Williams (LBL)

Outline

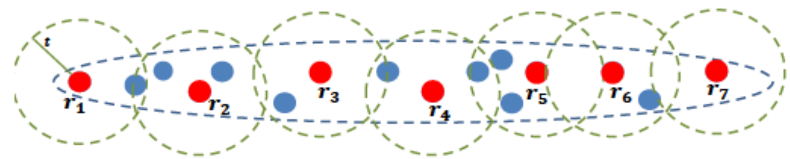
- A few sample applications
- Sparse matrices for graph algorithms
- Software: CombBLAS, KDT, QuadMat
- Challenges, issues, and questions

Large-scale genomic mapping and sequencing

[Strnadova, Buluc, Chapman, G, Gonzalez, Jegelska, Rokhsar, Oliker 2014]



(a) Linear Marker Structure



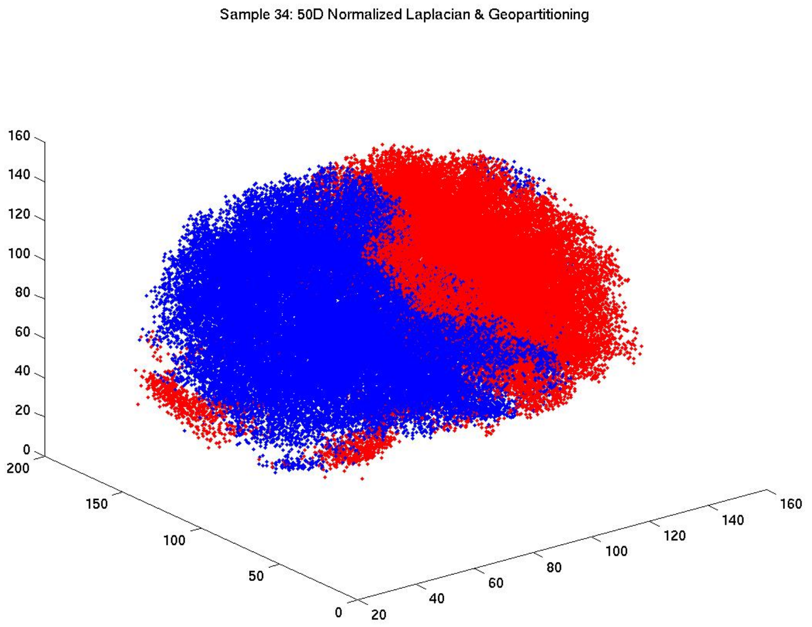
(b) Representative Points

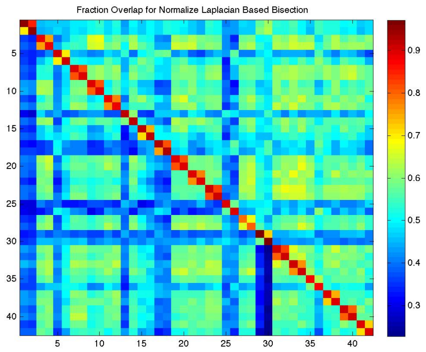
- Problem: scale to millions of markers times thousands of individuals, with “unknown” rates > 50%
- Tools used or desired: spanning trees, approximate TSP, incremental connected components, spectral and custom clustering, k-nearest neighbors
- Results: using more data gives better genomic maps

UCSB

Alignment and matching of brain scans

[Conroy, G, Kratzer, Lyzinski, Priebe, Vogelstein 2014]



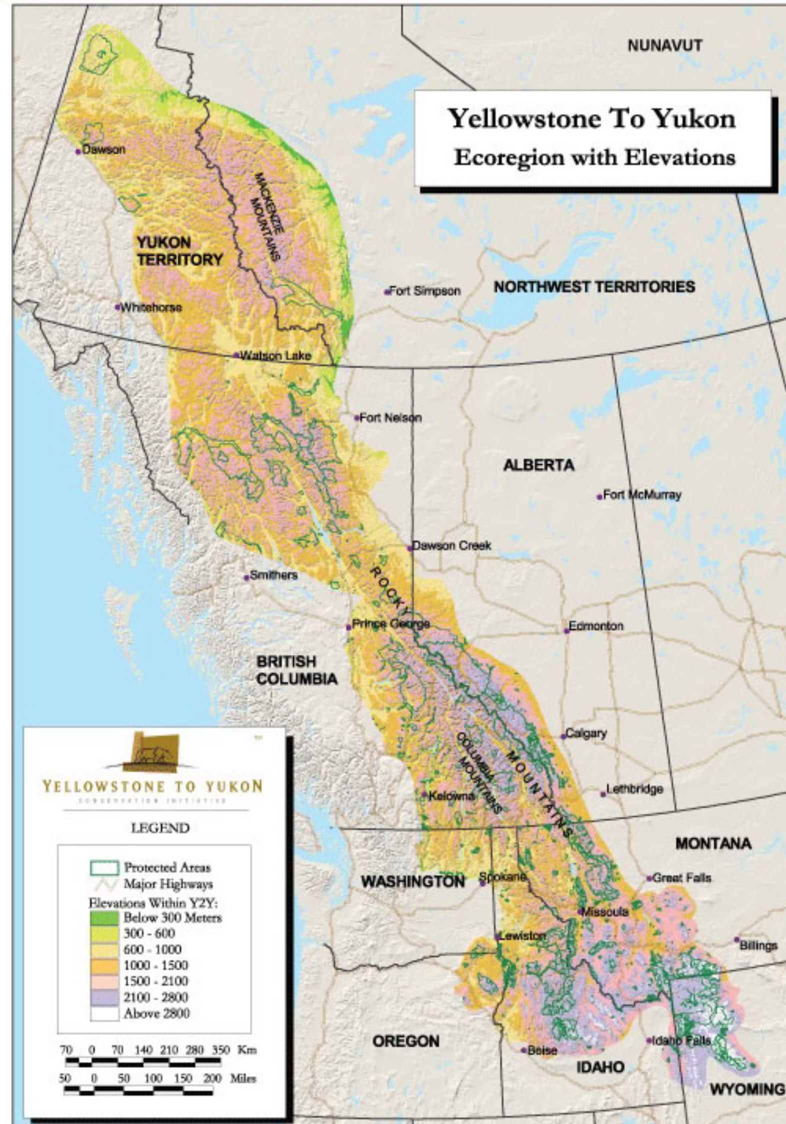


– Problem: match functional regions across individuals
– Tools: Laplacian eigenvectors, geometric spectral partitioning, clustering, and more. . .

Landscape connectivity modeling

[McRae et al.]

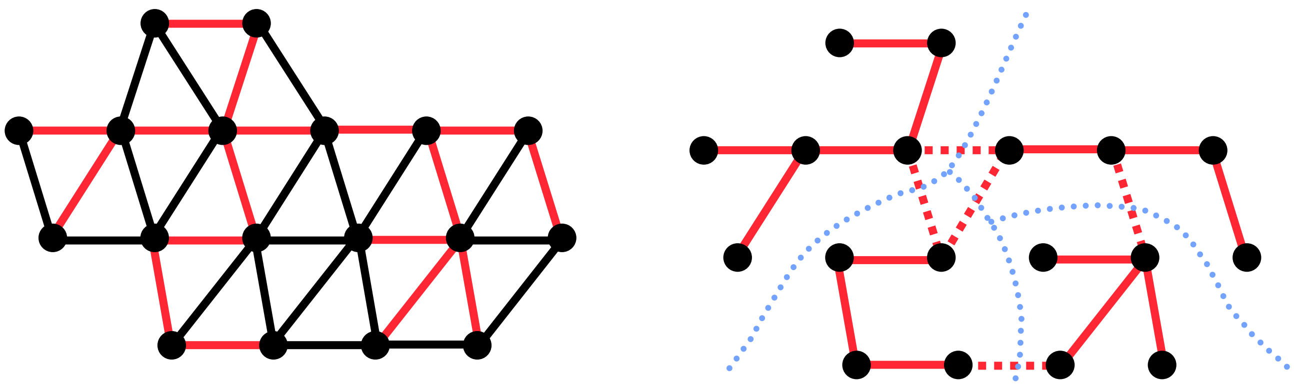
- Habitat quality, gene flow, corridor identification, conservation planning
- Targeting larger problems: Yellowstone-to-Yukon corridor
- Tools: Graph contraction, connected components, Laplacian linear systems



Figures courtesy of Brad McRae, NCEAS

Combinatorial acceleration of Laplacian solvers

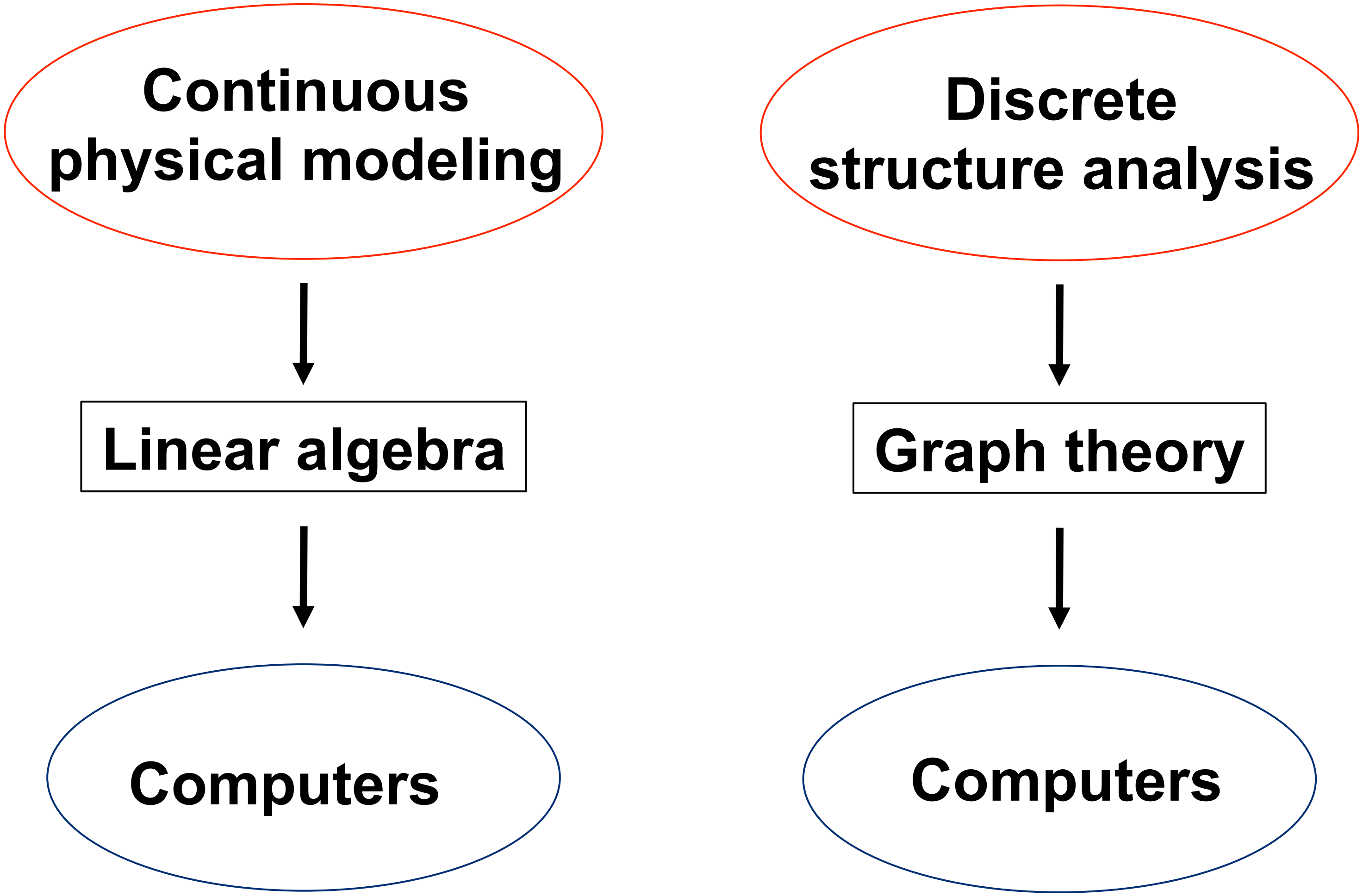
[Boman, Deweese, G 2014]



$$(B^{-1/2} A B^{-1/2}) (B^{1/2} x) = B^{-1/2} b$$

- Problem: approximate target graph by sparse subgraph
- $Ax = b$ in nearly linear time in theory [ST08, KMP10, KOSZ13]
- Tools: spanning trees, subgraph extraction and contraction, breadth-first search, shortest paths, . . .

The middleware challenge for graph analysis



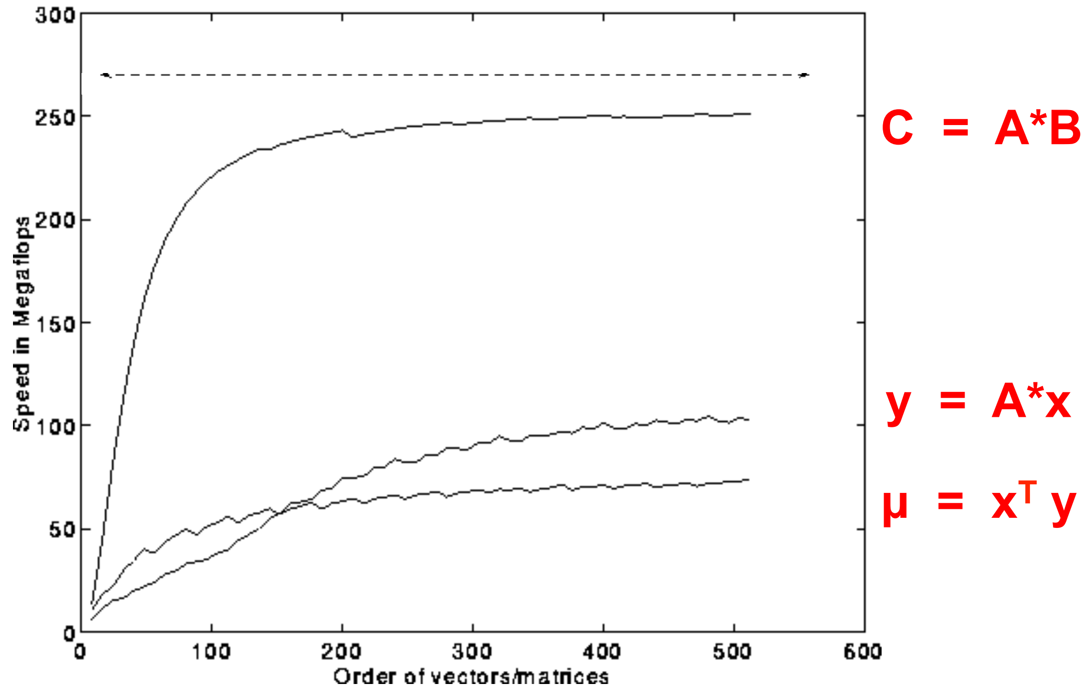
UCSB

The middleware challenge for graph analysis

- By analogy to numerical scientific computing. . .

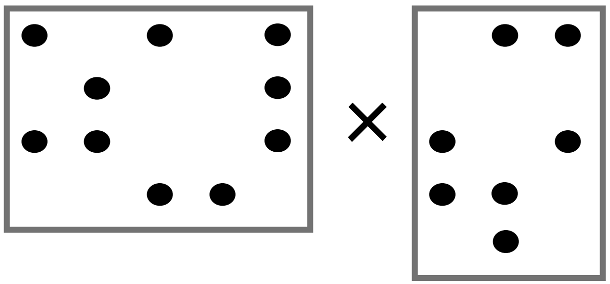
- What should the combinatorial BLAS look like?

Basic Linear Algebra Subroutines (BLAS): Ops/Sec vs. Matrix Size

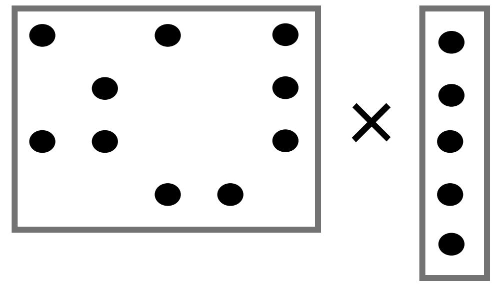


Sparse array primitives for graph manipulation

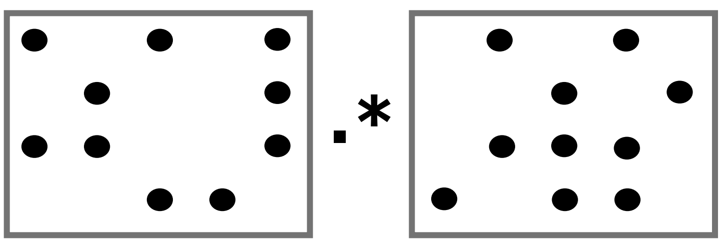
Sparse matrix-matrix multiplication (SpGEMM)



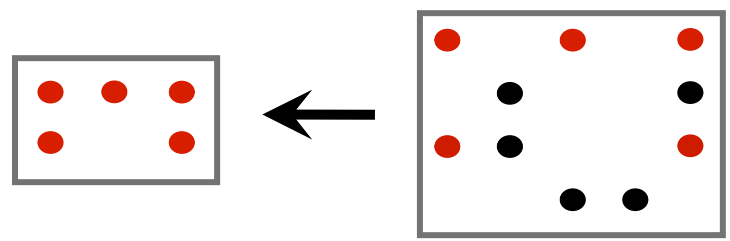
Sparse matrix-dense vector multiplication



Element-wise operations



Sparse matrix indexing



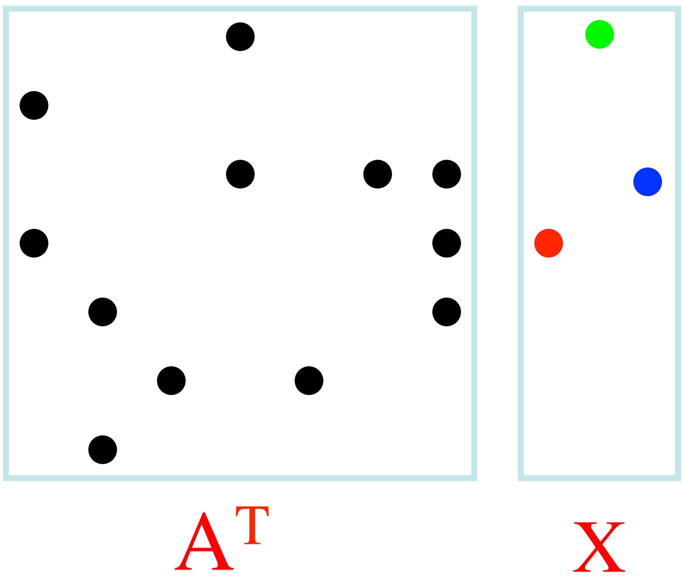
Matrices over various semirings: (+ . x), (min . +), (or . and), …

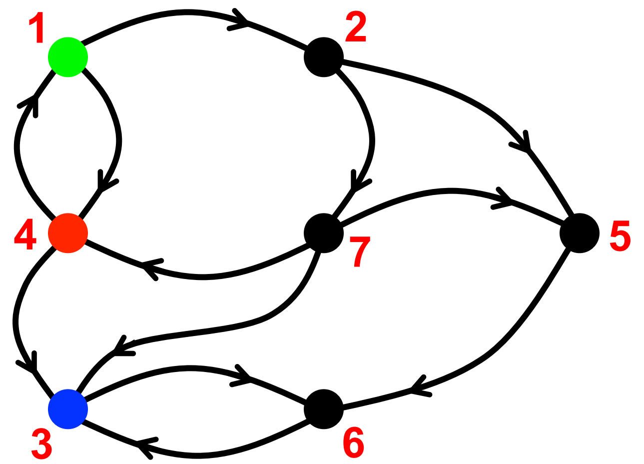
Examples of semirings in graph algorithms

Real field: (R, +, x)	Classical numerical linear algebra
Boolean algebra: ({0 1}, |, &)	Graph traversal
Tropical semiring: (R U {∞}, min, +)	Shortest paths
(S, select, select)	Select subgraph, or contract nodes to form quotient graph
(edge/vertex attributes, vertex data aggregation, edge data processing)	Schema for user-specified computation at vertices and edges

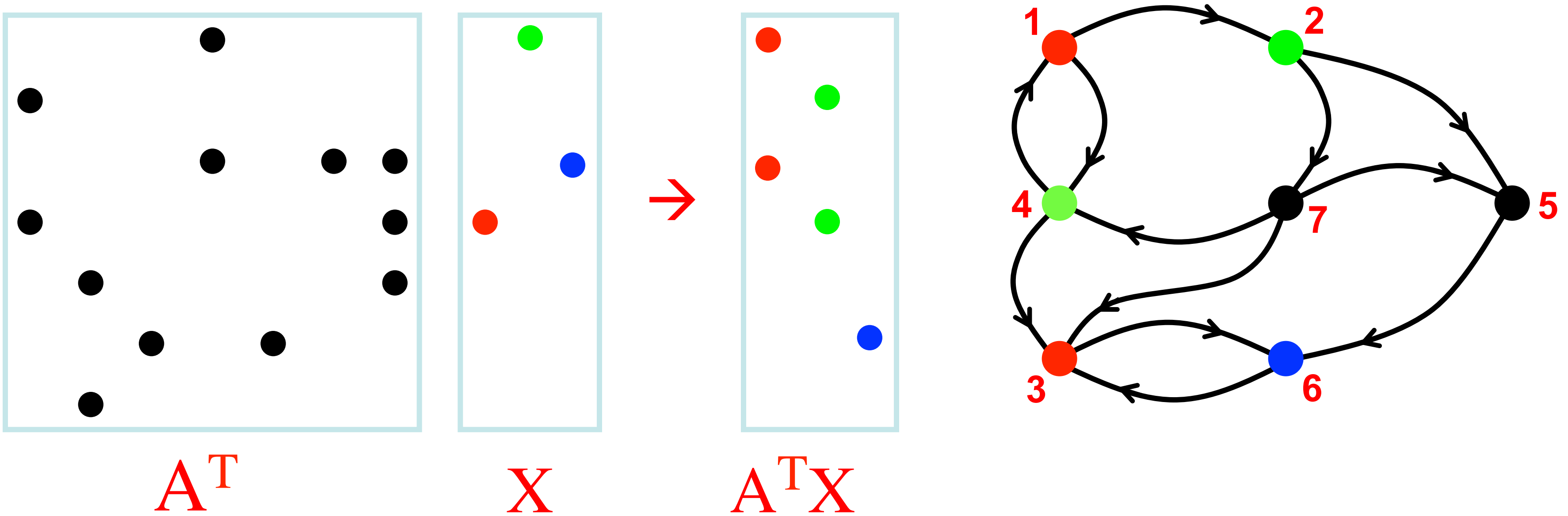
UCSB

Multiple-source breadth-first search



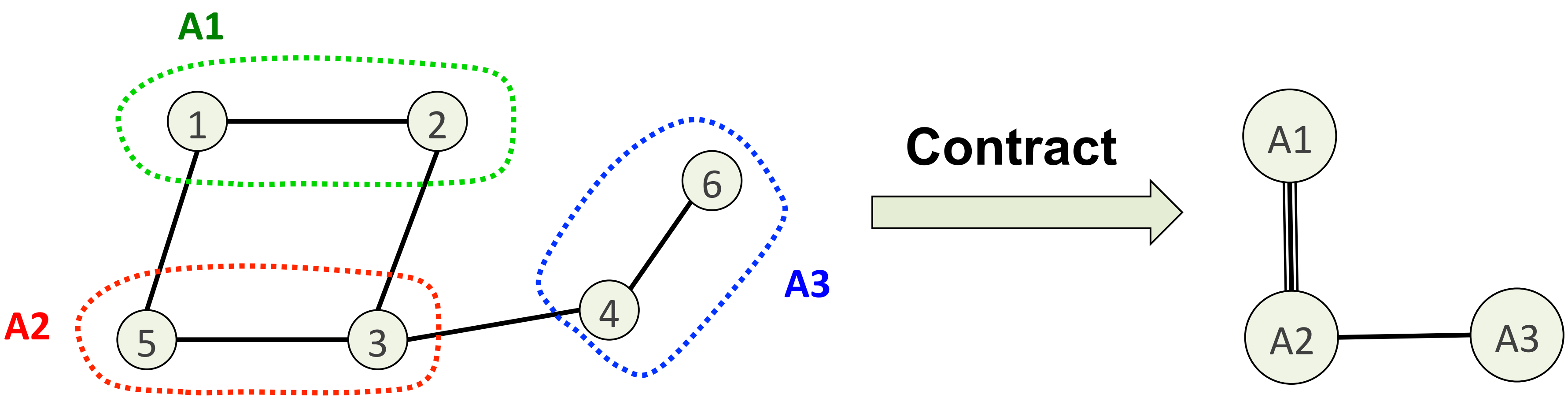


Multiple-source breadth-first search



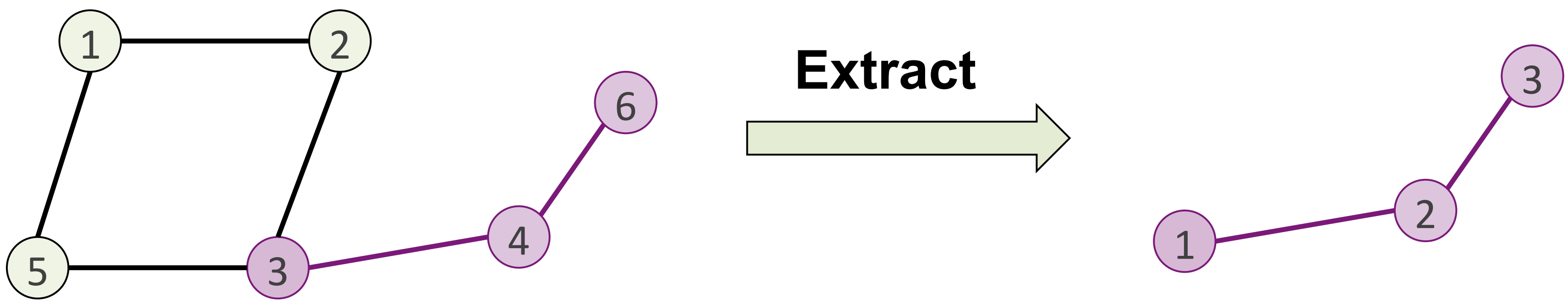
- Sparse array representation => space efficient
- Sparse matrix-matrix multiplication => work efficient
- Three possible levels of parallelism: searches, vertices, edges

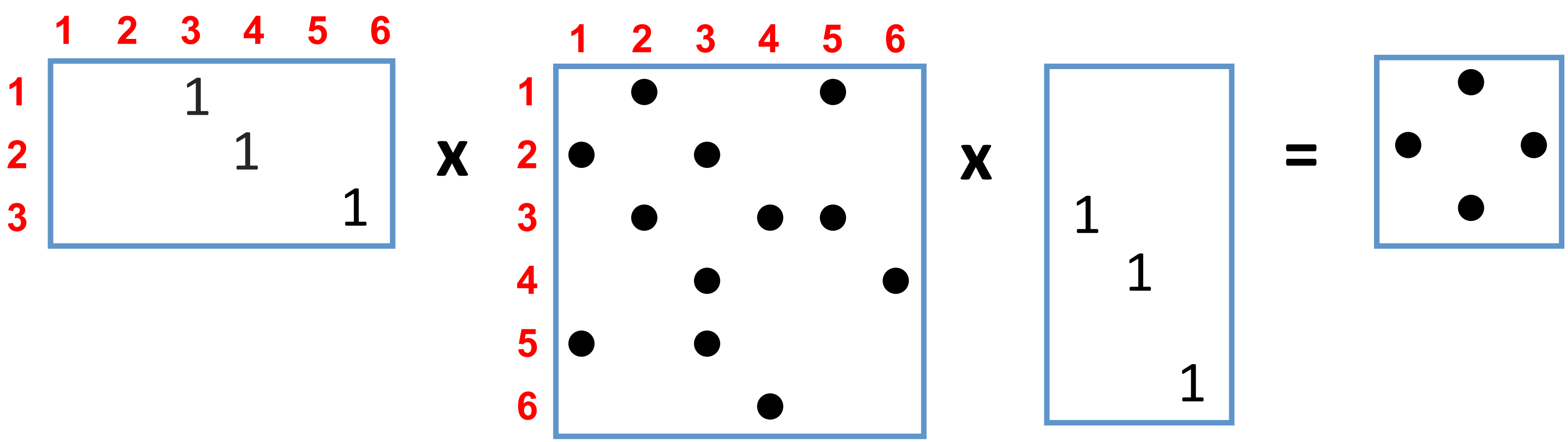
Graph contraction via sparse triple product



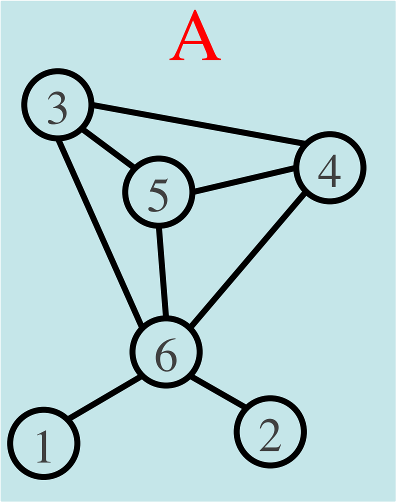
$$
\begin{array}{c|cccccc}
 & 1 & 2 & 3 & 4 & 5 & 6 \\
\hline
1 & 1 & 1 & & & & \\
2 & & & 1 & & 1 & \\
3 & & & & 1 & & 1
\end{array}
\quad \times \quad
\begin{array}{c|cccccc}
 & 1 & 2 & 3 & 4 & 5 & 6 \\
\hline
1 & & \bullet & & & \bullet & \\
2 & \bullet & & \bullet & & & \\
3 & & \bullet & & \bullet & \bullet & \\
4 & & & \bullet & & & \bullet \\
5 & \bullet & & \bullet & & & \\
6 & & & & \bullet & &
\end{array}
\quad \times \quad
\begin{bmatrix}
1 & & \\
1 & & \\
 & 1 & \\
 & & 1 \\
 & 1 & \\
 & & 1
\end{bmatrix}
\quad = \quad
\begin{bmatrix}
 & \bullet & \\
\bullet & & \bullet \\
 & \bullet &
\end{bmatrix}
$$

Subgraph extraction via sparse triple product





Counting triangles (clustering coefficient)

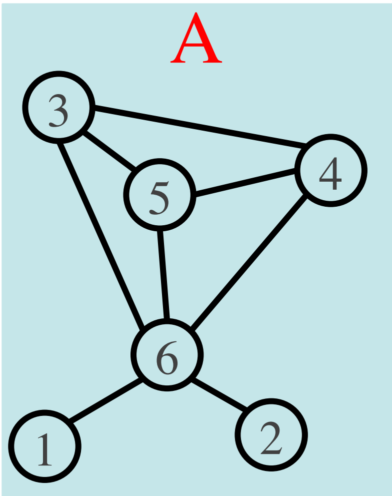


Clustering coefficient:

- 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

UCSB

Counting triangles (clustering coefficient)

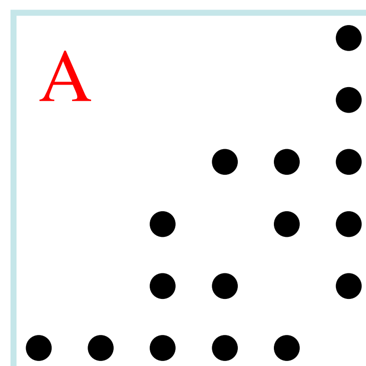


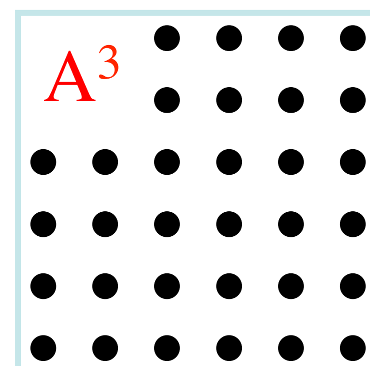
Clustering coefficient:

- 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

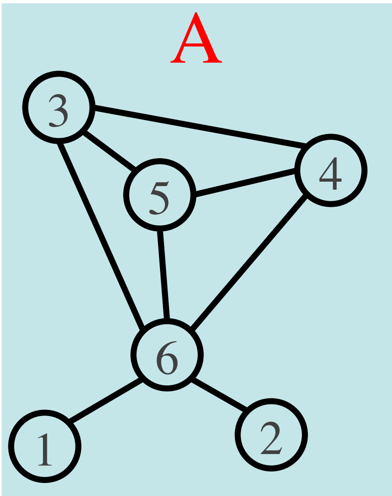
Inefficient way to count triangles with matrices:

- A = adjacency matrix
- # triangles = trace(A^3) / 6
- but A^3 is likely to be pretty dense





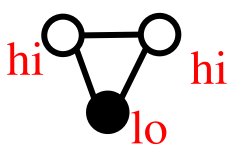
Counting triangles (clustering coefficient)



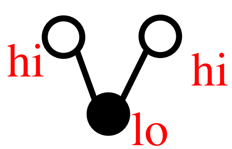
Clustering coefficient:

- 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

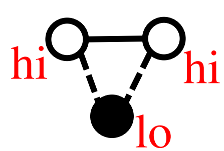
Cohen's algorithm to count triangles:



- Count triangles by lowest-degree vertex.

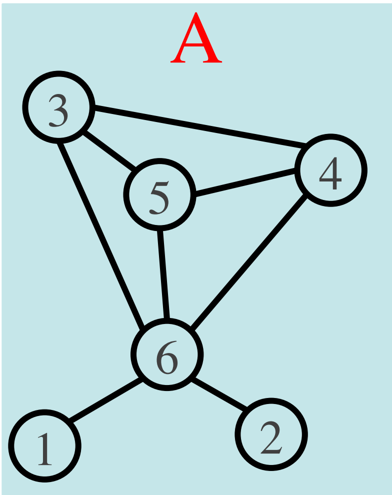


- Enumerate "low-hinged" wedges.



- Keep wedges that close.

Counting triangles (clustering coefficient)

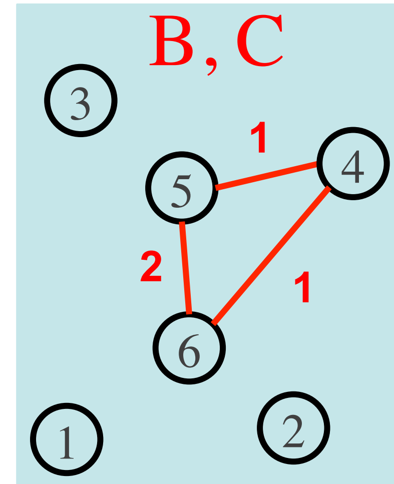


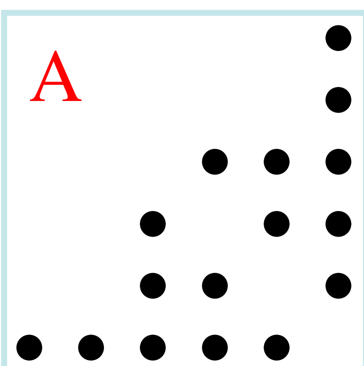
$A = L + U$ (hi->lo + lo->hi)

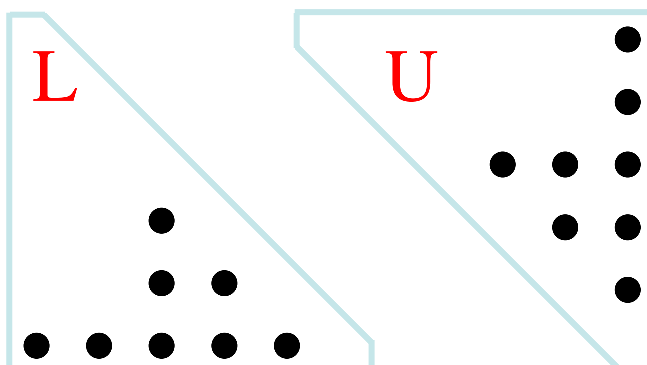
$L \times U = B$ (wedge, low hinge)

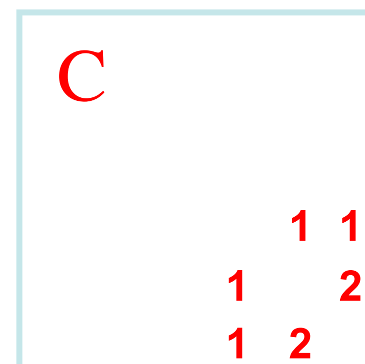
$A \wedge B = C$ (closed wedge)

sum(C)/2 = **4 triangles**









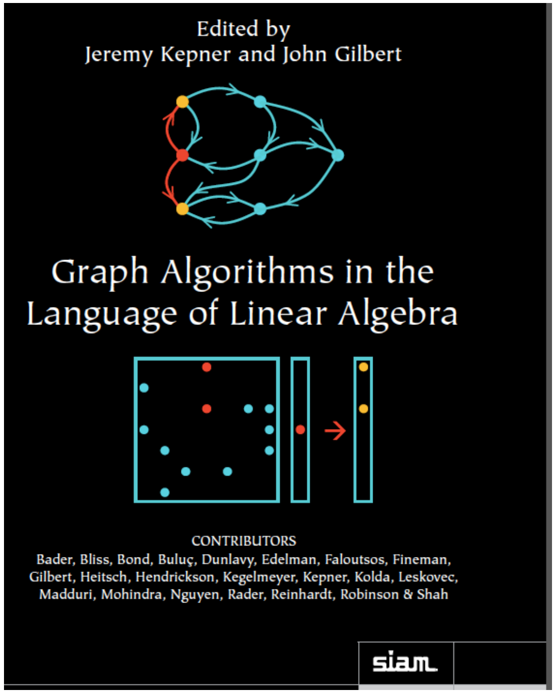
A few other graph algorithms we've implemented in linear algebraic style

- Maximal independent set (KDT/SEJITS) [BDFGKLOW 2013]
- Peer-pressure clustering (SPARQL) [DGLMR 2013]
- Time-dependent shortest paths (CombBLAS) [Ren 2012]
- Gaussian belief propagation (KDT) [LABGRTW 2011]
- Markoff clustering (CombBLAS, KDT) [BG 2011, LABGRTW 2011]
- Betweenness centrality (CombBLAS) [BG 2011]
- Hybrid BFS/bully connected components (CombBLAS) [Konolige, in progress]
- Geometric mesh partitioning (Matlab ☺) [GMT 1998]

UCSB

Graph algorithms in the language of linear algebra

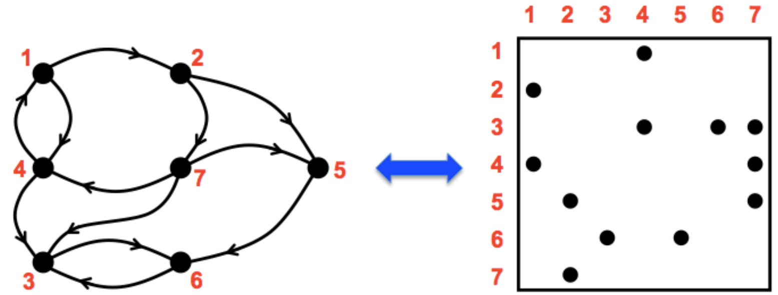
- Kepner et al. study [2006]: fundamental graph algorithms including min spanning tree, shortest paths, independent set, max flow, clustering, …
- SSCA#2 / centrality [2008]
- Basic breadth-first search / Graph500 [2010]
- Beamer et al. [2013] direction-optimizing breadth-first search, implemented in CombBLAS



UCSB

Combinatorial BLAS

http://gauss.cs.ucsb.edu/~aydin/CombBLAS



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

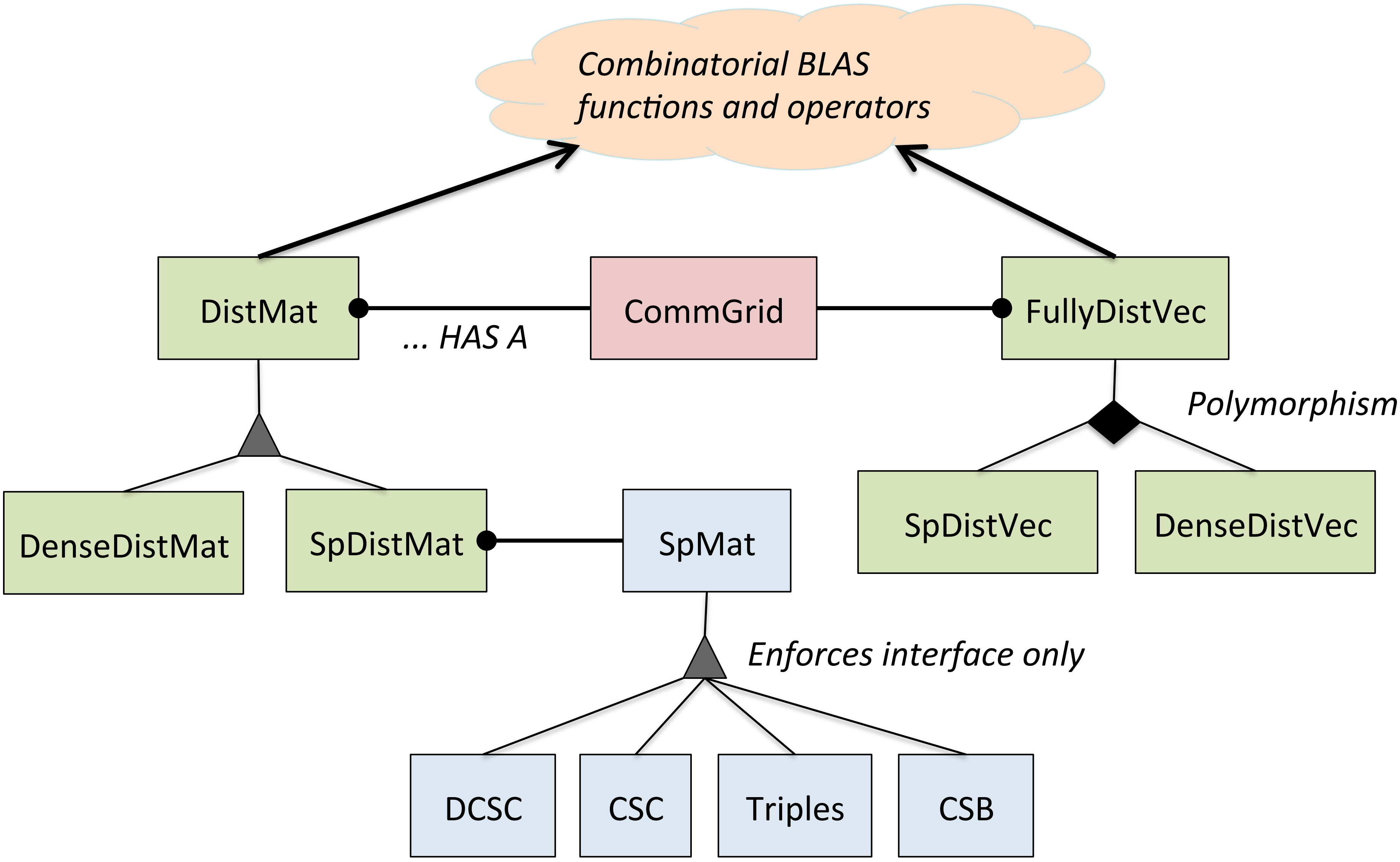
- Aimed at graph algorithm designers/programmers who are not expert in mapping algorithms to parallel hardware.
- Flexible templated C++ interface.
- Scalable performance from laptop to 100,000-processor HPC.

- Open source software.
- Version 1.4.0 released January 16, 2014.

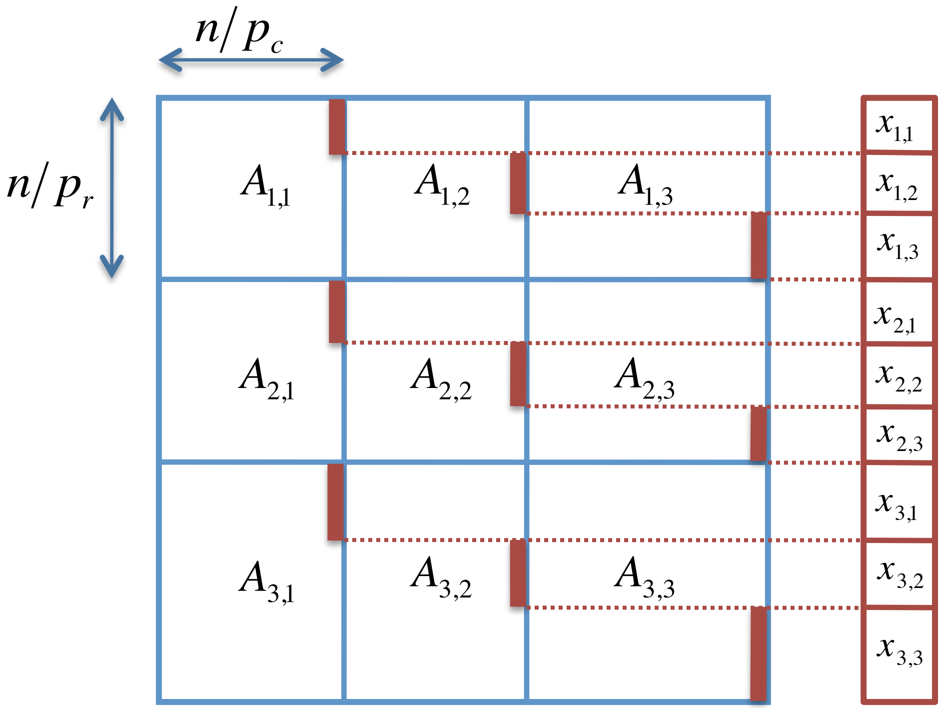
Some Combinatorial BLAS functions

Function	Parameters	Returns	Math Notation
SpGEMM	- sparse matrices **A** and **B** - unary functors (op)	sparse matrix	**C** = op(**A**) * op(**B**)
SpM{Sp}V **(Sp: sparse)**	- sparse matrix **A** - sparse/dense vector **x**	sparse/dense vector	**y** = **A** * **x**
SpEWiseX	- sparse matrices or vectors - binary functor and predicate	in place or sparse matrix/vector	**C** = **A** .* **B**
Reduce	- sparse matrix **A** and functors	dense vector	**y** = sum(**A**, op)
SpRef	- sparse matrix **A** - index vectors **p** and **q**	sparse matrix	**B** = **A**(**p**,**q**)
SpAsgn	- sparse matrices **A** and **B** - index vectors **p** and **q**	none	**A**(**p**,**q**) = **B**
Scale	- sparse matrix **A** - dense matrix or vector **X**	none	check manual
Apply	- any matrix or vector **X** - unary functor (op)	none	op(**X**)

Combinatorial BLAS: Distributed-memory reference implementation



2D layout for sparse matrices & vectors



Matrix/vector distributions, interleaved on each other.

Default distribution in **Combinatorial BLAS**.

Scalable with increasing number of processes

- 2D matrix layout wins over 1D with large core counts and with limited bandwidth/compute
- 2D vector layout sometimes important for load balance

Combinatorial BLAS "users" (Sep 2013)

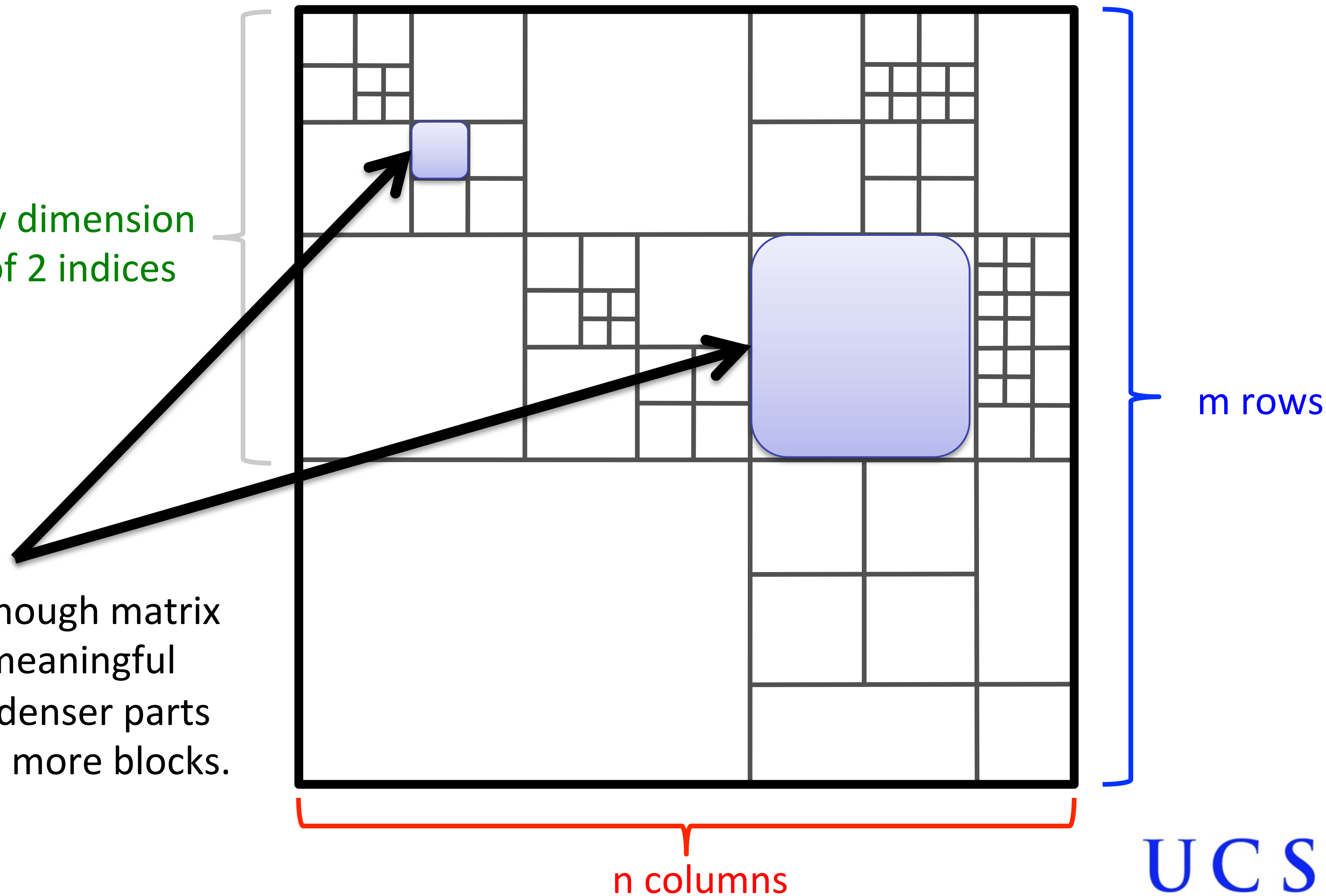
- IBM (T.J. Watson, Zurich, & Tokyo)
- Microsoft
- Intel
- Cray
- Stanford
- UC Berkeley
- Carnegie-Mellon
- Georgia Tech
- Ohio State
- Columbia
- U Minnesota
- King Fahd U
- Tokyo Inst of Technology
- Chinese Academy of Sciences
- U Ghent (Belgium)
- Bilkent U (Turkey)
- U Canterbury (New Zealand)
- Purdue
- Indiana U
- Mississippi State
- UC Merced

UCSB

QuadMat shared-memory data structure

[Lugowski, G]

subdivide by dimension on power of 2 indices



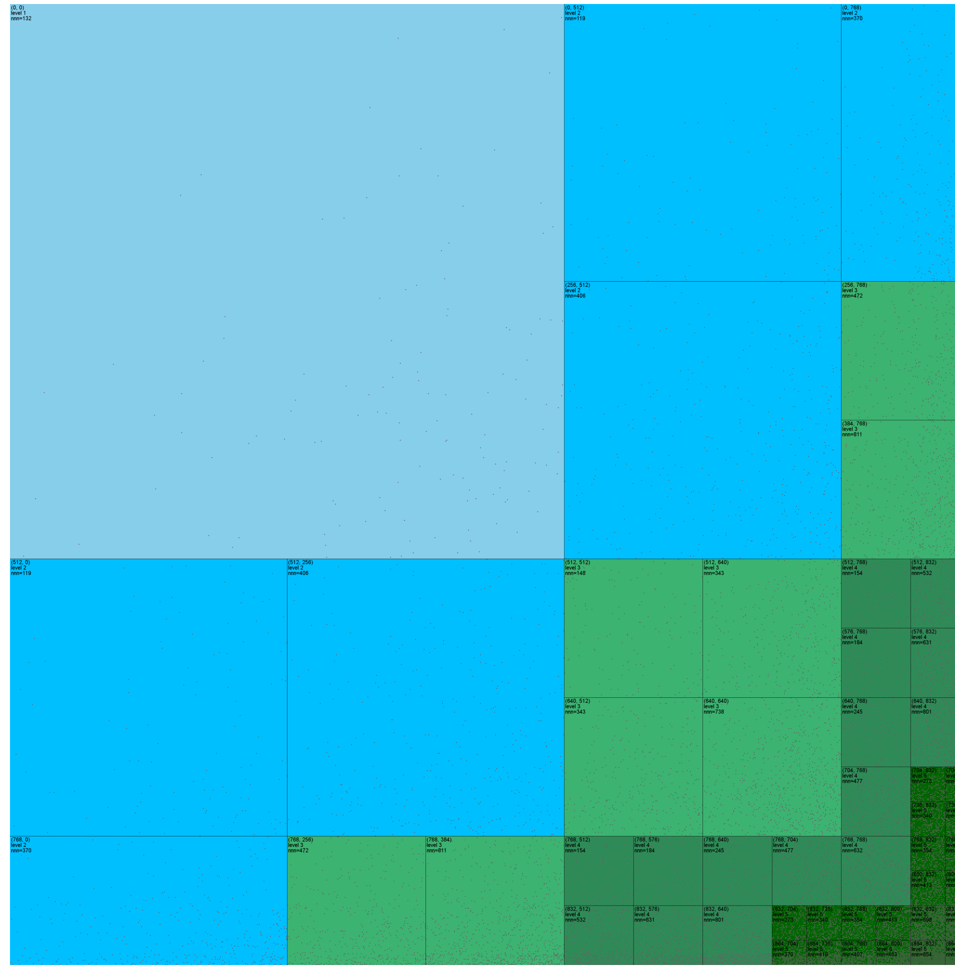
Blocks store enough matrix elements for meaningful computation; denser parts of matrix have more blocks.

UCSB

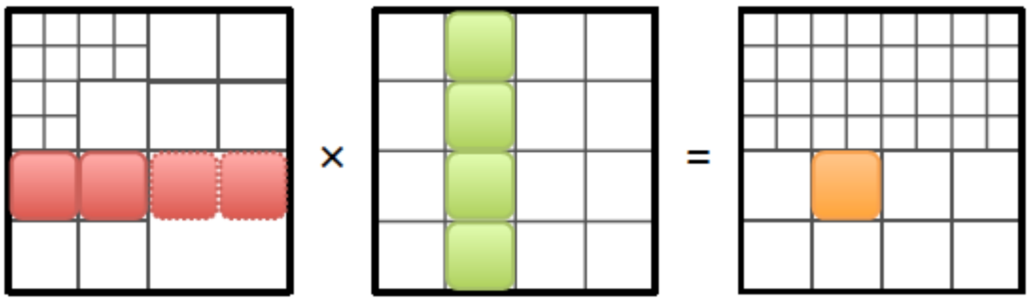
QuadMat example: Scale-10 RMAT

Scale 10 RMAT
(887x887, 21304 non-nulls)
up to 1024 non-nulls per block
In order of increasing degree

Blue blocks: uint16_t indices
Green blocks: uint8_t indices

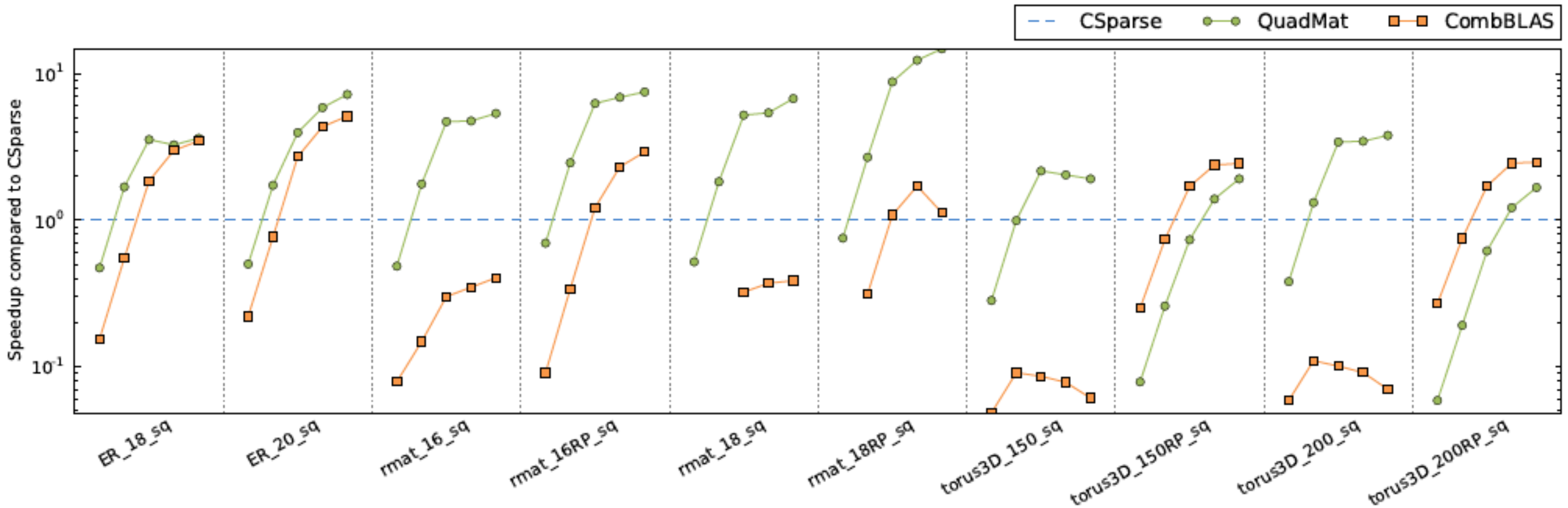


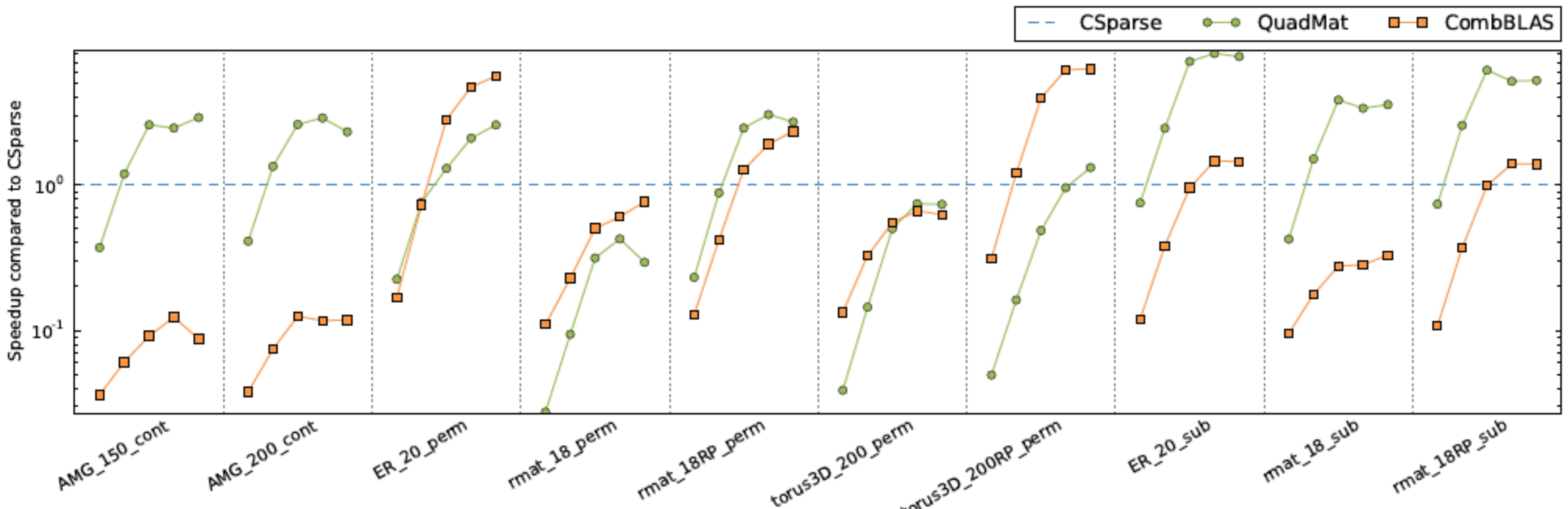
Pair-List QuadMat SpGEMM algorithm



- <u>Problem</u>: Natural recursive matrix multiplication is inefficient due to deep tree of sparse matrix additions.
- <u>Solution</u>: Rearrange into block inner product *pair lists.*
- A single matrix element can participate in pair lists with different block sizes.
- Symbolic phase followed by computational phase
- Multithreaded implementation in Intel TBB

QuadMat compared to Csparse & CombBLAS



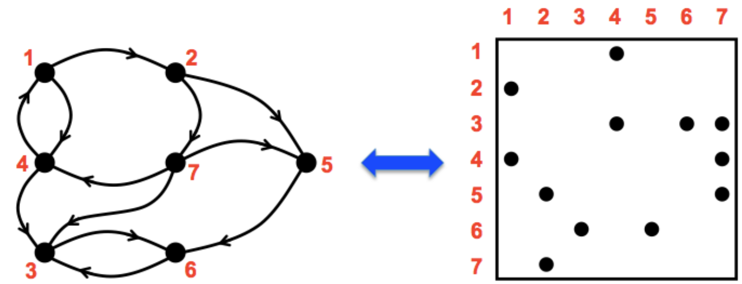


Knowledge

Discovery

Toolbox

http://kdt.sourceforge.net/



A general graph library with operations based on linear algebraic primitives

- Aimed at domain experts who know their problem well but don't know how to program a supercomputer
- Easy-to-use Python interface
- Runs on a laptop as well as a cluster with 10,000 processors

- Open source software (New BSD license)
- V3 release April 2013 (V4 soon)

Attributed semantic graphs and filters

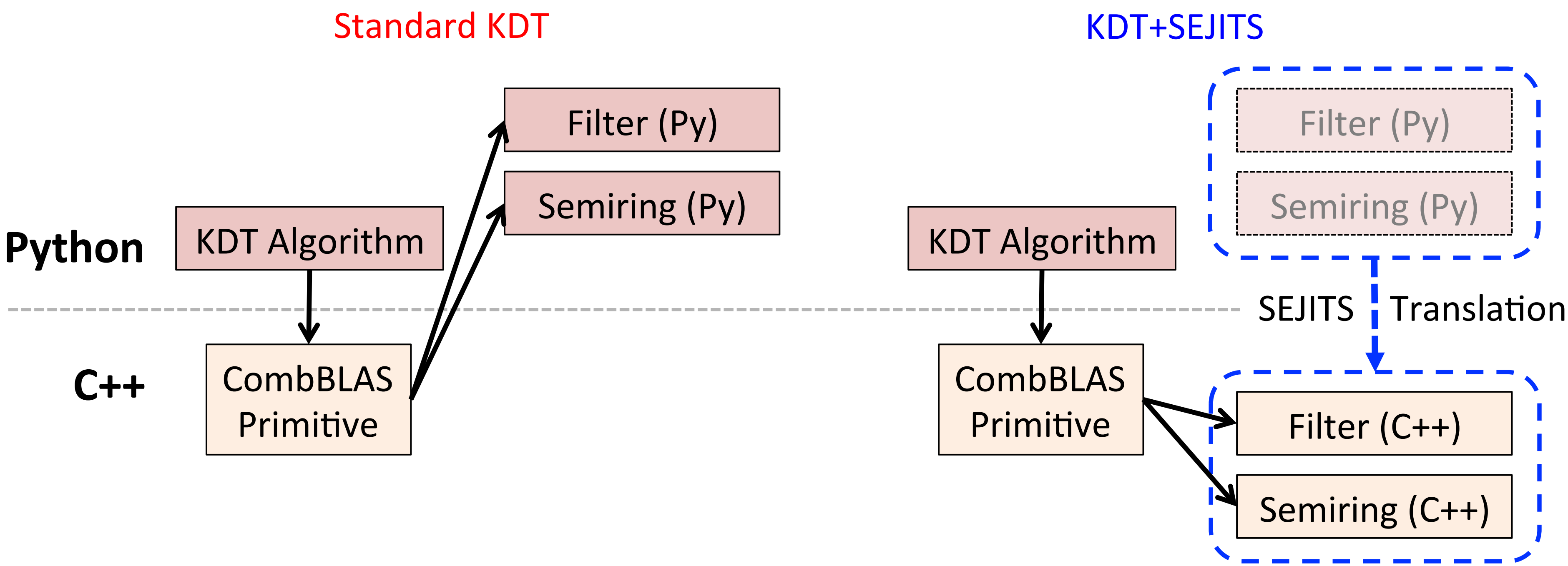
Example:

- Vertex types: Person, Phone, Camera, Gene, Pathway
- Edge types: PhoneCall, TextMessage, CoLocation, SequenceSimilarity
- Edge attributes: Time, Duration

- Calculate centrality just for emails among engineers sent between given start and end times

```
def onlyEngineers (self):
    return self.position == Engineer

def timedEmail (self, sTime, eTime):
    return ((self.type == email) and
            (self.Time > sTime) and
            (self.Time < eTime))


G.addVFilter(onlyEngineers)
G.addEFilter(timedEmail(start, end))

# rank via centrality based on recent
email transactions among engineers

bc = G.rank('approxBC')
```

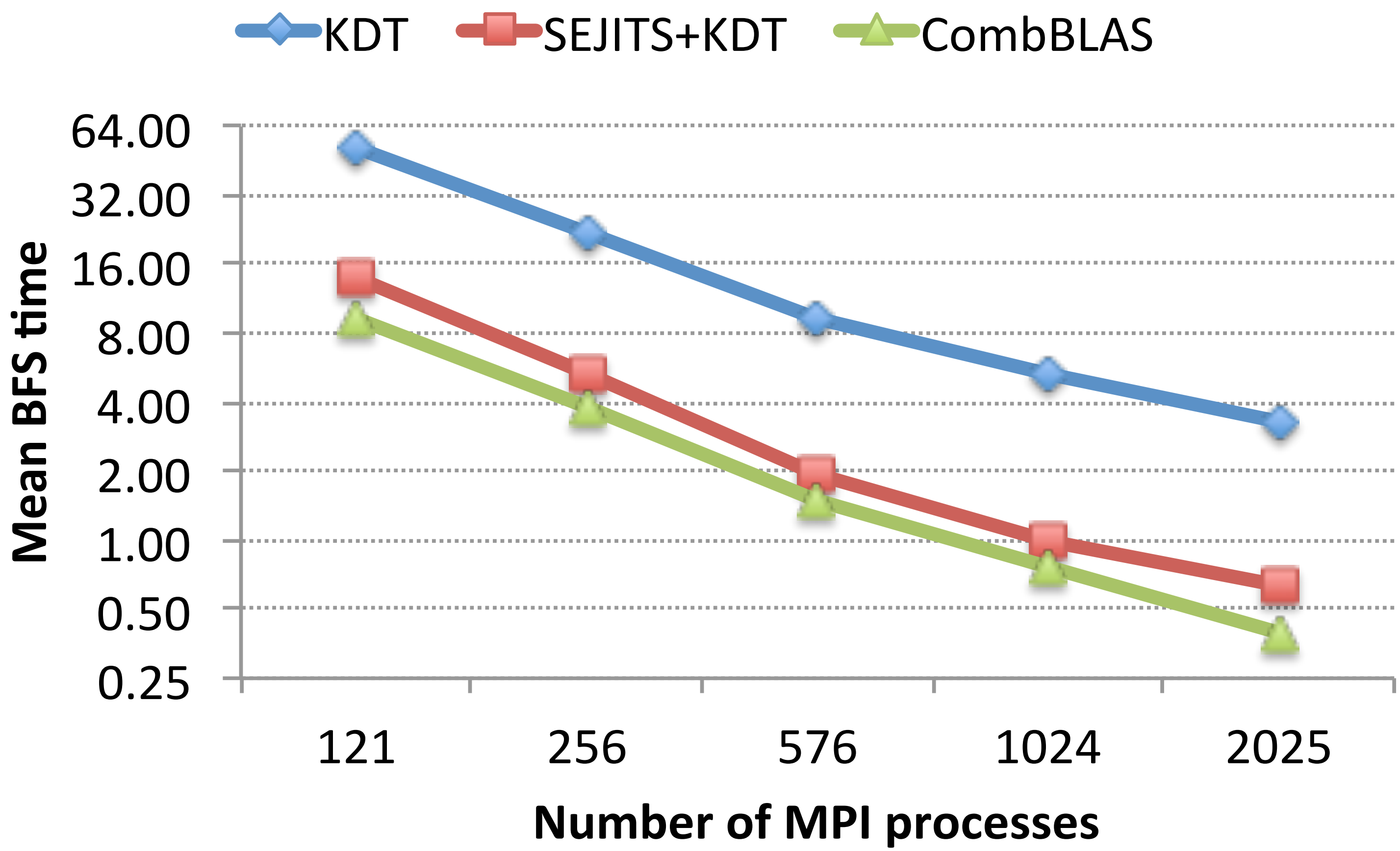
SEJITS for filter/semiring acceleration



Embedded DSL: Python for the whole application

- Introspect, translate Python to equivalent C++ code
- Call compiled/optimized C++ instead of Python

Filtered BFS with SEJITS



Time (in seconds) for a single BFS iteration on scale 25 RMAT (33M vertices, 500M edges) with 10% of elements passing filter. Machine is NERSC's Hopper.

What do we wish we had?

- Laplacian linear solvers and eigensolvers
  - Many applications: spectral clustering, ranking, partitioning, multicommodity flow, PDE's, control theory, ….
- Fusing sequences of operations instead of materializing intermediate results
  - Working on some of this, e.g. matrix triple products in QuadMat
- Priority-queue algorithms: depth-first search, Dijkstra's shortest paths, strongly connected components
  - These are hard to do in parallel at all
  - But sometimes you want to do them sequentially

A few questions for the Graph BLAS Forum

- How (or when) does the API let the user specify the "semiring scalar" objects and operations?
  - How general can the objects be?
  - What guarantees do the operations have to make?
  - Maybe there are different levels of compliance for an implementation, starting with just (double, +, *)

UCSB

A few questions for the Graph BLAS Forum

- How does the API let the user “break out of the BLAS” when they need to?
  - In dense numeric BLAS and in sparse Matlab (but not in Sparse BLAS), the user can access the matrix directly, element-by-element, with a performance penalty.
  - Graph BLAS needs something like this too, or else it’s only useful to programmers who commit to it 100%.
  - “for each edge e incident on vertex v do …”
  - “for each endpoint v of edge e do …”
  - Add or delete vertex v or edge e.

UCSB

Can we standardize a “Graph BLAS”?

No, it’s not reasonable to define a universal set of building blocks.

- Huge diversity in matching graph algorithms to hardware platforms.
- No consensus on data structures or linguistic primitives.
- Lots of graph algorithms remain to be discovered.
- Early standardization can inhibit innovation.

Yes, it *is* reasonable to define a common set of building blocks…
… for graphs as linear algebra.

- Representing graphs in the language of linear algebra is a mature field.
- Algorithms, high level interfaces, and implementations vary.
- But the core primitives are well established.

UCSB