Parallel Combinatorial BLAS and Applications in Graph Computations

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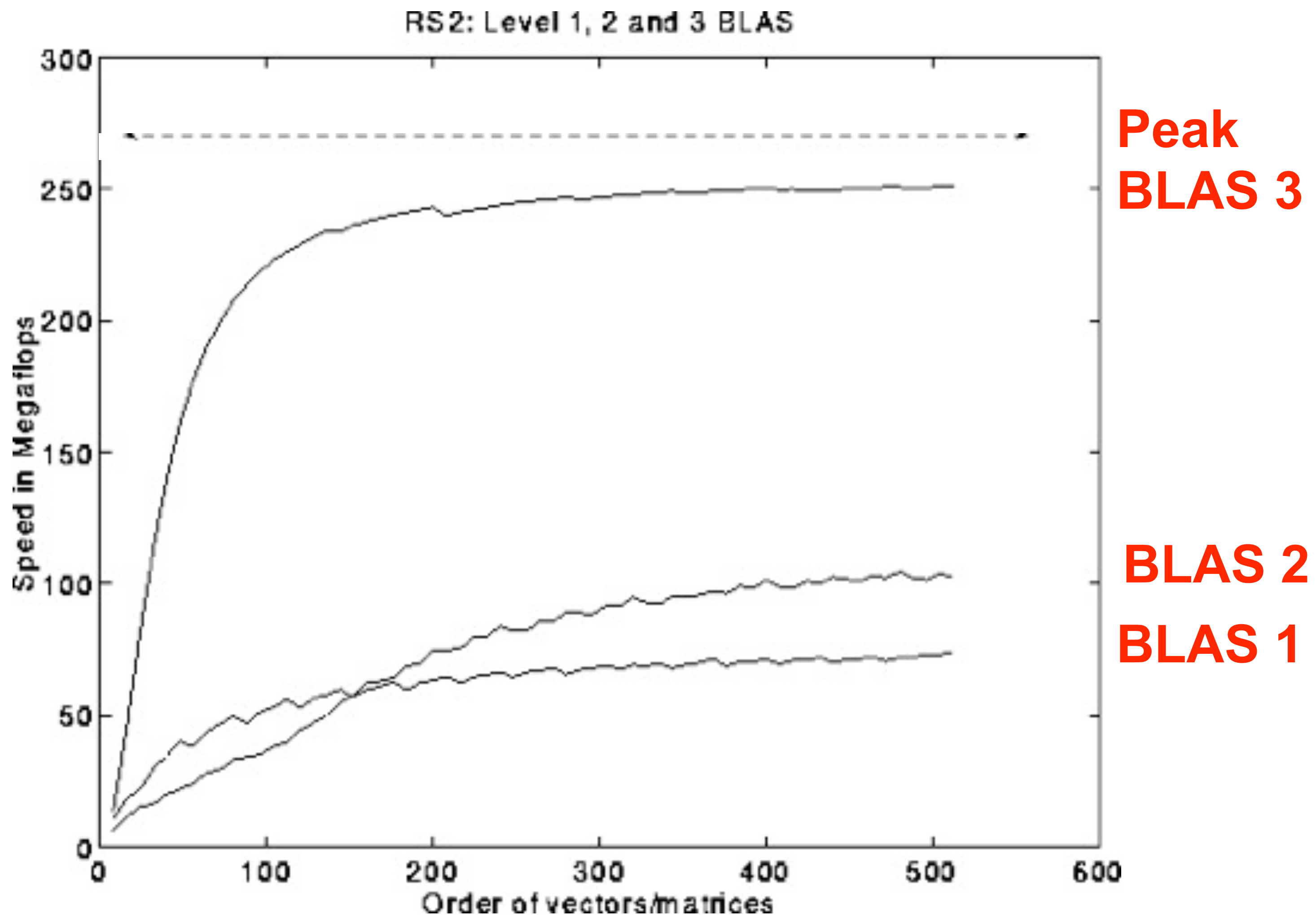
Primitives for Graph Computations

- By analogy to numerical linear algebra,

- What would the combinatorial BLAS look like?

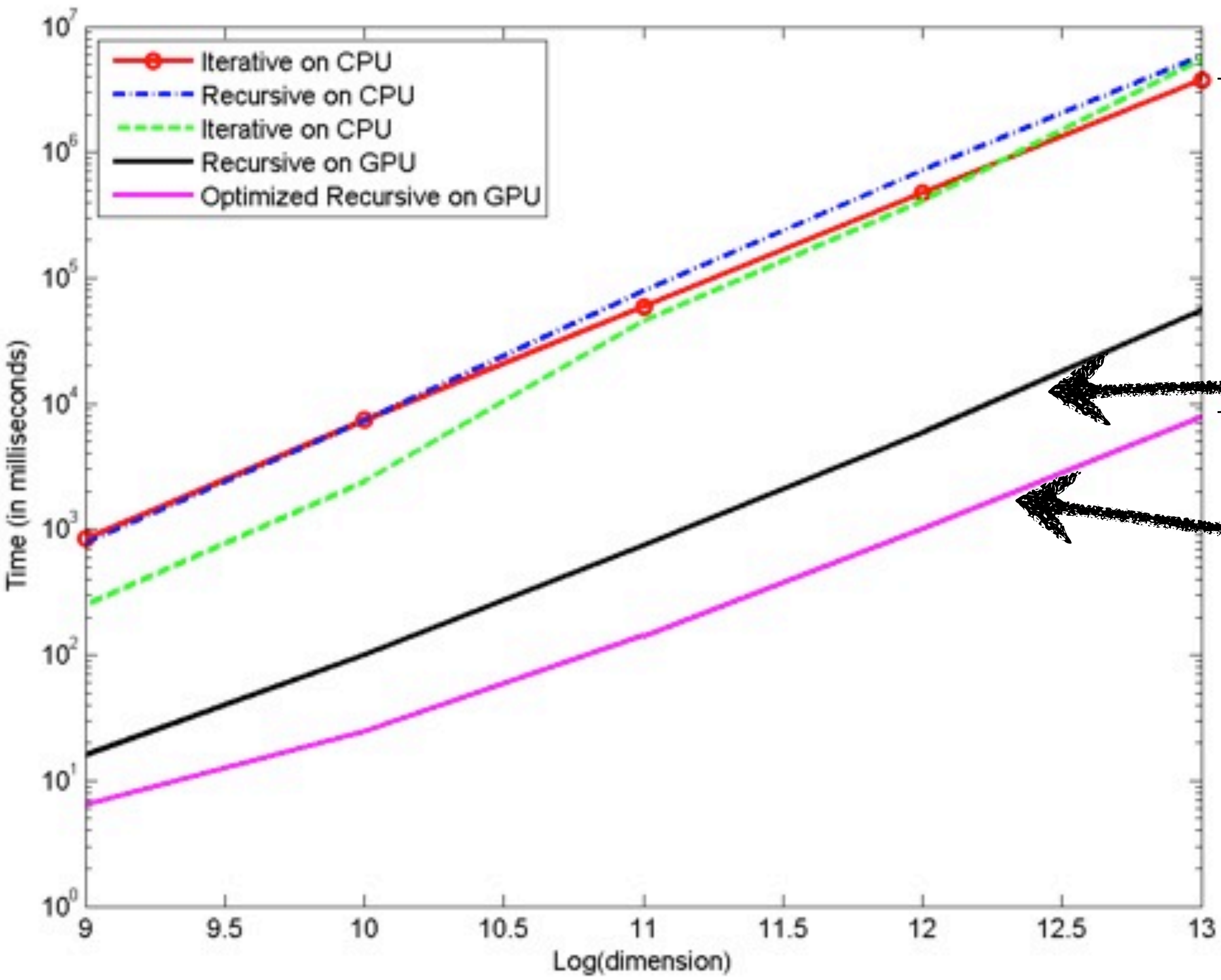


BLAS 3 (n-by-n matrix-matrix multiply)
BLAS 2 (n-by-n matrix-vector multiply)
BLAS 1 (sum of scaled n-vectors)

The Case for Primitives

It takes a “certain” level of expertise to get any kind of performance in this jungle of parallel computing

- I think you’ll agree with me by the end of the talk :)



What’s bandwidth anyway?

480x

I can just implement it (w/ enough coffee)

The right primitive !

All pairs shortest paths on the GPU

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The Case for Sparse Matrices

- Many irregular applications contain sufficient coarse-grained parallelism that can ONLY be exploited using abstractions at proper level.

Traditional graph computations	**Graphs in the language of linear algebra**
Data driven. Unpredictable communication patterns	Fixed communication patterns. Overlapping opportunities
Irregular and unstructured. Poor locality of reference	Operations on matrix blocks. Exploits memory hierarchy
Fine grained data accesses. Dominated by latency	Coarse grained parallelism. Bandwidth limited

Identification of Primitives

- Sparse matrix-matrix multiplication (SpGEMM)
  - Most general and challenging parallel primitive.
- Sparse matrix-vector multiplication (SpMV)
- Sparse matrix-transpose-vector multiplication (SpMVT)
  - Equivalently, multiplication from the left
- Addition and other point-wise operations (SpAdd)
  - Included in SpGEMM, “proudly” parallel
- Indexing and assignment (SpRef, SpAsgn)
  - A(I,J) where I and J are arrays of indices
  - Reduces to SpGEMM

Matrices on semirings, e.g. (×, +), (and, or), (+, min)

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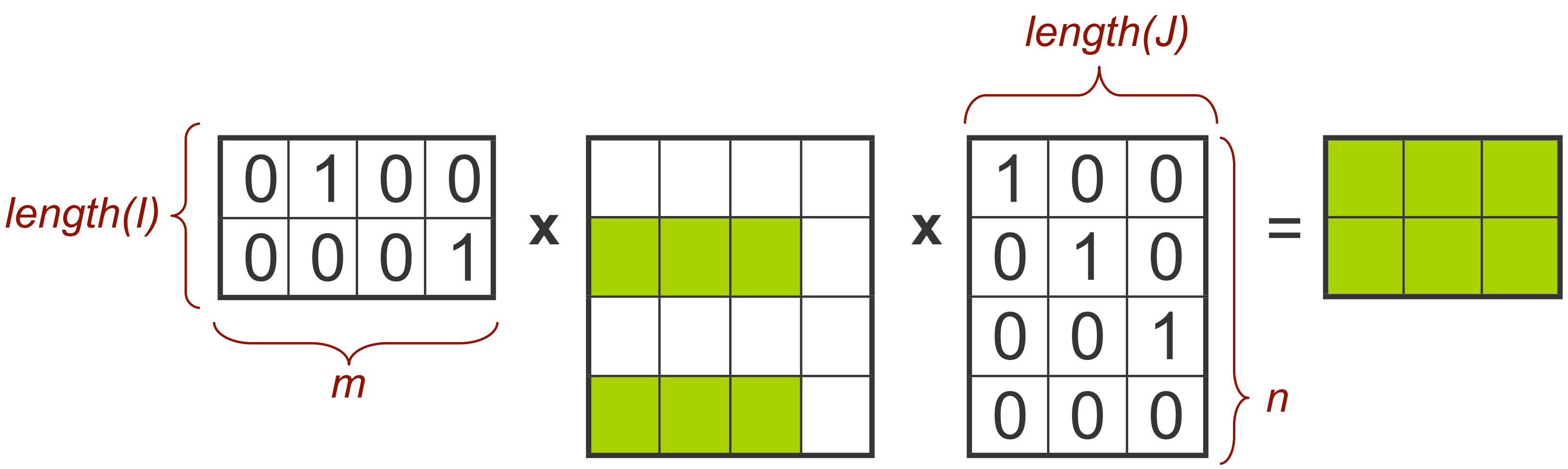
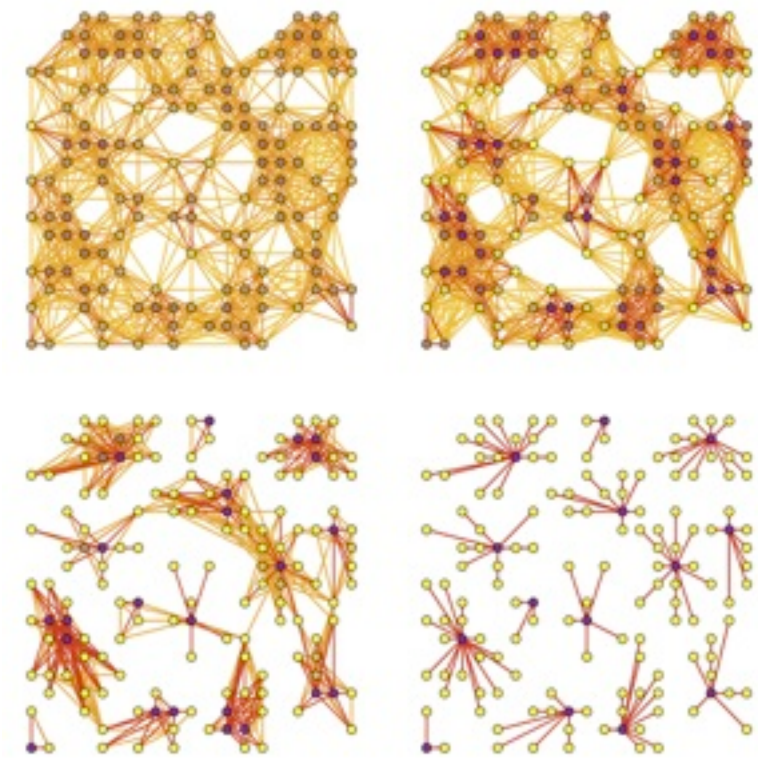
Why focus on SpGEMM?





- Graph clustering (Markov, peer pressure)
- Shortest path calculations
- Betweenness centrality
- Subgraph / submatrix indexing
- Graph contraction
- Cycle detection
- Multigrid interpolation & restriction
- Colored intersection searching
- Applying constraints in finite element computations
- Context-free parsing ...

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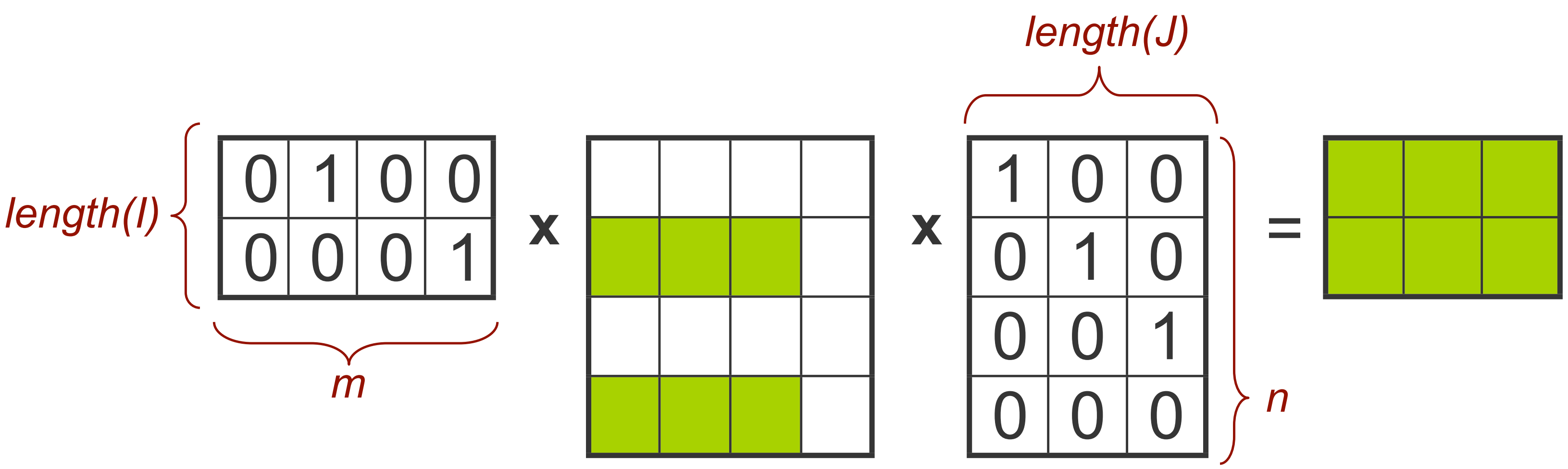

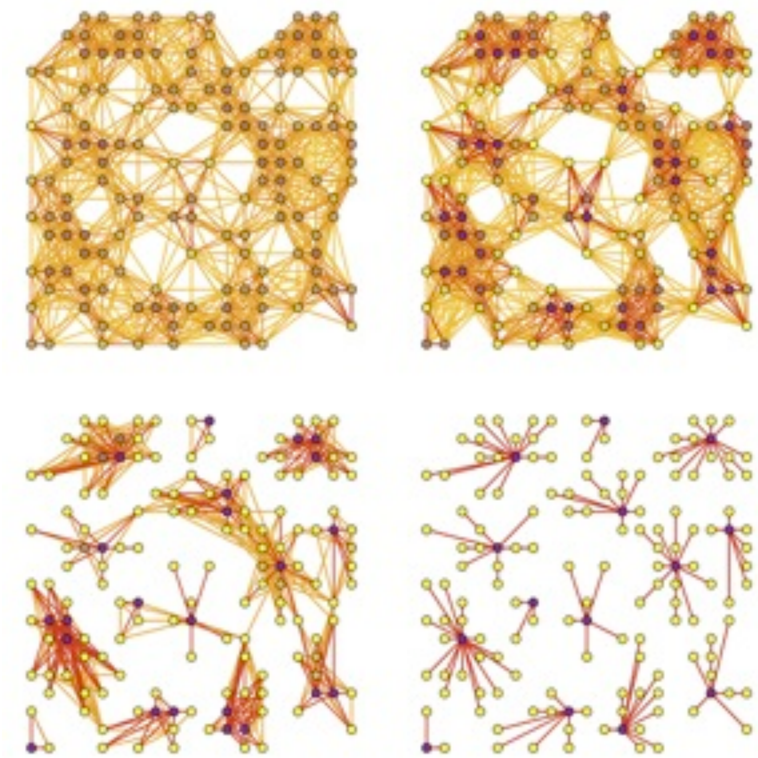

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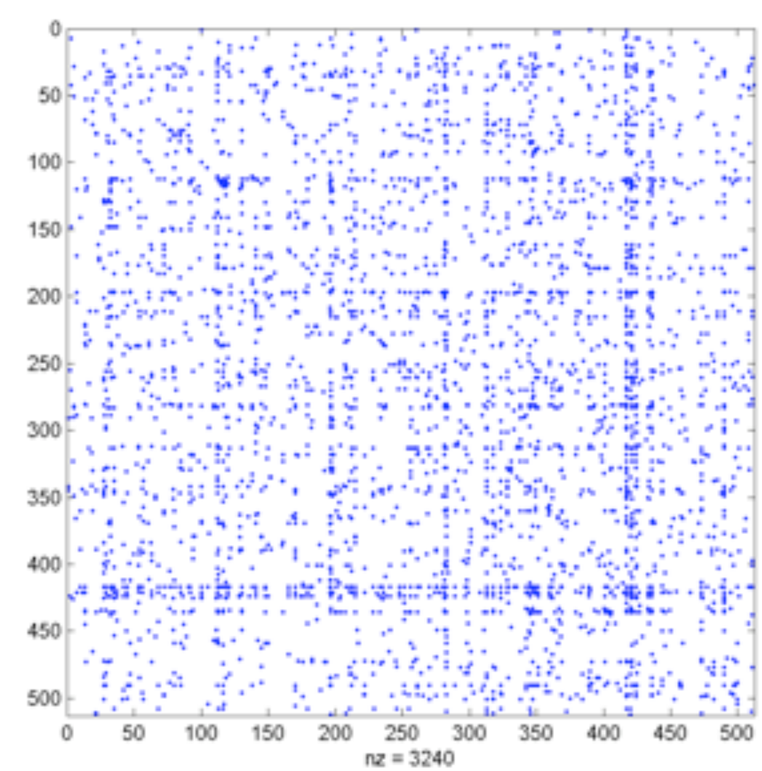

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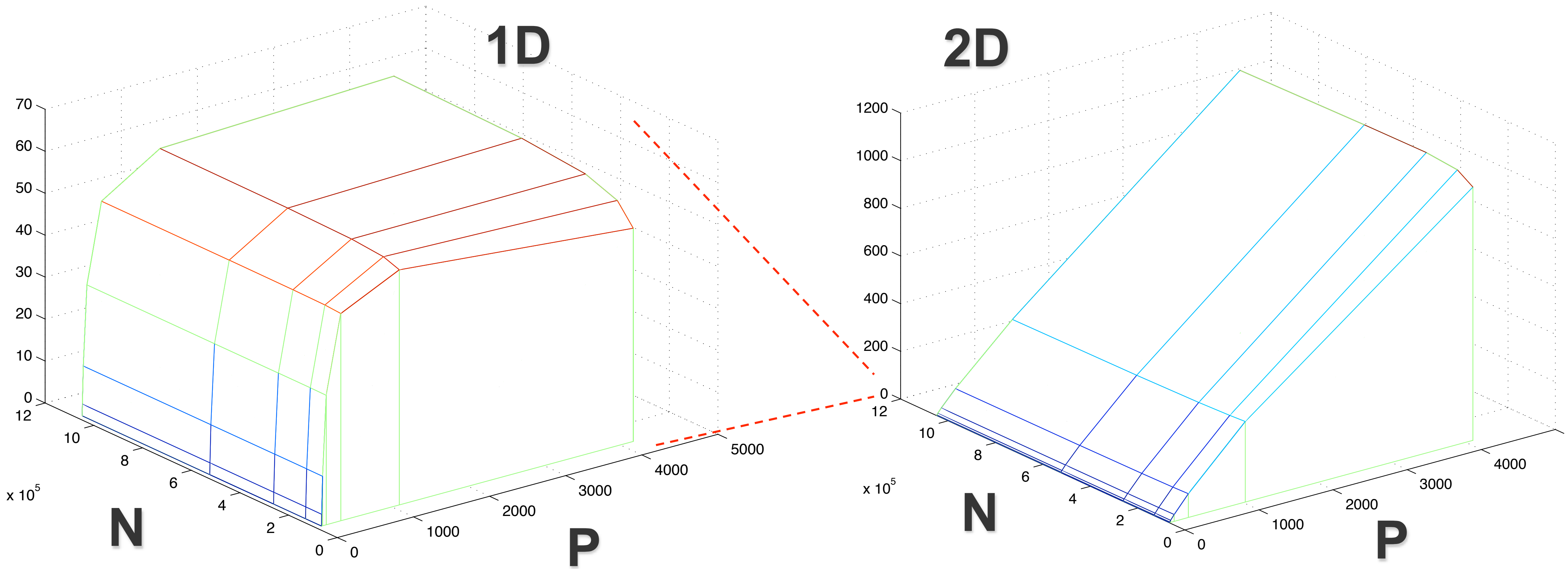
Vitals of Combinatorial BLAS

1. **Scalability**, in the presence of increasing *processors*, *problem size*, and *sparsity*.



In practice, 2D algorithms have <u>the potential</u> to scale, if implemented correctly. Overlapping communication, and maintaining load balance are crucial.

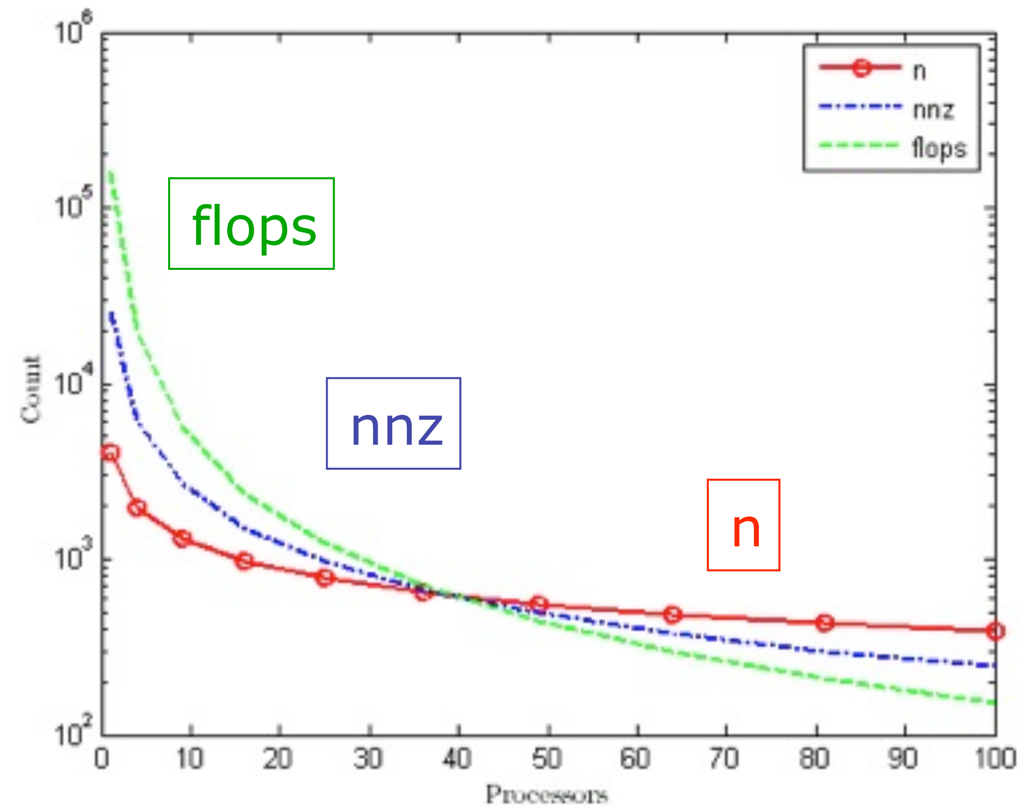
Sequential Kernel

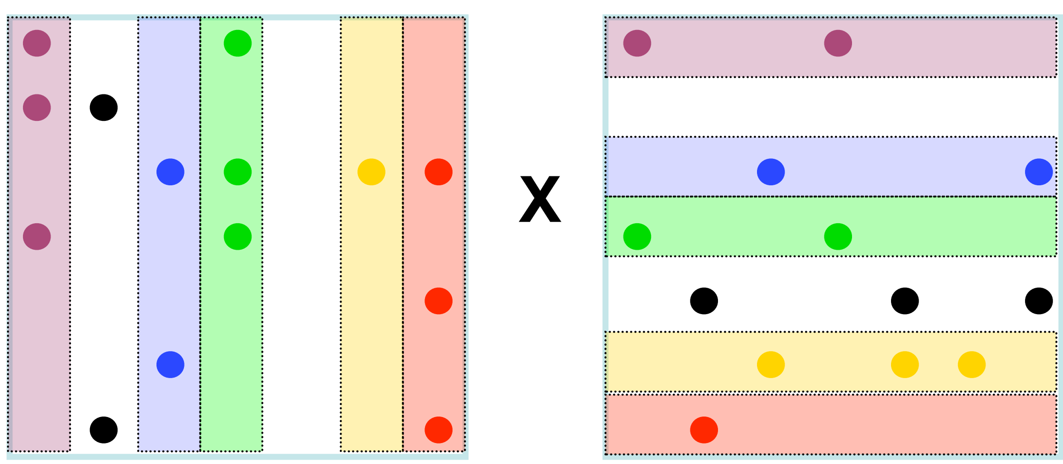
Standard algorithm is *O(nnz+ flops+n)*

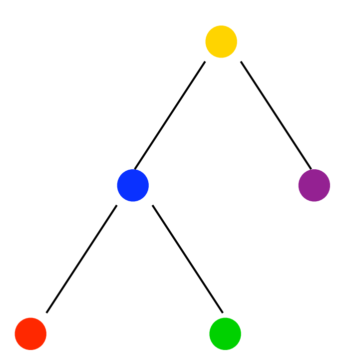
$$n'(\text{dimension}) \approx \frac{n}{\sqrt{p}}$$

$$flops'(\text{work}) \approx \frac{flops}{p\sqrt{p}}$$

$$nnz'(\text{data size}) \approx \frac{nnz}{p}$$







- Strictly *O(nnz)* data structure
- Outer-product formulation
- Work-efficient

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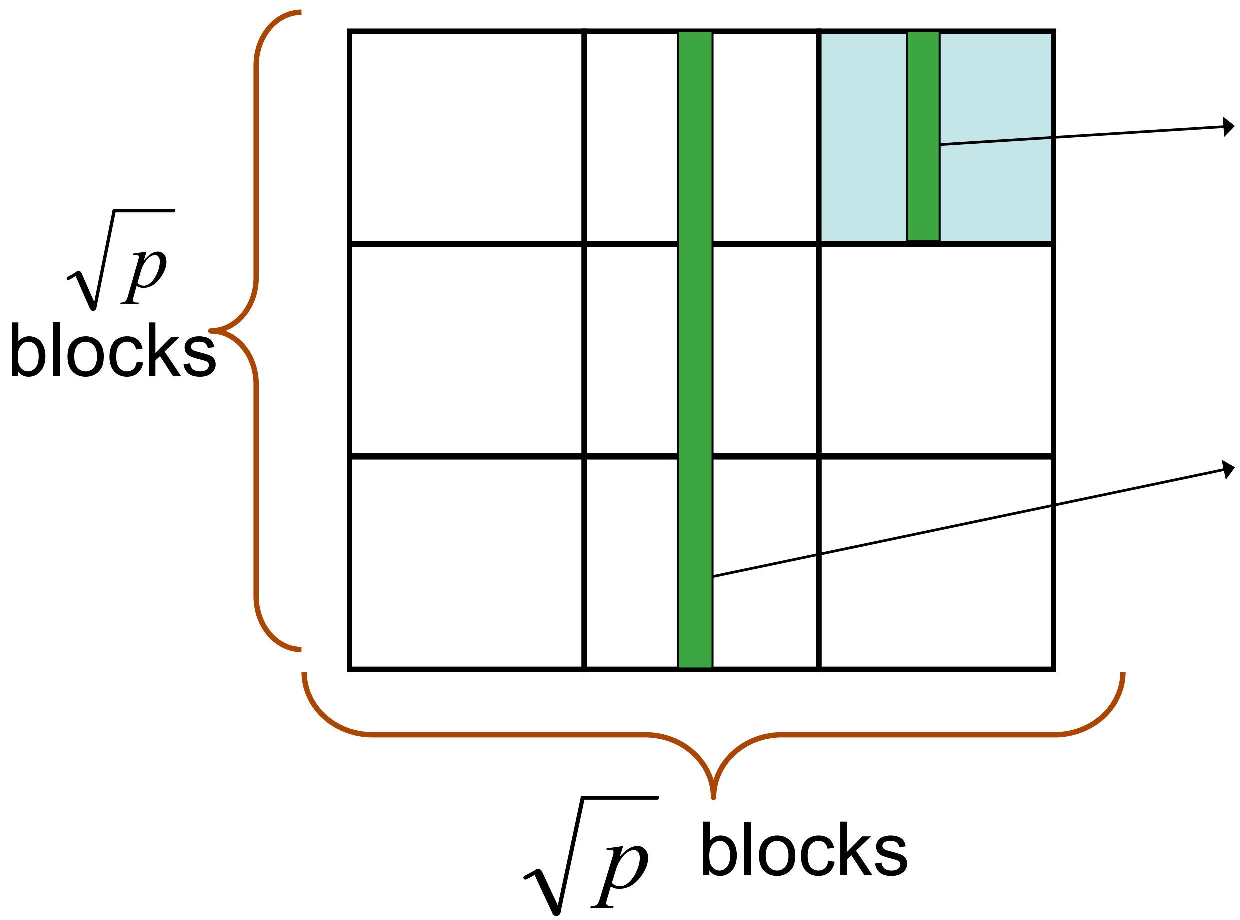
Node Level Considerations

Submatrices are *hypersparse* *(i.e. nnz << n)*



$$nnz' = \frac{c}{\sqrt{p}} \rightarrow 0$$

Average of c nonzeros per column

<u>Total Storage</u>:

$$O(n + nnz) \Rightarrow O(n\sqrt{p} + nnz)$$

- A data structure or algorithm that depends on the matrix dimension n (e.g. CSR or CSC) is asymptotically too wasteful for submatrices

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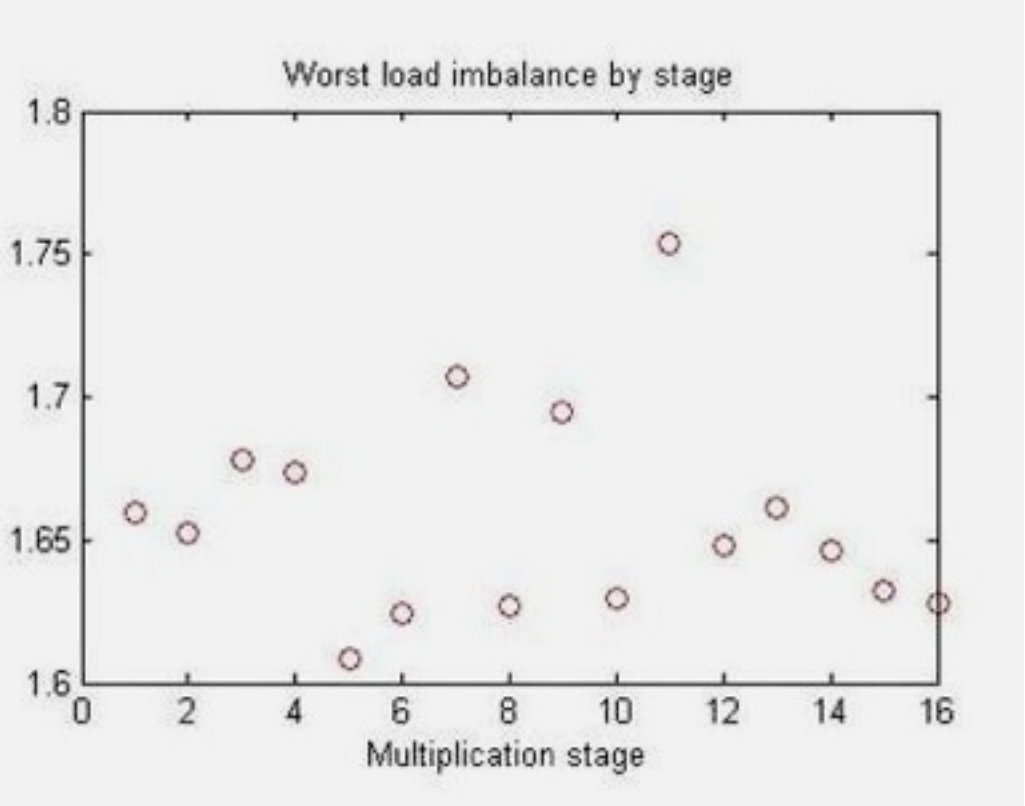
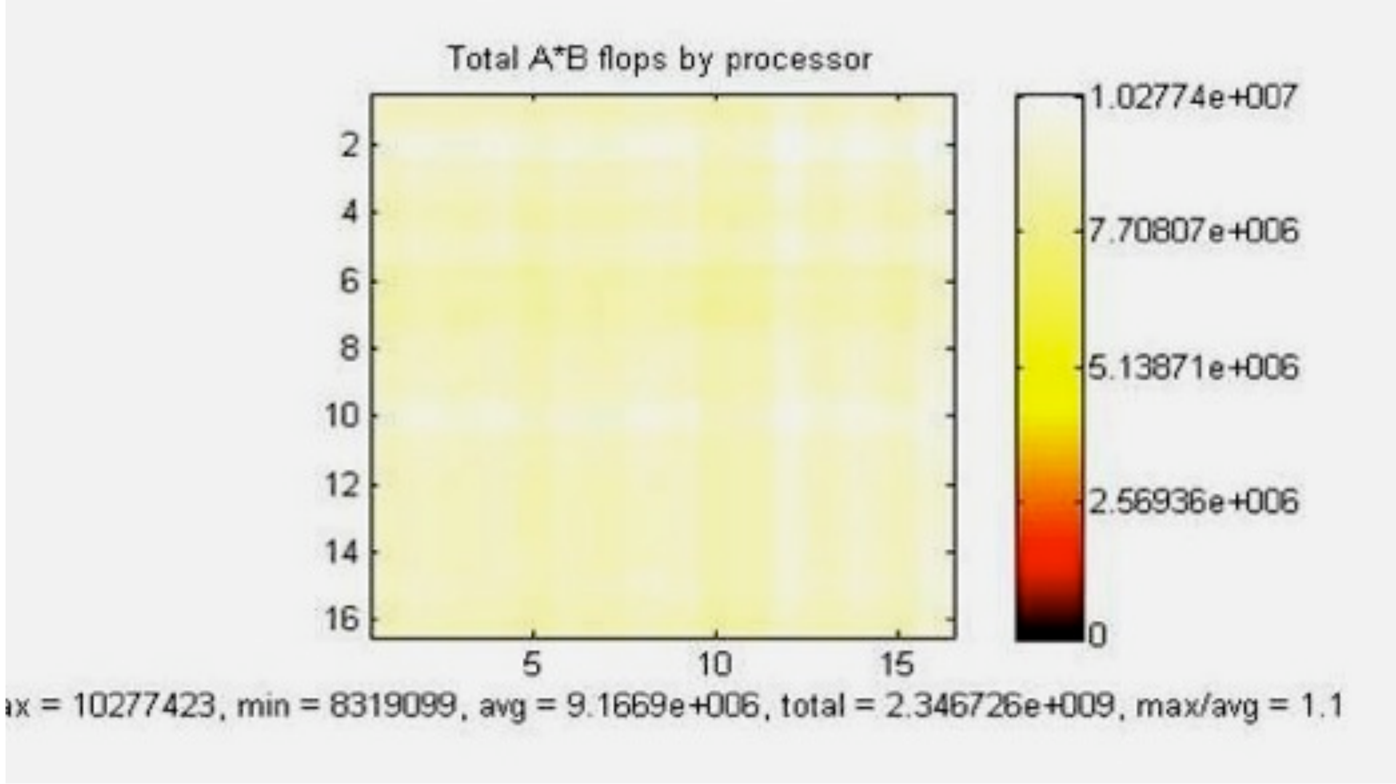
Addressing the Load Balance

RMat: Model for graphs with high variance on degrees

- Random permutations are useful. But...
- Bulk synchronous algorithms may still suffer:



- Asynchronous algorithms have no notion of stages.
- Overall, no significant imbalance.



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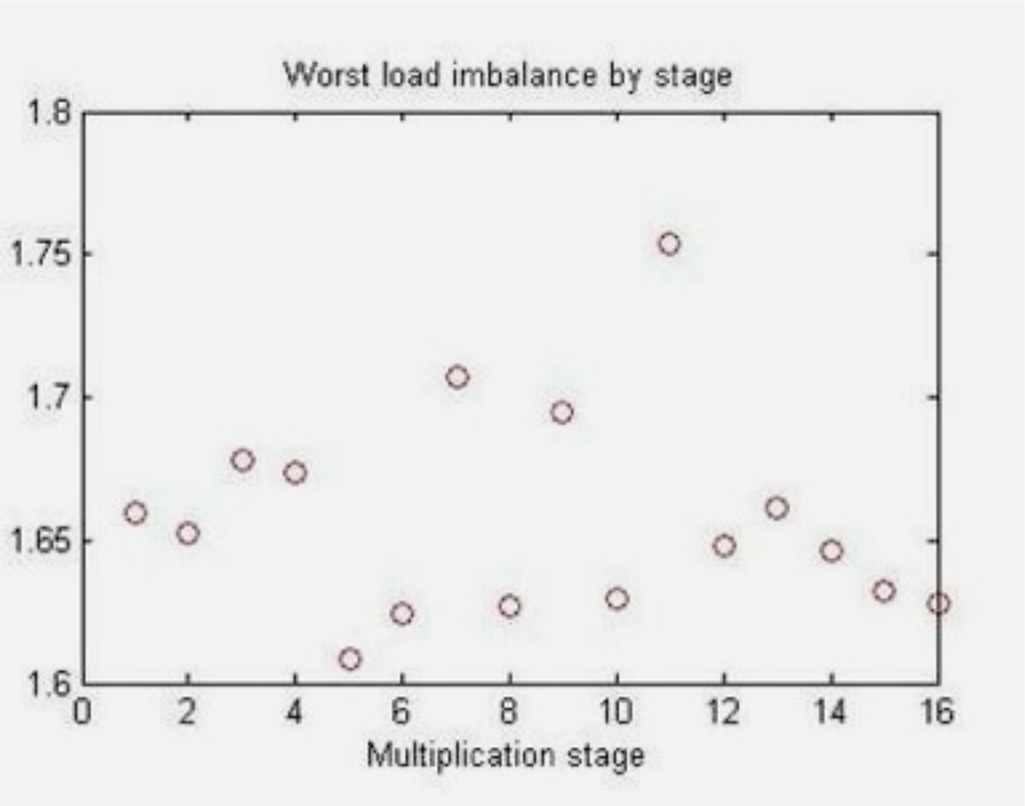

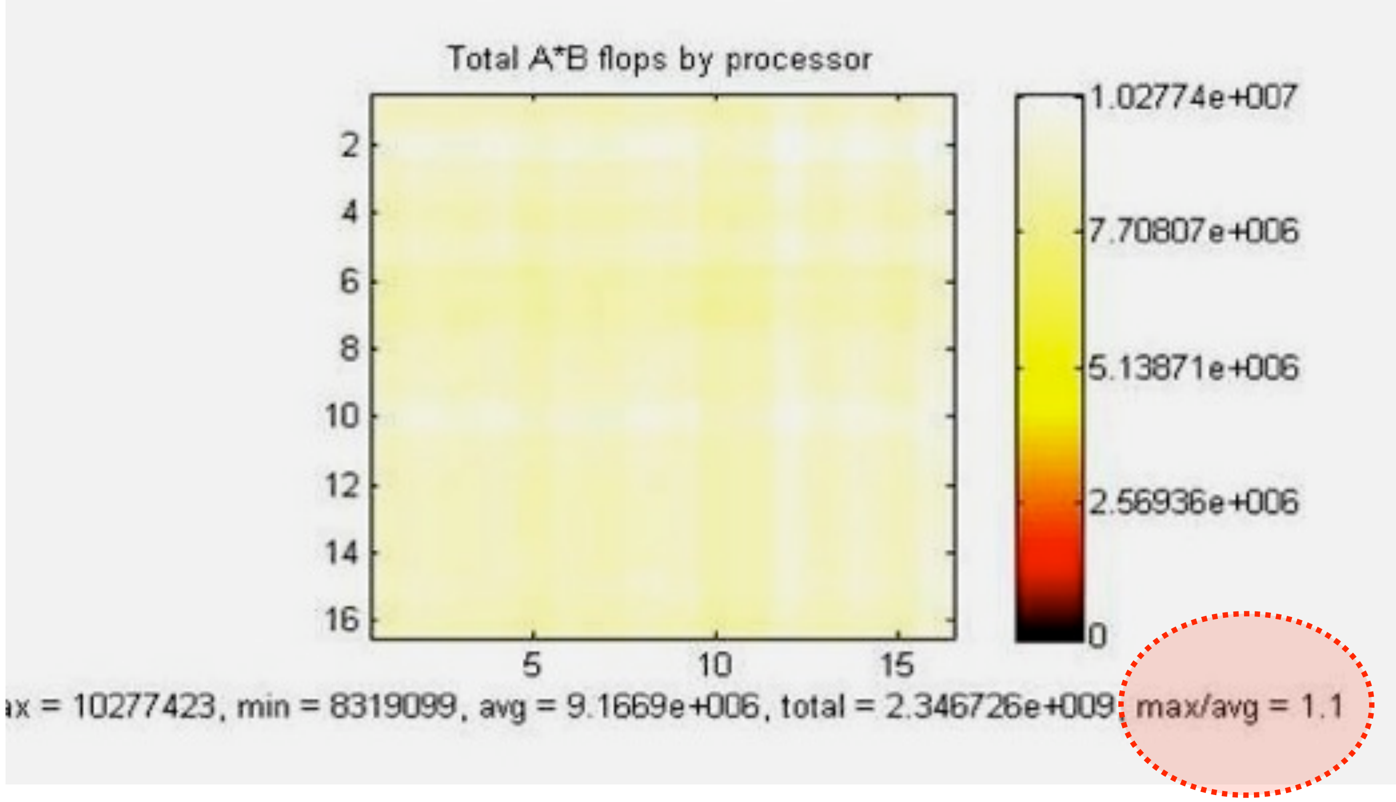

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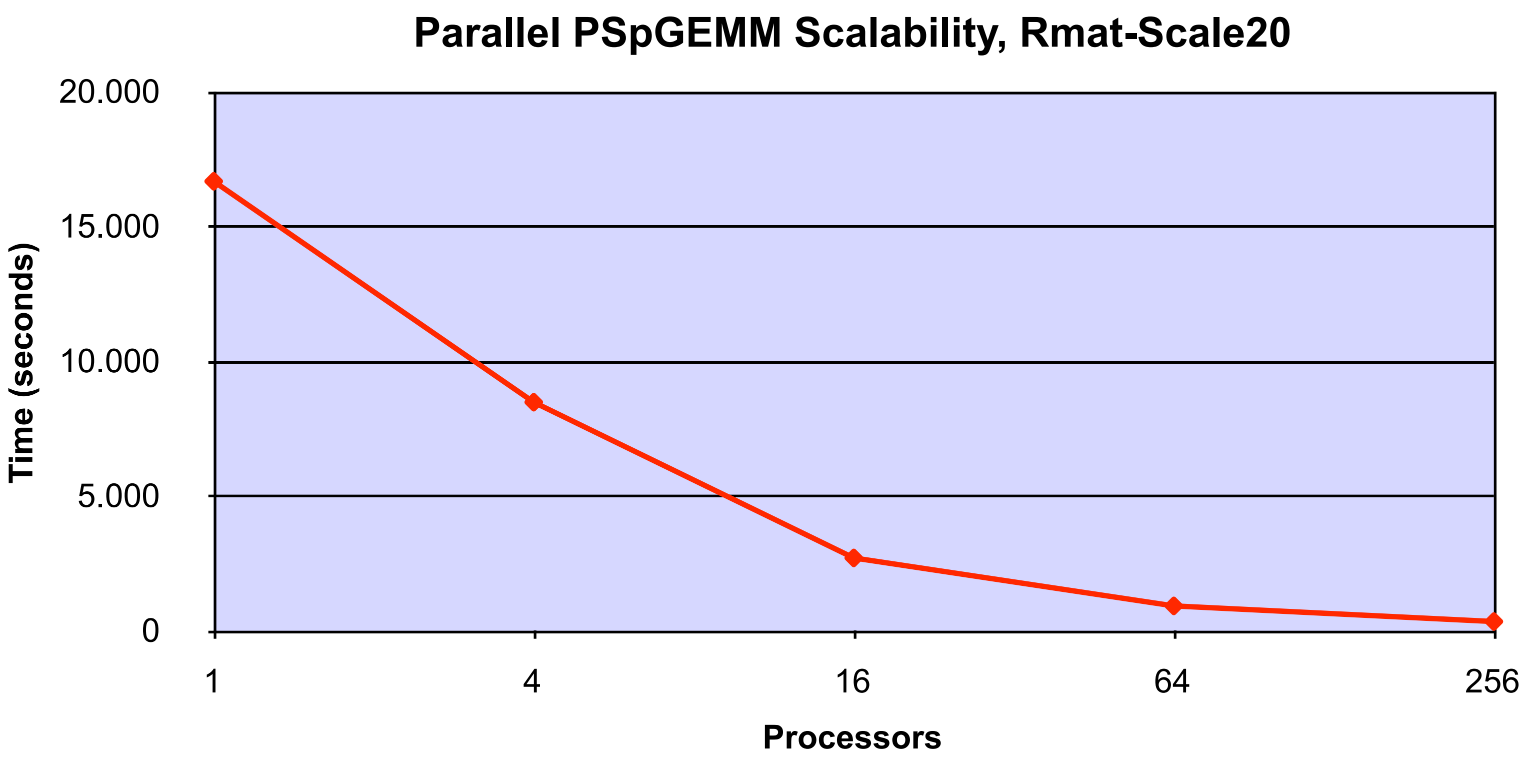
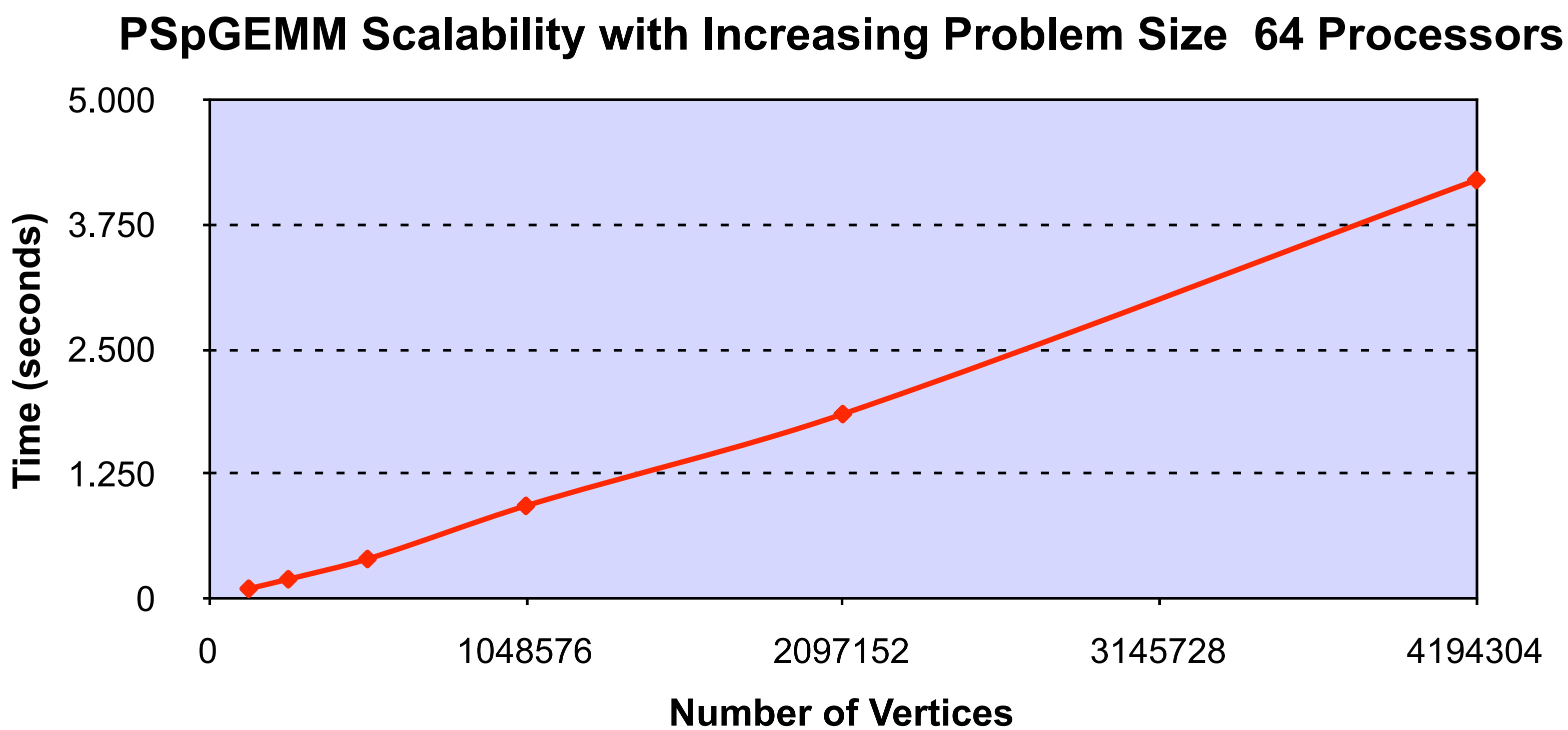
Scaling Results for SpGEMM





- Asynchronous implementation
  One-sided MPI-2
- Runs on TACC's Lonestar cluster
- Dual-core dual-socket
  Intel Xeon 2.66 Ghz
- RMat X RMat product
  Average degree (nnz/n) ≈ 8

Vitals of Combinatorial BLAS

2. **Generality**, of the numeric type of matrix elements, algebraic operation performed, and the library interface.

   Without the language abstraction penalty: C++ Templates

```
template <class IT, class NT, class DER>
class SpMat;
```

- Achieve mixed precision arithmetic: Type traits
- Enforcing interface and strong type checking: CRTP
- General semiring operation: Function Objects

➡ *Abstraction penalty is not just a programming language issue.*

➡ *In particular, view matrices as indexed data structures and stay away from single element access (Interface should discourage)*

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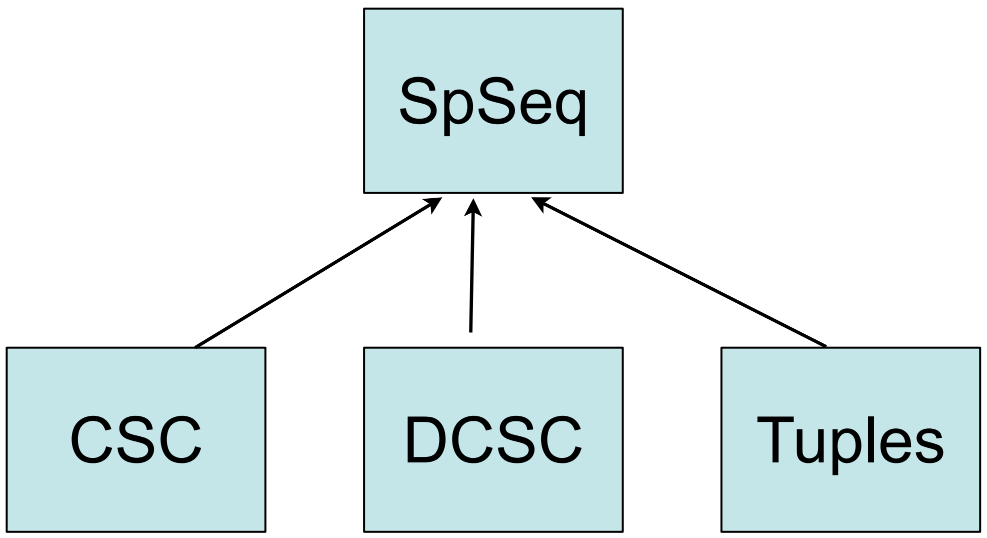
Vitals of Combinatorial BLAS

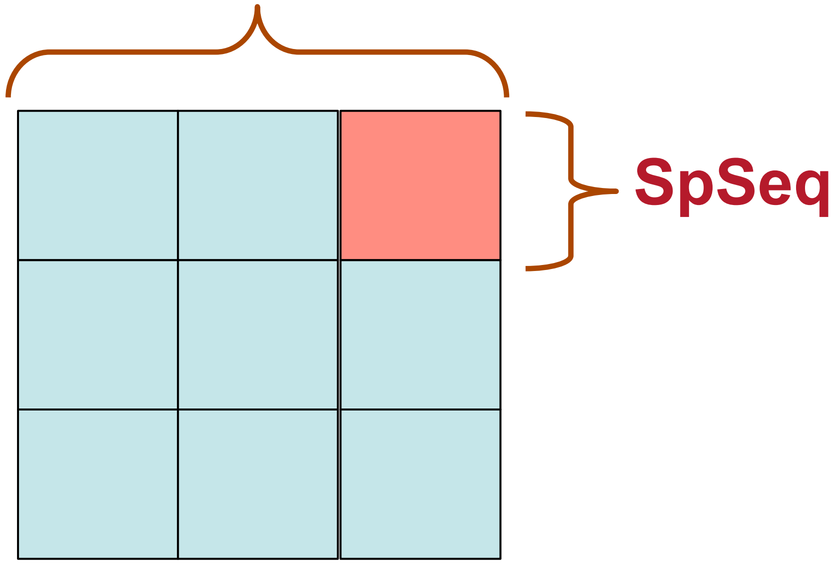
3. **Extendability,** of the library while maintaining compatibility and seamless upgrades.
   - ➡ Decouple parallel logic from the sequential part.
   - ➡ Even Boost' serializable concept might be restrictive (and slow)

Commonalities:
- Support the sequential API
- Composed of a **number of arrays**

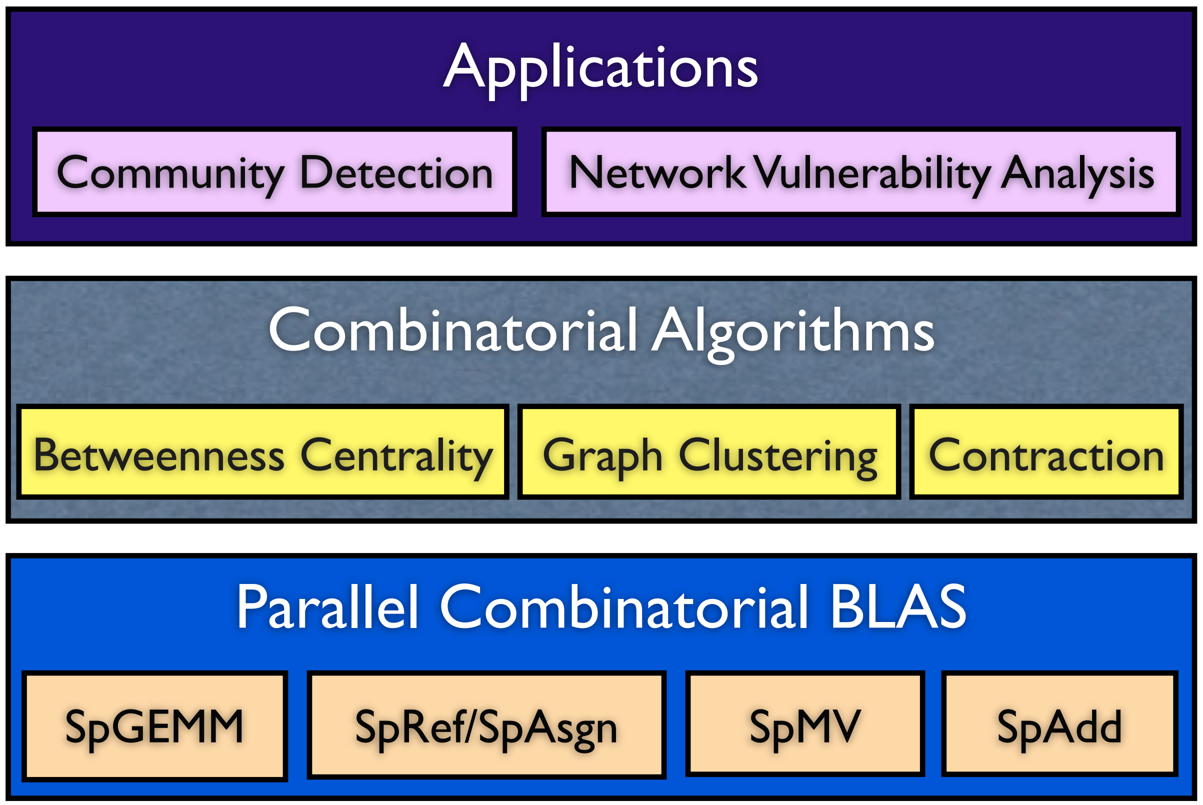


Any parallel logic:
asynchronous, bulk synchronous, etc

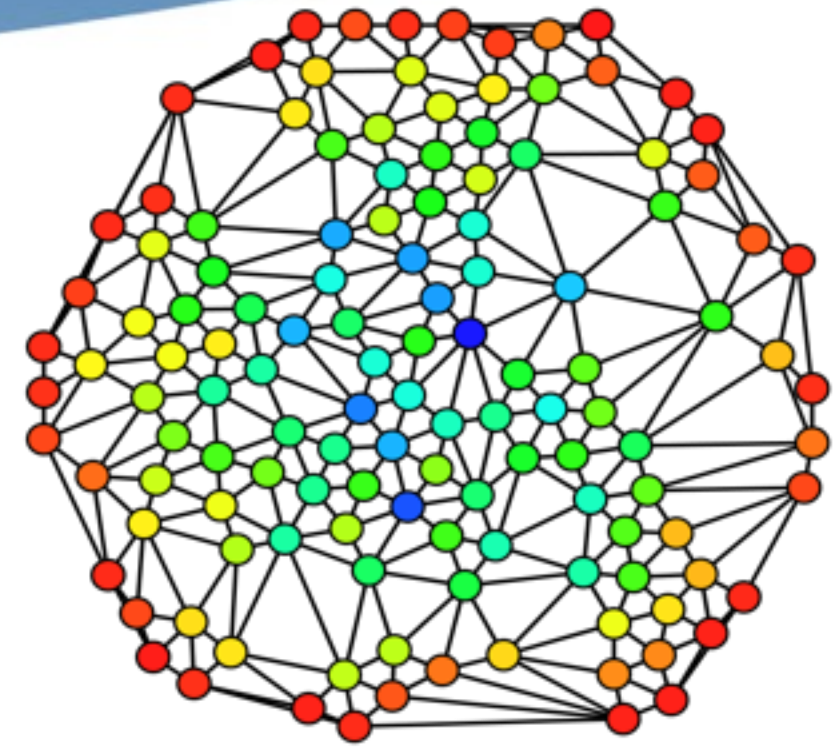
SpPar<Comm, SpSeq>



Applications and Algorithms



A typical software stack for an application enabled with the Combinatorial BLAS



Betweenness Centrality

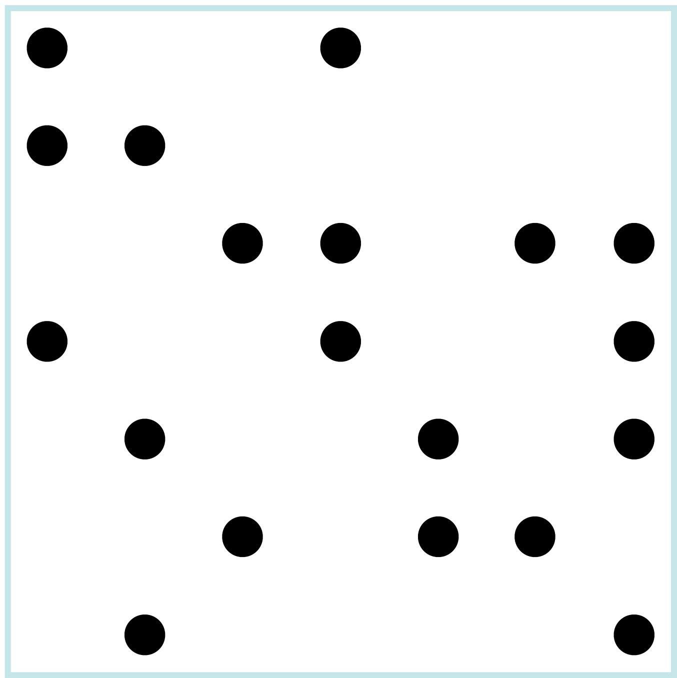
$C_B(v)$: Among all the shortest paths, what fraction of them pass through the node of interest?

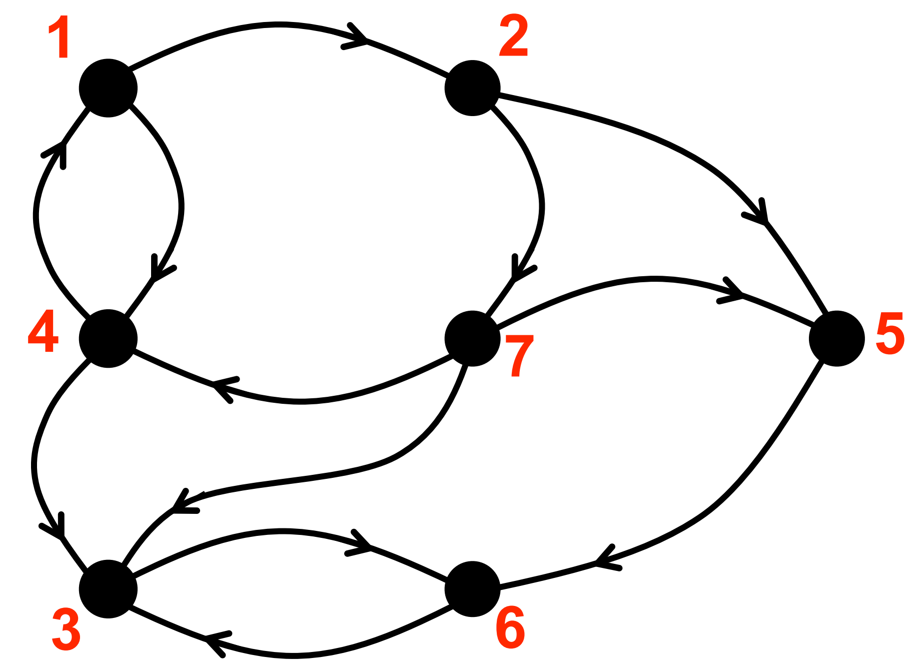
$$C_B(v) = \sum_{\substack{s \neq v \neq t \in V \\ s \neq t}} \frac{\sigma_{st}(v)}{\sigma_{st}}$$

Brandes' algorithm

Betweenness Centrality using Sparse Matrices [Robinson, Kepner]

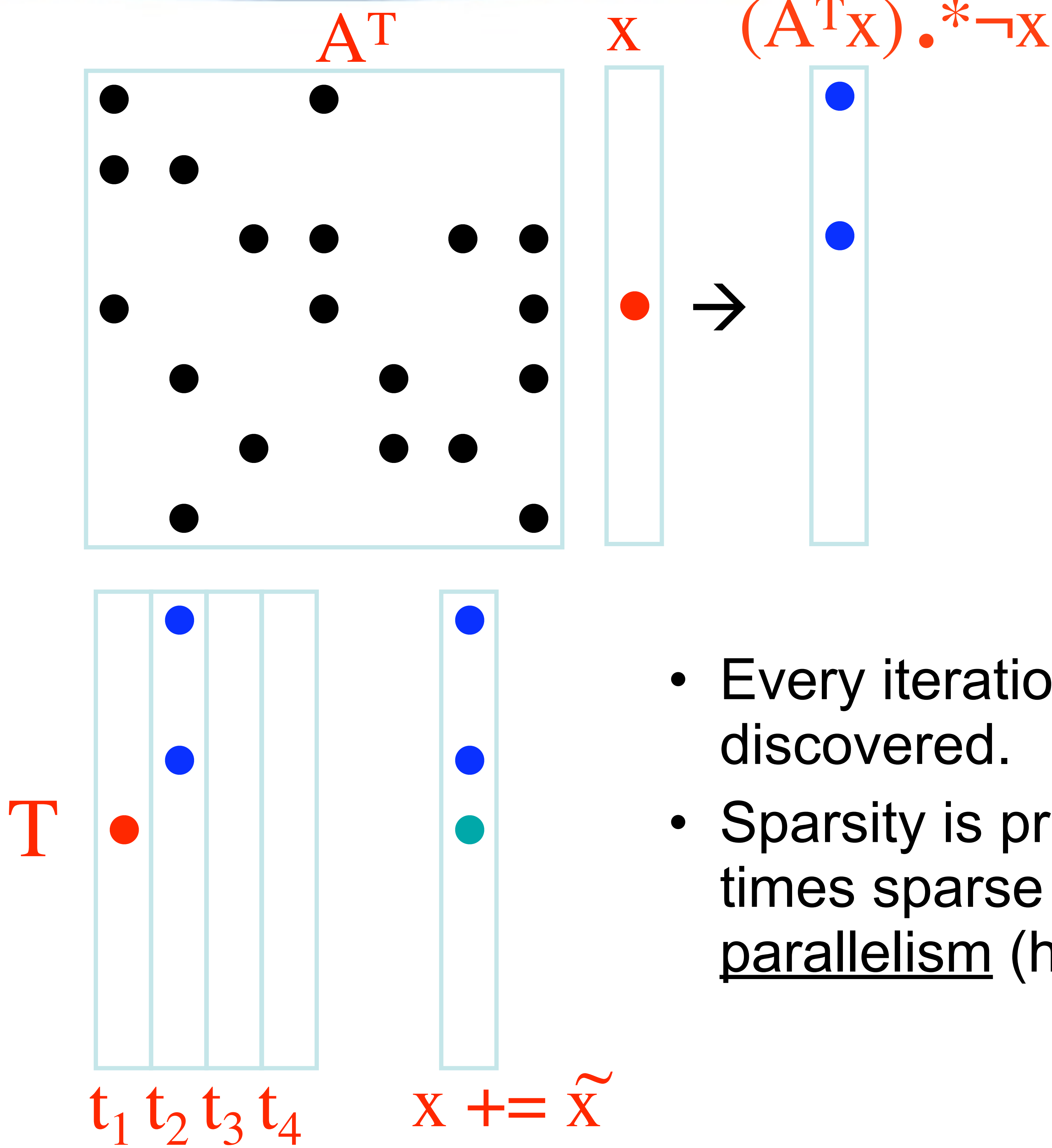
A^T

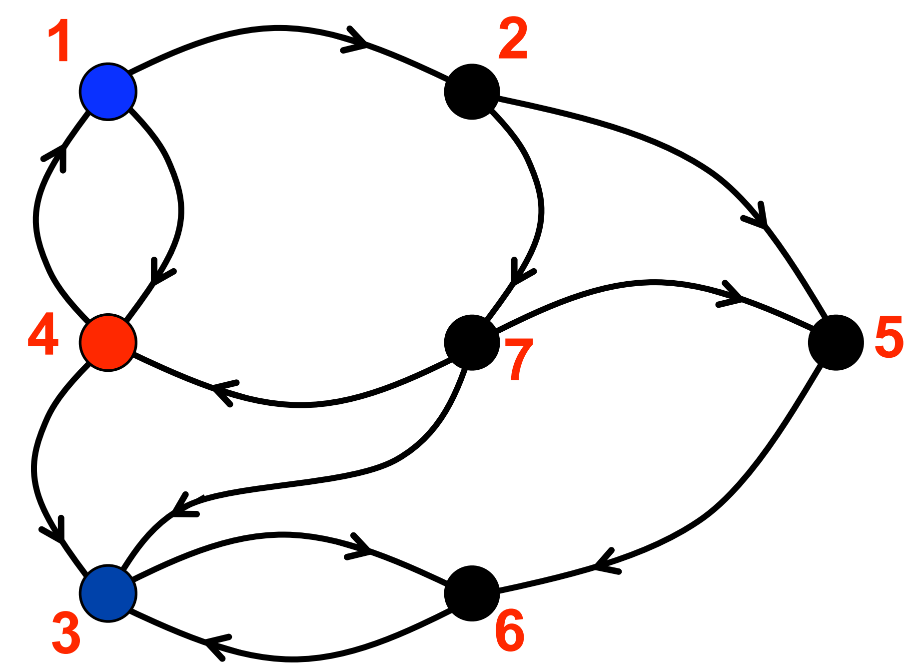




- Adjacency matrix: sparse array w/ nonzeros for graph edges
- Storage-efficient implementation from sparse data structures
- Betweenness Centrality Algorithm:
  1. Pick a starting vertex, v
  2. Compute shortest paths from v to all other nodes
  3. Starting with most distant nodes, roll back and tally paths

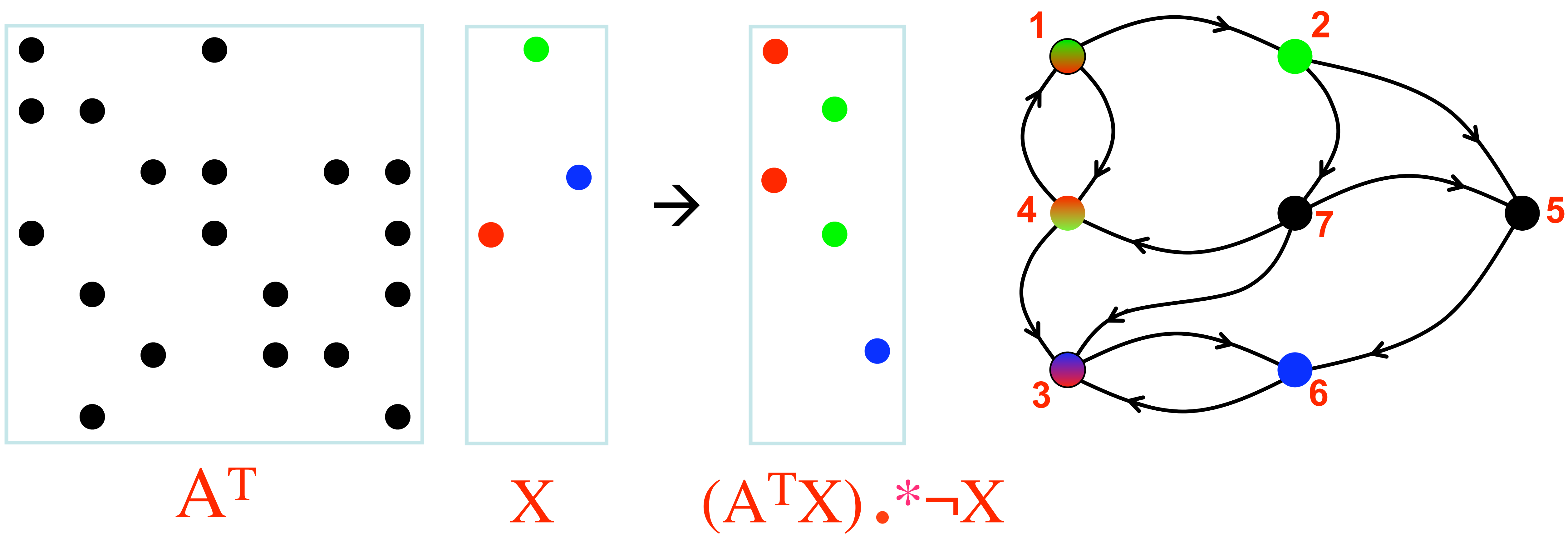
Betweenness Centrality using BFS





- Every iteration, another level of the BFS is discovered.
- Sparsity is preserved, but sparse matrix times sparse vector has <u>very little potential parallelism</u> (has *o(nnz)* work)

Parallelism: Multiple-source BFS

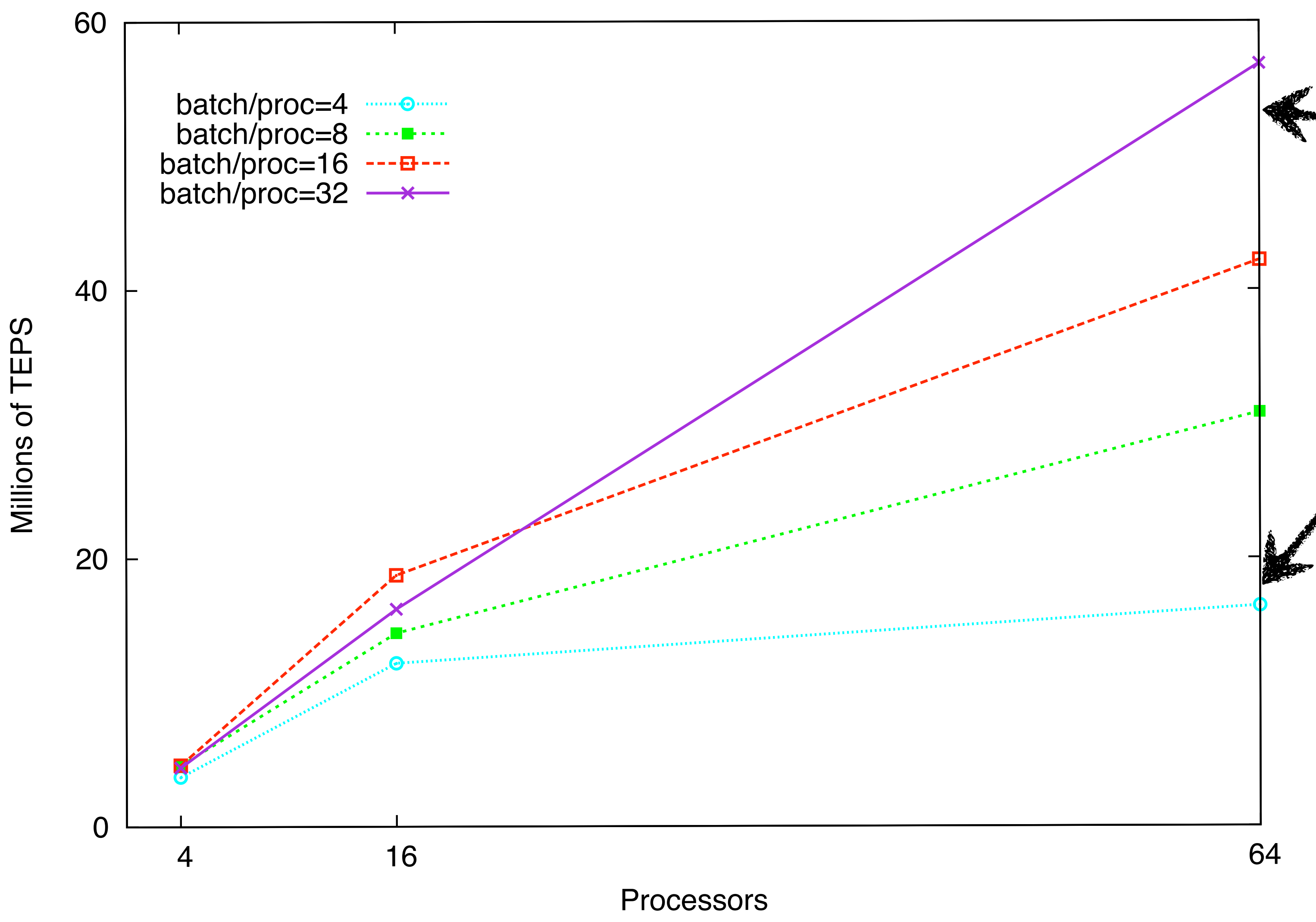


- Batch processing of multiple source vertices
- Sparse matrix-matrix multiplication => work efficient
- Potential parallelism is much higher
- Same applies to the tallying phase

Betweenness Centrality on Combinatorial BLAS

- <u>Semi-basic implementation:</u> *2D matrices*, synchronous matrix multiplication, no overlapping of communication with computation, *some remote DMA, mixed type arithmetic,* no template specialization for boolean matrices

Fundamental trade-off:
Parallelism vs memory usage



Batch processing greatly helps for large p

Input: RMAT scale 17
~1M edges only
• Likely to perform better on large inputs
• Code only a few lines longer than Matlab version

Thank You !

Questions?

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