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Task Parallel Approach to the Linear Algebra-Based Implementation of miniTri

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Center for Computing Research

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Sandia National Laboratories

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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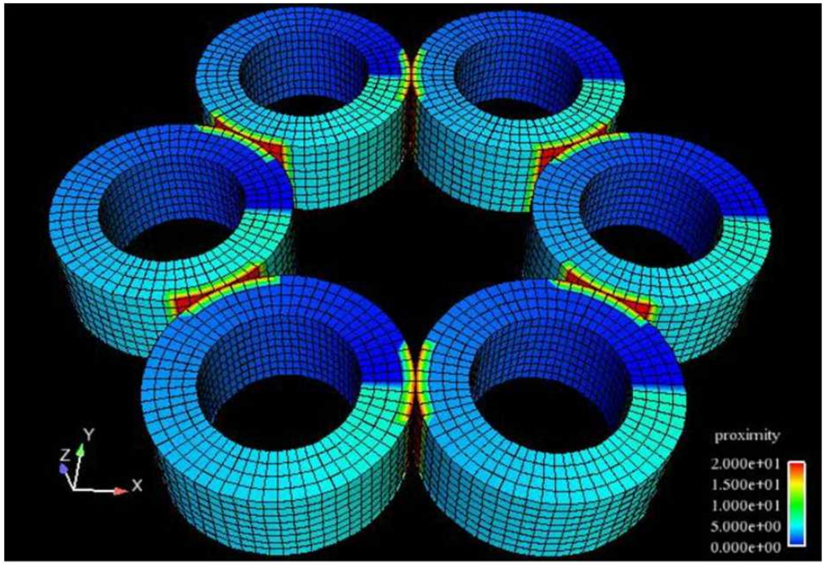
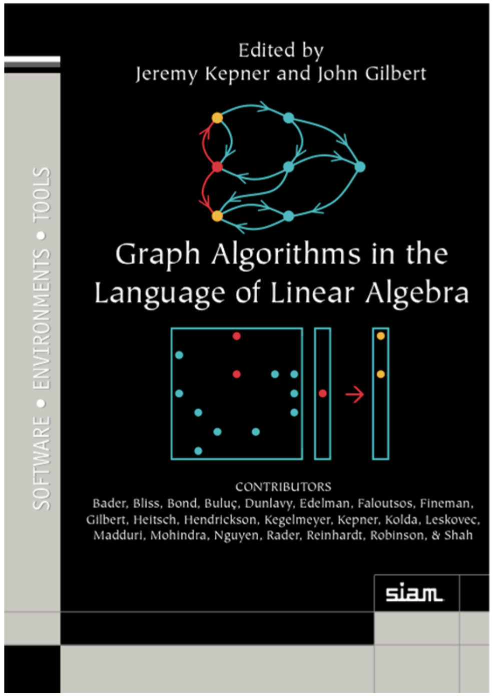
Miniapps



phdMesh (Mantevo)

- Small, self contained applications
- Proxy for important characteristics of full applications
- Important co-design tool: performance analysis
  - Target 1: existing applications on new and future architectures
  - Target 2: new applications on existing architectures
  - Strong partnership with industry
- Mantevo MiniApp Suite (Sandia): mantevo.org

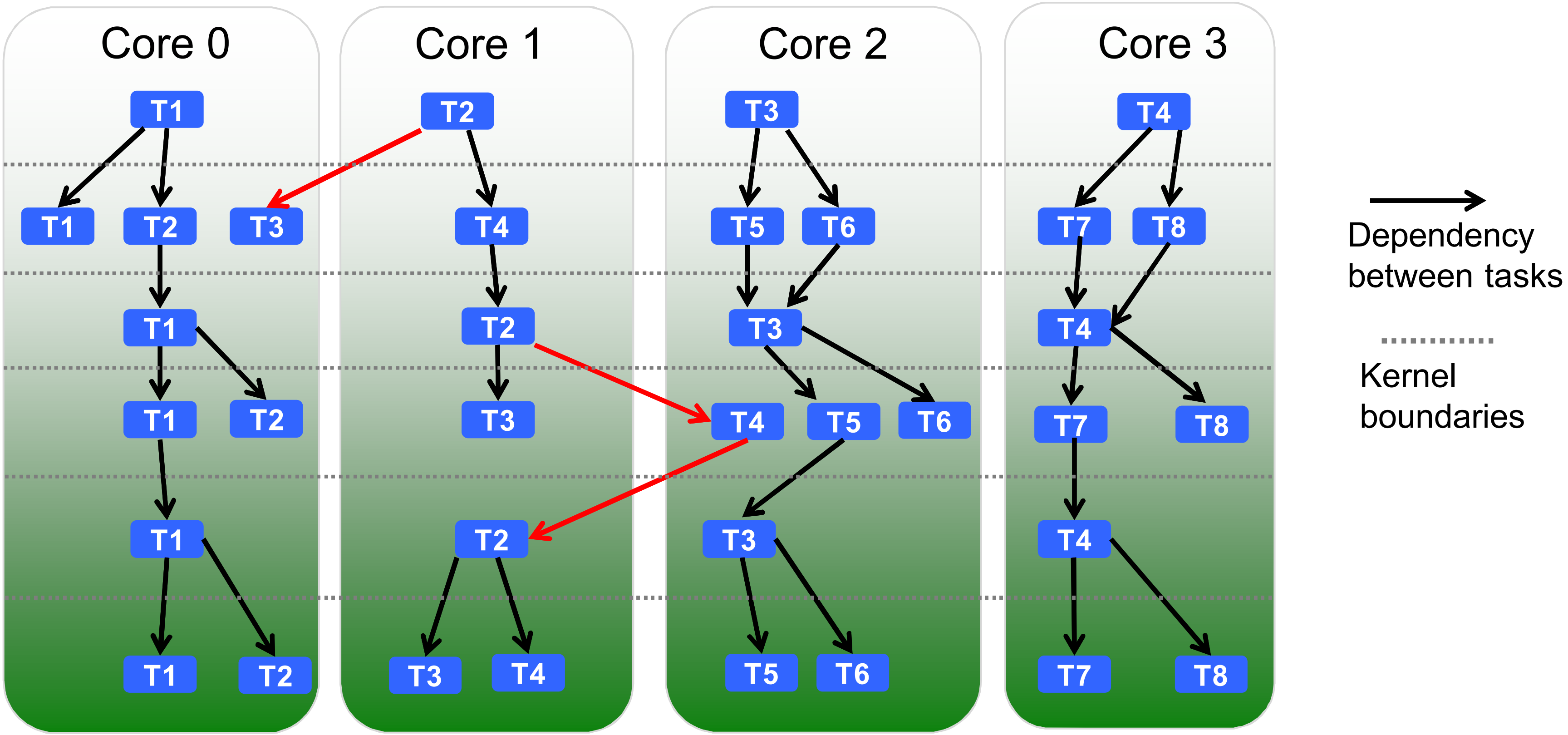
Graph BLAS



Eds. Kepner, Gilbert

- Effort to standardize building blocks for graph algorithms in language of linear algebra
  - Overloaded linear algebra kernels express most graph computations
  - Matrix-graph duality – highly impactful in CS&E (partitioning, solvers,…)
  - Promising for data sciences but many challenges

Task Parallelism



- Dataflow of application expressed through tasks/dependencies (Avoid explicit barriers between kernels)
- Overdecomposition of problem into tasks (# tasks > #cores)
- Tasks scheduled and moved to appropriate compute resources

Task Parallelism

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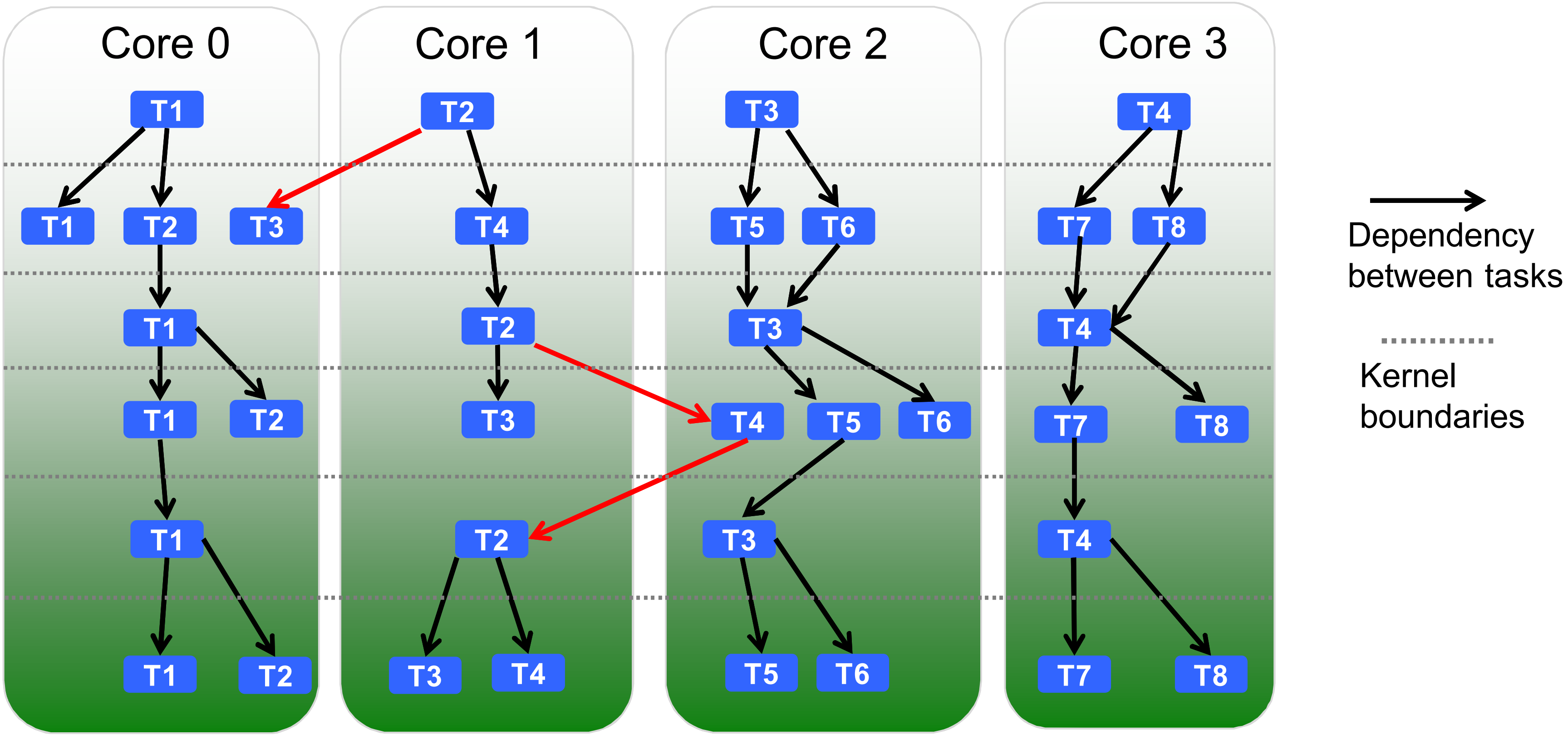
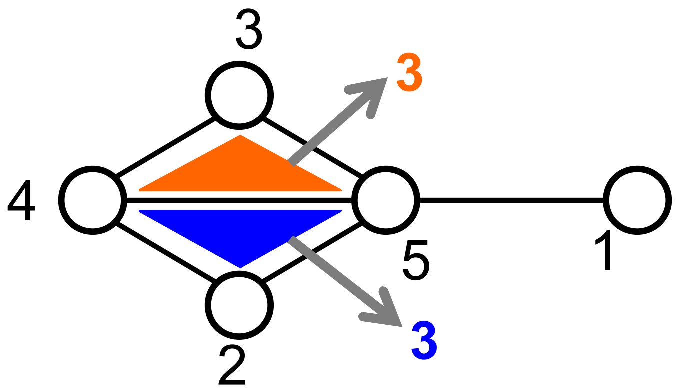


- Natural for data analytics (model intrinsically data-centric)
- Several task parallel models/libraries: **HPX**, **Kokkos/Qthreads**, Uintah, Legion, OCR, …

Outline

- Background
- ➡ miniTri
- Linear Algebra-Based miniTri (miniTriLA)
- Task Parallel Approach to miniTriLA
  - HPX
  - Kokkos/Qthreads
- Memory-Constrained Task Parallelism
- Summary

miniTri: Data Analytics Miniapp



k:

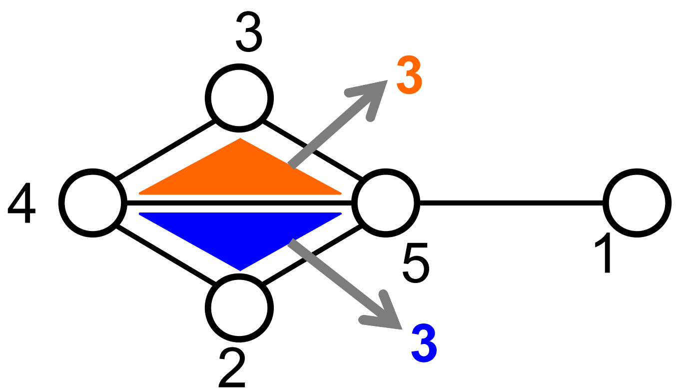
$$\arg\max_k \{(\min_{v \in t} t_v \geq \binom{k-1}{2}) \cap (\min_{e \in t} t_e \geq k-2)\}$$

Max clique size of given triangle

- Proxy for triangle based data analytics (Mantevo)
- Uses **triangle enumeration** + vertex/edge properties
- Key uses: **dense subgraph detection**, characterizing graphs, improving community detection, generating graphs
- Related applications in **cyber security**, **intelligence**, **functional biology**

miniTri is more application relevant than standard data analytics benchmarks such as Graph 500

miniTri: Overview



k:

$$\arg\max_k \{(\min_{v \in t} t_v \geq \binom{k-1}{2}) \cap (\min_{e \in t} t_e \geq k-2)\}$$

- miniTri Steps:
  - For each triangle, calculate triangle degrees for vertices and edges
  - For each triangle, calculate integer **k** given triangle degree info
- Developed 20+ variants
  - Different methods: buckets data structure, set intersection, linear algebra
  - Different programming models: OpenMP, MPI, HPX, Kokkos/Qthreads
- **Focus of talk:** linear algebra-based miniTri, task parallel models

Challenge: Can miniTri be implemented efficiently using Graph BLAS-like building blocks?

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Linear Algebra Based miniTri (miniTriLA)

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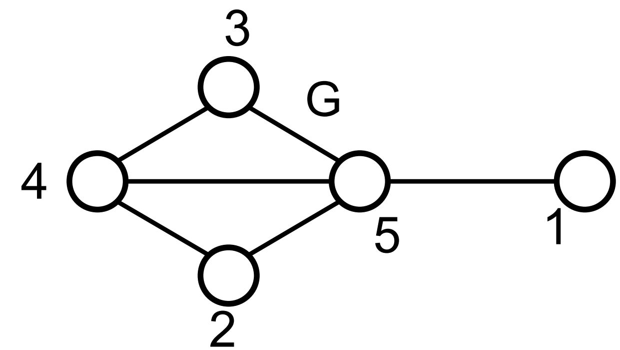
<u>miniTri</u>

$C = A * B$

$t_v = C * 1$

$t_e = C^T * 1$

$kcount(C, t_v, t_e)$



$$A = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 \end{pmatrix}$$

Adjacency matrix of G

$$B = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 & 1 \end{pmatrix}$$

Incidence matrix of G

- Developed Graph BLAS-like formulation of miniTri
- Important stressor of Graph BLAS

A = adjacency matrix for graph, B = incidence matrix for graph,
1 = vector of ones

miniTriLA: Triangle Enumeration

<u>miniTri</u>

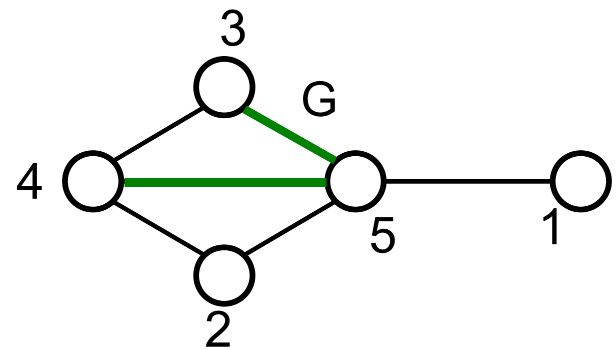
$C = A * B$

$t_v = C * 1$

$t_e = C^T * 1$

$kcount(C, t_v, t_e)$

Enumerates each triangle 3 times (once: C=L*B, where L is lower triangle part of A)



$$C = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 \end{pmatrix} * \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \emptyset & \emptyset & \emptyset & \emptyset & \emptyset & \emptyset \\ \emptyset & \emptyset & \emptyset & \emptyset & \emptyset & \{2,4,5\} \\ \emptyset & \emptyset & \emptyset & \emptyset & \emptyset & \{3,4,5\} \\ \emptyset & \{4,2,5\} & \{4,3,5\} & \emptyset & \emptyset & \emptyset \\ \emptyset & \emptyset & \emptyset & \{5,3,4\} & \{5,2,4\} & \emptyset \end{pmatrix}$$

Adjacency matrix of G — Incidence matrix of G — Matrix of Triangles

- Wedges implicitly stored in rows of A
  - Adj matrix: wedges = pairwise combinations of nonzero column ids + row #
  - E.g., row 5 wedges: {1,5,2}, {1,5,3}, {1,5,4}, {2,5,3}, {2,5,4}, {3,5,4}

A = adjacency matrix for graph, B = incidence matrix for graph, 1 = vector of ones

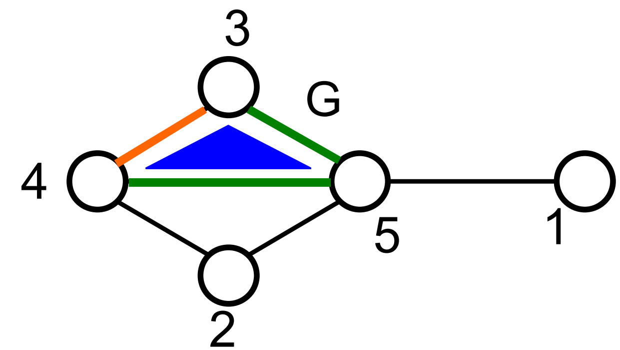
SPGEMM = Sparse Matrix Multiplication

miniTriLA: Triangle Enumeration

miniTri

```
C = A * B
t_v = C * 1
t_e = C^T * 1
kcount(C, t_v, t_e)
```

Enumerates each triangle 3 times (once: C=L*B, where L is lower triangle part of A)



$$C = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 \end{pmatrix} * \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \emptyset & \emptyset & \emptyset & \emptyset & \emptyset & \emptyset \\ \emptyset & \emptyset & \emptyset & \emptyset & \emptyset & \{2,4,5\} \\ \emptyset & \emptyset & \emptyset & \emptyset & \emptyset & \{3,4,5\} \\ \emptyset & \{4,2,5\} & \{4,3,5\} & \emptyset & \emptyset & \emptyset \\ \emptyset & \emptyset & \emptyset & \{5,3,4\} & \{5,2,4\} & \emptyset \end{pmatrix}$$

Adjacency matrix of G — Incidence matrix of G — Matrix of Triangles

- Columns of B tell us whether wedge is "closed" to form triangle
- Overloaded SpGEMM yields triangle enumeration:
  - If $A_{i,x}=A_{i,y}=1$ and $B_{x,j}=B_{y,j}=1$ (or equivalently $A_{i,*}B_{*,j}=2$), $C_{i,j}$ = triangle {i,x,y}
  - Else, no triangle

A = adjacency matrix for graph, B = incidence matrix for graph, 1 = vector of ones

SPGEMM = Sparse Matrix Multiplication

miniTriLA: Triangle Degree Calculation

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<u>miniTri</u>

C = A * B
$t_v = C * 1$
$t_e = C^T * 1$
kcount(C, t_v, t_e)

$$C=\begin{pmatrix} \emptyset & \emptyset & \emptyset & \emptyset & \emptyset & \emptyset \\ \emptyset & \emptyset & \emptyset & \emptyset & \emptyset & \{2,4,5\} \\ \emptyset & \emptyset & \emptyset & \emptyset & \emptyset & \{3,4,5\} \\ \emptyset & \{4,2,5\} & \{4,3,5\} & \emptyset & \emptyset & \emptyset \\ \emptyset & \emptyset & \emptyset & \{5,3,4\} & \{5,2,4\} & \emptyset \end{pmatrix}$$

$$t_v = \begin{pmatrix} \emptyset & \emptyset & \emptyset & \emptyset & \emptyset & \emptyset \\ \emptyset & \emptyset & \emptyset & \emptyset & \emptyset & \{2,4,5\} \\ \emptyset & \emptyset & \emptyset & \emptyset & \emptyset & \{3,4,5\} \\ \emptyset & \{4,2,5\} & \{4,3,5\} & \emptyset & \emptyset & \emptyset \\ \emptyset & \emptyset & \emptyset & \{5,3,4\} & \{5,2,4\} & \emptyset \end{pmatrix} * \mathbf{1} = \begin{pmatrix} 0 \\ 1 \\ 1 \\ 2 \\ 2 \end{pmatrix}$$

Triangles with v_4

$$t_e = \begin{pmatrix} \emptyset & \emptyset & \emptyset & \emptyset & \emptyset & \emptyset \\ \emptyset & \emptyset & \emptyset & \emptyset & \emptyset & \{2,4,5\} \\ \emptyset & \emptyset & \emptyset & \emptyset & \emptyset & \{3,4,5\} \\ \emptyset & \{4,2,5\} & \{4,3,5\} & \emptyset & \emptyset & \emptyset \\ \emptyset & \emptyset & \emptyset & \{5,3,4\} & \{5,2,4\} & \emptyset \end{pmatrix}^T * \mathbf{1} = \begin{pmatrix} 0 \\ 1 \\ 1 \\ 1 \\ 1 \\ 2 \end{pmatrix}$$

Triangles with $e_{4,5}$

Overloaded SpMV to count triangles in rows

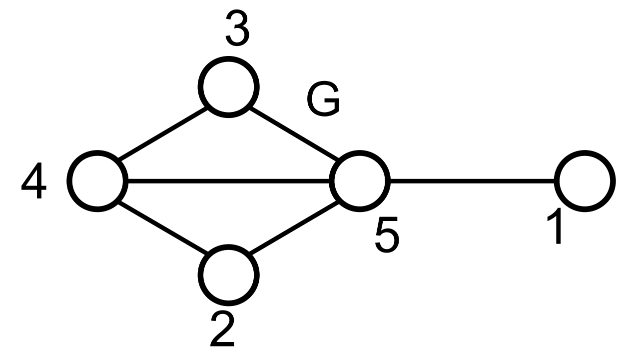
- Triangle degree calculation
  - Each triangle represented once in C for each of its edges and vertices
  - Triangle vertex and edge degrees are number of nz in rows and columns

A = adjacency matrix for graph, B = incidence matrix for graph,
1 = vector of ones

miniTriLA: Kcounts

<u>miniTri</u>

```
C = A * B
t_e = C * 1
t_v = C^T * 1
kcount(C, t_e, t_v)
```



k:

$$\arg\max_k \{(\min_{v \in t} t_v \geq \binom{k-1}{2}) \cap (\min_{e \in t} t_e \geq k-2)\}$$

K	1	2	3
triangle count	0	0	2

- Compute **k** for each triangle (summarize in table)
- **k**-count table gives us upper bound on largest clique in graph
  - Largest *c* such that Comb(*c*,3) triangles have *k*-counts at least *c*

A = adjacency matrix for graph, B = incidence matrix for graph,
1 = vector of ones

miniTriLA: Challenges

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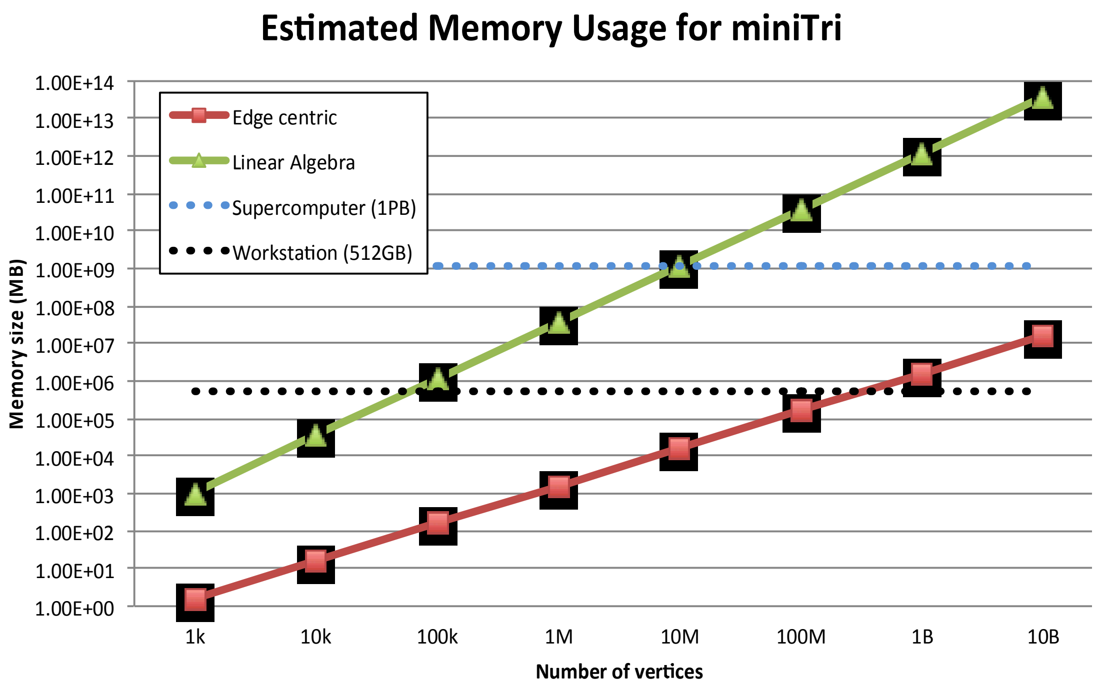
miniTri

```
C = A * B
t_e = C * 1
t_v = C^T * 1
kcount(C, t_e, t_v)
```



- Challenge 1: Computation difficult to load-balance
- Challenge 2: Typical Graph BLAS approach forms C, which means storing all triangles in graph
  - Worst case: $O(|E|^{3/2})$ triangles in graph, typical: 100-1000 triangles/edge
  - Severely limits size of graph

A = adjacency matrix for graph, B = incidence matrix for graph,
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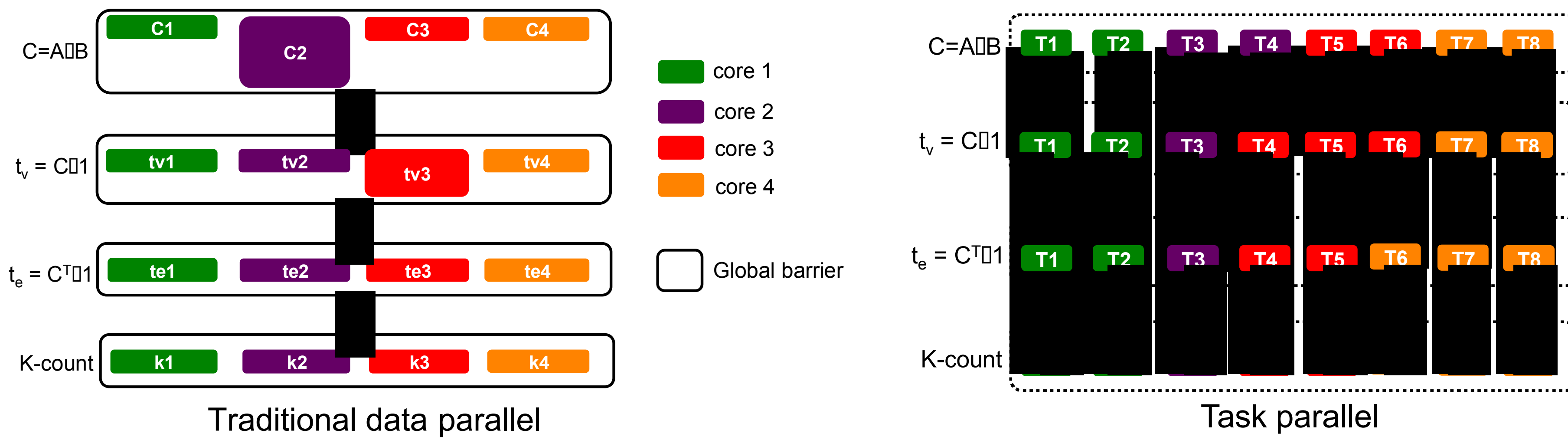
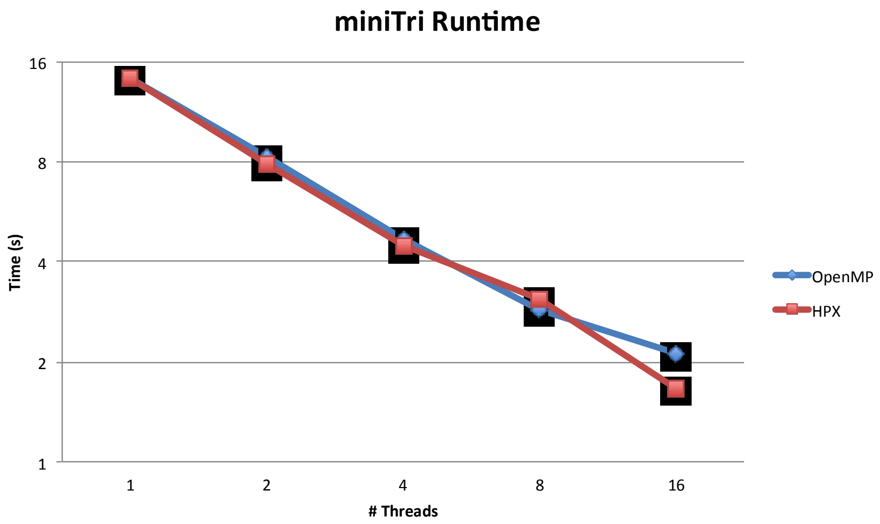
Task Parallel Approach

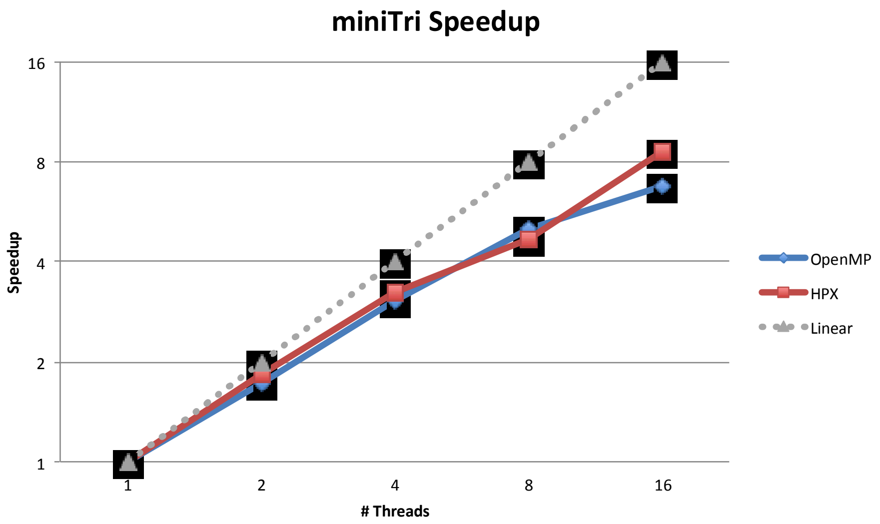


Illustrative Example of GraphBLAS Approaches

- Each block of linear algebra operations assigned to a task
  - Block of rows, 2D block of elements
- Global barriers between kernels removed
  - Replaced by dependencies between tasks
  - Tasks in subsequent kernels can start/finish before first kernel finishes

HPX-3 Implementation

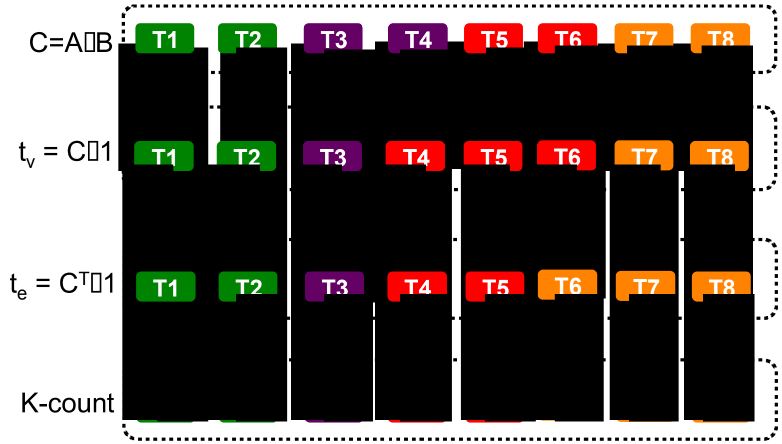




- HPX-3 (LSU)
  - General purpose C++ runtime system
  - Supports both on-node and inter-node tasks parallelism
  - Active global address space (AGAS)
  - Lightweight control objects instead of global barriers

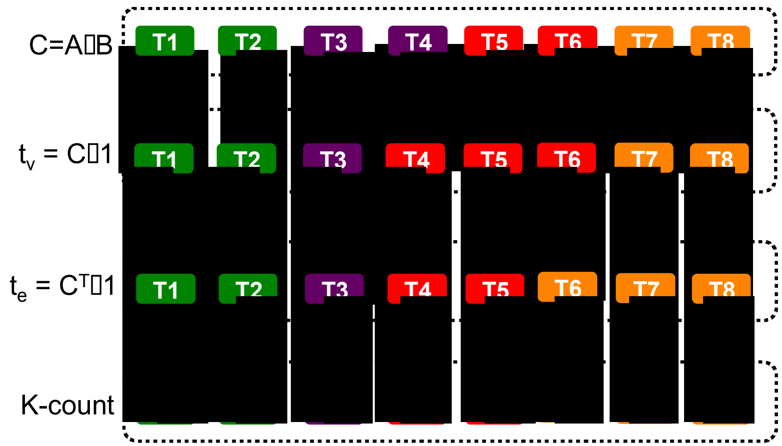
Preliminary results show similar performance of task parallel and data parallel approaches

Kokkos/Qthreads Implementation



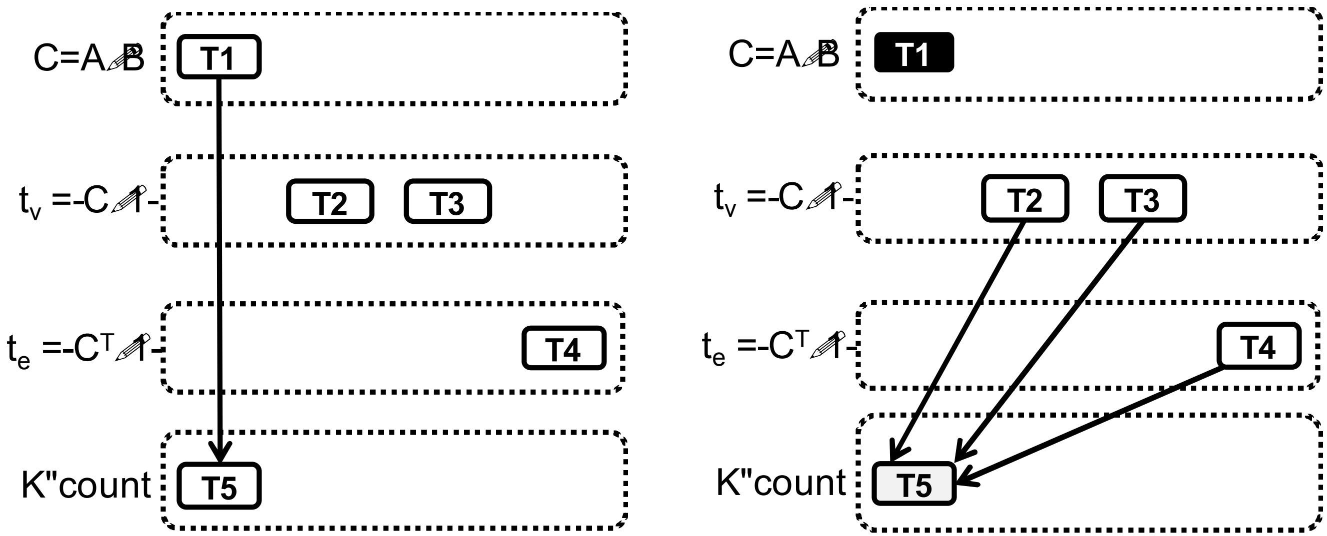
- Kokkos
  - Performance portable programming model and C++ library implementation for intra-node (shared memory) parallelism
  - Supports diverse manycore architectures (GPUs, CPUs, Intel MIC, …)
  - **policy** manages how tasks are scheduled using task-DAG pattern
- Qthreads
  - C-based multithreading library inspired by MTA/XMT architectures
  - Runtime system to execute Kokkos API's task-DAG pattern

Kokkos Task Parallel API



- Task Creation
  - f = policy.create(func);
  - f – future; func – functor that creates/executes tasks
- Setting Dependencies
  - policy.add_dependence(f1, f2);
  - f1, f2 – futures such that task corresponding to f1 depends on task corresponding to f2
- Launch Tasks
  - policy.spawn(f); // f is future

Dynamic Task Dependencies of miniTri



T5 initially spawned | T5 respawned once T1 complete

- Complication with asynchronous task parallel miniTri
  - kcount task (e.g., T5) dependencies not known until after corresponding triangle enumeration task (e.g., T1) is complete
- Kokkos provides respawn functionality
  - Relaunches task
  - Necessary for portability to GPUs (tasks can't yield to other tasks)
  - miniTri exploits this feature to handle dynamic dependencies

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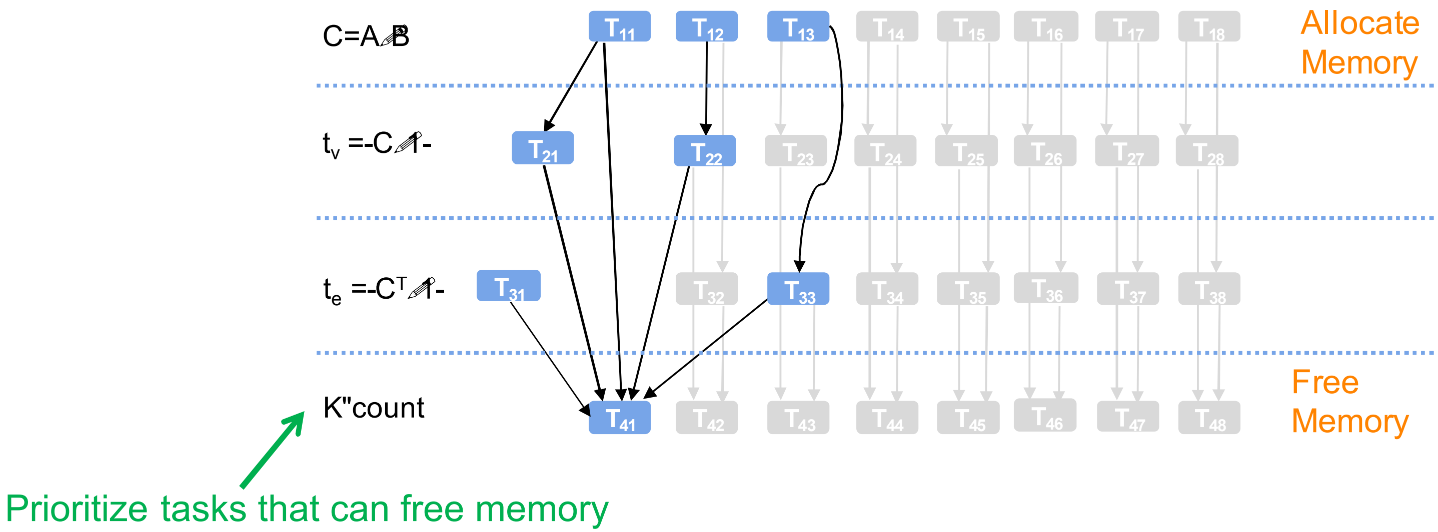
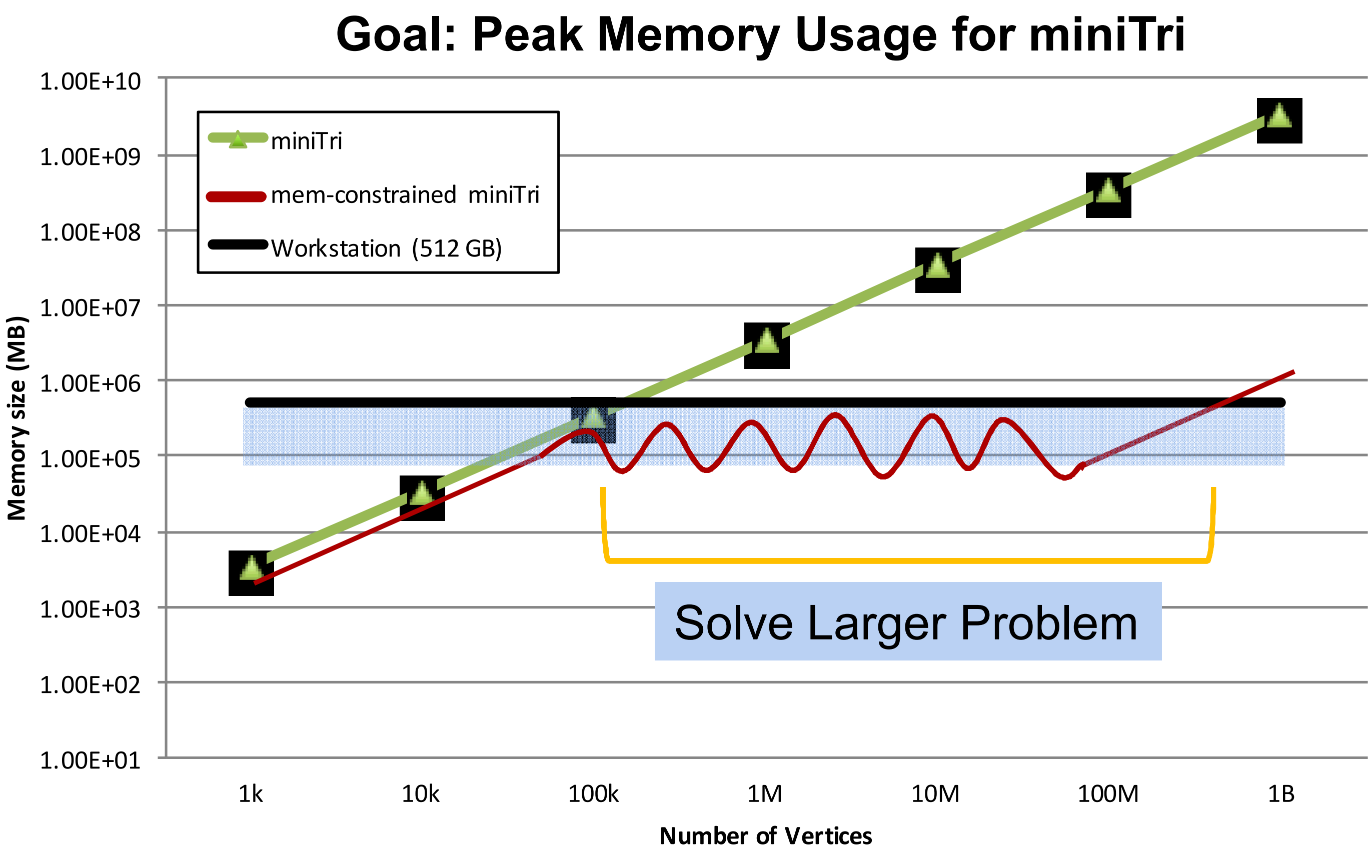
Addressing Challenge #2 with Memory-Constrained Task Parallelism



- Key insight: Tasks can be scheduled asynchronously to free temporary memory early
  - Prioritize k-count tasks to free blocks of triangles from memory
  - **Need runtime system to support advanced resource management/priorities (on-going effort: Kokkos/Qthreads and HPX)**

Asynchrony can be exploited to reduce peak memory of application

Memory-Constrained Task Parallelism



Task parallelism with memory-constrained scheduling allows solution of larger problems

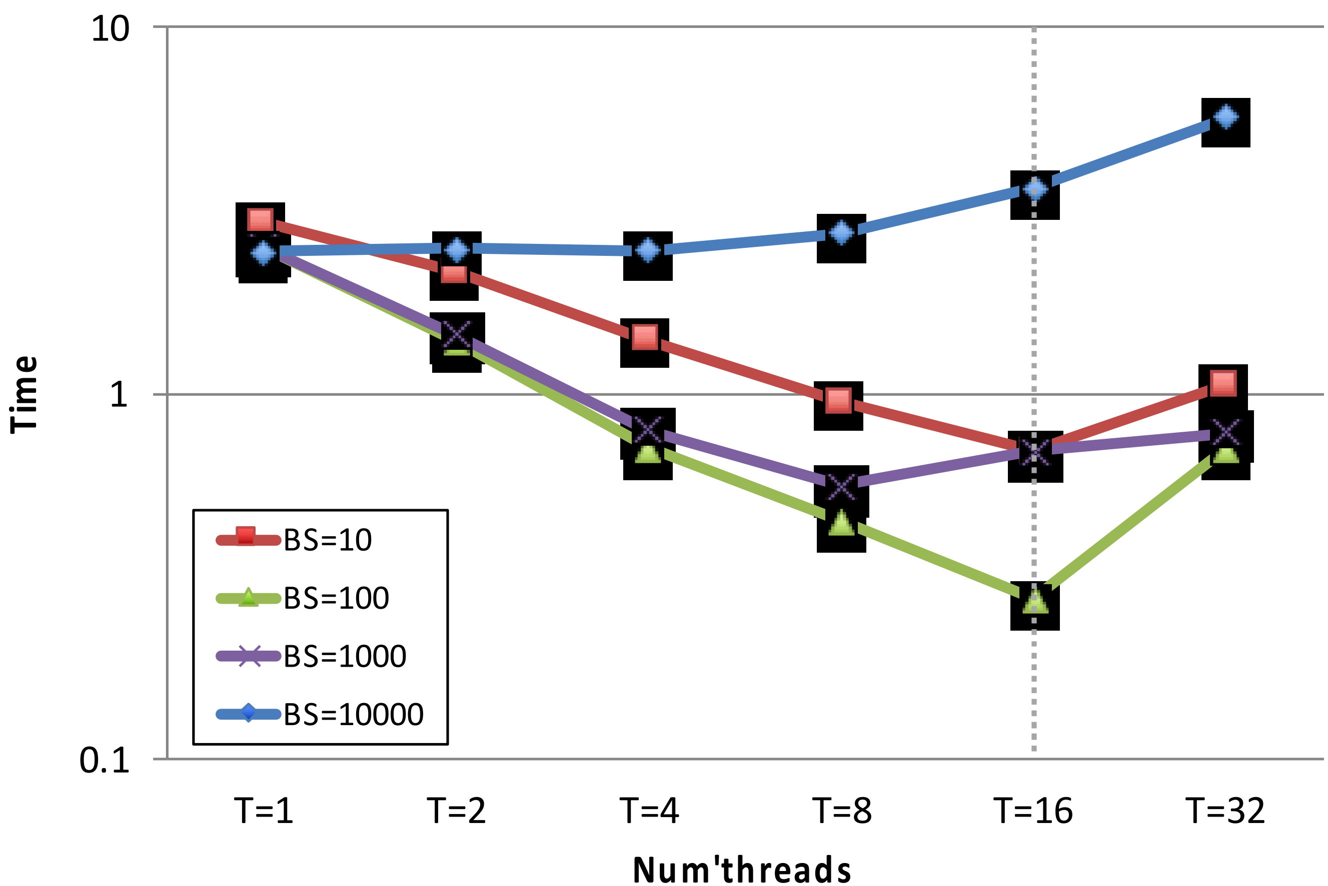
Kokkos/Qthreads miniTri Experiments

Graph	|V|	|E|	|T|	|T|/|E|
Oregon-1	11174	23409	19894	0.85
email-Enron*	36692	183831	727044	3.95
ca-AstroPh*	18772	198110	1352469	6.87
com-Youtube	1157827	2987624	3056386	1.02

- 16 core workstation with 64 GB of memory (dual processor Intel Xeon E5-2630 v3 @ 2.40 GHz)
- SNAP datasets (http://snap.stanford.edu)
  - Oregon-1: autonomous system dataset
  - email-Enron: Enron email network
  - ca-AstroPh: Arxiv Astro Physics collaboration network
  - com-Youtube: social network dataset

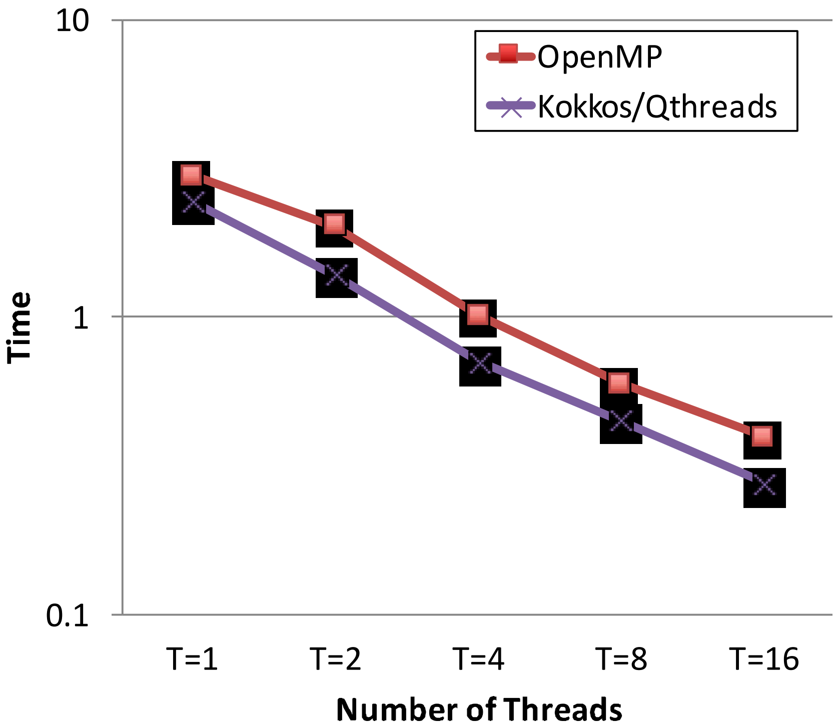
* University of Florida Sparse Matrix Collection

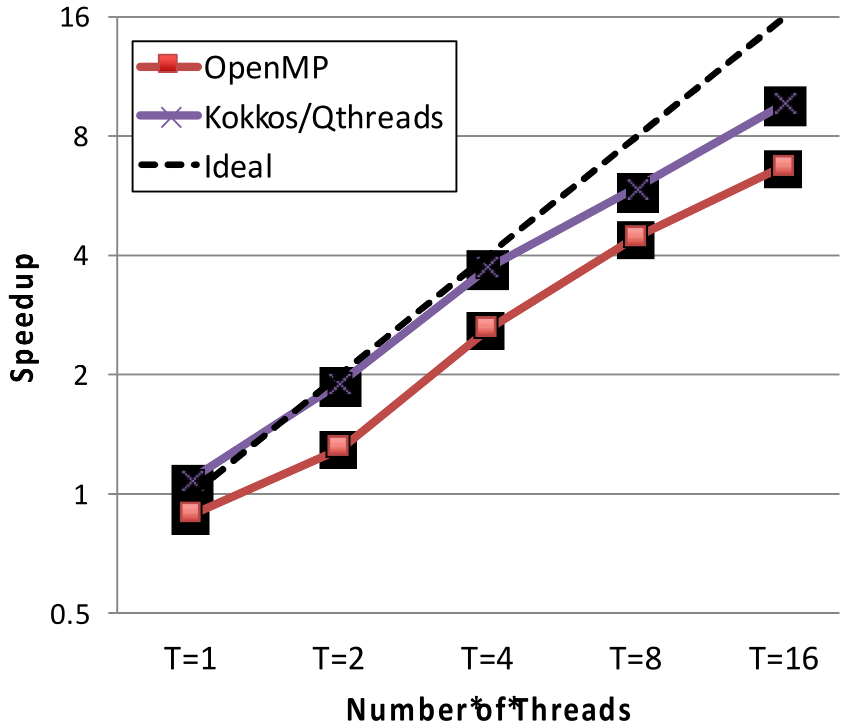
Oregon-1: Kokkos/Qthreads



Improvements in runtimes up to 16 threads for block sizes of 100

Oregon-1: Kokkos vs. OpenMP





Kokkos/Qthreads performs significantly better than OpenMP

email-Enron: Kokkos vs. OpenMP

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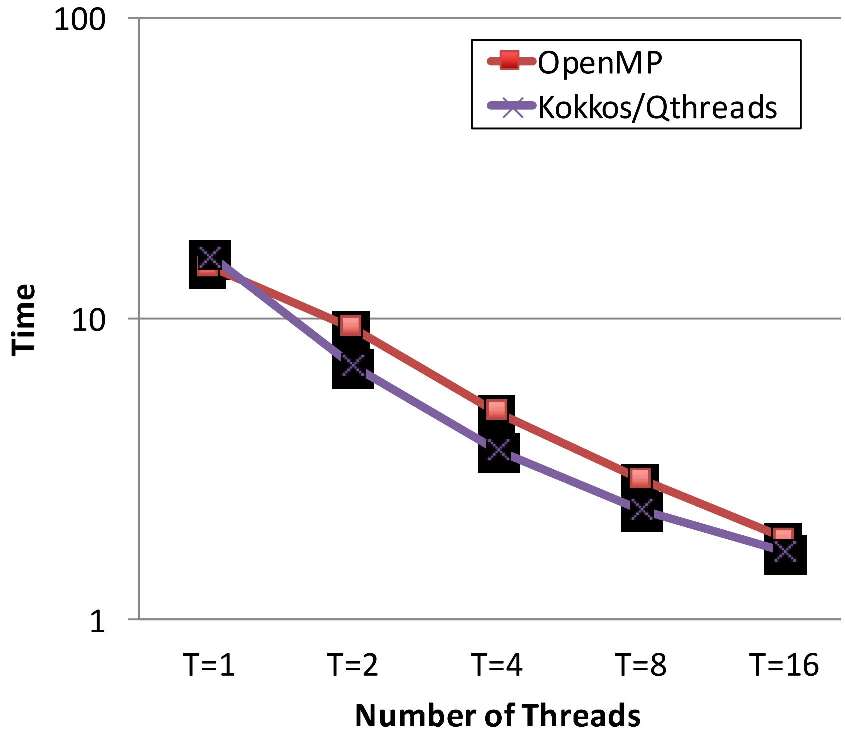
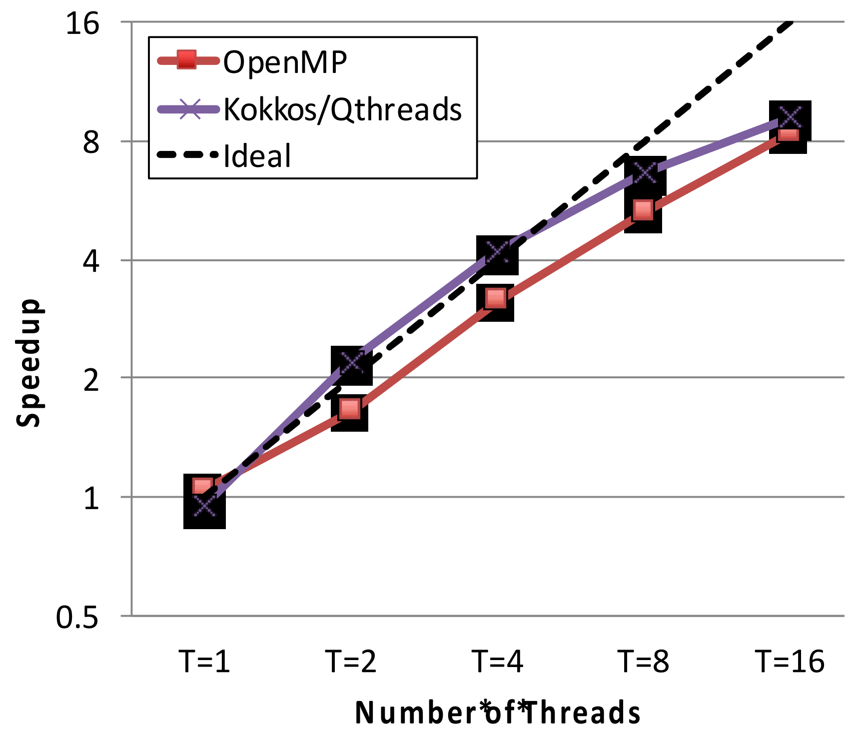
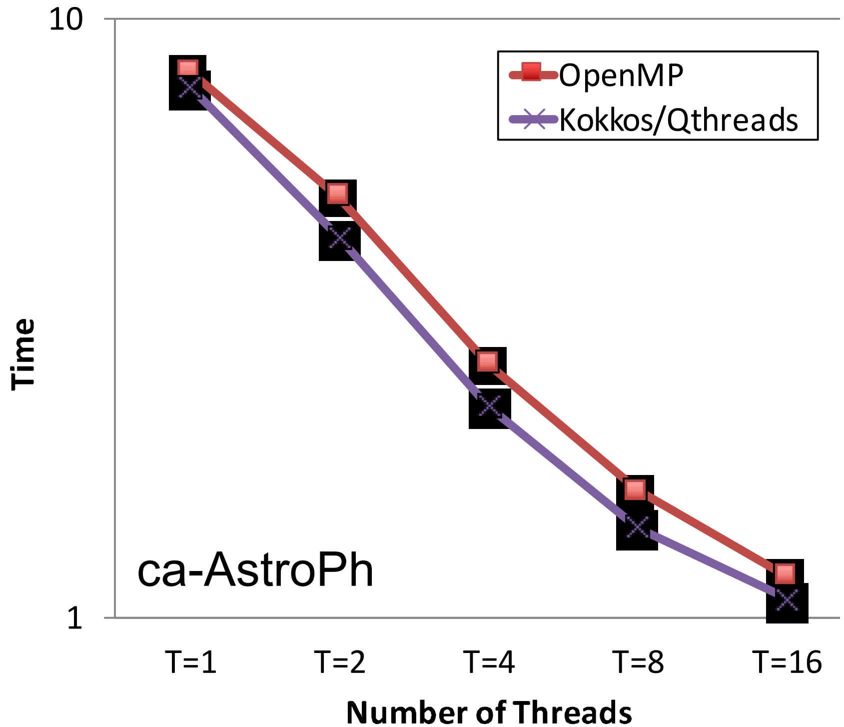
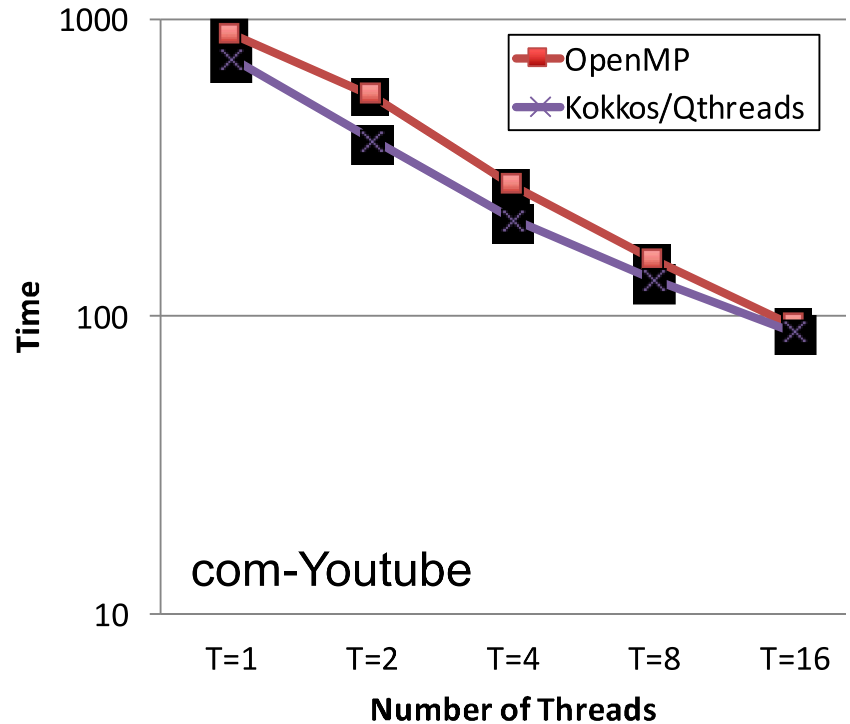




Kokkos/Qthreads performs slightly better than OpenMP

Kokkos vs. OpenMP: ca-AstroPh, com-Youtube





Kokkos/Qthreads performs slightly better than OpenMP

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Summary/Conclusions

- Overview of new data analytics miniapp **miniTri**
  - Application relevant, released as part of Mantevo
- Presented linear algebra-based formulation of miniTri
  - miniTri in 4 compact linear algebra-based operations
  - Asynchronous, task parallel approach for constraining memory usage
- Described Kokkos/Qthreads task parallel implementation that outperforms data parallel (OpenMP) implementation
- Graph BLAS powerful approach for expressing graph algorithms
  - However, significant challenges exist for implementing certain graph applications efficiently (e.g., miniTri)
  - Linear algebra kernels should exploit **asynchrony** for more flexibility (e.g., solving larger problems) and better future performance – task parallelism helps here

Acknowledgements

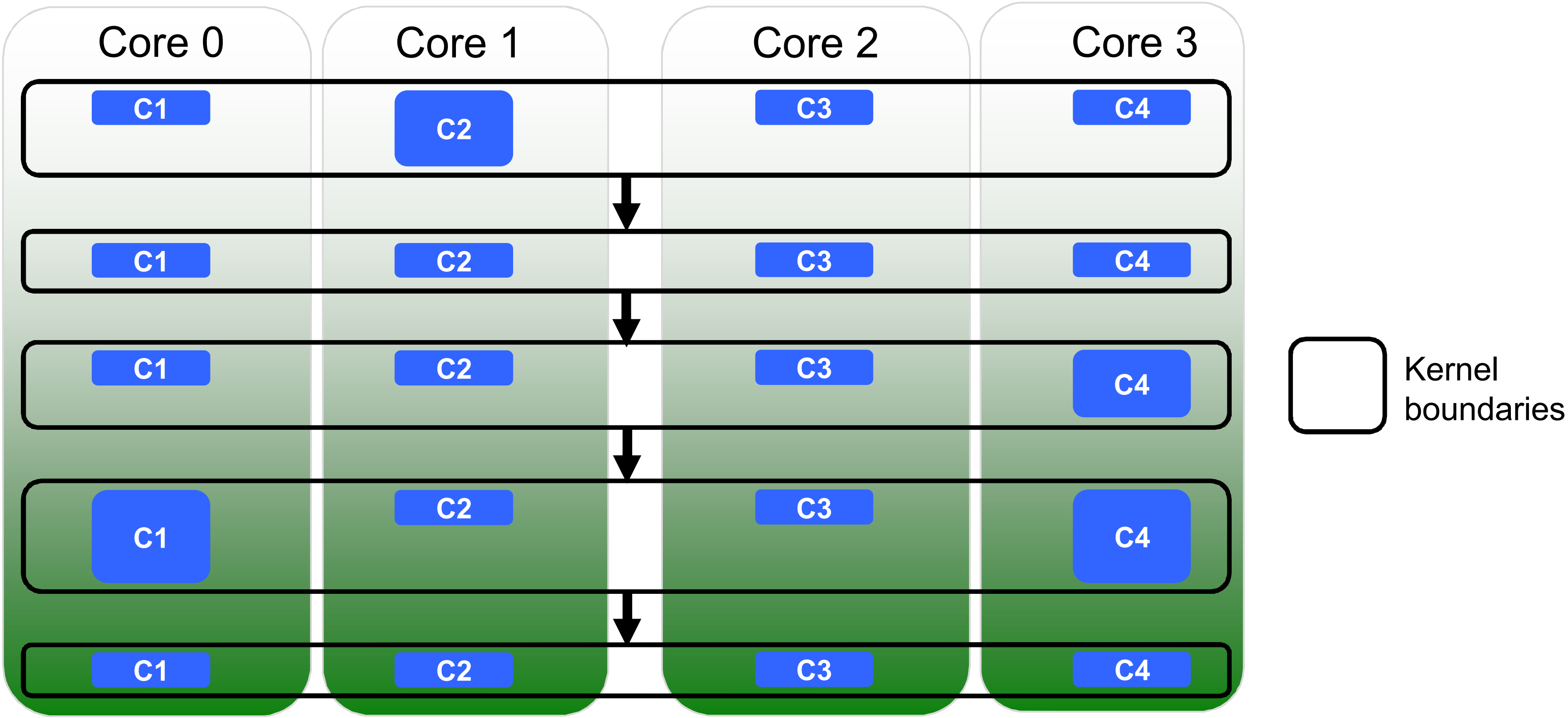
- Jon Berry (SNL)
  - Co-author of miniTri
- Carter Edwards (SNL)
  - Kokkos Lead
- Stephen Olivier (SNL)
  - Qthreads Lead
- Hartmut Kaiser, Daniel Bourgeois (LSU)
  - HPX

Additional Info/Resources

- miniTri now released under Mantevo repo
  - mantevo.org
  - Repo moving to github: **https://github.com/mantevo**
- Related publications
  - Wolf, Berry, Stark: "A Task-Based Linear Algebra Building Blocks Approach for Scalable Graph Analytics," *2015 IEEE HPEC*.
  - Wolf, Edwards, Olivier: "Kokkos/Qthreads Task-Parallel Approach to Linear Algebra Based Graph Analytics," *2016 IEEE HPEC* (to appear)
- Kokkos
  - https://github.com/kokkos
- Qthreads
  - https://github.com/Qthreads/qthreads

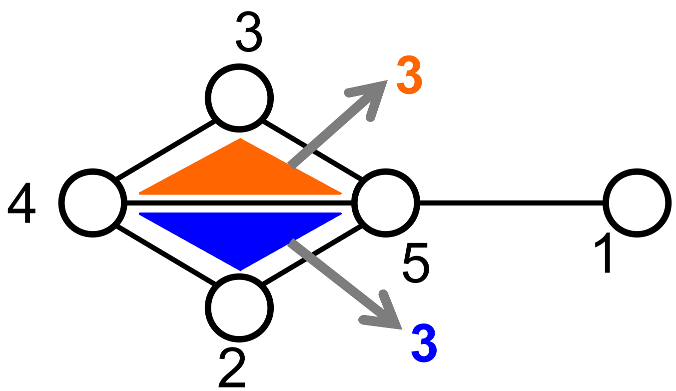
Extra

Traditional Data Parallelism



- **Data distributed across cores**
- **Global barriers between kernels**

kcount



k:

$$\arg\max_k \{(\min_{v \in t} t_v \geq \binom{k-1}{2}) \cap (\min_{e \in t} t_e \geq k-2)\}$$

- Upper bound on largest clique in graph = largest *c* such that Comb(*c*,3) triangles have *k*-counts at least *c*
  - Any v of *k*-clique, incident on Comb(*k*-1,2) triangles of that clique
  - Any e of *k*-clique, incident on *k*-2 triangles of that clique
  - argmax selects the largest *k* satisfying these condition (largest clique containing triangle)

miniTriLA: Challenges

miniTri

$C = A * B$
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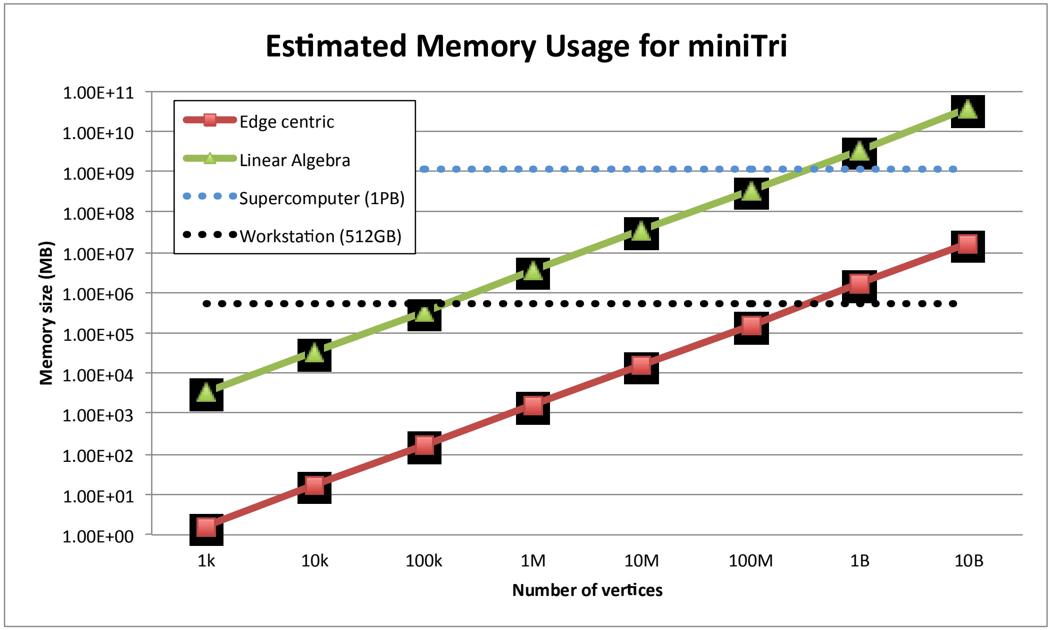
$t_v = C^T * 1$
$kcount(C, t_e, t_v)$



- Challenge 1: Computation difficult to load-balance
- Challenge 2: Graph BLAS approach forms C, which means storing all triangles in graph
  - Worst case: $O(|E|^{3/2})$ triangles in graph, typical: 100-1000 triangles/edge
  - Severely limits size of graph

A = adjacency matrix for graph, B = incidence matrix for graph,
1 = vector of ones

Summary

- Overview of new data analytics miniapp **miniTri**
  - Will be released soon as part of Mantevo
- Presented linear algebra-based formulation of miniTri
  - miniTri in 4 compact linear algebra-based operations
  - Graph Algorithm Building Block (GABB) for triangle enumeration
  - GABBs for calculating triangle vertex and edge degree
- miniTri poses challenges for Graph BLAS-like implementations
  - Load balancing, Memory usage
- Presented task parallel approach that addresses these challenges
  - Asynchrony is key
  - Can use task priorities to constrain memory usage