Parallel Combinatorial Computing and Sparse Matrices

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Outline

Fundamental question: What performance metrics are right?

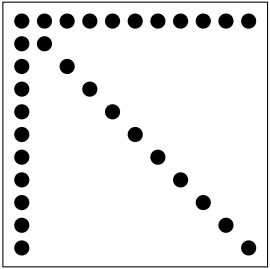
Background

Algorithms
  - Sparse Transpose
  - Weighted Bipartite Matching

Setting Performance Goals

Ordering Ideas

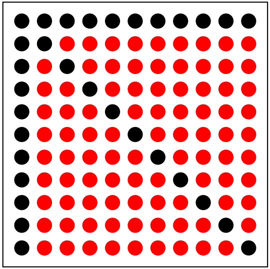
App: Sparse *LU* Factorization



Characteristics:

- Large quantities of numerical work.
- Eats memory and flops.
- Benefits from parallel work.
- And needs combinatorial support.

App: Sparse *LU* Factorization



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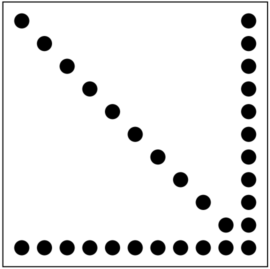


Combinatorial support:

- Fill-reducing orderings, pivot avoidance, data structures.
- Numerical work is distributed.
- Supporting algorithms need to be distributed.
- Memory may be cheap ($100 GB), moving data is costly.

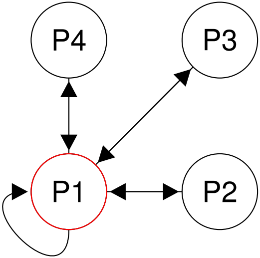
Sparse Transpose

Data structure manipulation

- Dense transpose moves numbers, sparse moves numbers and re-indexes them.
- Sequentially space-efficient "algorithms" exist, but disagree with most processors.
  - Chains of data-dependent loads
  - Unpredictable memory patterns

If the data is already distributed, an unoptimized parallel transpose is better than an optimized sequential one!

Parallel Sparse Transpose



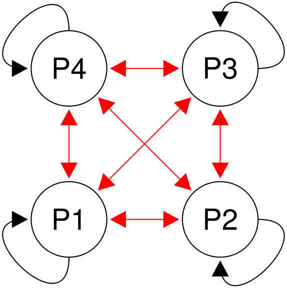
Many, many options:

- Send to root, transpose, distribute.
- Transpose, send pieces to destinations.
- Transpose, then rotate data.
- Replicate the matrix, transpose everywhere.

Communicates most of matrix twice. Node stores whole matrix.

Note: We should compare with this implementation, not purely sequential.

Parallel Sparse Transpose



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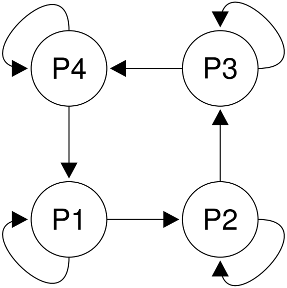
All-to-all communication. Some parallel work.

Parallel Sparse Transpose



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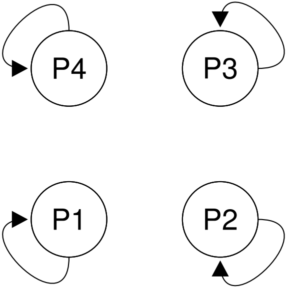
Serial communication, but may hide latencies.

Parallel Sparse Transpose



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Useful in some circumstances.

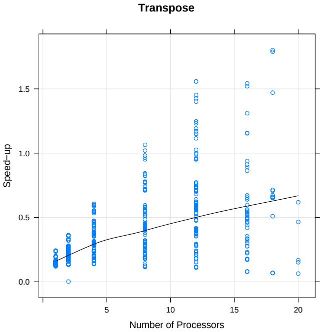
What Data Is Interesting?

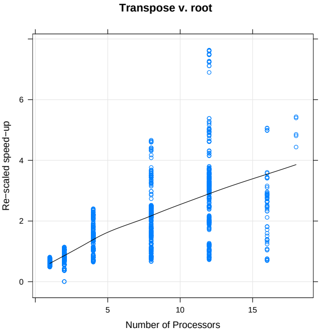
- Time

What Data Is Interesting?

- Time (to solution)
- How much data is communicated.
- Overhead and latency.
- Quantity of data resident on a processor.

Parallel Transpose Performance

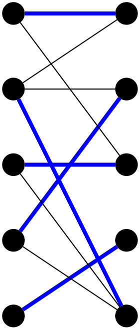




- All-to-all is slower than pure sequential code, but distributed.
- Actual speed-up when the data is already distributed.
- Hard to keep constant size / node when performance varies by problem.

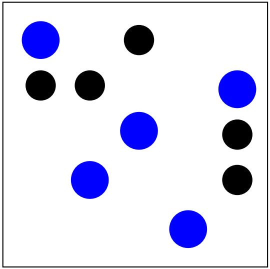
Data from CITRIS cluster, Itanium2s with Myrinet.

Weighted Bipartite Matching



- Not moving data around but finding where it should go.
- Find the “best” edges in a bipartite graph.
- Corresponds to picking the “best” diagonal.
- Used for static pivoting in factorization.
- Also in travelling salesman problems, *etc*.

Weighted Bipartite Matching



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Algorithms

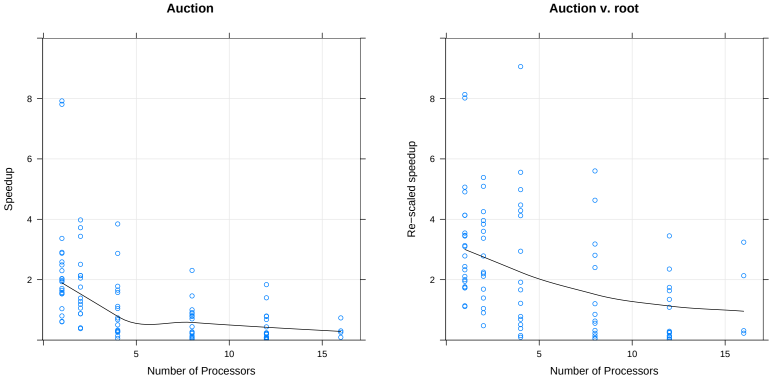
Depth-first search

- Reliable performance, code available (MC64)
- Requires A and A^T.
- Difficult to compute on distributed data.

Interior point

- Performance varies wildly; many tuning parameters.
- Full generality: Solve larger sparse system.
- Auction algorithms replace solve with iterative bidding.
- Easy to distribute.

Parallel Auction Performance



Compare with running an auction on the root, a parallel auction achieves slight speed-up.

Proposed Performance Goals

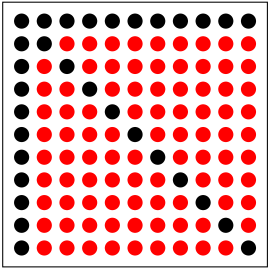
When is a distributed combinatorial algorithm (or code) successful?

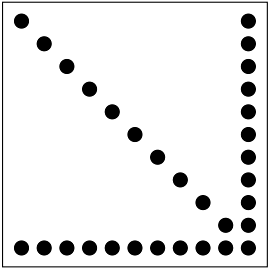
- Does not redistribute the data excessively.
- Keeps the data distributed.
- No process sees more than the whole.
- Performance is competitive with the on-root option.

Pure speed-up is a great goal, but not always reasonable.

Distributed Matrix Ordering

Finding a permutation of columns and rows to reduce fill.





NP-hard to solve, difficult to approximate.

Sequential Orderings

Bottom-up

- Pick columns (and possibly rows) in sequence.
- Heuristic choices:
  - Minimum degree, deficiency, approximations
- Maintain symbolic factorization

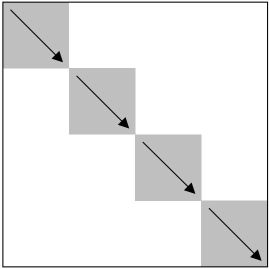
Top-down

- Separate the matrix into multiple sections.
  - Graph partitioning: $A + A^T$, $A^T \cdot A$, A
- Needs vertex separators: Difficult.

Top-down Hybrid

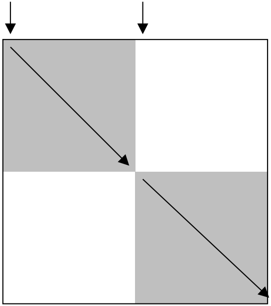
- Dissect until small, then order.

Parallel Bottom-up Hybrid Order



1. Separate the graph into chunks.
    - Needs an edge separator,
    - and knowledge of the pivot.
2. Order each chunk separately.
    - Forms local partial orders.
3. Merge the orders.
    - What needs communicated?

Merging Partial Orders



Respecting partial orders

- Local, symbolic factorization done once.
- Only need to communicate quotient graph.
  - Quotient graph: Implicit edges for Schur complements.
- No node will communicate more than the whole matrix.

Preliminary Quality Results

Merging heuristic

- Pairwise merge.
- Pick the head pivot with least worst-case fill (Markowitz cost).

Small (tiny) matrices: performance not reliable.

Matrix	Method	NNZ increase
west2021	AMD $(A + A^T)$	1.51×
	merging	1.68×
orani678	AMD	2.37×
	merging	6.11×

Increasing the numerical work drastically spends any savings from computing a distributed order. Need better heuristics?

Summary

- Meeting classical expectations of scaling is difficult.
  - Relatively small amounts of computation for much communication.
  - Problem-dependent performance makes equi-size scaling hard.
- But consolidation costs when data is already distributed.

In a supporting role, don't sweat the speed-up.
Keep the problem distributed.

Open topics

- Any new ideas for parallel ordering?