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Sparse Communication Avoiding Pivoting

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25th Biennial Numerical Analysis Conference
June 2013

Communication avoiding pivoting: why?

Now:

- K10 GPU has 16,384 threads for 1,536 "cores" (or 48 warps)
- Xeon Phi has 240 threads for 60 cores
- Typical workstation 32 threads for 16 cores

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- More, less powerful, lower clocked cores
- Multiple threads per core to hide latencies

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More cores = More communication

Communication isn't getting (that much) faster

Sparse direct solvers

Solve:

$$Ax = b$$

Where A is

- Large
- Sparse

and for this talk

- Symmetric

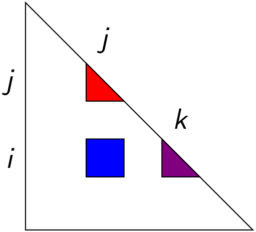
Using the factorization

$$A = LDL^T$$

LDL^T factorization

Work by blocks:

- Factorize dense blocks on diagonal using dense algorithm $A_{jj} = L_{jj} D_{jj} L_{jj}^T$
- "Divide" remainder of column by diagonal block $L_{ij} = A_{ij} L_{jj}^{-T}$
- Update matrix to right as $A_{ik} = A_{ik} - L_{ij} D_{jj} {L_{kj}}^T$



Threshold Partial Pivoting

For backwards stability:

- Sufficient to bound entries of L
- Threshold test such that $L_{ij} = A_{ij}L_{jj}^{-T}$ yields $l_{ij} \leq u^{-1}$
- Need to consider whole column

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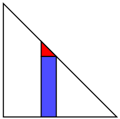
1×1 pivot test

$$|a_{jj}| \geq u \max_{i>j} |a_{ij}|$$



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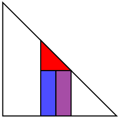

2×2 pivot test

$$\left| \begin{pmatrix} a_{jj} & a_{j(j+1)} \\ a_{j(j+1)} & a_{(j+1)(j+1)} \end{pmatrix}^{-1} \right| \begin{pmatrix} \max_{i>j+1} |a_{ij}| \\ \max_{i>j+1} |a_{i(j+1)}| \end{pmatrix} \leq \begin{pmatrix} u^{-1} \\ u^{-1} \end{pmatrix}$$

Alternatives

Various a priori treatments to reduce/eliminate need for pivoting:

- Scaling. “Normalize” entries of A

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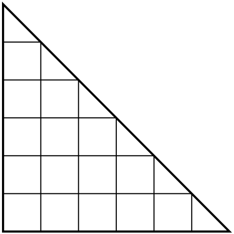
A combination of these approaches works for 95% of real matrices.

For the other 5% we need pivoting!

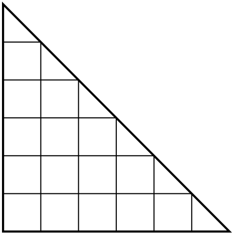
Parallel decomposition

- Apply 2D data decomposition



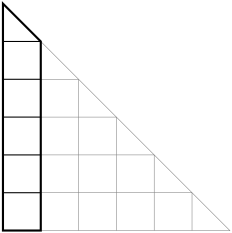
Parallel decomposition

- Apply 2D data decomposition
- Update step parallelizes nicely as per _gemm

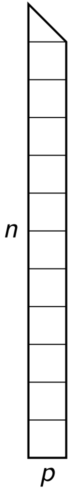


Parallel decomposition

- Apply 2D data decomposition
- Update step parallelizes nicely as per `_gemm`
- For pivoting equivalent to 1D on tall skinny matrix



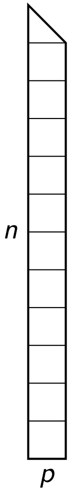
Parallel Variants



Various options:

- Restricted pivoting: only pivot within diagonal block
- Assume all pivots are valid, check L maxima a posteriori
- Traditional TPP

Parallel Variants



Various options:

- Restricted pivoting: only pivot within diagonal block
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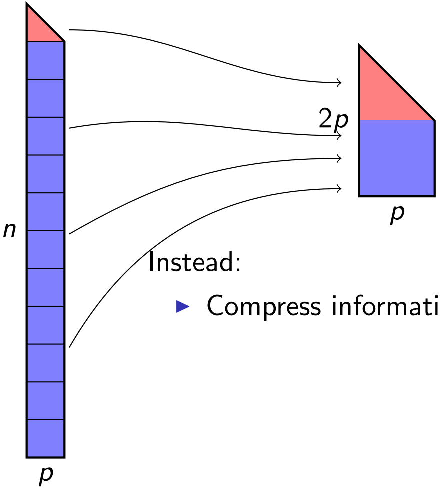
Parallel variant TPP:

- **Either** one thread owns the diagonal block
- **or** each thread has its own copy of diagonal block
- Regardless, needs a reduction for every pivot
- $O(p \log n)$ messages

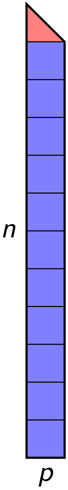
Compressed pivoting

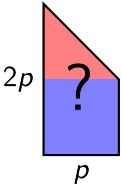


Instead:

- Compress information into small matrix

Compressed pivoting





Instead:

- Compress information into small matrix
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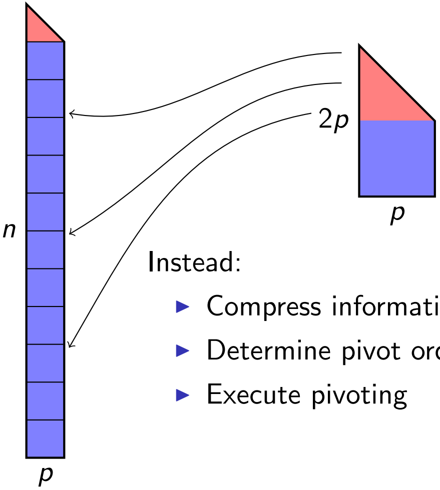

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- Compress information into small matrix
- Determine pivot order
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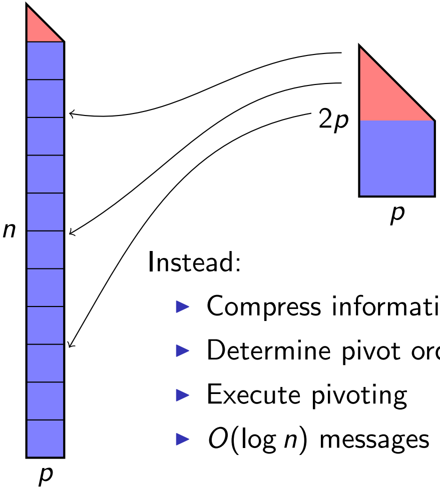

Instead:

- Compress information into small matrix
- Determine pivot order
- Execute pivoting
- $O(\log n)$ messages rather than $O(p \log n)$

Strict Compressed Pivoting

1. Partition rows into sets by column of maximum $|a_{ij}|$

$$\begin{pmatrix} 12 & 10 & 10 \\ 2 & 3 & 4 \\ & 10 & -3 \\ 4 & -5 & 4 \\ & -6 & 8 \end{pmatrix}$$

Partitioned rows

Strict Compressed Pivoting

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Compressed matrix

Strict Compressed Pivoting

1. Partition rows into sets by column of maximum $|a_{ij}|$
2. Represent each set by single row: take maximum $|a_{ij}|$
3. Update using a "worst-case" formula

$$\begin{pmatrix} 12 & 10 & 10 \\ 2 & 3 & 4 \\ & 10 & -3 \\ 4 & -5 & 4 \\ & -6 & 8 \end{pmatrix}$$

Partitioned rows

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Compressed matrix

- Provably backwards stable
- Sometimes too pessimistic

Relaxed example

1. For each column, pick a "representative" row: largest $|a_{ij}|$
2. Apply standard threshold partial pivoting.

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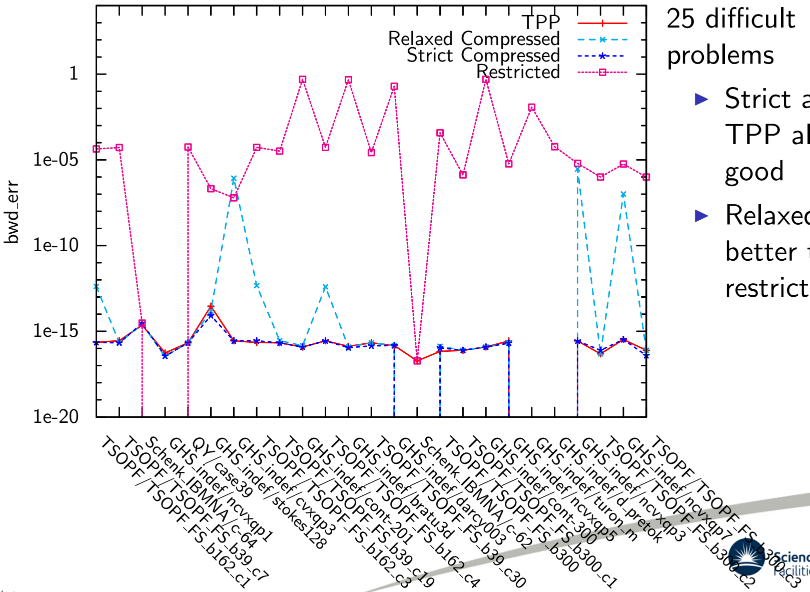
Compressed matrix

- Not backwards stable!
- Stable in practice (see results)

Results: numerical stability



25 difficult problems

- Strict and TPP always good
- Relaxed better than restricted

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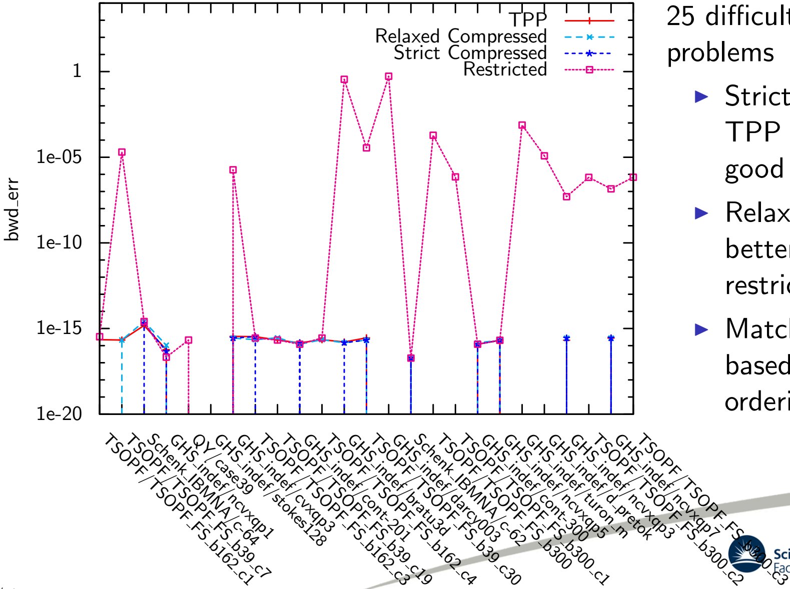
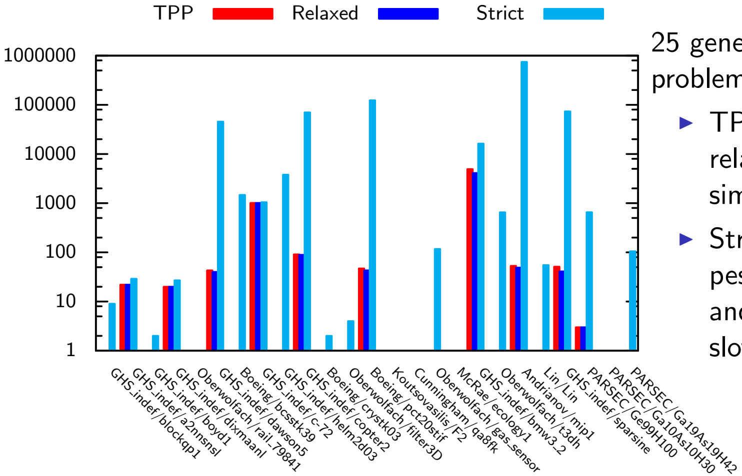


25 difficult problems

- Strict and TPP always good
- Relaxed better than restricted
- Matching-based ordering helps

Results: delays



25 general problems

- TPP and relaxed very similar
- Strict very pessimistic and hence slow

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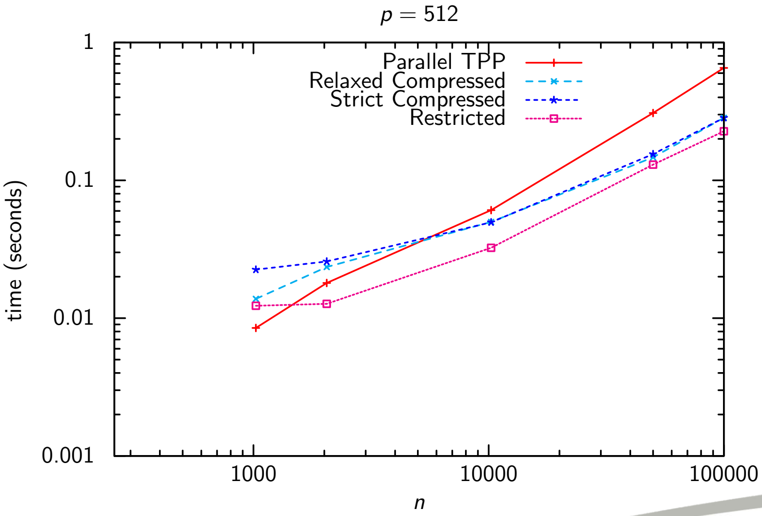
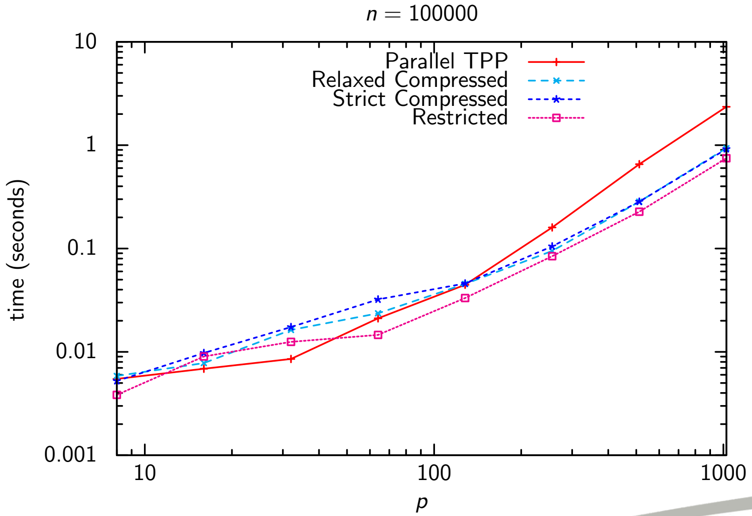
Results: speed $p = 512$



Results: speed $n = 100000$



Conclusions

Summary

- CPU compressed pivoting 2+ times faster on large problems
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- Factorize without pivoting and check L
- If too large, roll-back factorization and...
- ...use compressed pivoting to minimize communication

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Now do it on a GPU!

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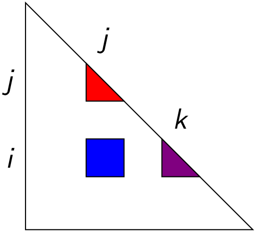
Thank you!

Stability



- What if diagonal block is **singular**?
- What if off-diagonal entries **much larger** than diagonal entries?

Then factorization is **not** backwards stable