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Challenges in Parallel Sparse Direct Linear Solvers

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Perspectives on Parallel Numerical Linear Algebra
18th July 2012

Sparse Direct Solvers

Solve

$$Ax = b$$

where A is Sparse.

Direct Methods Factorize $A = LU$, solve $Ly = b$, $Ux = y$.

Black-box, robust, **compute-bound**.

Memory-hungry⇒ slow for large matrices?.

Iterative Methods CG, GMRES, BiCGStab, etc.

Matrix-free. Fast? Efficient? **memory-bound**.

Non-robust, performance depends on preconditioner.

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Sparse Direct Solvers

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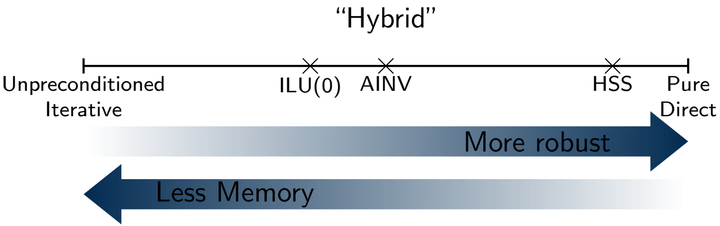
New view: Spectrum



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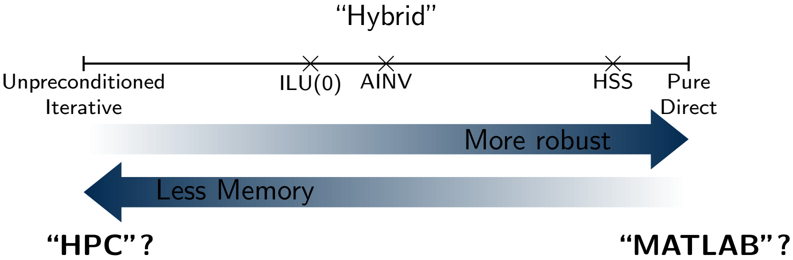
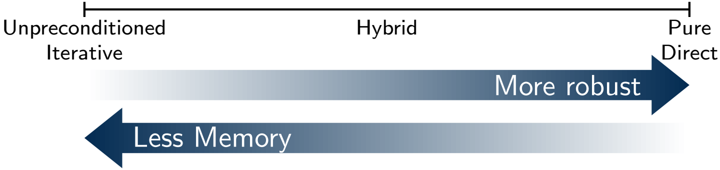


Horses for Courses



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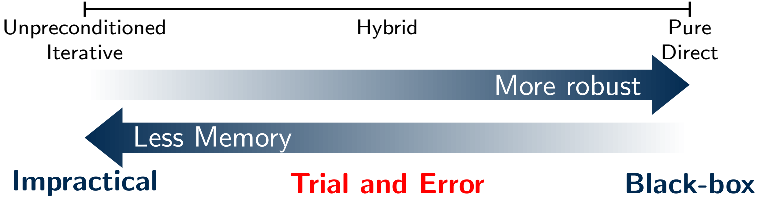

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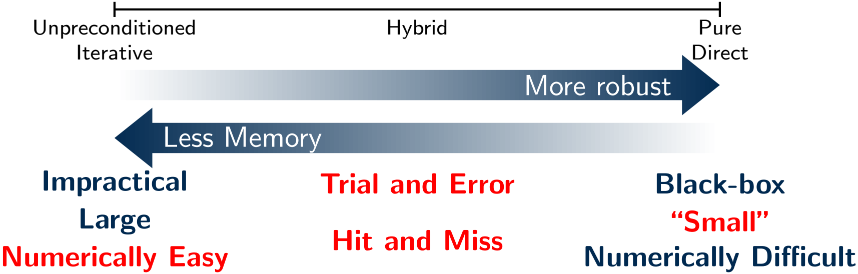

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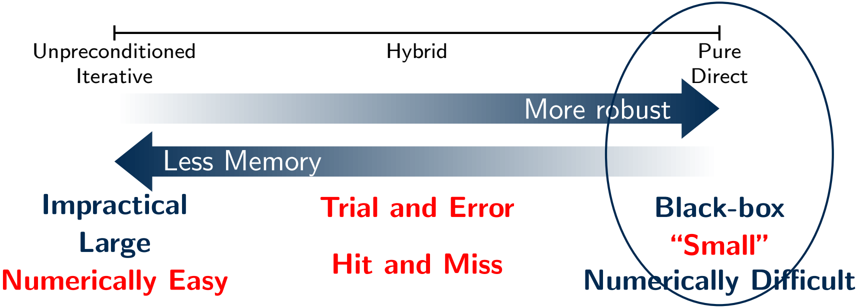

Challenge: + Parallel

Challenge #1: **“Small” + Parallel**

We need to achieve strong scaling.

Example

Non-linear optimization solver, unknown problem origin
$\Rightarrow$ Preconditioning difficult (at best)!

Direct solver: solves 100 systems ($n = 35000$) to reach solution in 5 seconds. 95% of time in linear solver.
$\Rightarrow$ 0.05s per serial factorization
Maybe 2 million flops with 250,000 non-zeroes (8 flops/non-zero)

2015 desktop: 16 CPU cores + 1024 GPU cores?
$\Rightarrow$ Fewer than 250 non-zeroes per core!

Challenge #1: **"Small" + Parallel**

We need to achieve strong scaling.

8 flops/non-zero ⇒ Communication is King!
Work by *Laura Grigori*, *Jim Demmel* and others:
Communication avoiding algorithms

A small world:
Avoid fine-grained communication — latency hurts.

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Assume flops are (almost) free: what can we do?

- Generic compression [bandwidth]
- Low-rank approximation (HSS preconditioning) [bandwidth]
- Speculative assumptions on numerical stability [latency]

Generic Compression

J.D. Hogg and J.A. Scott
A note on the solve phase of a multicore solver
RAL-TR-2010-007

Idea:
Compress data blocks before storing factors, decompress into cache before use. Otherwise 1 flops/non-zero in solve phase.

LZO Compression Library Higher compression than GZIP, *much* faster.

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Outcome:

Performance matched that of original algorithm:
Wait for more flops/unit bandwidth.

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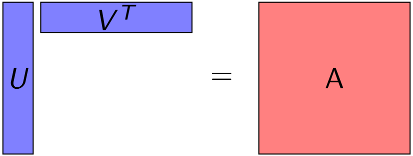
Low-rank approximation

Multiple works by *J. Xia, S. Chandrasekaran, M. Gu, X.S. Li* et al.

Idea:

Communicate low rank approximations not large dense matrices

Rank-revealing QR:



Flops are cheap!

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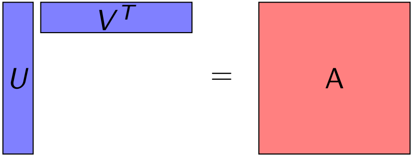

Flops are cheap!

Outcome:

Good *preconditioner* for some classes of matrix.

More work needed!

Speculative assumptions on numerical stability

PARDISO: *O. Schenk* et al.
Static pivoting, weighted matchings: *I.S. Duff* and others.

Idea:
Assume no pivoting is needed; don't do pivoting.

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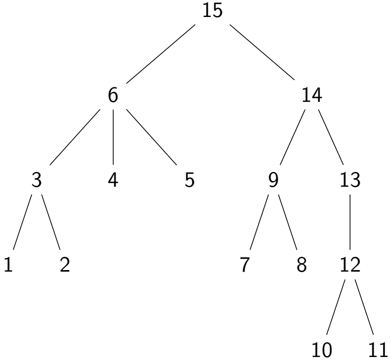
Outcome:
Works for majority of matrices.
But: Not for some *difficult* matrices — what direct solvers are for!

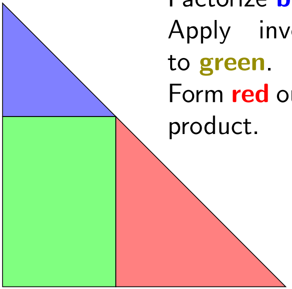
Challenge #2: **Numerically difficult + Parallel**

Need to do **pivoting** for stability — in parallel.

Sparse Direct Primer:

Organises into tree of dense linear algebra + sparse scatters





Factorize **blue**. Apply inverse to **green**. Form **red** outer product.

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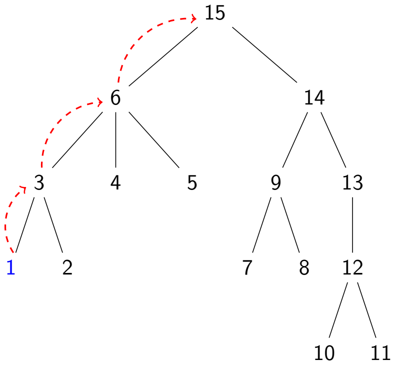

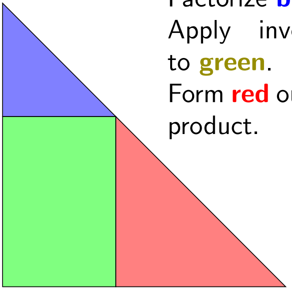

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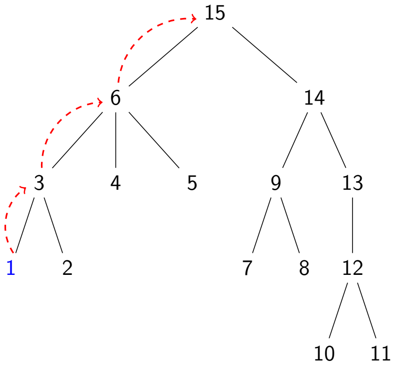

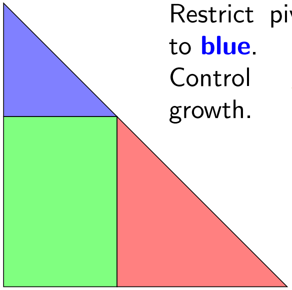

Restrict pivoting to **blue**.

Control **green** growth.

Challenge #2: **Numerically difficult + Parallel**

Need to do **pivoting** for stability — in parallel.

Observations:

- Want to start factorization of diagonal block *before* rest of column is ready.
- Even for difficult matrices, delayed pivots generally restricted to few subtrees.
- Assume pivoting will work; backtrack if it doesn't.
- Achieve the best of both worlds?

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Challenge #2: **Numerically difficult + Parallel**

Need to do **pivoting** for stability — in parallel.

Otherwise:

- Currently test 1×1 and 2×2 pivots
- Use larger block pivots?
- Sparse analog to tournament pivoting?

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Challenge #3: Bit-compatibility?

Bit-compatibility: Getting the same answer twice.

$$1 + (\epsilon/2 + \epsilon/2) \neq (1 + \epsilon/2) + \epsilon/2$$

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Why would we not do this?

- If we don't, answers are still equally valid
- Less efficient: restrict parallelism, optimization
- More difficult to achieve
- Must be achieved by all libraries used

Challenge #3: Bit-compatibility?

Bit-compatibility: Getting the same answer twice.

$$1 + (\epsilon/2 + \epsilon/2) \neq (1 + \epsilon/2) + \epsilon/2$$

But it's very attractive

- Hard to debug without it: make it an option?
- Confuses non-expert users no end
- Methods built on top may behave unexpectedly:

  e.g. Different local maxima found for non-linear optimization
  Different iteration counts

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Achieving bit-compatibility

Option #1: Add up in the same order

J.D. Hogg and J.A. Scott, **HSL_MA97**

Enforce ordering on additions:

$$((1+2)+3)+4 \qquad \text{or} \qquad (1+2)+(3+4).$$

Option #2: Add up in high precision

Use quad or double-double precision to store intermediate results

Ideally requires sufficient cache to hold intermediate results.

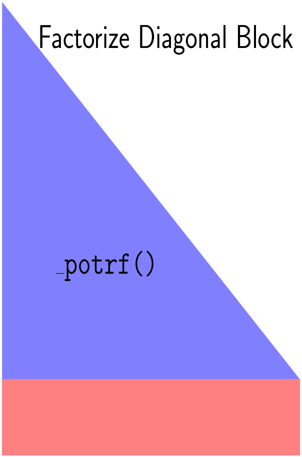
Task-based

Sparse task-based implementation *exist*: `HSL_MA86`, `HSL_MA87`, `PaStiX`.

Problems:

- Block alignments — need dynamic reblocking for best efficiency.
- Building on top of LAPACK/PLASMA — dynamic reblocking on same data desirable.
- Building on top of LAPACK/PLASMA — can we use the same task scheduler?
- Dynamic task sizing — splitting/merging across levels.
- Bit-compatibility?

Supernodal method



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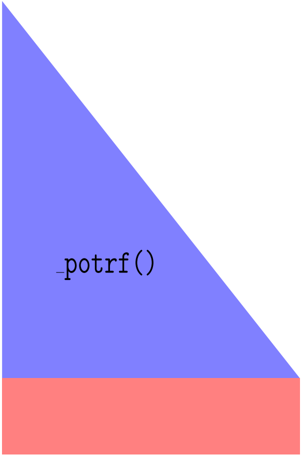
Supernodal method



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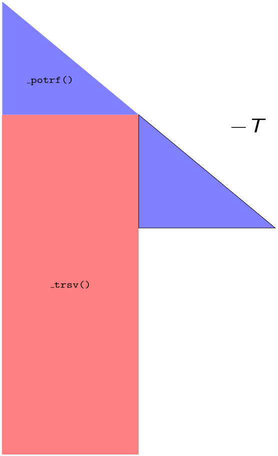

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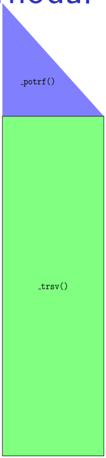

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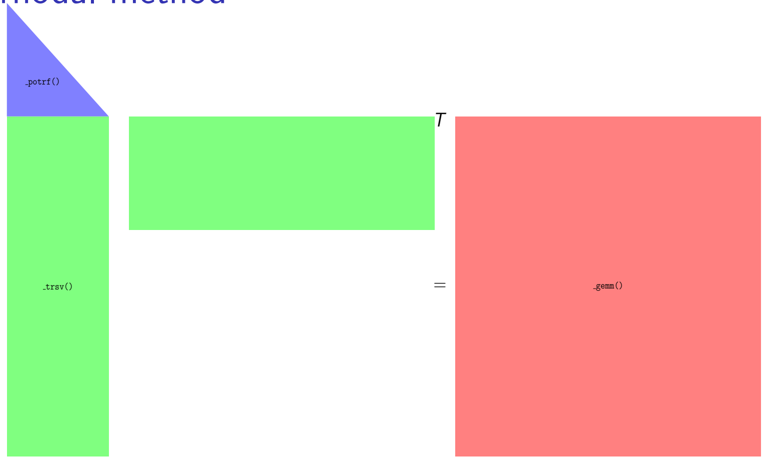

Tasking

- Each task may have its own way of blocking.
- Run in parallel — different optimal block sizes.
- Want to compose libraries.

Summary

“Direct” Methods Still required:

- Black-box solution
- Small problems
- Numerically difficult problems

Challenges:

1. Small + Parallel (strong scaling)
2. Accurate + Parallel (communication avoiding pivoting)
3. Bit-compatiblity (software/user education)
4. Interface to rest of software stack (up *and* down)

But iterative methods aren't perfect either...

Iterative methods challenges

If Matrix-vector product is main cost:

- Already Memory-bound
- Look for ways to use spare cycles $\Rightarrow$ More expensive preconditioning?
- 2 or 4 M-v product not much more expensive than 1 M-v. Can you exploit this?

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Existing Efforts:

- *Mark Hoemmen* (Berkeley), Communication Avoiding Krylov Methods
- Computes $[v, Av, A^2v, ..., A^sv]$ simultaneously
- Uses QR for orthogonalize
- Need to use Chebyshev basis for stability

Thank you!