Improving the performance of direct solvers for sparse symmetric indefinite linear systems

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Sparse indefinite system

Solve

$$Ax = b$$

with A large, sparse, symmetric and indefinite.

For example, systems arise in a number of important applications

$$\begin{pmatrix} H & B^T \\ B & \delta I \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} b \\ c \end{pmatrix}$$

(see next talk).

Direct method

- Compute explicit factorization

$$A = LDL^T$$

where L (unit) is lower triangular, D (block) diagonal.

- Complete solution by performing triangular solves.

Test examples

In this talk, we focus on tough indefinite systems only.

Examples from University of Florida Sparse Matrix Collection.

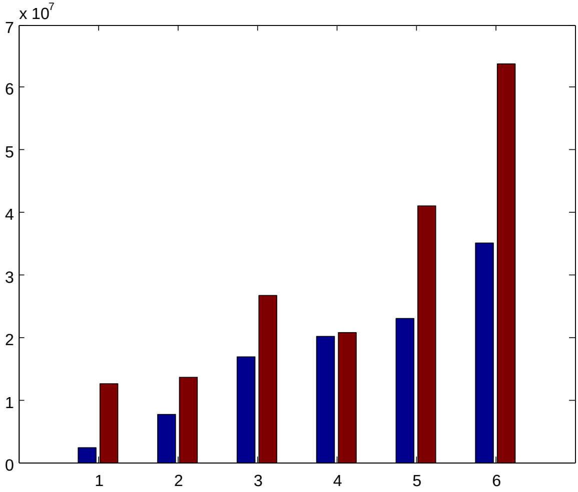
Identifier	n	$nz(A)$	$nz(L)$	*flops*
1. GHS_indef/ncvxqp1	12 111	73 963	1.68×10^6	7.28×10^8
2. GHS_indef/bratu3d	27 792	173 796	6.28×10^6	4.42×10^9
3. GHS_indef/cont-300	180 895	988 195	1.17×10^7	2.96×10^9
4. GHS_indef/d_pretok	182 730	1 641 672	1.46×10^7	5.06×10^9
5. TSOPF/TSOPF_FS_b300_c2	56 814	8 767 466	2.14×10^7	8.96×10^9
6. TSOPF/TSOPF_FS_b300_c3	84 414	13 135 930	3.31×10^7	1.43×10^{10}

* $nz(L)$ and *flops* are for positive definite equivalent with nested dissection ordering

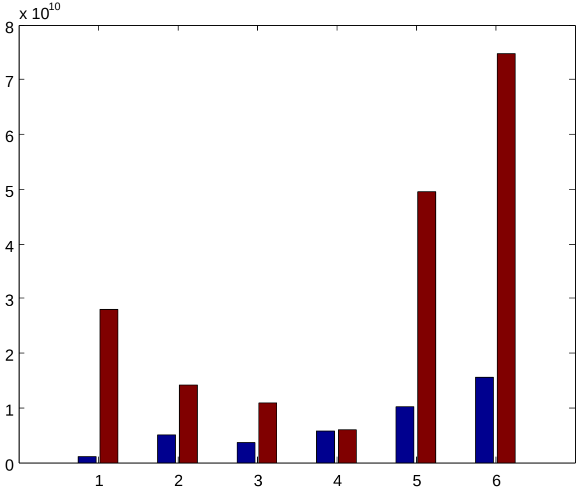
Let's look at the problem ...

- Run indefinite solver.
- Put large entries on diagonal and run positive definite solver.
- Compare the performance.

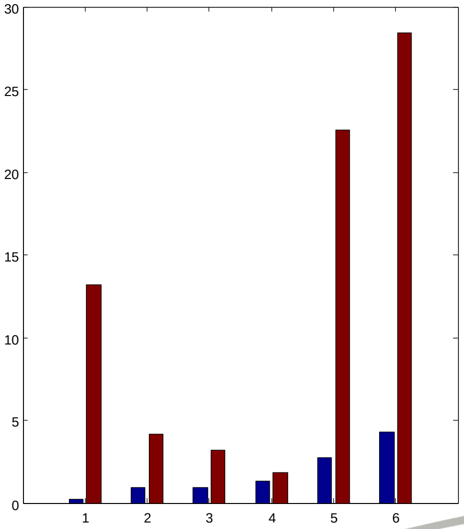
Positive definite versus indefinite $nz(L)$



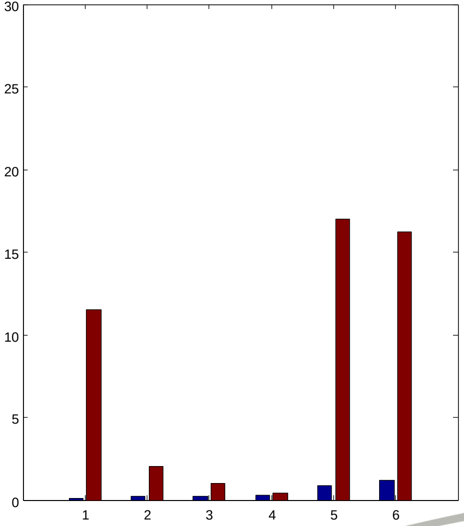
Positive definite versus indefinite flops



Positive definite versus indefinite time (serial)



Positive definite versus indefinite time (8 cores)



Why the differences?

- May not be able to use pivot sequence in supplied order.
- Rejected pivots $\Rightarrow$ more flops and denser factors.
- Extra data movement.
- Less scope for parallelism.

Our aim: improve indefinite performance without compromising stability or the computation of the inertia.

Note: indefinite solver designed on assumption of few rejected pivots so we need to reduce rejected pivots.

The heart of a direct solver

Elimination (pivot) order pre-selected to reduce fill in.

At each stage of factorization, the solver works with dense $m \times m$ submatrix ($m \ll n$)

$$\begin{pmatrix} F_1 & F_2^T \\ F_2 & E \end{pmatrix}.$$

Only rows/columns of F_1 are ready for elimination.

- Factorization: $F_1 = L_1 D L_1^T$
- Solve: $L_2 = F_2 L_1^{-1}$. (L_1, L_2) are computed columns of L.
- Update: $E \leftarrow E - L_2 (L_2 D)^T$ (BLAS 3).

Achieving good solver performance

Key is efficiency of partial dense factorizations.

In positive-definite case:

- Pivots can be selected from diagonal of F_1 in turn ... allows data structures to be fixed before factorization commences (simplifies code and reduces data movement).
- Factorization of F_1 can begin before all updates to F_2 have been made (improves scope for parallelism ... work with block tasks).

Indefinite case

For good performance want to use the supplied pivot sequence.

But

- Zero (or small) diagonal entries cannot be used as pivots.
- Necessary to incorporate numerical pivoting.
- 1×1 and 2×2 pivots needed to retain symmetry.
- Standard approach: threshold partial pivoting.

Threshold partial pivoting

Involves checking that the candidate pivot is 'large' compared to the other entries in its column(s).

Test for 1×1 pivot:

$$|a_{q+1,q+1}| > u \max_{q+1<i\leq n} |a_{i,q+1}|.$$

Corresponding test for 2×2 pivot:

$$\left| \begin{pmatrix} a_{q+1,q+1} & a_{q+1,q+2} \\ a_{q+1,q+2} & a_{q+2,q+2} \end{pmatrix}^{-1} \right| \begin{pmatrix} \max_{q+2<i\leq n} |a_{i,q+1}| \\ \max_{q+2<i\leq n} |a_{i,q+2}| \end{pmatrix} < \begin{pmatrix} u^{-1} \\ u^{-1} \end{pmatrix}.$$

Threshold partial pivoting

- u is threshold parameter, typical default value 0.01. This was used in our earlier tests.
- Larger u favours stability; smaller u means fewer rejects.
- If a pivot fails test, may have to be delayed until later in factorization. This is what we want to avoid.

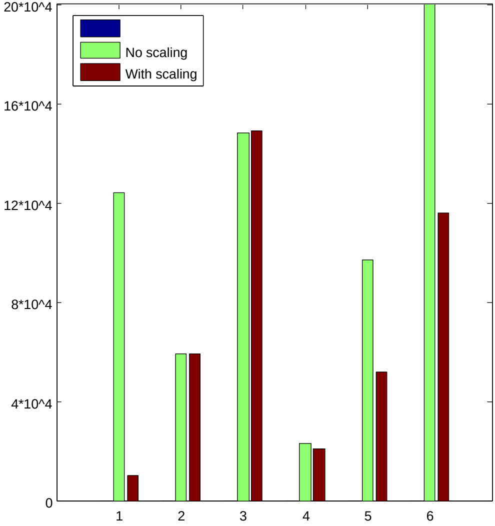
How can we reduce delays?

First remedy: scaling

- In particular, use symmetrized version of `MC64` (Duff and Koster, Duff and Pralet), which is based on maximum weighted matchings.

- Entries in scaled matrix SAS that are in the matching have absolute value 1 while rest have absolute value ≤ 1.

Effect of scaling on delayed pivots



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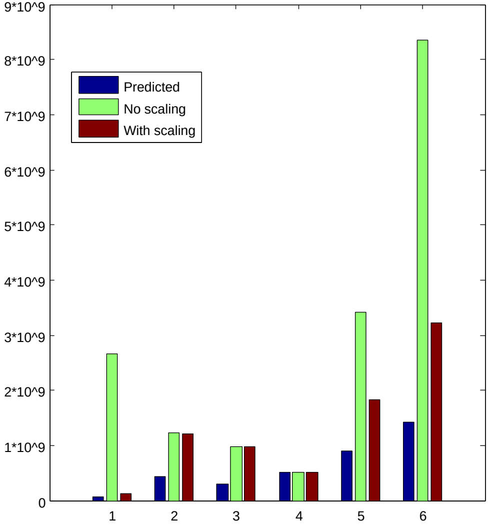
Effect of scaling on flops

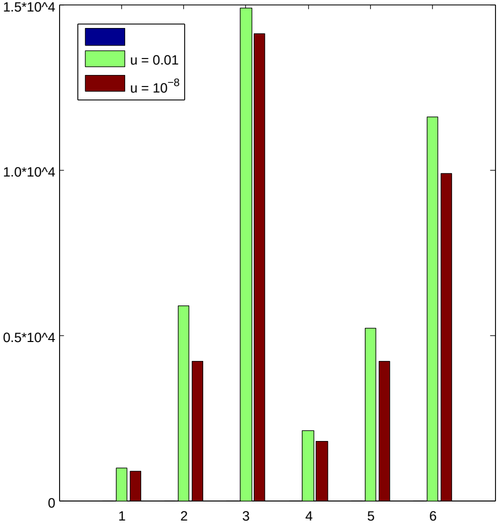


Next remedy: small u

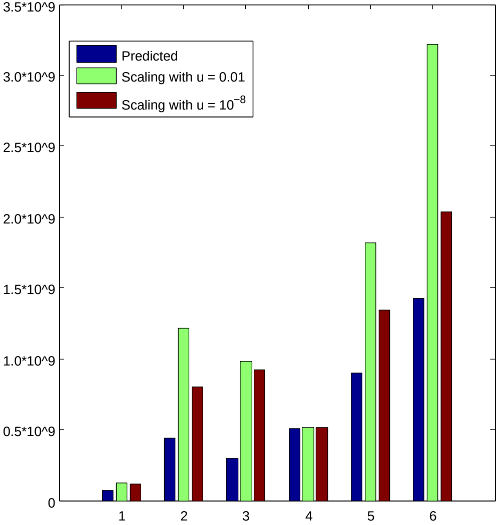
- Use a smaller threshold u to weaken stability test.
- If necessary, use iterative refinement or FGMRES to recover accuracy.
- If u too small, entries of L can become unbounded.
- Here we use $u = 10^{-8}$.

Note: in this and all other experiments, we prescale.

Effect of small u on delayed pivots



Effect of small u on flops



Story so far:

- Good scaling can really help.
- Small u may also help ... but may need additional solves.

So what else?

Try preselecting 2×2 pivots?

An approach that does this is MA47 (Duff and Reid):
sparse indefinite solver that uses structured 2×2 pivots.

Experiments show can work really well for matrices of form

$$\begin{pmatrix} 0 & B^T \\ B & 0 \end{pmatrix}$$

but more generally leads to much denser factors
(without eliminating delayed pivots).

What else? Constraint ordering

Proposed (Bridson) for systems of form

$$\begin{pmatrix} H & B^T \\ B & C \end{pmatrix}$$

with H symmetric positive definite, B rectangular, and C symmetric positive semi-definite.

Only order a C-node after its H-node neighbours have been ordered.

Advantages: able to use modified Cholesky code with no delays (although stability not guaranteed, works in practice).

But: too restrictive so that generally much denser factors and more flops (can require order of magnitude more flops).

So what else? Matching orderings

Aim: permute large off-diagonal entries a_{ij} close to diagonal so that 2×2 block

$$\begin{pmatrix} a_{ii} & a_{ij} \\ a_{ij} & a_{jj} \end{pmatrix}$$

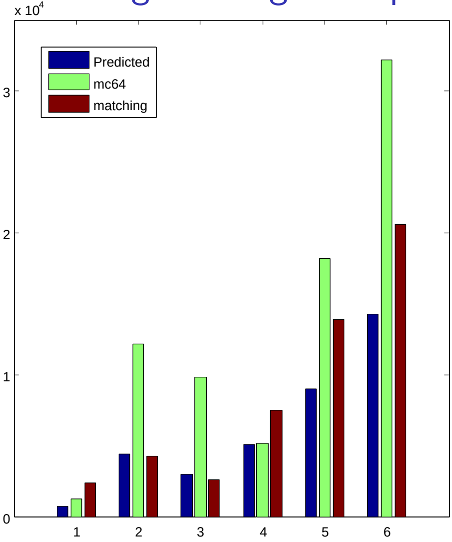
is potentially good 2×2 candidate pivot.

Use cycle structure of permutation associated with unsymmetric maximum weighted matching $\mathcal{M}$ to obtain such a permutation

(Duff and Gilbert, also Duff and Pralet, Schenk *et. al.*).

Combines scaling with ordering in single step.

Effect of matching ordering on flops



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Effect of matching ordering

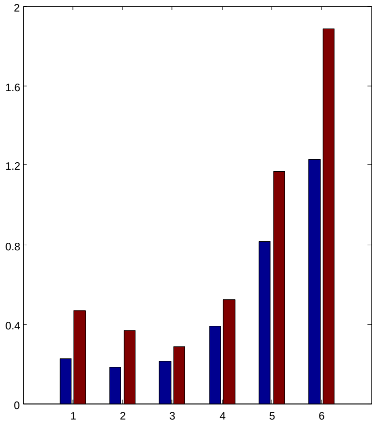
- Predicted values in last plot were for default ordering.
- Predicted values for matching ordering are typically 50 to 100% greater.

  But for the matching ordering, (almost) no delays and, most importantly,

  $$\text{predicted flops (and } nz(L)) \approx \text{actual flops (and } nz(L))$$

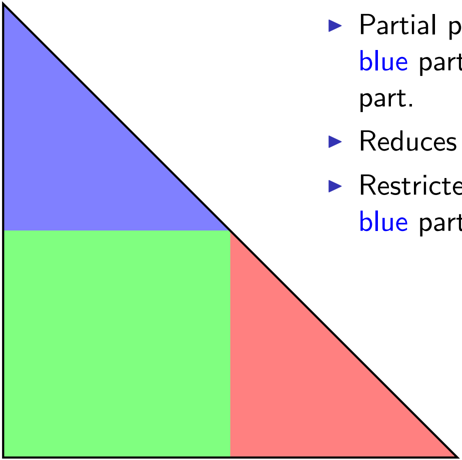
- Also, matching ordering stable (single step of refinement sufficient with $u = 0.01$ and 10^{-8}).

Positive definite versus indefinite time (matching ordering)



Difference now is down to pivot searches that restrict parallelism.

Restricted pivoting



- Partial pivoting — when factorizing blue part, takes into account green part.
- Reduces scope for parallelism.
- Restricted pivoting: just pivot within blue part.

Restricted pivoting

- Found that used just with scaling can lead to numerical instability (accuracy not recovered by refinement).
- If combined with matching ordering, works well for many problems
- But does not give stable factorization in all cases so not recommended for black box solver (note: it is used within PARDISO).

Concluding remarks

- Strategies explored to reduce delayed pivots and hence improve performance of direct solvers for tough (non-singular) indefinite problems.
- Robust approach: matching ordering (used with scaling), combined with threshold partial pivoting.
- But matching is expensive so only use on tough problems.
- Still requires access to whole pivot column and so scope for parallelism less than in positive-definite case.
- For many problems can get away with cheaper strategies but for a robust solver, matching is a good fall back strategy.

More details, further suggestions and lots of results available in technical report RAL-TR-2012-009.

Thank you!

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