Parallel computation of entries of A^{-1}

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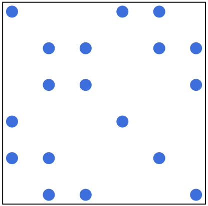
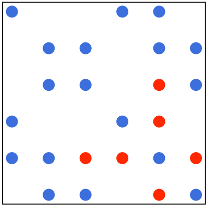
Computation of entries of A^{-1}

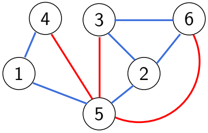
Problem

- Given a large sparse matrix A, compute a set of entries of A^{-1}.
- Many applications: linear least-squares, quantum-scale device simulation, short-circuit currents, astrophysics. . .
- Typical case: computation of the whole diagonal of A^{-1}.

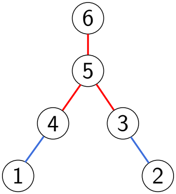
We rely on the pattern of A and its factors L and U such that $A = LU$.


Pattern of A.

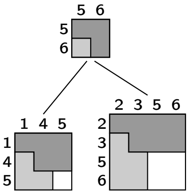

Pattern of $L + U$.



Graph of $L + U$.



Elimination tree.



Assembly tree.

Computing an entry in A^{-1}

The (i,j) entry of A^{-1} is computed as $a^{-1}_{i,j} = (A^{-1}e_j)_i$.
Using the LU factors,

$$\begin{cases} y = L^{-1}e_j \\ a^{-1}_{i,j} = (U^{-1}y)_i \end{cases}$$

Computing an entry in A^{-1}

The (i, j) entry of A^{-1} is computed as $a_{i,j}^{-1} = (A^{-1}e_j)_i$.
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$$\begin{cases} y = L^{-1}e_j & \Rightarrow \text{sparse right-hand side.} \\ a_{i,j}^{-1} = (U^{-1}y)_i & \Rightarrow \text{only one component needed.} \end{cases}$$

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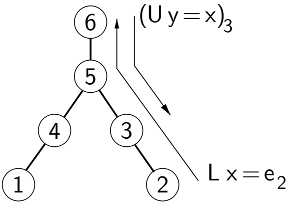
Sparsity of both the RHS and the solution is exploited to reduce the traversal of the tree:

For each requested entry $a^{-1}_{i,j}$,

(1) visit the nodes of the elimination tree from node j to the root: at each node access necessary parts of L,

(2) visit the nodes from the root to node i; this time access necessary parts of U.

$\Rightarrow$ "pruned tree"



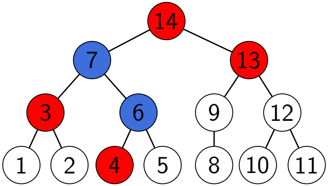
Computation of $a^{-1}_{3,2}$.

Computing a set of entries

In reality

We wish to compute a set R of requested entries. Usually $|R|$ is large and one cannot hold all the solution vectors in memory, even with a storage scheme that exploits sparsity. We assume that we process nb solution vectors at a time.

The way the requested entries are partitioned has a strong influence on the number of accesses to the nodes:



$[R = \{3, 4, 13, 14\},\ nb = 3]$

	Partition	Accesses
Π'	$R_1 = \{3, 13, 14\}$ $R_2 = \{4\}$	$R_1 : 3, 7, 13, 14$ $R_2 : 4, 6, 7, 14$
Π''	$R_1 = \{3, 4, 14\}$ $R_2 = \{13\}$	$R_1 : 3, 4, 6, 7, 14$ $R_2 : 13, 14$

Tree-partitioning problem in out-of-core

Tree-Partitioning problem (OOC version)

Given a set R of nodes of a node-weighted tree and a blocksize nb, find a partition $\Pi(R) = \{R_1, R_2, \ldots\}$ such that $\forall R_k \in \Pi, |R_k| \leq nb$, and has minimum cost

$$\mathrm{Cost}(\Pi) = \sum_{R_k \in \Pi} \mathrm{Cost}(R_k) \quad \text{where} \quad \mathrm{Cost}(R_k) = \sum_{i \in P(R_k)} w(i)$$

- We showed that it is NP-complete.
- There is a non-trivial lower bound.
- The case $nb = 2$ is special and can be solved in polynomial time.
- A simple algorithm, postorder, gives an approximation guarantee.
- We have a heuristic which gives extremely good results.
- We have hypergraph models that address the most general cases.

P. Amestoy, I. Duff, J.-Y. L'Excellent, Y. Robert, F.-H. R. and B. Uçar. On computing inverse entries of a sparse matrix in an out-of-core environment. Submitted to SIAM journal on Scientific Computing.

Parallel issues

Computing blocks in parallel ?

Computing (many) blocks is embarassingly parallel: one would like to compute all the blocks in parallel, but:

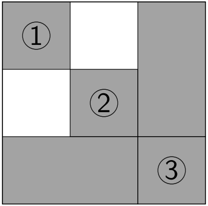
- In a distributed memory environment, this is not feasible without replicating the factors.
- In a shared-memory environment, this is feasible but might lead to poor performance (memory demanding).

Computational setting

Blocks are processed one by one:

- Sparsity is exploited between the blocks, i.e. the tree is pruned for each block.
- Sparsity is not exploited within the blocks, to benefit from dense kernels (BLAS).

Problem: any permutation aimed at reducing flops provides poor speed-ups.
Archetypal example: whole diagonal of A^{-1}, with $nb = N/3$.



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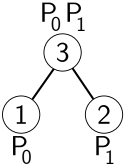

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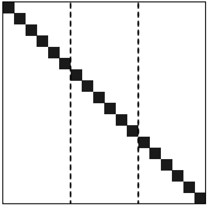

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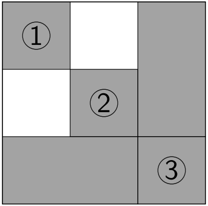

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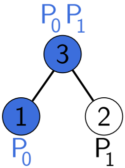

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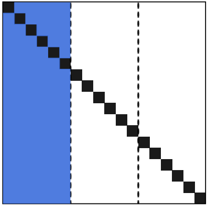

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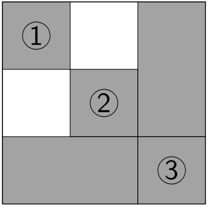

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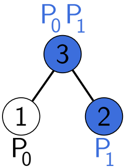

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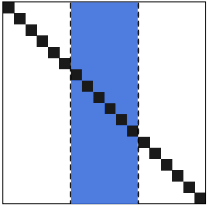

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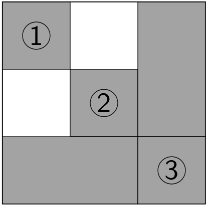

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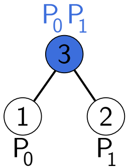

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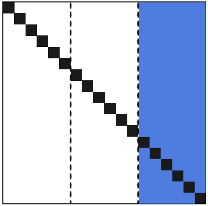

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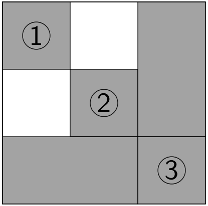

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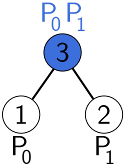

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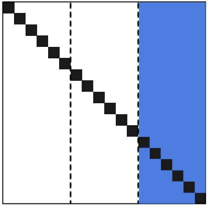

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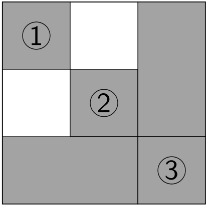
Few active procs at the bottom of the tree

$\Rightarrow$ poor speed-up.

An attempt (Slavova): interleave the requested entries over the processors.



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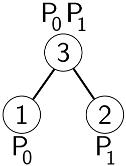

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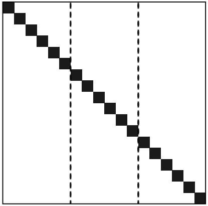

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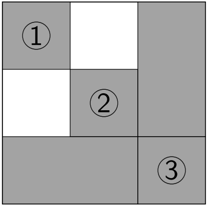

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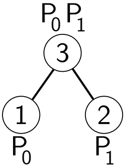

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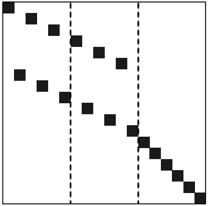

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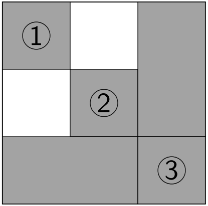

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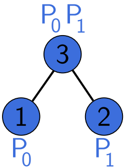

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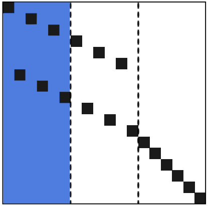

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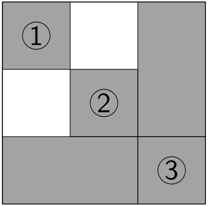

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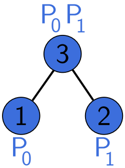

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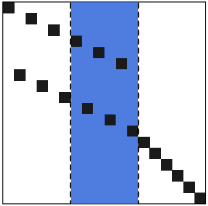

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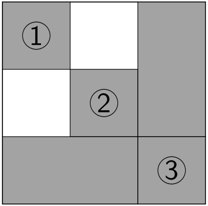

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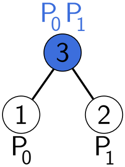

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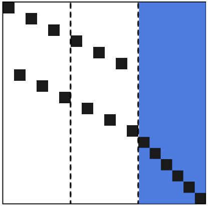

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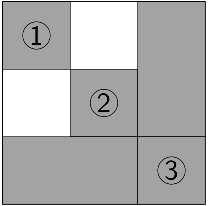

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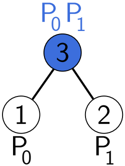

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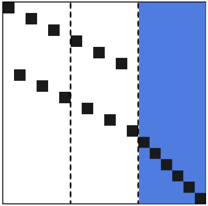

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More active procs but more flops !

$\Rightarrow$ no speed-up.

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Core idea

- Interleaving tends to cancel the benefits of a good permutation, since it groups together entries that are distant in the tree.

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  - Right-hand sides are still processed by blocks of nb
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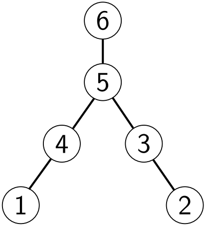
  - Dense computations are performed on subblocks of size called nb_{sparse}
- Each node of the tree is provided with the subscripts of the columns to process. We do not want to manage a list; to ensure efficiency, we rely on the interval that bounds the list of necessary columns.

Exploiting sparsity within the blocks - cont

Core idea - cont

- Intervals are computed in a two-step traversal of the tree:

Example: the block of right-hand sides is equal to $[e_2, e_4, e_5, e_6]$.



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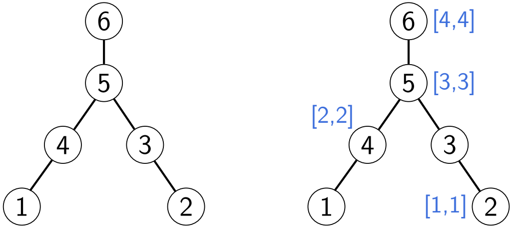

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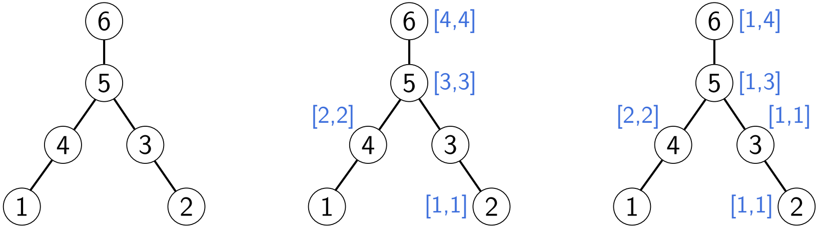

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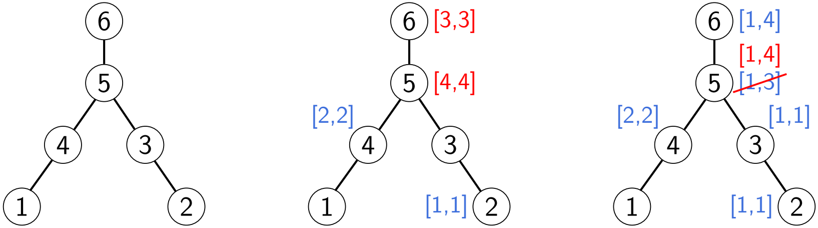
  1. Initialization: at each node, initialize with the target entries (columns) appearing at the node.
  2. Propagation: at each node, add the union of the intervals of its children.
- By postordering each block, this interval is reduced.

Example: with a non-postordered block $[e_2, e_4, e_6, e_5]$



Illustration

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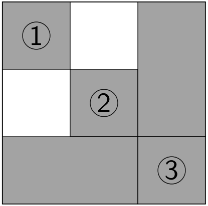

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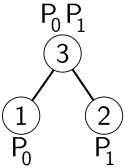

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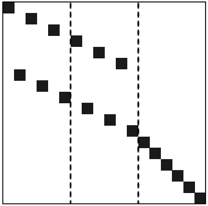

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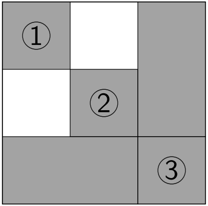
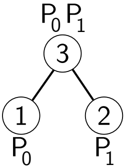
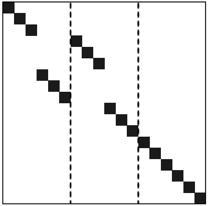


[Simple matrix...



...and its tree.]



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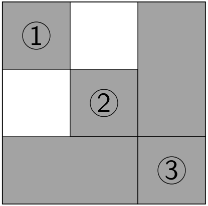

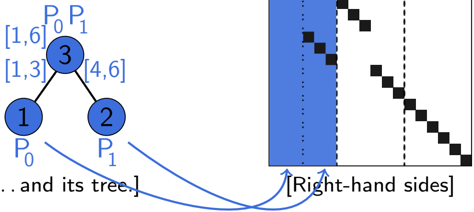

[Simple matrix. . . . . . and its tree.] [Right-hand sides]

1^{st} block: traverses all the nodes, P_0 and P_1 active at the bottom of the tree.
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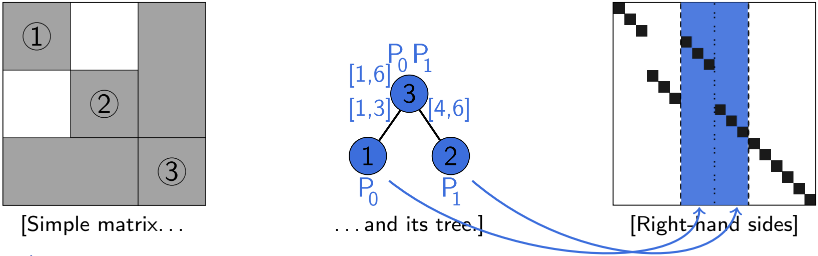

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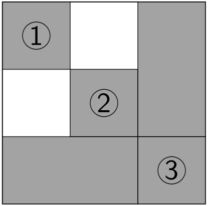

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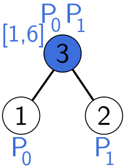

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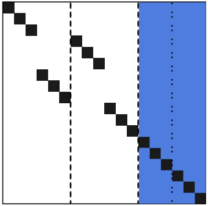

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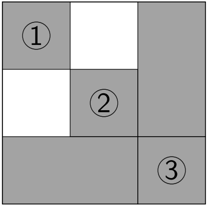

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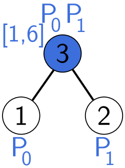

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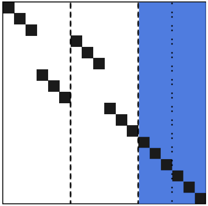

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2^{nd} block: traverses all the nodes, P_0 and P_1 active at the bottom of the tree.
At node 1, flops are performed on $N/6$ vectors only. Same at node 2.

All procs are active, and flops have not increased !

$\Rightarrow$ good speed-up.

The different strategies are compared. The average number of active processors at leaf nodes of the pruned tree is used as a measure of tree parallelism.

Computation of 10% diagonal entries, 11-point discretization of a $200 \times 200 \times 20$ grid, blocks of size 512:

<table>
<tr><th>Procs</th><th colspan="2">Strategy</th><th>Time (seconds)</th><th>Operation (TFlops)</th><th>Active procs</th></tr>
<tr><td>1</td><td colspan="2">-</td><td>1667</td><td>16.2</td><td>1</td></tr>
<tr><td rowspan="3">4</td><td>IL off</td><td>nb_{sparse} off</td><td>1366</td><td>16.2</td><td>1.10</td></tr>
<tr><td rowspan="2">IL on</td><td>nb_{sparse} off</td><td>2028</td><td>45.4</td><td rowspan="2">3.92</td></tr>
<tr><td>nb_{sparse} on</td><td>659</td><td>15.2</td></tr>
<tr><td rowspan="3">8</td><td>IL off</td><td>nb_{sparse} off</td><td>1241</td><td>13.3</td><td>1</td></tr>
<tr><td rowspan="2">IL on</td><td>nb_{sparse} off</td><td>1508</td><td>61.0</td><td rowspan="2">7.76</td></tr>
<tr><td>nb_{sparse} on</td><td>418</td><td>12.4</td></tr>
</table>

Influence of the block size on the same problem:

Procs	Strategy		Block size			
			64	128	512	1024
1 proc	-		1518	1432	1667	2002
8 procs	IL on	nb_{sparse} on	555	466	418	379

Conclusion

Exploiting sparsity within a block...

...can be done without sacrificing efficiency (BLAS kernels optimally used).

...increases parallelism when combined with interleaving.

...is interesting even in the sequential case (it reduces flops).

...gives some leeway for the backward phase (off-diagonal case): each block can be reordered following a permutation that will have a good effect for backward targets.

Conclusion - cont

Further work

- Still some effort to make to reach the scalability of the dense solve.
- Several improvements upon interleaving: management of type 2 nodes, management of sequential subtrees...
- Minimize nb_{sparse}-sized intervals in the general case, i.e. find a good permutation within each block (postorder works fine for diagonal entries...).

Next release of MUMPS

- Compressed solution space when exploiting sparse right-hand sides.
- Use of sparsity within blocks of sparse right-hand sides.

Thank you for your attention!

Any questions?