# Parallel computation of entries of $A^{-1}$

François-Henry Rouet
ENSEEIHT-IRIT, Université de Toulouse, France

Joint work with: P. Amestoy, I. Duff, J.-Y. L'Excellent & B. Uçar

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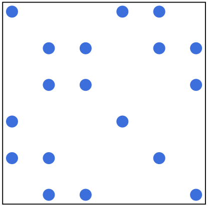
# Computation of entries of $A^{-1}$

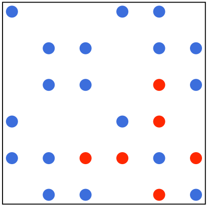
## Problem

- 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 $A^{-1}$.

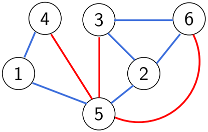
We rely on the pattern of $A$ and its factors $L$ and $U$ such that $A = LU$.



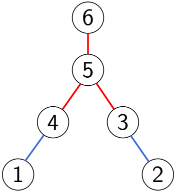
Pattern of $A$.



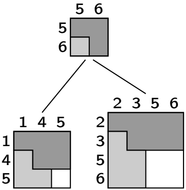
Pattern of $L + U$.




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,

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

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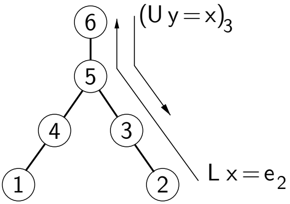
Sparsity of both the RHS and the solution is exploited to reduce the traversal of the tree:

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"



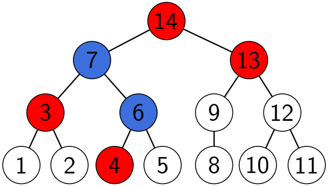

Computation of $a^{-1}_{3,2}$.

# 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 |
|---|---|---|
| $\Pi'$ | $R_1 = \{3, 13, 14\}$<br>$R_2 = \{4\}$ | $R_1 : 3, 7, 13, 14$<br>$R_2 : 4, 6, 7, 14$ |
| $\Pi''$ | $R_1 = \{3, 4, 14\}$<br>$R_2 = \{13\}$ | $R_1 : 3, 4, 6, 7, 14$<br>$R_2 : 13, 14$ |

# 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).

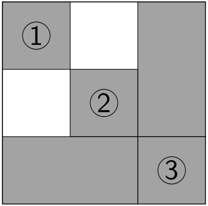
## Computational setting

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).

# Parallel issues - cont

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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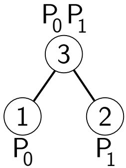


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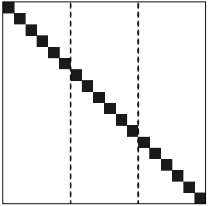

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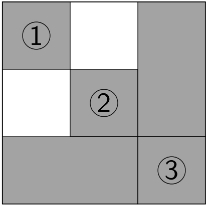


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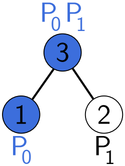


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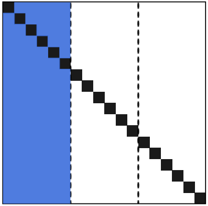

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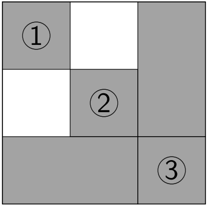


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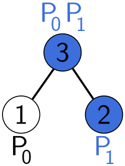


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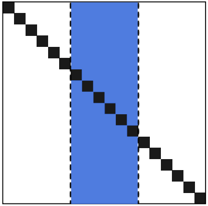

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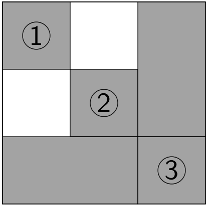


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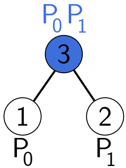


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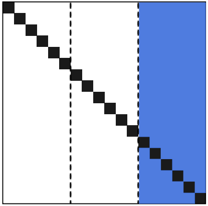

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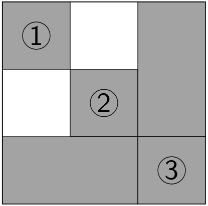


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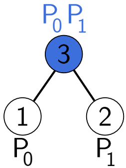


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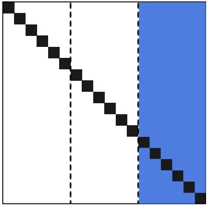

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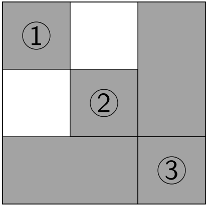
Few active procs at the bottom of the tree

$\Rightarrow$ poor speed-up.

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

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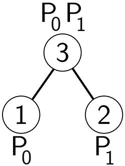


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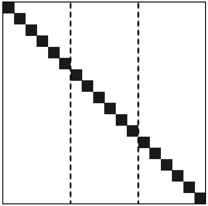

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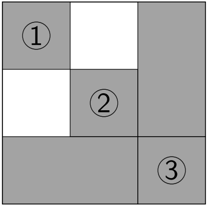

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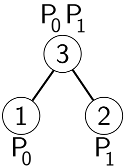

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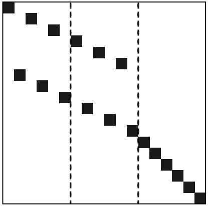
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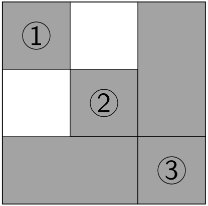


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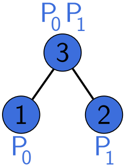


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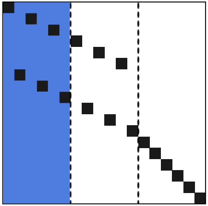

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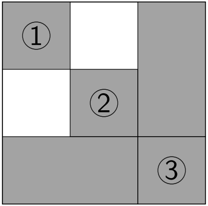


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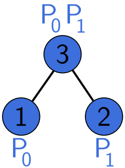


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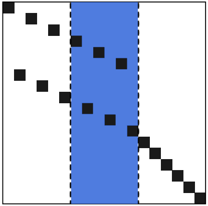

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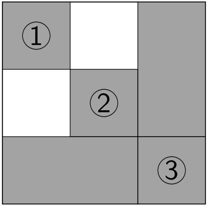


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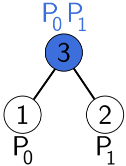


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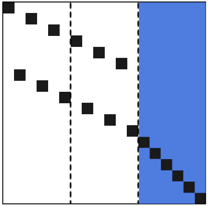

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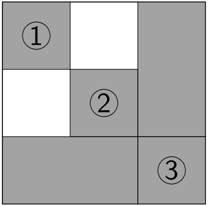


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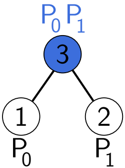


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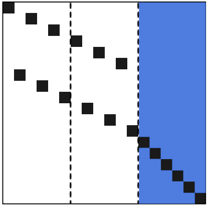

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More active procs but more flops !

$\Rightarrow$ no speed-up.

# Exploiting sparsity within the blocks

## Core idea

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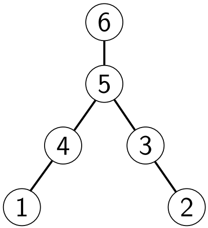
  - Dense computations are performed on subblocks of size called $nb_{sparse}$
- Each node of the tree is provided with the subscripts of the columns to process. We do not want to manage a list; to ensure efficiency, we rely on the interval that bounds the list of necessary columns.

# 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 $[e_2, e_4, e_5, e_6]$.



# Exploiting sparsity within the blocks - cont

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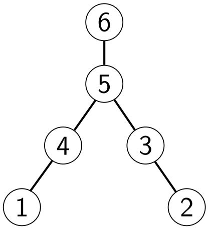


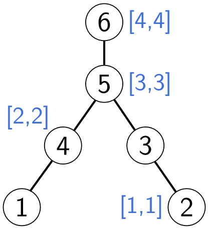

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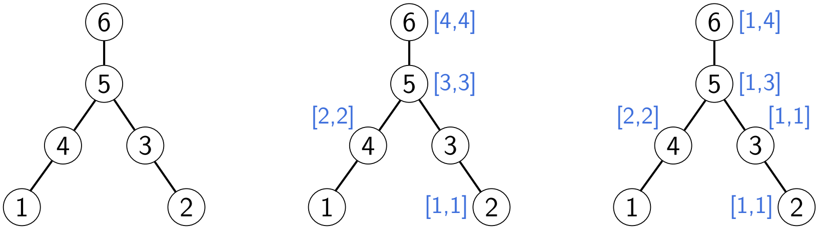

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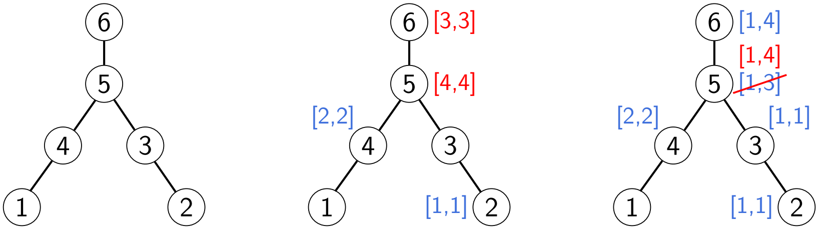
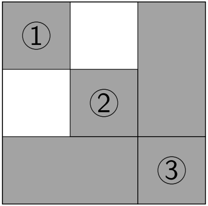
  1. Initialization: at each node, initialize with the target entries (columns) appearing at the node.
  2. Propagation: at each node, add the union of the intervals of its children.
- By postordering each block, this interval is reduced.

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



# Illustration

Back to the first example: $nb = N/3$, we use interleaving and blocks are postordered; when computing a block, compute for each node the interval to process.

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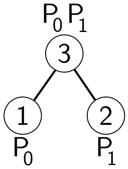
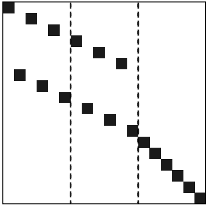


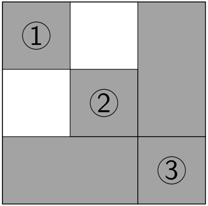

...and its tree.]



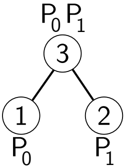
[Right-hand sides]

# Illustration

Back to the first example: $nb = N/3$, we use interleaving and blocks are postordered; when computing a block, compute for each node the interval to process.




[Simple matrix. . .

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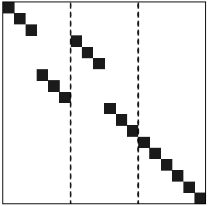

[Right-hand sides]

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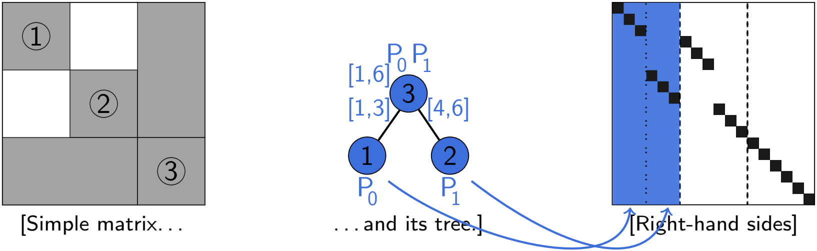


[Simple matrix. . . . . . and its tree.] [Right-hand sides]

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

# Illustration

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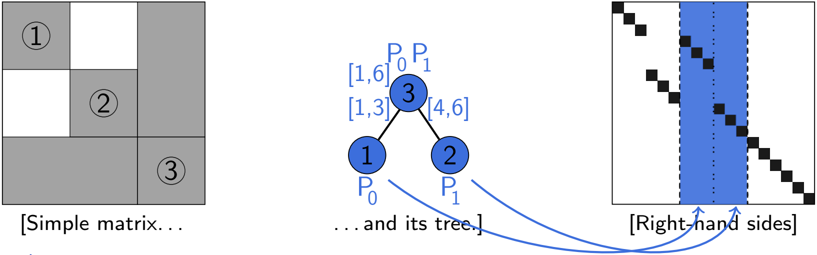


[Simple matrix... ...and its tree.] [Right-hand sides]

1st 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.

2nd 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.

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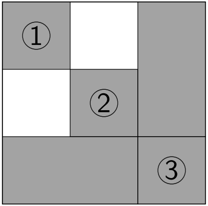


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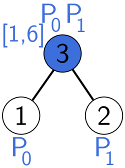
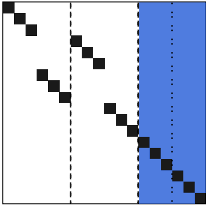



. . . and its tree.]



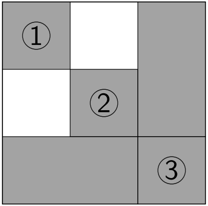
[Right-hand sides]

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

**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.

# Illustration

Back to the first example: $nb = N/3$, we use interleaving and blocks are postordered; when computing a block, compute for each node the interval to process.

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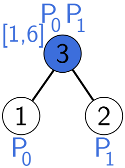


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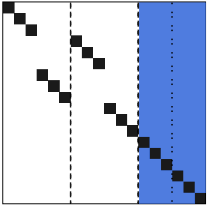

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**1$^{st}$ block:** traverses all the nodes, $P_0$ and $P_1$ active at the bottom of the tree.
At node 1, flops are performed on $N/6$ vectors only. Same at node 2.

**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:

| Procs | Strategy | | Time (seconds) | Operation (TFlops) | Active procs |
|---|---|---|---|---|---|
| 1 | - | | 1667 | 16.2 | 1 |
| 4 | IL off | $nb_{sparse}$ off | 1366 | 16.2 | 1.10 |
| | IL on | $nb_{sparse}$ off | 2028 | 45.4 | 3.92 |
| | | $nb_{sparse}$ on | 659 | 15.2 | |
| 8 | IL off | $nb_{sparse}$ off | 1241 | 13.3 | 1 |
| | IL on | $nb_{sparse}$ off | 1508 | 61.0 | 7.76 |
| | | $nb_{sparse}$ on | 418 | 12.4 | |

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?