Grouping variables in Frontal Matrices to improve Low-Rank Approximations in a Multifrontal Solver

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Preconditioning 2011, May 16, 2011

Joint work with Patrick Amestoy , Cleve Ashcraft, Olivier Boiteau, Alfredo Buttari and Jean-Yves L'Excellent.

PhD started on October 1st, 2010 and financed by EDF.

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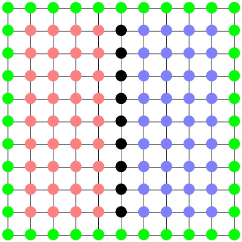
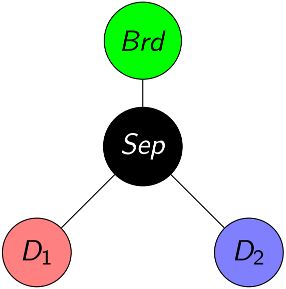
⇒ Try to combine these two notions to improve multifrontal solvers, in particular the `MUMPS` multifrontal solver

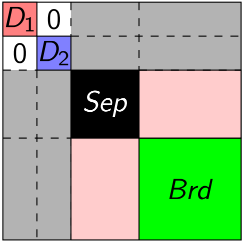
The multifrontal method

I. S. Duff and J. K. Reid, The multifrontal solution of indefinite sparse symmetric linear systems, ACM Transactions on Mathematical Software, 1983.

Idea







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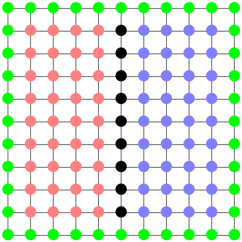
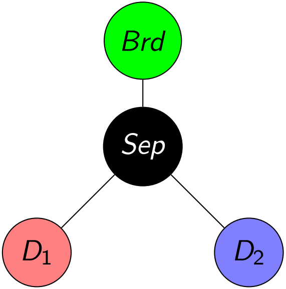
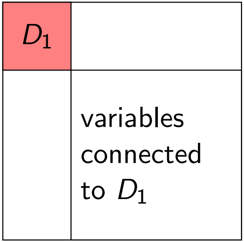
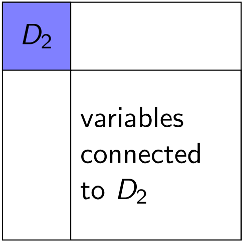
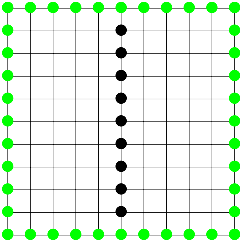


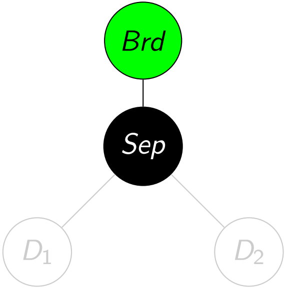

Brd
Sep
D_1
D_2


D_1
variables connected to D_1

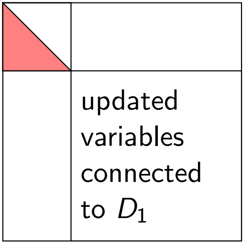

D_2
variables connected to D_2

Idea

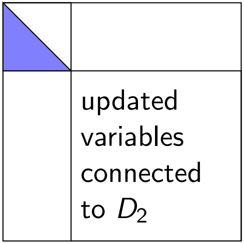




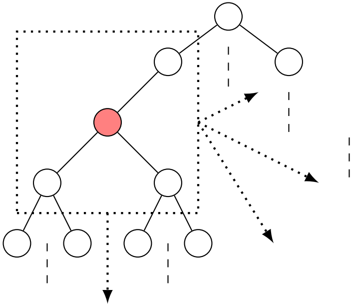
Brd
Sep
D_1
D_2



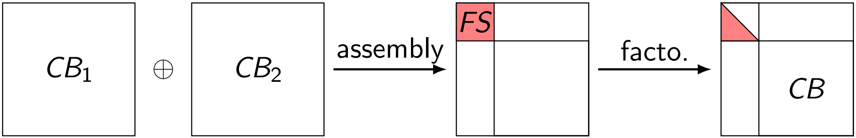
updated variables connected to D_1



updated variables connected to D_2



At each node, an incomplete factorization of the frontal matrix is performed :



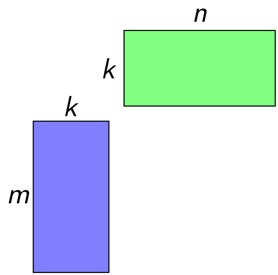
Low-rank theory

General idea

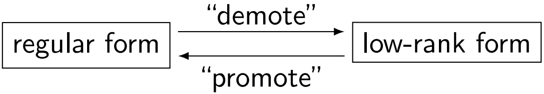
Outer-product form

Let $A \in \mathbb{R}^{m \times n}$ be a matrix of rank k . Let $U \in \mathbb{R}^{m \times k}$ and $V \in \mathbb{R}^{n \times k}$ be two matrices. The *outer-product form* of A is :

$$A = UV^T$$



- storage : $k(m+n)$ vs mn
- if $k < \frac{mn}{m+n} \longrightarrow$ low-rank form



Advantages and Drawbacks

- **Drawbacks**
  - Each outer-product form requires the computation of a *SVD* or a *QR* decomposition
  - More sophisticated data to store and manipulate (Householder vectors)

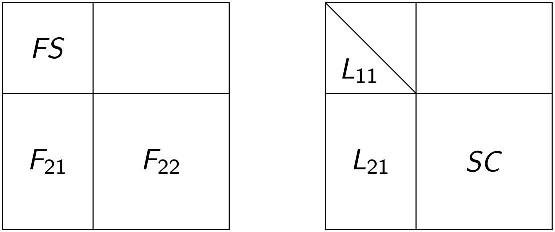
- **Advantages**
  - Reduction of the quantity of information stored
  - Basic algebra operations can be done more efficiently
  - Accuracy of the approximation directly controlled by a numerical parameter

Implementation of low-rank methods within a multifrontal solver

- J. Xia, S. Chandrasekaran, M. Gu and X. S. Li, Superfast Multifrontal Method for Large Structured Linear Systems of Equations, SIAM Journal on Matrix Analysis and Applications.
- M. Bebendorf, Hierarchical Matrices: A Means to Efficiently Solve Elliptic Boundary Value Problems, Springer.
- L. Grasedyck, R. Kriemann and S. Le Borne, Parallel black box $\mathcal{H}$-LU preconditioning for elliptic boundary value problems, Computing and Visualization in Science.

Complete front processing (Cholesky)

- " FSU " factorization of the front :



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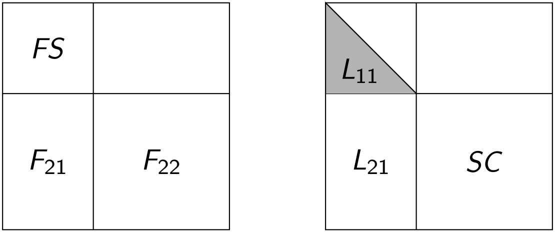

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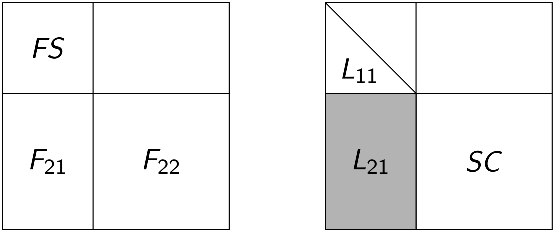

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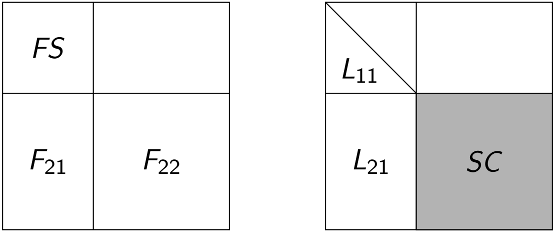

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Link with the low-rank approximations

The UPDATE(SYRK) and SOLVE(TRSM) phases can be performed using low-rank operations !

- LR-**U**pdate $(L_{21} = U \cdot V^T)$: $SC = F_{22} - U \cdot (V^T \cdot V) \cdot U^T$
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The fronts of the multifrontal tree are FULL rank

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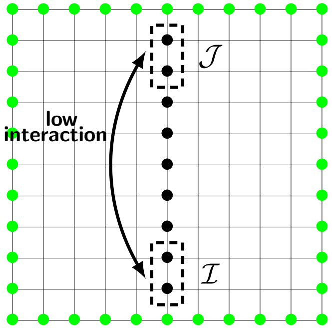
Solution :

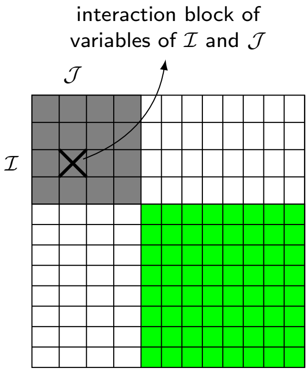
Group variables to obtain low-rank *subblocks*

The low-rank method

"How to find low-rank subblocks ?"

$$\boxed{min\{diam(\mathcal{I}), diam(\mathcal{J})\} < \eta \cdot dist(\mathcal{I}, \mathcal{J})}$$ *(Bebendorf)*



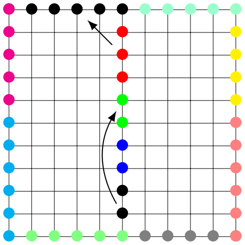


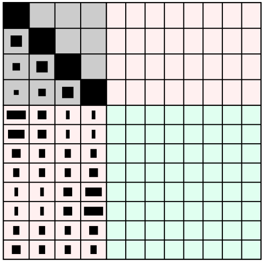
Variables of $\mathcal{I}$ and $\mathcal{J}$ well separated $\Rightarrow$ $L(\mathcal{I}, \mathcal{J})$ has a low numerical rank

Objective : define groups of well separated variables

First way : geometric partitioning

- geometric reordering : Geometric properties are taken into account
- Laplacian problem on square 500 × 500 domain



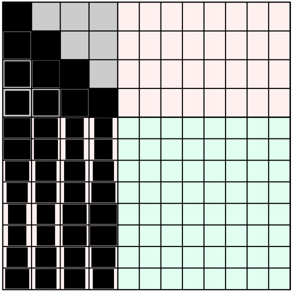


(density proportional to the rank)

Objective : define groups of well separated variables

Second way : random partitioning

- Random reordering : geometry is not taken into account
- Laplacian problem on square 500 × 500 domain



(density proportional to the rank)

Grouping algorithm

$\Rightarrow$ VERY important to have a good grouping of the variables

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Implemented algorithm :

- Halo-based algorithm to catch the geometry
- Coupled with a third party partitioning tool

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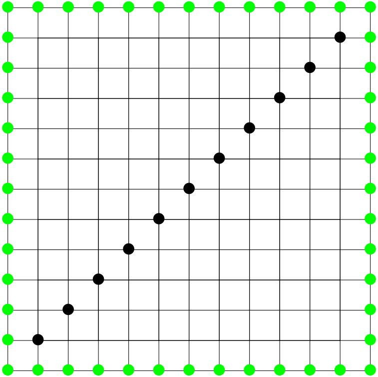

1. The separator

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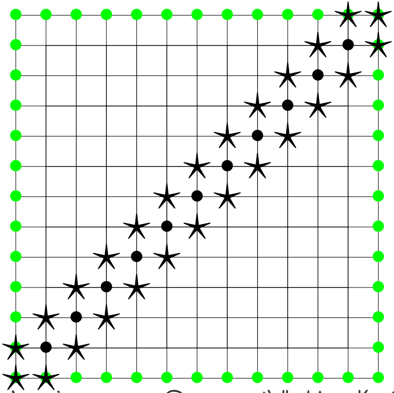

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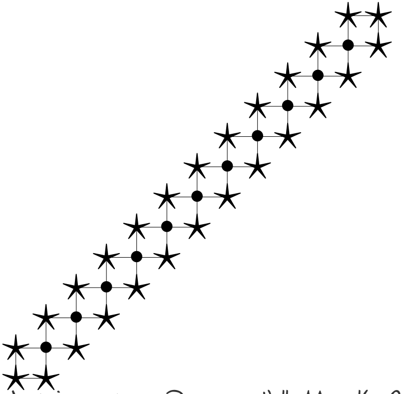

1. The separator
2. The halo
3. Extraction of the halo

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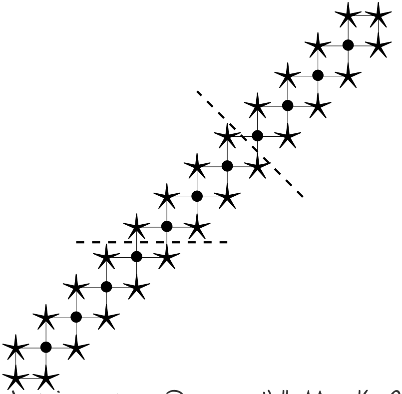

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3. Extraction of the halo
4. Partition of the halo

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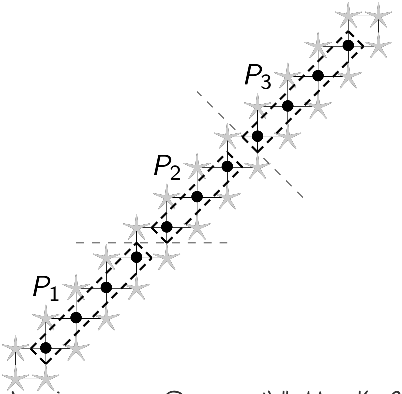


1. The separator
2. The halo
3. Extraction of the halo
4. Partition of the halo
5. Partition of the separator

Strategies

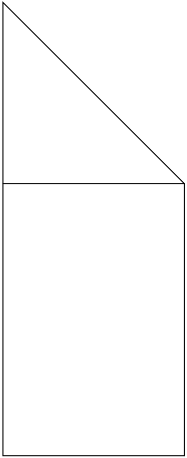
Remains to define how to use the low-rank operations within a front

$\Rightarrow$ 4 strategies to process a front :

- Strategy FSU**D**
- Strategy FS**D**U
- Strategy **panel** FS**D**U
- (Strategy F**D**SU)

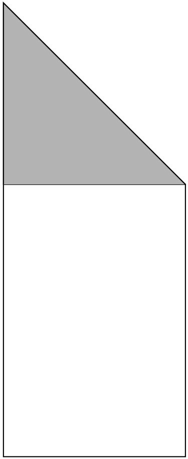
Note : we do not use low-rank within the Schur complements yet

Strategy FSUD



1. We consider all the fully summed variables

Strategy FSUD



1. We consider all the fully summed variables
2. **F***actor* the entire diagonal block

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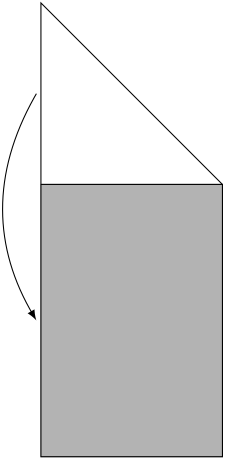

1. We consider all the fully summed variables
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3. **S***olve* operation on the off-diagonal block

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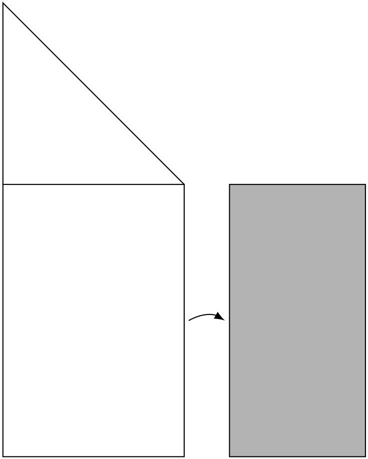

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2. **F***actor* the entire diagonal block
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4. **U***pdate* the Schur complement

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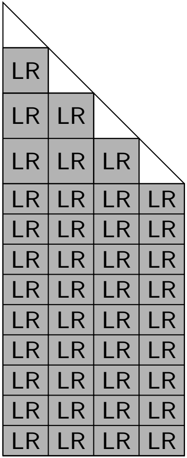
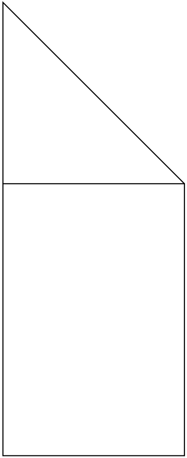


1. We consider all the fully summed variables
2. **F***actor* the entire diagonal block
3. **S***olve* operation on the off-diagonal block
4. **U***pdate* the Schur complement
5. **D***emote* each block of grouped variables within the factor

Strategy FSDU



1. We process the entire fully summed variables block

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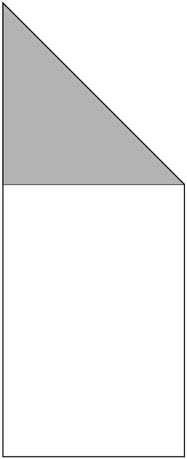

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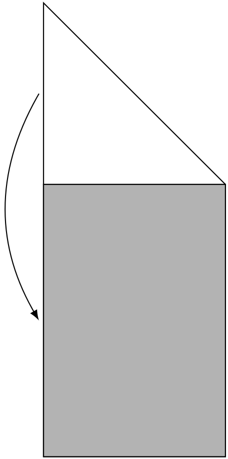

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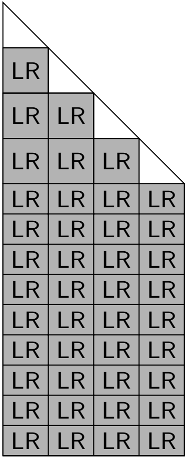

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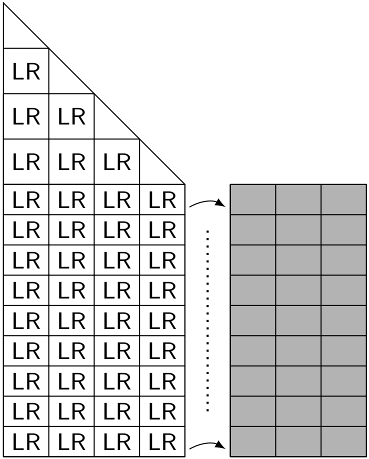

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2. **F***actor* the entire diagonal block
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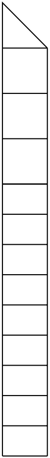
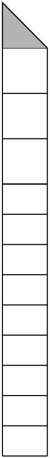
4. **D***emote* each block of grouped variables
5. *LR*-**U***pdate* the Schur complement blockwise

Strategy panel FSDU

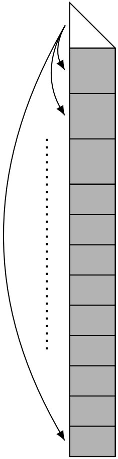


1. We process the fully summed variables block **panel***wise*



1. We process the fully summed variables block **panel**_wise_
2. **F**_actor_ the entire diagonal subblock

Strategy panel FSDU



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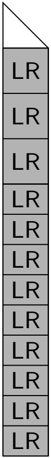
2. **F***actor* the entire diagonal subblock
3. **S***olve* operation on the off-diagonal subblocks

Strategy panel FSDU



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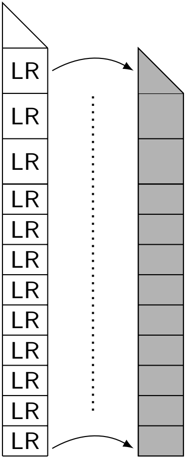

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2. **F***actor* the entire diagonal subblock
3. **S***olve* operation on the off-diagonal subblocks
4. **D***emote* each off-diagonal subblock
5. *LR*-**U***pdate* the trailing panels

Set of matrices

Matrix	N	NZ	Type	CSR
tpll01a_r6_t	66,053	295,947	thermic	6.4E-16
tpll01a_r7_t	263,173	1,181,707	thermic	8.6E-16
tpll01a_r8_t	1,050,629	4,722,699	thermic	1.3E-15
tpll01a_r6_m	132,106	1,117,719	mechanic	8.3E-16
tpll01a_r7_m	526,346	4,463,639	mechanic	1.8E-15
tpll01a_r8_m	2,101,258	17,840,151	mechanic	2.0E-15

- 2D problems
- thermo-mechanical simulations from Code_Aster (by EDF)
- different mesh refinements
- work still in progress on 3D problems
- Componentwise Scaled Residual $CSR = \frac{|\mathbf{b} - \mathbf{A}\bar{\mathbf{x}}|_i}{(|\mathbf{b}| + |\mathbf{A}|\ |\bar{\mathbf{x}}|)_i}$.

Strategy FSUD : results ($\varepsilon = 10^{-14}$)

Matrix	# of fronts	*L*	*MEMORY*	*OPS*	*CSR*
tpll01a_r6_t	6	10.3 %	49.9 %	–	9.2E-16
tpll01a_r7_t	22	17.4 %	35.7 %	–	9.1E-15
tpll01a_r8_t	111	28.2 %	29.4 %	–	3.6E-15
tpll01a_r6_m	100	22.2 %	58.0 %	–	1.5E-16
tpll01a_r7_m	423	45.1 %	59.9 %	–	1.8E-15
tpll01a_r8_m	468	40.1 %	41.7 %	–	1.0E-13

Features

- Focus on memory compression of the factorization
- No flop reduction during the factorization
- No error propagation within the factorization of the front
- Can be done "off-line" (solution phase, OOC)

Strategy FSDU : results ($\varepsilon = 10^{-14}$)

Matrix	# of fronts	*L*	*MEMORY*	*OPS*	*CSR*
tpll01a_r6_t	6	10.3 %	49.9 %	78.8 %	9.3E-16
tpll01a_r7_t	22	17.4 %	35.7 %	56.7 %	1.8E-15
tpll01a_r8_t	111	28.2 %	29.4 %	45.9 %	3.7E-14
tpll01a_r6_m	100	22.2 %	58.0 %	75.5 %	9.7E-15
tpll01a_r7_m	423	45.1 %	59.9 %	65.0 %	5.3E-15
tpll01a_r8_m	468	40.1 %	41.7 %	50.3 %	2.6E-13

- Memory compression for the storage of the factor
- More efficient update of the Schur complement thanks to the *LR-update* operation

Strategy panel FSDU : results ($\varepsilon = 10^{-14}$)

Matrix	# of fronts	*L*	*MEMORY*	*OPS*	*CSR*
tpll01a_r6_t	6	10.3 %	49.9 %	61.7 %	9.6E-16
tpll01a_r7_t	22	17.4 %	35.7 %	39.9 %	2.0E-15
tpll01a_r8_t	111	28.2 %	29.4 %	28.2 %	1.2E-14
tpll01a_r6_m	100	22.2 %	58.0 %	65.0 %	5.8E-15
tpll01a_r7_m	423	45.1 %	59.9 %	52.1 %	1.7E-15
tpll01a_r8_m	468	40.1 %	41.7 %	34.5 %	2.3E-13

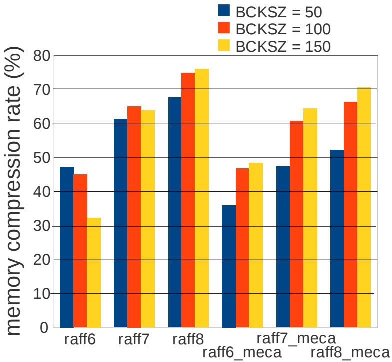
- Memory compression for the storage of the factor
- More efficient factorization due to *LR-updates* within the factor
- More efficient update of the Schur complement thanks to the *LR-update* operation

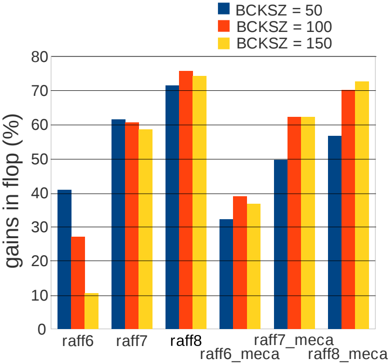
Comparison

	OPS (%)			ERROR				COND.
	FSUD	FSDU	panel FSDU	MUMPS	FSUD	FSDU	panel FSDU	
tpll01a_r6_t	–	78.8	61.7	6.4E-16	9.2E-16	9.3E-16	9.6E-16	4.0E+5
tpll01a_r7_t	–	56.7	39.9	8.6E-16	9.1E-15	1.8E-15	2.0E-15	1.7E+6
tpll01a_r8_t	–	45.9	28.2	1.3E-15	3.6E-15	3.7E-14	1.2E-14	6.9E+6
tpll01a_r6_m	–	75.5	65.0	8.3E-16	1.5E-16	9.7E-15	5.8E-15	7.4E+6
tpll01a_r7_m	–	65.0	52.1	1.8E-15	1.8E-15	5.3E-15	1.7E-15	3.3E+7
tpll01a_r8_m	–	50.3	34.5	2.0E-15	1.0E-13	2.6E-13	2.3E-13	1.5E+8

- not much error propagation from panel to panel
- Strategy panel FSDU is the most efficient
- need to process more fronts with the same efficiency

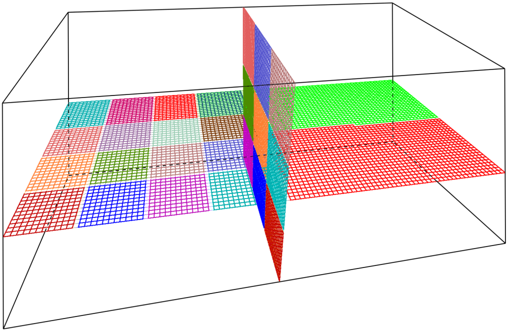
Influence of the block size





- stability for a large enough block size
- efficient block size depends on the front size
- will ease parallelism adaptation

3D target grouping (7-pts stencil, laplacian)



- hand-made separators (2 levels) and partitioning
- grouping results are close to this
- efficient on 2D separators
- problems with irregular separators

Error and accuracy

Local error on blocks : $\boxed{\frac{\|B - B_k\|_F}{\|B\|_F} \leq \varepsilon}$

Global error on solution : $\boxed{\sim \varepsilon}$

No propagation observed !

Summarizing

- → Strong link between structural and numerical aspects
- → Several gain spots

Summarizing

→ Strong link between structural and numerical aspects

→ Several gain spots

Two approaches

Summarizing

→ Strong link between structural and numerical aspects

→ Several gain spots

Two approaches

1 : PSEUDO-EXACT

- $\varepsilon \sim 10^{-16}$
- little accuracy lost
- typically used to accurately solve linear systems

Summarizing

→ Strong link between structural and numerical aspects

→ Several gain spots

Two approaches

1 : PSEUDO-EXACT

- $\varepsilon \sim 10^{-16}$
- little accuracy lost
- typically used to accurately solve linear systems

2 : APPROXIMATED

- $\varepsilon \gg 10^{-16}$
- typically used to compute preconditioners
- can replace mixed precision iterative refinement

Conclusion

- Efficient method for 2D problems
- Work still in progress for 3D problems
- An important step : the partitioning of the separator

Further works

- Pivoting, OOC, parallelism . . .
- Need to study the error propagation
- Theoretical work to have a better understanding of how the grouping should work
- 3D separator quality and partitioning

Questions

Thank you for your attention !

Any question ?