High performances methods for solving large sparse linear systems: Direct and Incomplete factorization

NEGST (NExt Grid Systems and Techniques)

REDIMPS Workshop
Tokyo, May 28-29 2007

P. Hénon, P. Ramet, J. Roman
LaBRI, UMR CNRS 5800, Université Bordeaux I
Projet ScAlApplix, INRIA Futurs

INRIA

Collaborations with MUMPS team (Bordeaux, Toulouse, Lyon)

Outlines

- Introduction (motivation for hybrid approach)
- Direct solvers
- Methods to get dense blocks in ILU(k)
- Experiments
- Others approaches (MUMPS, HIPS)

Motivation of this work

- A popular choice as an algebraic preconditioner is an ILU(k) preconditioner (level-of-fill based inc. facto.)

- BUT
- ➢ Parallelization is not easy

- ➢ Scalar formulation does not take advantage of superscalar effect (i.e. BLAS)
  => Usually a low value of fill is used (k=0 or k=1)

- ➢ Many people are working on hybrid methods
  (Luc Giraud at IRIT, David Keyes at Livermore, …)

Motivation of this work

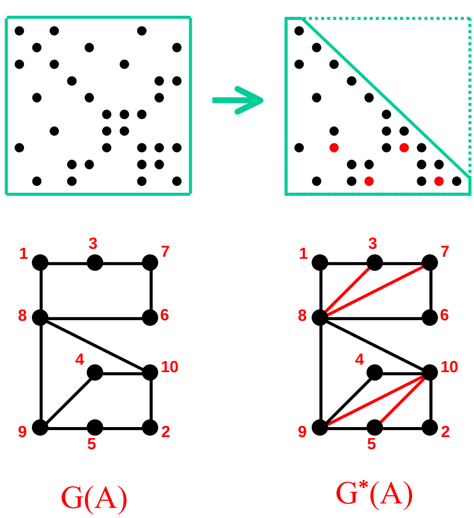
ILU + Krylov Methods	Direct methods
Based on scalar implementation	BLAS3 (mostly DGEMM) Thread/SMP, Load Balance…
Difficult to parallelize (mostly DD + Schwartz additive => # of iterations depends on the number of processors)	Parallelization job is done (MUMPS, PASTIX, SUPERLU…)
Low memory consumption	High memory consumption : very large 3D problems are out of their league (100 millions unknowns)
Precision ~ 10^-5	Great precision ~ 10^-18

We want a trade-off !

PaSTiX solver

- Current development team (SOLSTICE)
  - F. Pellegrini (assistant professor LaBRI/INRIA)
  - P. Hénon (researcher INRIA)
  - P. Ramet (assistant professor LaBRI/INRIA)
  - J. Roman (professor, leader of ScAlApplix INRIA project)
- PhD student
  - M. Faverge (NUMASIS project)
- Others contributors since 1998
  - D. Goudin (CEA-DAM)
  - D. Lecas (CEA-DAM)
- Main users
  - Electomagnetism & structural mechanics codes at CEA-DAM CESTA
  - MHD Plasma instabilities for ITER at CEA-Cadarache (ASTER)
  - Fluid mechanics at MAB Bordeaux

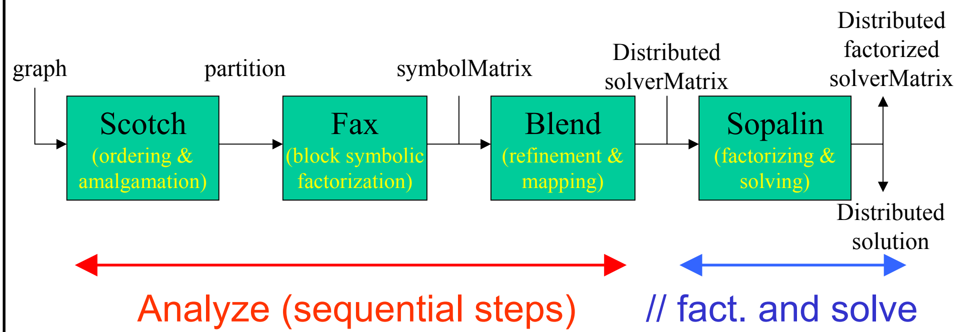
Graphs and Sparse Matrices:
Cholesky factorization



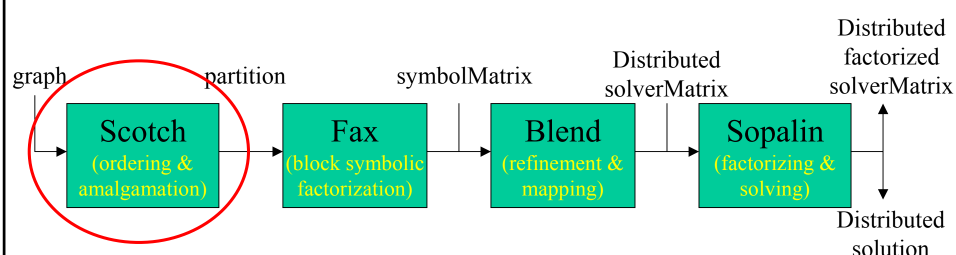
Fill: new nonzeros in factor

Symmetric Gaussian elimination:
for j = 1 to n
add edges between j's
higher-numbered neighbors

Direct solver chain (in PaStiX)



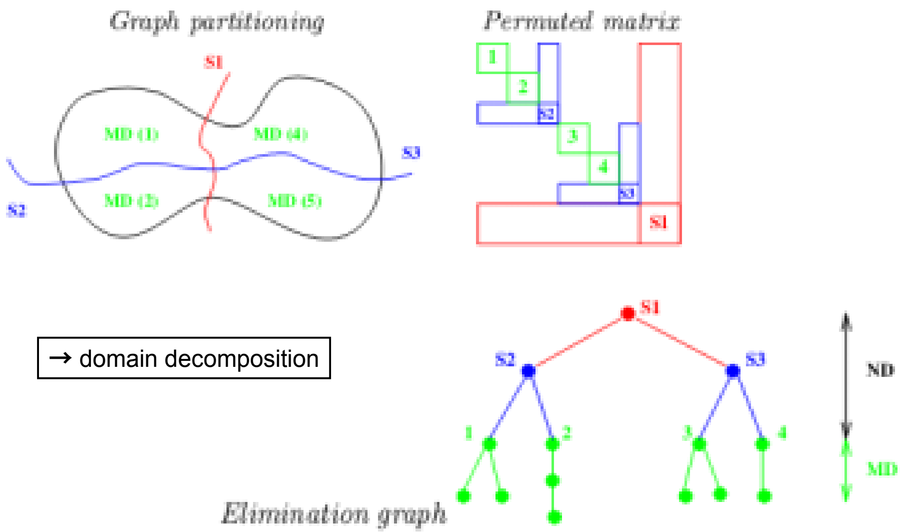
Direct solver chain (in PaStiX)



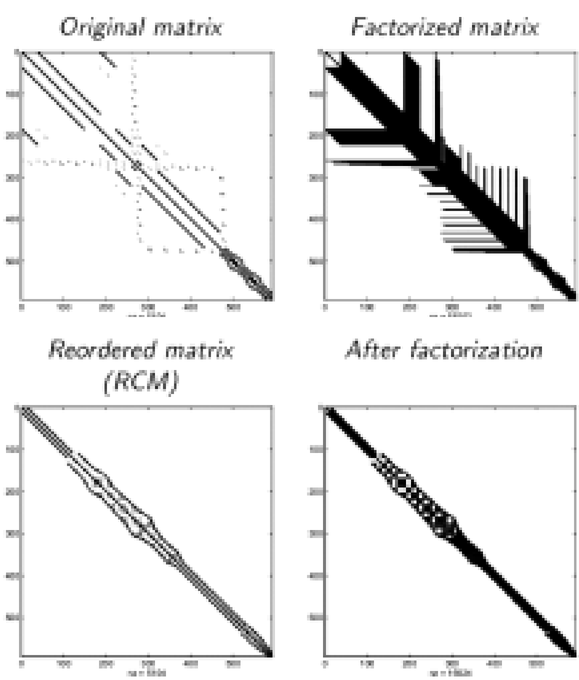
Sparse matrix ordering (minimizes fill-in)

- Scotch: an hybrid algorithm
  - incomplete Nested Dissection
  - the resulting subgraphs being ordered with an Approximate Minimum Degree method under constraints (HAMD)

Partition and Block Elimination Tree



→ domain decomposition



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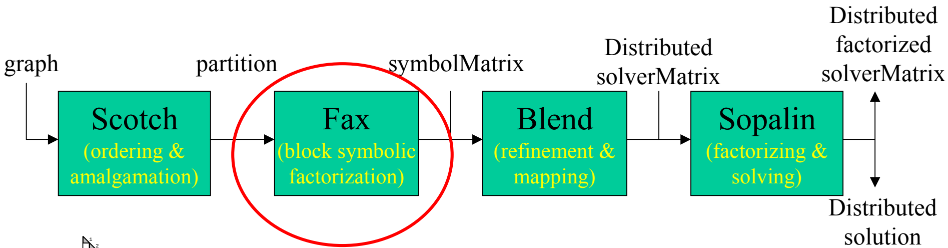
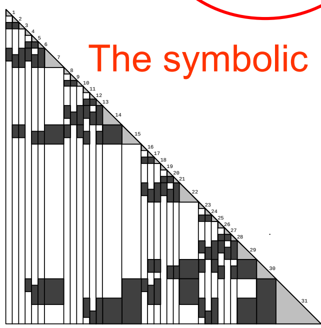




The symbolic block factorization

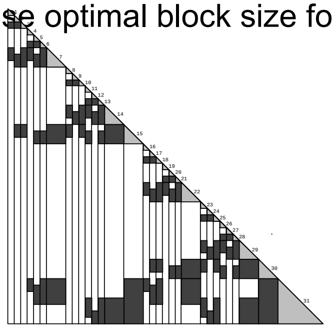
- ***Q(G,P)→Q(G,P)*=Q(G*,P) => linear in number of blocks!***
- Dense block structures → only a extra few pointers to store the matrix

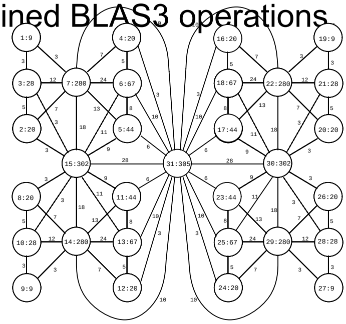
Matrix partitioning and mapping

⇒ Manage parallelism induced by sparsity (block elimination tree).

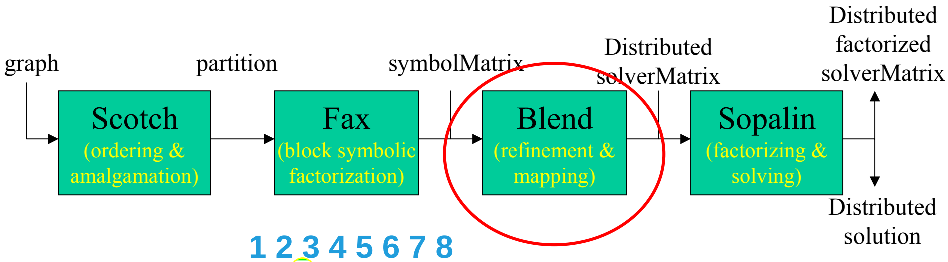
⇒ Split and distribute the dense blocks in order to take into account the potential parallelism induced by dense computations .

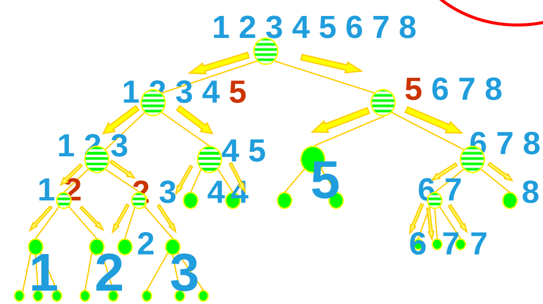
⇒ Use optimal block size for pipelined BLAS3 operations





Direct solver chain (in PaStiX)

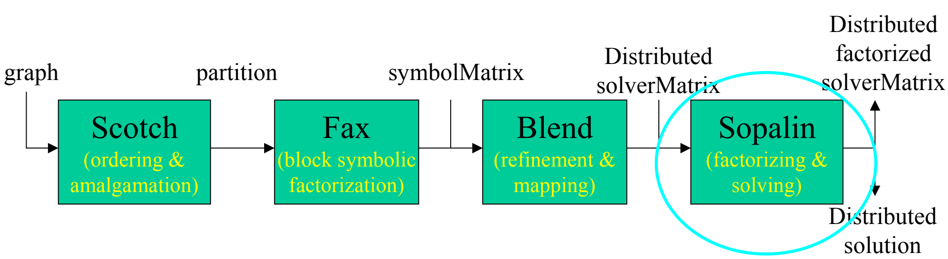




CPU time prediction

Exact memory ressources

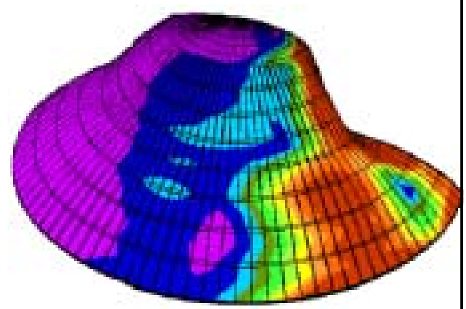
Direct solver chain (in PaStiX)



- Modern architecture management (SMP nodes) : hybrid Threads/MPI implementation (all processors in the same SMP node work directly in share memory)
- ➢ Less MPI communication and lower the parallel memory overcost

Numerical experiments (TERA1)

- Successful approach for a large collection of industrial test cases (PARASOL, Boeing Harwell, CEA) on IBM SP3
- TERA1 supercomputer of CEA Ile-de-France (ES45 SMP 4 procs)
- COUPOLE40000 :
  26.5 10^6 of unknowns
  1.5 10^{10} NNZL and 10.8Tflops
    - 356 procs: 34s
    - 512 procs: 27s
    - 768 procs: 20s



- (>500Gflop/s about 35% peak perf.)

Numerical experiments (TERA10)

- Successful approach on 3D mesh problem with about 30 millions of unkowns on TERA10 supercomputer
- But memory is the bottleneck !!!

MPI/Threads implementation for SMP clusters

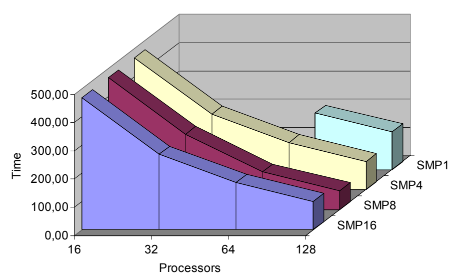
- **Mapping by processor**
  Static scheduling by processor
- Each processor owns its local part of the matrix (**private user space**)
- Message passing (**MPI or MPI_shared_memory**) between any processors
- Aggregation of all contributions is done per processor
- Data coherency insured by MPI semantic

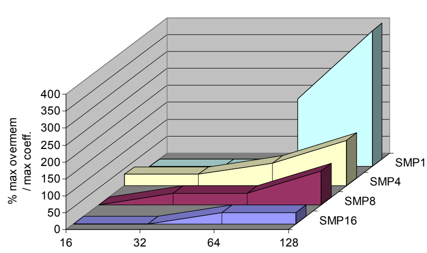
- **Mapping by SMP node**
  Static scheduling by thread
- All the processors on a same SMP node share a local part of the matrix (**shared user space**)
- Message passing (**MPI**) between processors on different SMP nodes

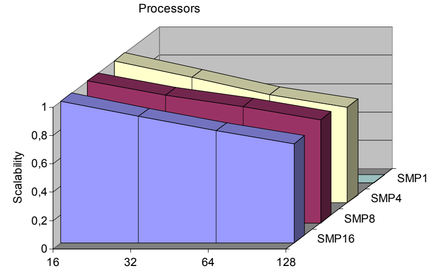
  Direct access to shared memory (**pthread**) between processors on a same SMP node
- Aggregation of non local contributions is done per node
- Data coherency insured by explicit mutex

SP3 : AUDI ; $N=943.10^{3}$; $NNZ_L=1,21.10^{9}$; 5,3 TFlops

Num. of threads / MPI process	Processors	16	32	64	128
	16	481,96	270,16	152,58	86,07
	8	476,40	265,09	145,19	81,90
	4	472,67	266,89	155,23	87,56
	1			(211,35)	(134,45)







AUDI : 943.10^3 (symmetric)

no meaning

- SP4 : 32 ways Power4+ (with 64Go)

Procs		32	64
Num. of threads / MPI process	32	94,21	60,03
	16	**93,14**	47,80
	8	96,31	**47,28**
	4	100,40	51,02

- SP5 : 16 ways Power5 (with 32Go)

Procs		2	4	8	16	32	64
Num. of threads / MPI process	16	-	-	-	**91**	59,7	34,1
	8	-	-	**177**	98,6	57,7	**31,3**
	4	-	**368**	182	99,7	**55,3**	-
	2	**686**	373	185	95	-	-

pb. alloc.

MHD1 : 485.10^3 (unsymmetric)

- SP4 : 32 ways Power4+ (with 64Go)

Procs		32	64
Num. of threads / MPI process	32	199,17	115,97
	16	**187,89**	**111,99**
	8	197,99	115,79
	4	202,68	117,80

- SP5 : 16 ways Power5 (with 32Go)

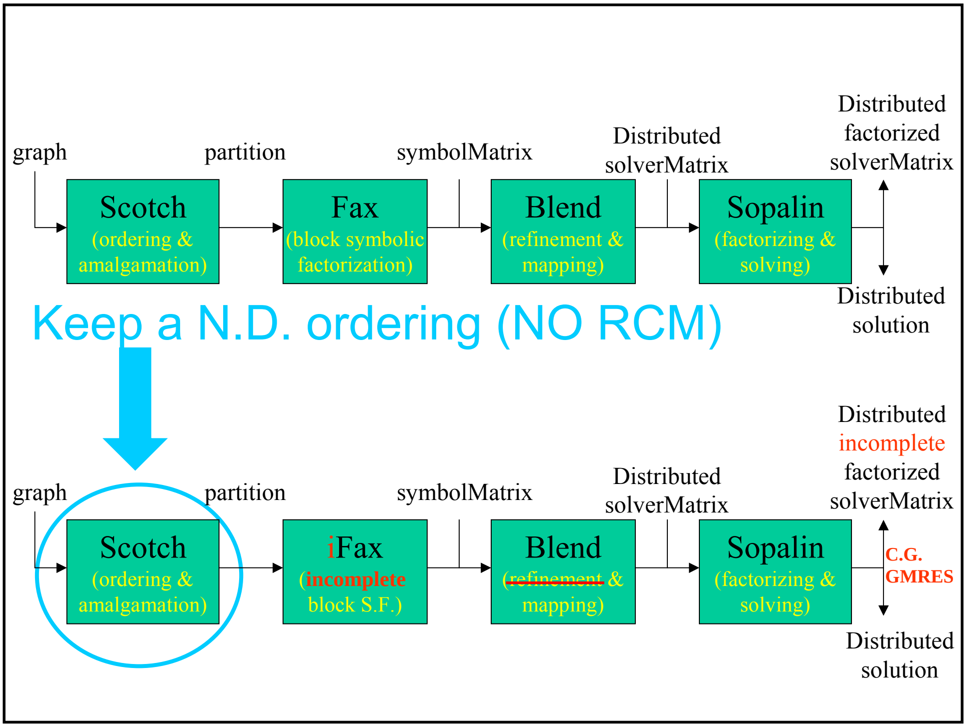
Procs		2	4	8	16	32	64
Num. of threads / MPI process	16	-	-	-	139	84,2	63,4
	8	-	-	**261**	141	**78,3**	-
	4	-	**505**	262	**136**	-	-
	2	**977**	506	265	-	-	-

How to reduce memory resources

- Goal: we want to adapt a (supernodal) parallel direct solver (PaStiX) to build an incomplete block factorization and benefit from all the features that it provides:
  - Algorithmic is based on linear algebra kernels (BLAS)
  - Load-balancing and task scheduling are based on a fine modeling of computation and communication
  - Modern architecture management (SMP nodes) : hybrid Threads/MPI implementation

Incomplete factorization outlines

- Which modifications in the direct solver?
- The symbolic incomplete factorization
- An algorithm to get dense blocks in ILU
- Experiments


graph
partition
symbolMatrix
Distributed solverMatrix
Distributed factorized solverMatrix
Scotch (ordering & amalgamation)
Fax (block symbolic factorization)
Blend (refinement & mapping)
Sopalin (factorizing & solving)
Distributed solution
Keep a N.D. ordering (NO RCM)
graph
partition
symbolMatrix
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Distributed incomplete factorized solverMatrix
Scotch (ordering & amalgamation)
iFax (incomplete block S.F.)
Blend (~~refinement~~ & mapping)
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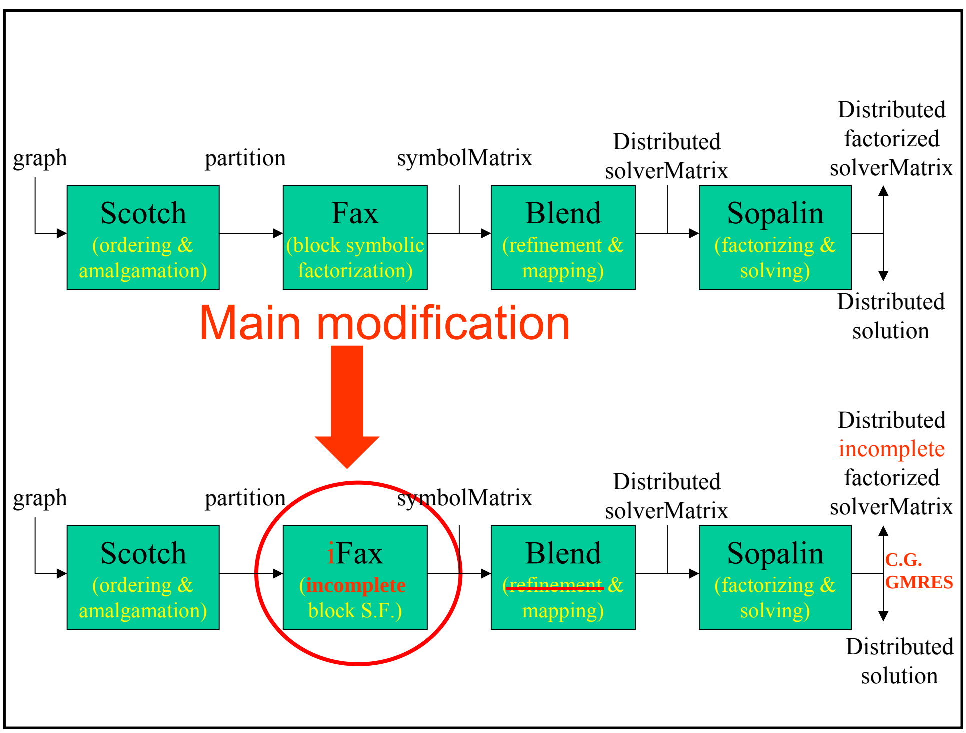
C.G.
GMRES
Distributed solution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Main modification
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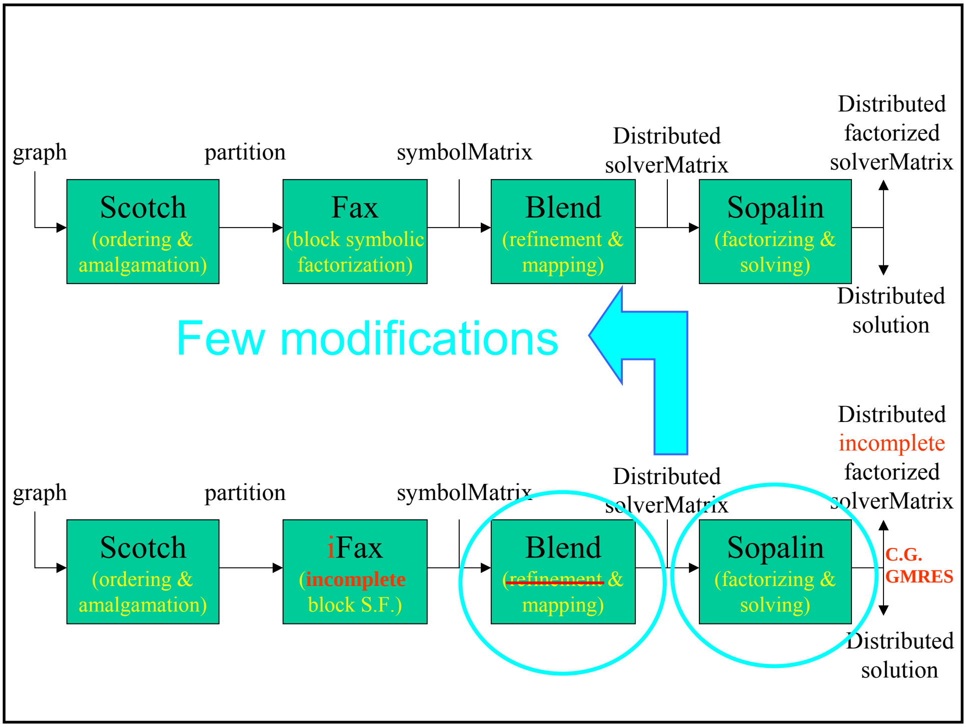
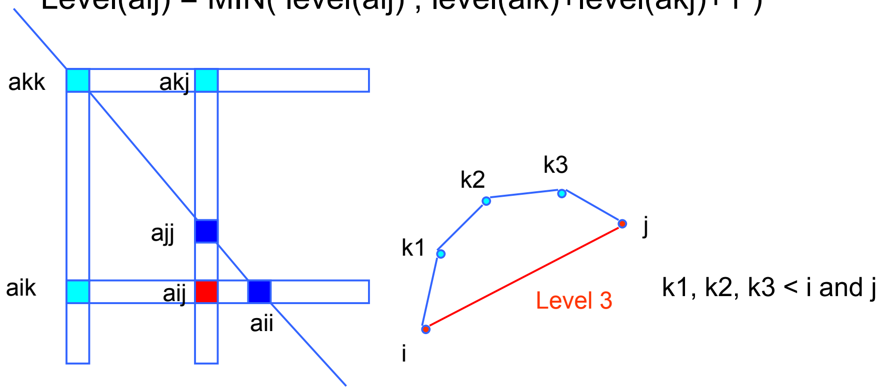


Incomplete factorization outlines

- Which modifications in the direct solver?
- ➢ The symbolic incomplete factorization
- An algorithm to get dense blocks in ILU
- Experiments

Level based ILU(k)

- Scalar formulation of the level-of-fill:
  Non zero entries of A have a level 0.
  Consider the elimination of the k^{th} unknowns during the fact.
  then:
  Level(aij) = MIN(level(aij) , level(aik)+level(akj)+1)



Level-of-fill metric

- Scalar formulation of the level-of-fill:
  - A fill-path, in the graph associated with the matrix A, is a path between two nodes i and j such that the nodes in this path have smaller number than i and j
  - There is a fill-in value (i,j), at the end of the Gauss elimination, iff there is a fill-path between i and j
  - At the end of the factorization, the level-of-fill value (i,j) is p iff there is a shortest fill-path of length p+1 between i and j (0 for terms in A)

Level based ILU(k)

- The scalar incomplete factorization have the same asymptotical complexity than the Inc. Fact.
- BUT: it requires much less CPU time
- D. Hysom and A. Pothen gives a practical algorithm that can be easily // (based on the search of elimination paths of length <= k+1) [Level Based Incompleted Factorization: Graphs model and Algorithm (2002)]

Level based ILU(k)

- In a FEM method a mesh node corresponds to several Degrees Of Freedom (DOF) and in this case we can use the node graph instead of the adj. graph of A i.e. :

  $Q(G,P) \rightarrow Q(G,P)^k = Q(G^k,P)$ *P = partition of mesh nodes*

- This means the symbolic factorization will have a complexity in the respect of the number of nodes whereas the factorization has a complexity in respect to the number of DOF.

Incomplete factorization outlines

- Which modifications in the direct solver?
- The symbolic incomplete factorization
- ➢ An algorithm to get dense blocks in ILU
- Experiments

How to build a dense block structure in ILU(k) factors ?

- First step: find the exact supernode partition in the ILU(k) NNZ pattern
- In most cases, this partition is too refined (dense blocks are usually too small for BLAS3)
- Idea: we allow some extra fill-in in the symbolic factor to build a better block partition
- ➢ Ex: How can we make bigger dense blocks if we allow 20% more fill-in ?

How to build a dense block structure in ILU(k) factors ?

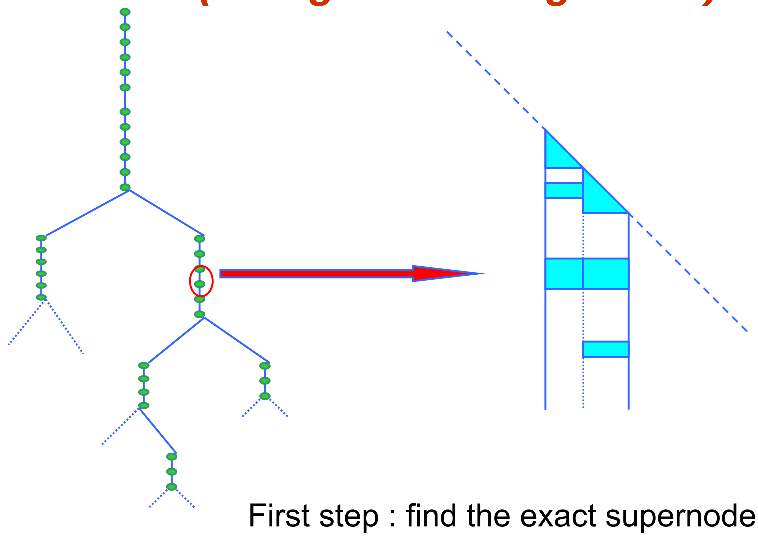
- We imposed some constraints:

➢ any permutation that groups columns with similar NNZ pattern should not affect G^k

➢ any permutation should not destroy the elimination tree structure

=> We impose the rule « merge only with your father… » for the supernode

Finding an approximated Supernodes Partition (amalgamation algorithm)



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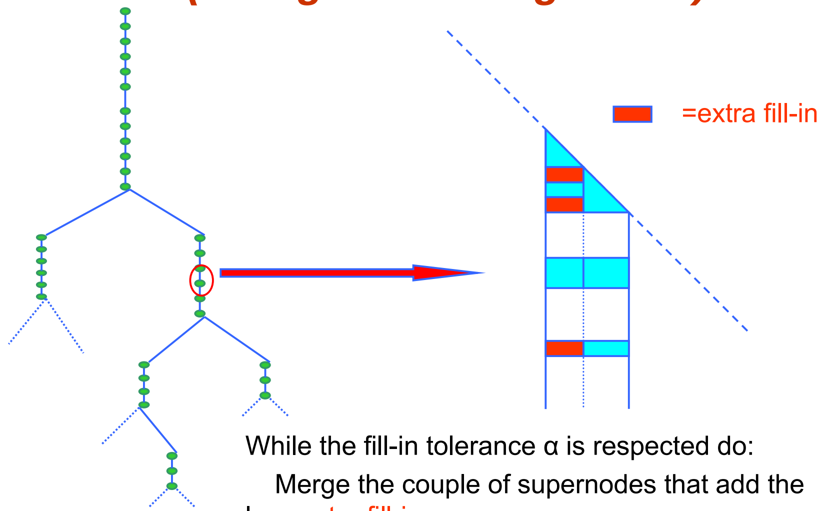
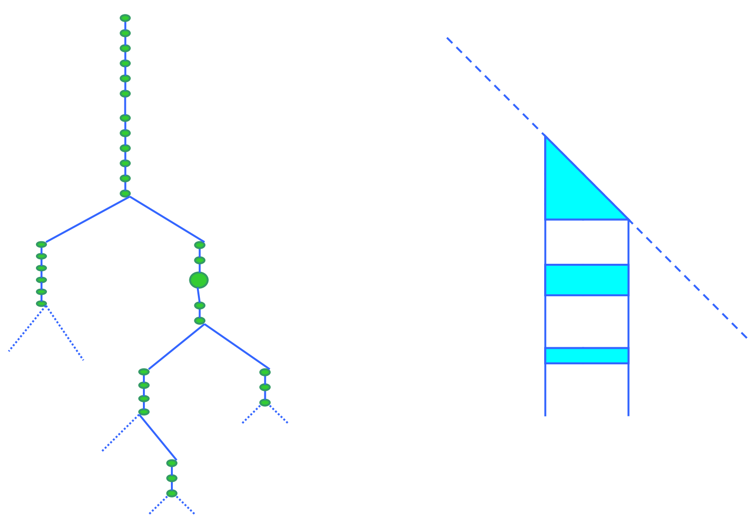
Finding an approximated Supernodes Partition (amalgamation algorithm)



While the fill-in tolerance α is respected do:

Merge the couple of supernodes that add the less extra fill-in

Finding an approximated Supernodes Partition (amalgamation algorithm)



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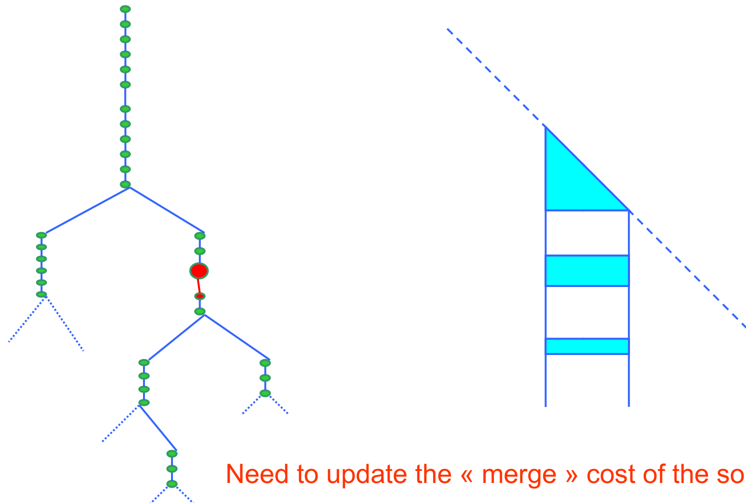

Need to update the « merge » cost of the son

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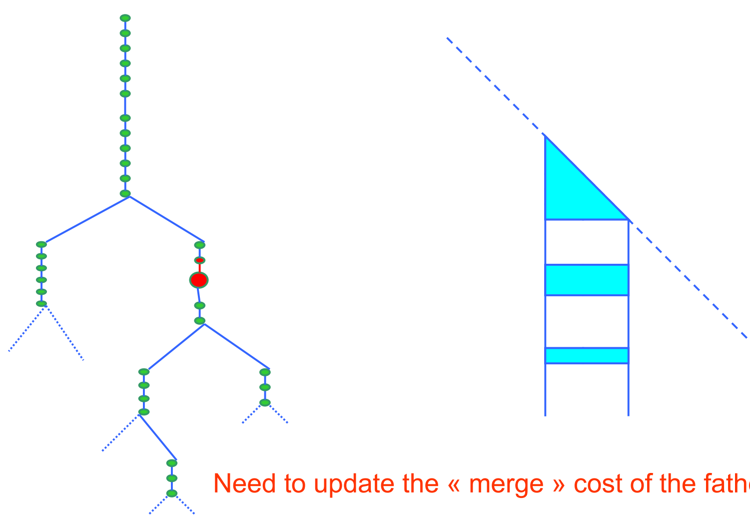

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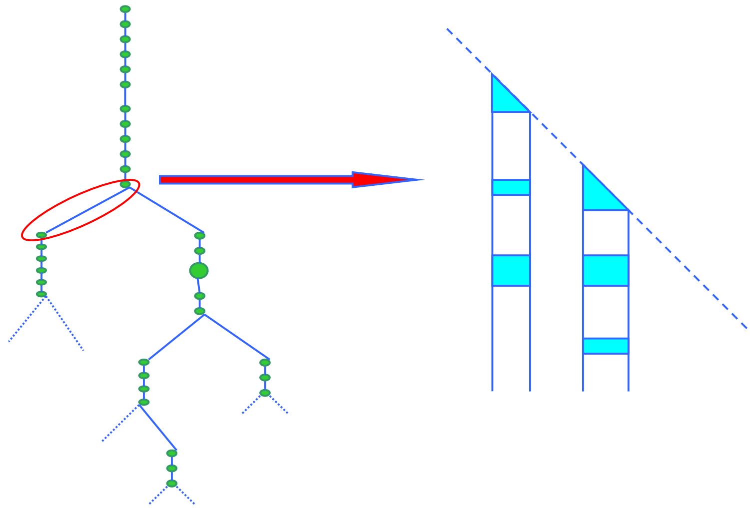

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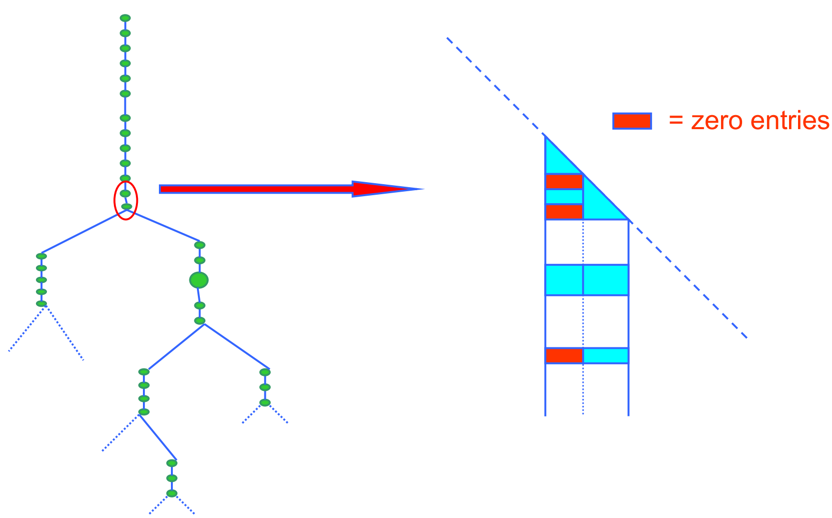

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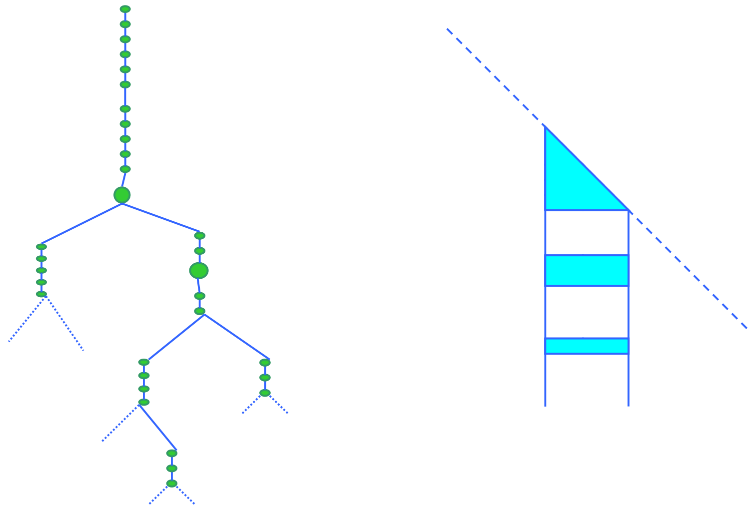

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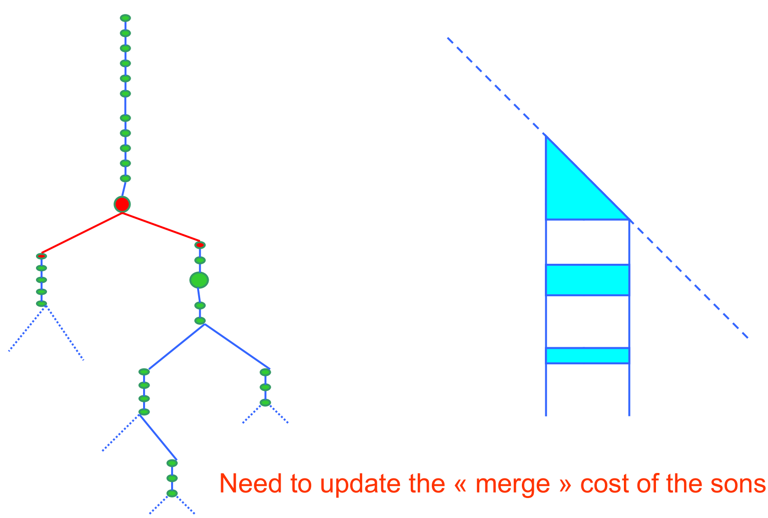

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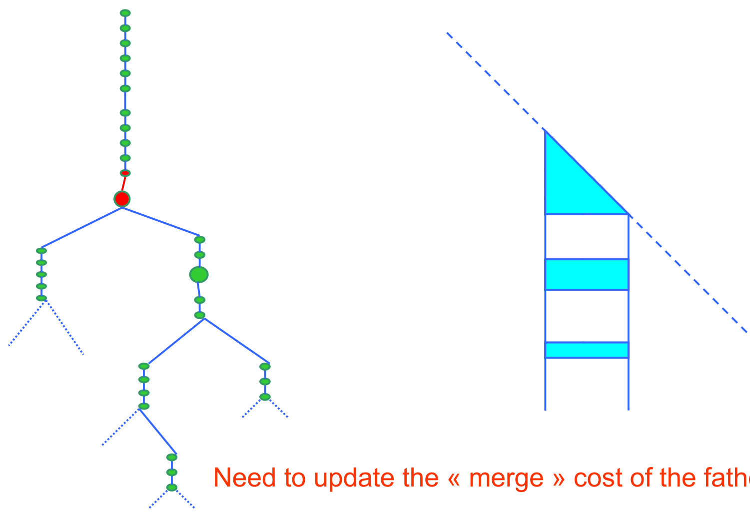

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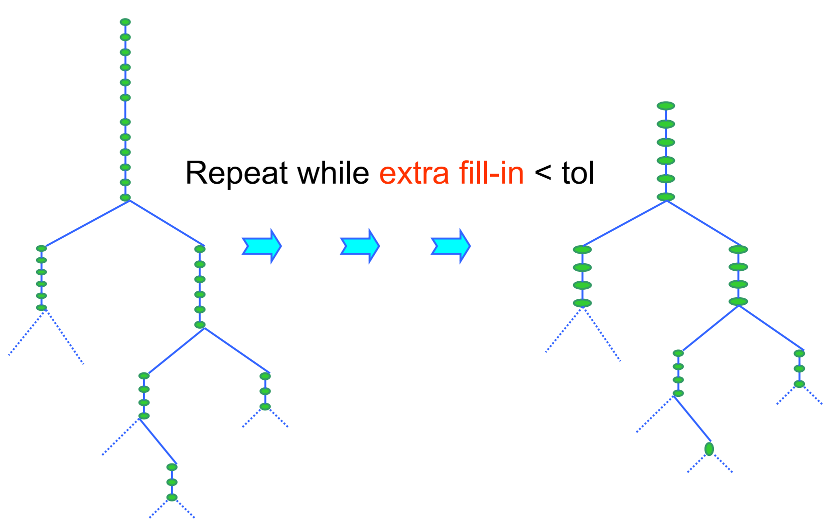


Cost of the algorithm

- The approximate supernode merging algorithm is really cheap compare to the other steps

➢ At each step: recompute fill-add for modified (son-father) couples and maintain the heap sort.

➢ Complexity bound by $O(D.N_0 + N_0.Log(N_0))$
N_0 : number of exact supernodes in ILU factors
D : maximum number of extradiagonal blocks in a block-column

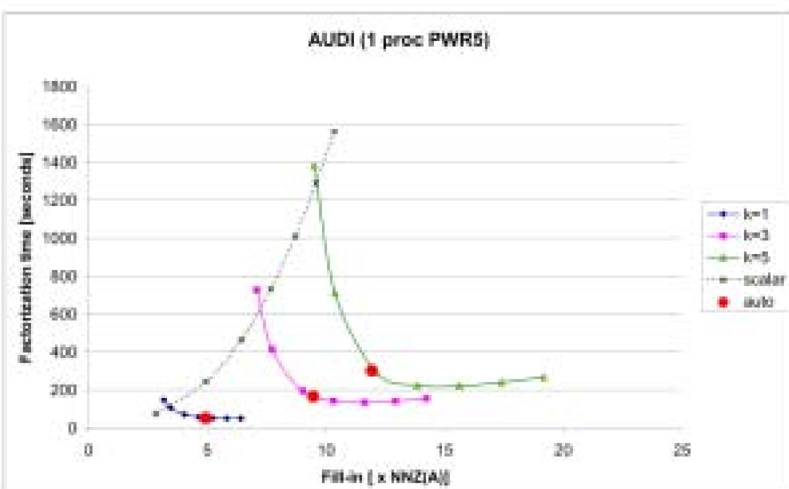
Numerical experiments

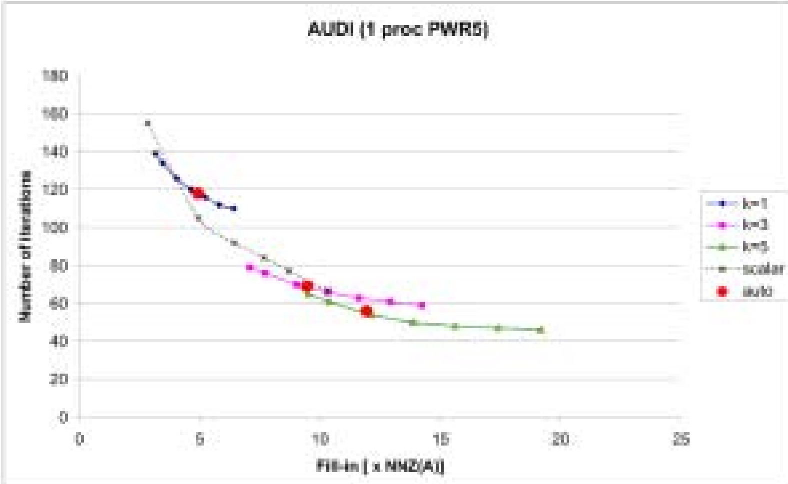
- Results on IBM power5 + Switch “Federation”
- All computations were performed in double precision
- Iterative accelerator was GMRES (no restart)
- Stopping criterion for iterative accelerators was a relative residual norm (||b-A.x||/||b||) of 1e-7

Test cases:

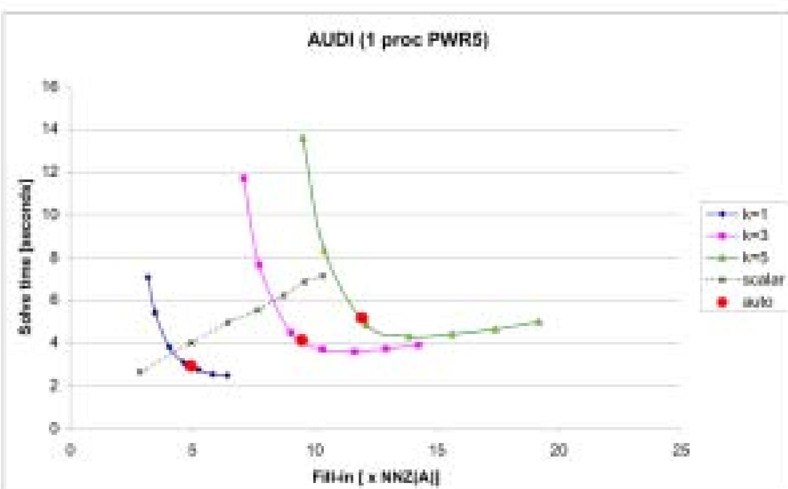
- AUDIKW_1 : Symmetric matrix (Parasol collection)
  n = 943,695   nnz(A) = 39,297,771
  With direct solver : nnz(L) = 30 x nnz(A)
  total solution in 91s on 16 procs
  ➔ 3D

- MHD : Unsymmetric matrix (Y. Saad collection)
  n = 485,597   nnz(A) = 24,233,141
  With direct solver : nnz(L) = 46 x nnz(A)
  total solution in 139s on 16 procs
  ➔ 3D

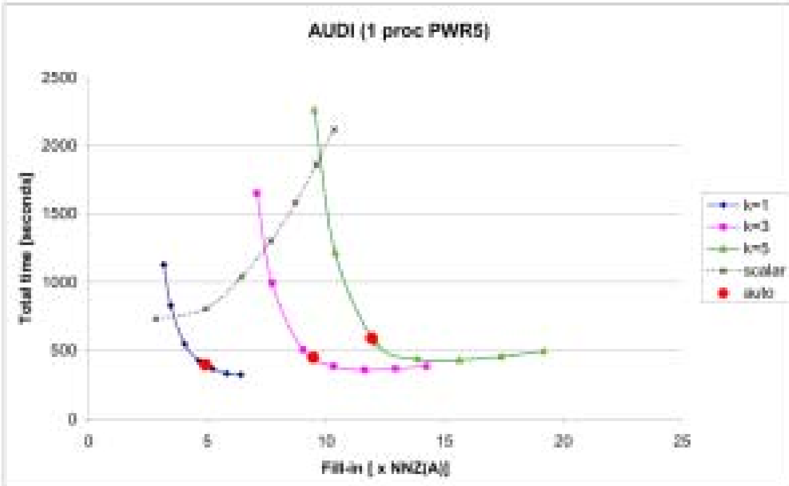




AUDI (1 proc PWR5)
Number of iterations
Fill-in [x NNZ(A)]
k=1
k=3
k=5
scalar
auto



AUDI (1 proc PWR5)
Solve time [seconds]
Fill-in [x NNZ(A)]
k=1
k=3
k=5
scalar
auto



Parallel Time: AUDI (Power5)

		1 processor			16 processors		
K	α	Fact	TR solv	Total	Fact	TR Solv	Total
1	20 %	74.5	4.59	690.1	21.4	0.51	91.5
1	40 %	56.4	4.44	620.3	12.7	0.42	67.0
3	20 %	331.1	7.97	936.8	39.2	0.91	108.7
3	40 %	194.6	7.57	732.0	18.6	0.66	65.7
5	20 %	518.5	8.86	1058.9	52.3	1.16	123.1
5	40 %	258.1	7.80	679.3	21.2	0.78	63.3

Table 3. Effect of amalgamation ratio α for MHD problem

k	α	# Supernodes	# Blocks	Fill-in	Amalg.	Inc. Fact.	Triang. Solve	Iterations	Total
1	∞	40215	528640	4.04	4.36	12.3	1.05	153	172
1	0	132615	1585901	1.77	1.51	16.0	2.04	172	366
1	10	103119	1199872	1.96	1.83	14.3	1.67	164	288
1	20	91975	1086335	2.16	1.92	13.7	1.55	164	267
1	40	71787	901500	2.57	2.15	12.7	1.36	162	233
1	60	56402	753112	2.98	2.33	12.1	1.22	158	204
1	80	43912	651356	3.41	2.48	12.2	1.12	156	186
1	100	33590	561447	3.81	2.62	12.4	1.05	153	173
1	120	26375	478080	4.19	2.76	12.8	0.97	149	**157**
3	∞	50361	803279	6.34	6.32	37.4	1.44	88	164
3	0	132485	3202800	3.69	2.20	85.6	3.52	100	437
3	10	93524	2290760	4.10	2.67	69.7	2.66	98	327
3	20	76199	1862555	4.51	2.93	57.8	2.30	97	280
3	40	53717	1390499	5.34	3.26	50.1	1.91	94	229
3	60	38617	1066834	6.15	3.53	46.5	1.67	92	200
3	80	27862	853927	6.96	3.75	44.6	1.49	89	177
3	100	20806	658369	7.74	3.92	43.8	1.35	86	159
3	120	16239	521220	8.57	4.05	44.2	1.27	83	**149**
5	∞	47646	932096	8.66	7.84	73.6	1.71	67	188
5	0	131806	4633544	5.42	2.76	237	4.83	79	596
5	10	83467	3215398	6.03	3.42	164	3.56	78	441
5	20	64718	2602706	6.65	3.69	145	3.12	77	385
5	40	41257	1811205	7.82	4.13	115	2.38	73	288
5	60	27553	1181086	8.97	4.45	94.3	1.93	69	226
5	80	19373	832068	10.15	4.68	85.5	1.65	66	194
5	100	14174	608861	11.35	4.84	80.4	1.53	64	176
5	120	10875	455535	12.51	4.96	79.6	1.48	61	**169**

Table 4. Performances on 1, 4, 8 and 16 processors PWR3 for 3 test α

AUDI						
	1 processor			4 processors		
k	Inc. Fact.	Triang. Solve	Total	Inc. Fact.	Triang. Solve	Total
1	53.7	2.91	397	14.2	0.84	113
3	167	4.12	451	43.1	1.23	126
5	304	5.19	592	78.2	1.53	163
	8 processor			16 processors		
k	Inc. Fact.	Triang. Solve	Total	Inc. Fact.	Triang. Solve	Total
1	7.86	0.51	68.4	6.34	0.39	52.2
3	22.4	0.73	73.8	12.8	0.52	48.4
5	40.8	0.91	91.7	22.1	0.76	64.9
MHD						
	1 processor			4 processors		
k	Inc. Fact.	Triang. Solve	Total	Inc. Fact.	Triang. Solve	Total
1	12.3	1.05	172	3.26	0.29	48.2
3	37.4	1.44	164	9.83	0.41	46.5
5	73.6	1.71	188	19.6	0.50	53.3
	8 processor			16 processors		
k	Inc. Fact.	Triang. Solve	Total	Inc. Fact.	Triang. Solve	Total
1	1.94	0.18	29.6	2.06	0.17	27.9
3	5.25	0.27	28.9	4.17	0.23	26.1
5	10.2	0.32	31.8	6.56	0.29	26.2

Table 5. Direct factorization on 16 processors

Name	#Columns	NNZ_L	Fill-in	Num. Fact.	Triang. Solve
AUDI	943695	39297771	30.1	91.4	1.21
MHD	485597	24233141	45.7	139	0.56

Prospects:

- Parallelization of the ordering (ParMetis, PT-Scotch) and of the Inc. Symbolic Factorization
- Perform more experiments to explore different classes of problems with symmetric and unsymmetric version
- Plug this solver in real simulations (CEA, ITER)

ASTER project

- ANR CIS 2006 Adaptive MHD Simulation of Tokamak ELMs for ITER (ASTER)
- The ELM (Edge-Localized-Mode) is MHD instability which localised at the boundary of the plasma
- The energy losses induced by the ELMs within several hundred microseconds are a real concern for ITER
- The non-linear MHD simulation code JOREK is under development at the CEA to study the evolution of the ELM instability
- To simulate the complete cycle of the ELM instability, a large range of time scales need to be resolved to study:
    - The evolution of the equilibrium pressure gradient (~seconds)
    - ELM instability (~hundred microseconds)

➢ a fully implicit time evolution scheme is used in the JOREK code

- This leads to a large sparse matrix system to be solved at every time step.
- This scheme is possible due to the recent advances made in the parallelized direct solution of general sparse matrices (MUMPS, PaStiX, SuperLU, ...)

NUMASIS project

- Middleware for NUMA architecture
- Application to seismology simulation

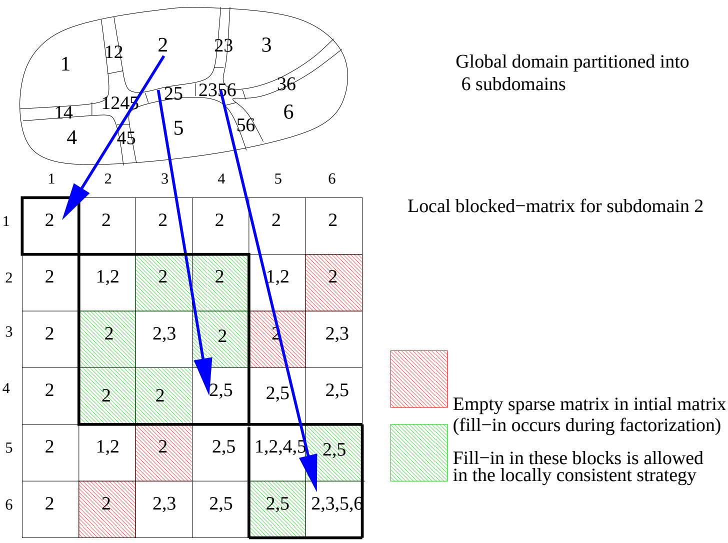
- New dynamic scheduling algorithm for solvers
- Take into account non-uniform acces to memory
- Use of MadMPI (R. Namyst)
  - Need a middleware to handle complexe architectures
  - Multi-Rails, packet re-ordering, …
- PhD of Mathieu Faverge (INRIA-LaBRI)

HIPS solver

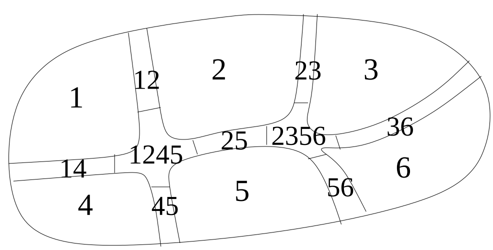
- Recent work of P. Hénon and J. Gaidamour (PhD student)
- Idea : build many subdomains that will be factorized with direct method
- Iterations on the Schur complement
- Use of a specific ordering to control fill-in based on Hierachical Interface Decomposition (HID) [Y. Saad, Phidal]
- Parallel implementation is achieved by mapping many subdomains on each processor

- A way to get an efficient solver on grid architecture ?

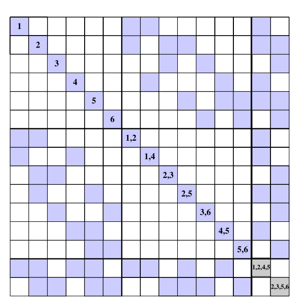
HIPS solver



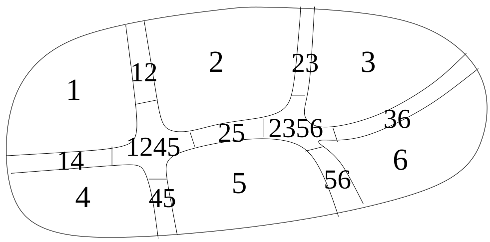
HIPS solver



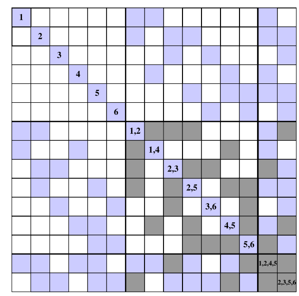
- Strictly consistant fill-in:
  - Fill-in is not allowed between connectors of a same level
  - Same structure of matrix A



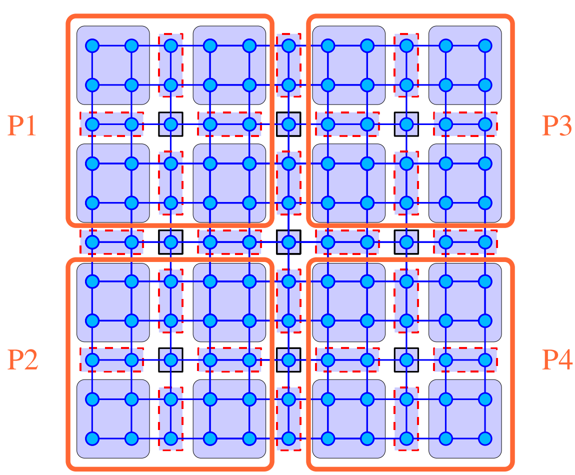
HIPS solver



- Locally consistant fill-in:
  - Fill-in is allowed between connectors that are adjacent to a same subdomain



HIPS solver



Links

- Scotch : http://gforge.inria.fr/projects/scotch
- PaStiX : http://gforge.inria.fr/projects/pastix
- MUMPS : http://mumps.enseeiht.fr/
  http://graal.ens-lyon.fr/MUMPS
- ScAlApplix : http://www.labri.fr/project/scalapplix

- ANR CIGC Numasis
- ANR CIS Solstice & Aster

- Latest publication : to appear in Parallel Computing : *On finding approximate supernodes for an efficient ILU(k) factorization*
- *For more publications, see : http://www.labri.fr/~ramet/*