Implementation of mulitfrontal method MULT_FRONT

Summarized:

One presents in this note, the data-processing description of the native version in Code_Aster, the linear solver multi-frontal, commonly called MULT_FRONT.

This version, developed at EDF R & D is stabilized, with an almost complete perimeter.

This note supplements the documentation of reference of Code_Aster: “Linear solver by the multi-frontal method” [R6.02.02].

One points out the principal notions used by the method: renumbering, shaft of elimination, super-nodes. One describes data-processing structures created by the algorithm. The data-processing main difficulties and characteristics are announced. The various possible developments are considered.

A report published except for is dedicated in an inventory of fixtures and the prospects for application maintenance: [RB12] “native multi-frontal Method in Code_Aster: prospect and inventory of fixtures”, CR-I23-2012-001.

Contents

1 Introduction

One describes in this note the data-processing implementation of the solver multifrontal, in Code_Aster. It is intended for the developers of the code and is not a “monopiece” document.

This method was developed in the shape of prototype within group ISA [RO93], and was in 1993 introduced then into *Code_Aster* in 1994, a form adapted to this code:
•Factorization of a matrix not necessarily in main memory (“out of core”), based on the package JEVEUX.
•Processing of the boundary conditions with Lagrange multipliers.
•One supposed moreover not to need to activate a search for pivot.

Initially, only a sequential version for symmetric real matrix was implemented in *Code_Aster*.

Thereafter the NON-symmetric and complex versions were introduced.

Complete parallelism was developed in prototype [RO95], it was not retained for the version developed in Code_aster. The reasons are the following ones:
•The priority purpose at the time was to optimize the memory requirements in order to treat linear systems of big size. However parallelism requires more memory than the sequential one.
•The parallelism of multi-frontal requires a management of the specific memory parallel to this method, which should have cohabited with the package JEVEUX, intrinsically sequential.
•Parallelism was not either a priority at that time where one had only calculators slightly parallel.

One will find a base theoretical on the method in [DU86], [AS87], [RO93] & [RO95], like in the documentation of reference of *Code_Aster* : “Linear solver by the Multi-Frontal method”, [R6.02.02].

The version double precision REAL*8 (resp. COMPLEX*16) is carried out by the call to routine FORTRAN MULFR8 (resp. MLFC16).

Thereafter one will describe in detail the version for symmetric matrix of real variable, of the paragraphs will be devoted to the versions asymmetric and complex. For more details on data structures of Code_Aster, one will refer to documentations [D4.06.07] (`sd_ nume_ddl`) and [D4.06.10] (`sd_matr_asse`).

1.1 General principles.

One wants to replace the factorization of a hollow matrix, by a continuation of factorization of full matrixes. It is the Cartesian principle: to replace a difficult problem by a set of simple problems.

For that one initially has an algorithm of renumbering of the variables of the system. This algorithm (of minimum degree, for example), makes it possible to minimize the order of the full matrixes to factorize, it is the first axis of effectiveness of the method.

Moreover, of this renumbering, one can extract the two following products:
•A shaft of elimination, obtained starting from the “hollow” (sparsity) of the initial matrix and optimum filling resulting from the renumbering. This graph (in the shape of tree structure) provides the order D `elimination of the variables and induces parallelism. (Indeed a node “wires” must be eliminated before a node “father”, but all the “wires” of the same “father” can be eliminated independently, i.e. in parallel.) This parallelism is the second axis of effectiveness of the method.
•Notion of super-node. This notion was conceived, initially, to minimize the cost (considerable) of the renumbering. While simplifying, one calls super-node, a set of nodes (within the meaning of the graph theory), having the same neighbors. The tree structure quoted above, in fact is formed by super-nodes whose size increases when one goes up in the tree structure, this increase is an illustration of the filling due to the method of elimination of Gauss. This regrouping has the following interest: one eliminates the variables by group, and not one by one, thus allowing the use of effective methods per block (using BLAS from level 2 or 3, produced matrice*vector or matrice*matrice). This work per block is the third axis of effectiveness.

In short, the 3 tension fields of the method are:
•A renumbering,
•a shaft of elimination,

•a regrouping of the variables.

Numerical factorization proceeds then as follows:

One traverses the shaft of elimination, with each stage (elimination of the super-node), one lays out of a matrix full partner with the super-node and with his neighbors, one carries out the elimination of Gauss limited to the variables of the super-node. One thus obtains on the one hand the columns of factorized final (variables of the super-node), and a frontal matrix modified and reduced to the neighbors (“complement of Schur”), who will be assembled in the frontal matrix of the variables of the super-node “father”.

1.2 Programming of the method.

In general, the programming of the multi-frontal method is divided into 2 phases:
•a phase of factorization known as “symbolic system”, including the renumbering,
•a phase of numerical factorization itself.

In *Code_Aster*, the renumbering and the first phase are carried out by the call to subroutine MLTPRE (called via MLFC16 and MULFR8, in the routines “hat” TLDLG2 and TLDLG3).

The second phase is carried out via the call to these routines MLFC16 and MULFR8, in the complex cases or realities.

2 Renumbering and factorization symbolic system: MLTPRE

By convenience, one omitted the prefix NU, in front of the structure names.

Data structures read.
Data structure: NUME_DDL, one extracts the records:

NUMÉRIQUE.DELG : indicate if the degree of freedom is of “Lagrange” or not.
NUMÉRIQUE.DEEQ ,
NUMÉRIQUE.NUEQ,
NUMÉRIQUE.PRNO : These 3 records and the draw up the restrains between the degrees of freedom subjected to a boundary condition Lagranges corresponding
The 3 following records describe a matrix “Morse”.
SMOS.SMHC : Number of column of term
SMOS.SMDI : Addresses of diagonal terms
SMOS.SMDE. : Many unknowns, and of terms of the matrix

written Data structures.
(Opposite each structure *Code_Aster*, one wrote the name of corresponding table FORTRAN, who will be used, thereafter for more conveniences.)
MLTF.ADNT ADINIT : addresses of the initial terms in factorized matrix
MLTF.LGBL LGBLOC : length of the blocks of factorized matrix
MLTF.LGSN LGSN : length of super-nodes
MLTF.LOCL LOCAL : used the assembly of the frontal matrixes, correspondence enters the local numbers of the super-nodes father and wires.
MLTF.ADRE ADRESS
MLTF.SUPN SUPND : definition of super-nodes
MLTF.FILS WIRES : wires of the super-nodes in the shaft of elimination
MLTF.FRER BROTHER: brother of the super-nodes in the shaft of elimination
MLTF.LGSN LGSN : length of super-nodes
MLTF.LFRN LFRONT : order of frontal matrixes (after elimination)
MLTF.NBAS NBASS : pointer related to the assembly of frontal matrixes
MLTF.ADPI ADPILE : addresses in the stack of frontal matrixes
MLTF.ANCI ANC : table reverses renumbering

MLTF.NBLI NBLIGN : order of frontal matrixes (before elimination)
MLTF.NCBL NCBLOC : many degrees of freedom of each block
MLTF.DECA DECAL : shift between the beginning of column D "a super-node and the beginning of the block JEVEUX which contains it
MLTF.SEQU SEQ : order D" elimination of the super-nodes (path of the tree structure).
These data structures will be described in the following paragraphs.

Description of the code.
One distinguishes 2 phases, the first consists of the renumbering, the second in what one calls in the language of the multi-frontal method, factorization symbolic system.

Data structure NUME_DDL describes a classification of NEQ degrees of freedom, including, most of the time, of the degrees of freedom known as of Lagrange. These degrees of freedom must satisfy the following relation of order:
(1) $L1 < U < L2$, if $L1$ and $L2$ are "Lagranges" associated with the boundary condition on U .

In order to preserve this order, one will not subject to the algorithm of renumbering only the degrees of freedom "Lagranges". The degrees of freedom "Lagranges are thus removed and the information with regard to them are stored in order to reinstate them in new classification, while satisfying (1).

Routines called (the first brief description of the code).

For the first phase, the routines called are the following ones:
PREML0: extraction of information on "Lagranges"
PREMLA: processing for "Lagranges" of standard linear relation
PREML1: pre processing and renumbering.
PREMLC : postprocessing of the renumbering (addition of "Lagranges").
PREMLD: idem

For the second:
PREML2: factorization symbolic system.

2.1 PREML0

One stores in the tables $LBD1$ $LBD2$, "Lagranges" of blocking, and in RL "Lagranges" of linear relation.

One obtains a new classification of 1 with $N2$ degrees of freedom without Lagrange, defined by:
P of $[1:\mathrm{NEQ}] \Rightarrow [1-N2]$, and Q Opposite of P .

For I 1 with NEQ , if I is a blocked degree of freedom $LBD1(I)$, (resp. $LBD2(I)$), is the number of its L1 (resp. $L2$).

In the case of NRL linear relations, one will have:
$RL(1,I)$: $L1$ relation I
$RL(2,I)$: $L2$ relation I .

N.B. Programming
In certain routines, one will use the name of variable $N1$ out of core of NEQ .

2.2 PREMLA

For all the degrees of freedom $L2$ of linear relation, (second "Lagrange"), its neighbors of lower number are known by extracting information from data structure SMOS.SMHC (table SADDLE-POINT).

From this information, PREMLA creates lists chained (tables DEB., SEE, FOLLOWS) for the degrees of freedom of linear relation $L2$.

That is to say J a degree of freedom included in a linear relation, $j0=DEB(j)$ is the address of the first neighbor of J in the table $VOIS$, $J1=SUIV(J0)$ is the address of the following neighbor, $J2=SUIV(J1)$ is the address of the following and so on.

This chained list will be used thereafter in PREML1, for the fabrication of $ADJNCY$.

N.B. Memory allocation
the chained list consists of 2 local structures, of names NOMVOI and NOMSUI, (created by WKVECT and destroyed at the end of the MLTPRE).
Their length: $LGLIST$, is estimated a priori by PREML0 (parameter of output LT), if it is insufficient, PREMLA provides an error code, and is called again with structures length 2 times larger.

2.3 PREML1

PREML1 calls the following routines:
PRMADJ, GENMMD, AMDBAR, ONMETL.

The crucial role of PREML1 is of launching the renumbering. This one, carried out with the choice by: METIS (method of dissection), GENMMD (minimum dismantles) or AMDBAR (minimum dismantles improved), require 2 preliminary actions.

2.3.1 Reconstitution of the nodes (within the meaning of the discretization by finite elements).

In a first version of the code, the algorithm of renumbering worked on $N2$ the degrees of freedom (without Lagranges).

One then wanted to preserve the internal order of the unknowns within the nodes of discretization finite element (for example ux uy uz, p).

A development was carried out for this purpose. **One subjects from now on to the algorithm of renumbering all the nodes and not $N2$ the degrees of freedom**.

One thus forms a new number of $NBND$ nodes and 2 associated pointers:
$NŒUD[1:N2]\Rightarrow[1:NBND]$, and the pointer reverses $DDL[1:NBND]$

One has 3 classifications thus:
•Initial classification of 1 with NEQ,
•That of the degrees of freedom without Lagranges 1 with $N2$,
•That of the nodes of interpolation 1 with $NBND$.

Provided with the tables P and Q between the first and the second, $NŒUD$ and DDL between the second and the third.

2.3.2 Creation of structure ($ADJNCY$, $XADJ$)

This structure is the standard structure of data of the algorithms of renumbering referred to above. There are 2 tables $ADJNCY$ and $XADJ$ defined as follows:

That is to say a node I, its neighbors are stored in the table $ADJNCY$, between the addresses $XADJ(I)+1$ and $XADJ(I+1)$.

One creates initially a structure $(ADJNCY, XADJ)$ relating to $N2$ the degrees of freedom, then routine PRMADJ transforms it into a structure $(ADJNCY, XADJD)$ relating to $NBND$ the nodes.

To create $ADJNCY$, one uses the chained list $(DEB, VOIS, SUIT)$ created by PREMLA, by forcing the degrees of freedom of a linear relation to being close. Thus these degrees of freedom will be in the same super node, just as them $L2$. The relation of order will be thus respected.

One carries out then the call to GENMMD, AMDBAR or METIS. One gets the usual results of this algorithm:

1) Renumbering,
2) Definition of the super-nodes,
3) Tree structure

the sources of these 3 methods are in the public domain.
Concerning the last 2 points, they should have been adapted. The renumbering relates to the nodes (1 with $NBND$), it has the shape of 2 tables opposite one of the other: $INVPND$ $PERMND$. ($INVPND(I)$ is the new number of the node I).

The tree structure, as for it, relates to the super-nodes created by the renumbering. The super-node SND is defined as follows: it is made up by the segment of nodes $[SPNDND(SND-1)+1, SPNDND(SND)]$. $SPNDND$ is thus an injection of the segment $[1 : NBSND]$ towards $[1 : NBND]$ $NBSND$: many super-nodes.

The tree structure is defined as follows: $PARENT(SND)$ "father" of the super-node is the node SND.

N.B. Programming
the tree structure of the super-nodes of multi-frontal, appears under 2 names: $PARENT$ and $PAREND$
the first contains the tree structure of SN except Lagrange, it is provided by renumbering (GENMMD/AMDBAR/METIS.)
The second is supplemented first by adding to it Lagranges, it is calculated by PREMLC starting from the first.

In the appealing program MLTPRE $PARENT$, which is an intermediary, is stored in ZI with the address SEQ, re-used later (space saver).

These preceding tables are defined according to $NBND$ the nodes of discretization of *Code_Aster*, (1 with $NBND$). They are rebuilt then in the classification of $N2$ the degrees of freedom not "Lagrange".
$INVPND$ becomes thus $INVP$, $PERMND$ becomes $PERM$ and $SPNDND$ becomes $SUPND$. (Cf loops 400.405.406 407 of PREML1).

N.B. Memory allocation

the structure $(XADJ, ADJNCY)$ of PREML1, is called $(XADJ2, ADJNC2)$ in MLTPRE. It is created before PREML1 and is destroyed afterwards. The length of $ADJNC2$ $LGADJN$, is estimated at $2\times(lmat-\mathrm{neq}+lglist)$, with $lglist$ = length of the list of the neighbors used in PREML0
$lmat$ = length of the initial matrix (provided by SMOS).
If $LGADJN$ is insufficient, PREML1 provides the length necessary in return code, and is started again.

NB. METIS

Before, one produced executable software MONGREL, writing in C, compiled and linké separately. This executable was called through APLEXT, layer of call of executable external by Code_Aster. From now on the routines of METIS are compiled and called by a call to ONMETL, function C appealing.

2.4 PREMLC

In output of PREML1, the results are expressed in term of degrees of freedom not "Lagrange" (1 with $N2$), routine PREMLC supplements the classification of 1 with $N2$ by adding "Lagrange" and by creating new super-nodes.

"Lagrange" are included thus in new classification:

For each $L1$, one creates a new super-node SN, made up of only one degree of freedom ($L1$), and wires of the first degrees of freedom of which it is "Lagrange" (blocked or linear relation). While being the wires of this degree of freedom, it will be eliminated before, which is the rule.

For $L2$, one does not create again SN, one is satisfied to add an additional degree of freedom ($L2$) to the super-node containing the degree of freedom (blocked or R.L.) of which it is "Lagrange".

In the event of linear relation, all the degrees of freedom of the relation are put by the algorithm in the same super-node. That is carried out in the preceding paragraph (PREML1), during the fabrication of structure $ADJNCY$, by forcing the degrees of freedom of the linear relations to being close between them, by means of the chained list (DEB $VOIS$, $SUIV$).

The new renumberings are obtained $NOUV$ and ANC on $[1:\mathrm{NEQ}]$, for all the degrees of freedom in new classification, $ANC(I)$ will provide its number in initial classification. $NOUV$ is the opposite table.

$NBSN$ the new number of super-nodes and $SUPND[1:nbsnd+1]$ defines these SN.
The super-node SN is made up by the segment of nodes $[SUPND(SN-1)+1, SUPND(SN)]$.
$SUPND$ is thus an application of the segment $[1:NBSN]$ towards $[1:\mathrm{NEQ}]$.

N.B. Memory allocation

$LGIND$ is the estimated length of the tables $GLOBAL$ AND $LOCAL$, (cf further 2.6) which are allocated before PREML2 ($NOPGLO$ and $NOPLOC$)
$LGIND$ is initially result of the renumbering, provided by PREML1 and increased by PREMLC according to the boundary conditions.

$LGIND$ is an overestimation of $GLOBAL$ and $LOCAL$ one does not want to preserve a too important structure.

Thus, after PREML2, one knows the real length of these tables, one redefines $LGIND$ with this value, and one recopies $GLOBAL$ and $LOCAL$ in structures $NOMGLO$ and $NOMLOC$ exact length.

2.5 PREMLD

It is a technical stage: this routine manufactures a structure of the type $ADJNCY$ like those used by the algorithms of renumbering, this time all the degrees of freedom of 1 with NEQ are taken into account.

N.B. Memory allocation

the structure $(XADJ, ADJNCY)$ manufactured by PREMLD, is called $(XADJ1, ADJNC1)$ in MLTPRE.
One uses the same length $LGADJN$ calculated previously.

2.6 PREML2

It is the second phase of MLTPRE: one carries out inter alia, the factorization symbolic system which is a simulation of real factorization, without floating operation, intended to facilitate the work of real factorization, by manufacturing certain pointers necessary.

PREML2 calls the following routines:

- FACSMB: factorization symbolic system itself.
- MLTPOS : fabrication of the sequence of factorization, i.e., gone up tree structure defined by the table $PAREND$, which thus defines the order of elimination of the super-nodes.

- MLTBLC : One defines here cutting in blocks of the factorized matrix, virtually “out of core”, because cut out in releasable blocks by the package JEVEUX .
- MLTPAS : One calculates here the address of the initial coefficients in the factorized matrix.

2.6.1 FACSMB

Given (They result from the renumbering):
$SUPND$
$PAREND$,
(And of initial topology):
$ADJNCY$.

Results :

$GLOBAL$
$LOCAL$
$ADRESS$
$NBASS$
$DEBFAC$
$DEBFSN$
$LGSN$
$LFRON$
$FILS$
$FRERE$.

These tables are described below.

$FILS$ and $FRERE$ are the tables “opposite” of the table $PAREND$, they allow to know all the super-nodes “wires” of a given super-node SN , it are $FILS(SN)$ $FRERE(FILS(SN))$, and so on. For the other results, it is necessary to reconsider the basic principles of the multi-frontal method, by means of the following figures:

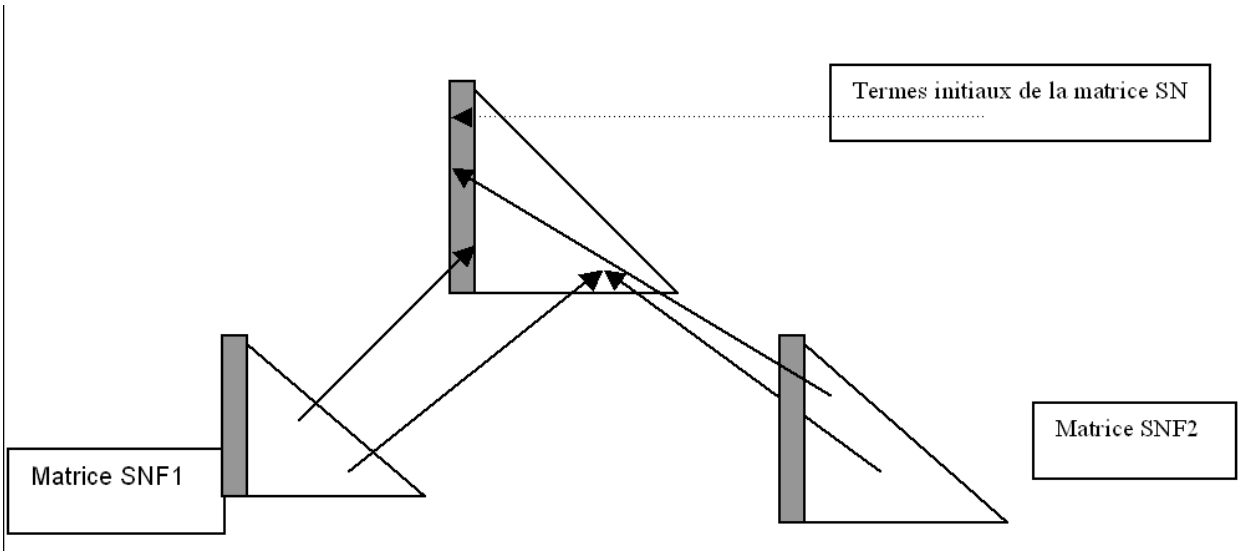


Figure 1 Assembly of 2 matrixes girls in a matrix mother

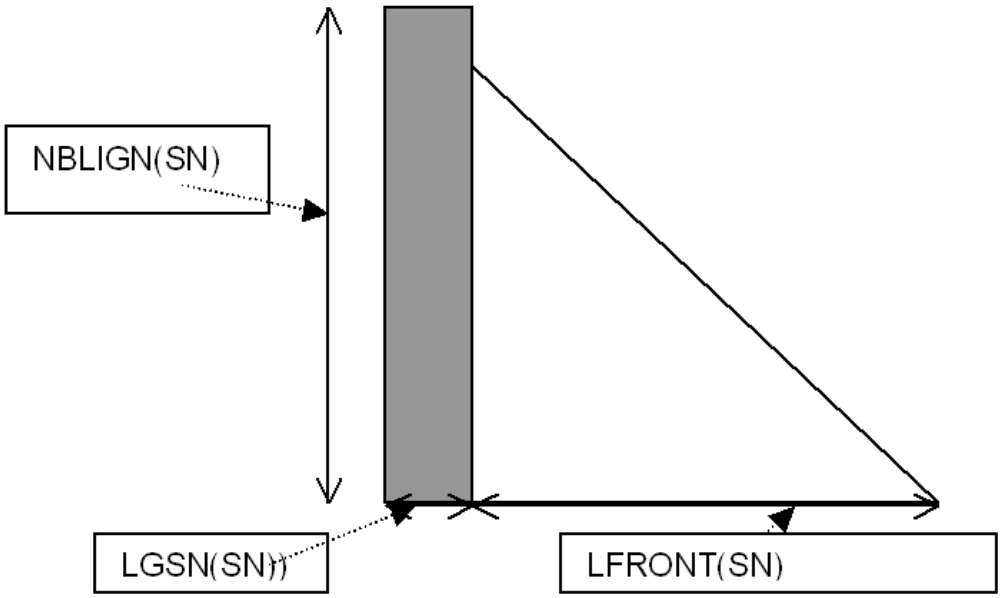


Figure 2 Stamps frontal SN

One sees on Figure 1, the matrix frontal SN (of the super-node SN), made up by the terms coming from the initial matrix, as well as terms coming from the matrixes girls $SNF1$ and SNF2, after elimination of the super-nodes $SNF1$ and $SNF2$. After elimination, the grayed part of the frontal matrix will constitute the columns of the factorized matrix, and the remaining white part arranged in the stack of the frontal matrixes, will agglomerate with the matrix mother during the assembly of the latter.

Factorization symbolic system carried out by FACSMB will simulate this process of assembly/elimination. For each super-node SN, one will manufacture a chained list containing the numbers of unknowns of the super node itself, as well as the numbers of unknowns of the neighbors of all the wires of SN. One includes the neighbors of the wires, but not the wires themselves which were eliminated.

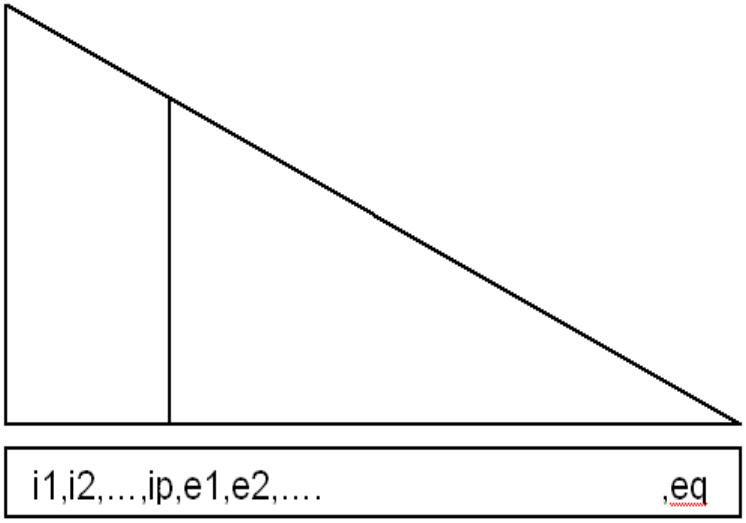
In language FORTRAN, FACSMB produces the following tables:

$LGSN(SN)$: many unknowns of the super-node SN (in fact = $supnd(sn+1)-supnd(sn)$)
$NBLIGN(SN)$: total number of unknowns of the frontal matrix SN
$LFRONT(SN)=NBLIGN(SN)-LGSN(SN)$, order of the frontal matrix after elimination which will be stored in the stack.

FACSMB manufactures also a table $GLOBAL$, provided with a table of pointers $ADRESS$.
$GLOBAL$ contains the numbers of the unknowns of the frontal matrix SN (before elimination), between the addresses $ADRESS(SN)$ and $ADRESS(SN+1)-1$.

These unknowns are with the number of $NBLIGN(SN)=(ADRESS(SN+1)-ADRESS(SN))$.
One reaches the table $LOCAL$ like $GLOBAL$, by means of the table $ADRESS$. Either $FSN1$ the super-node "wires" of the super-node SN, as on the figure above, and or I an index understood enters $ADRESS(FSN1)+LGSN(FSN1)$ and $ADRESS(FSN1+1), LOCAL(I)$ will be the local number (including enters 1 and $NBLIGN(SN)$) of this unknown in the matrix of the super-node "father" SN (one a) $PAREND(FSN1)=SN$.

$LOCAL$ will be used in the assembly of the frontal matrix "girl" in the frontal matrix "mother", it gives the TO address directly. One illustrates this using the following example:



The frontal matrix SN has $(p+q)$ unknown: $i1, i2, .., ip, e1, e2, ..., eq$, with

$NBLIGN(SN)=p+q$
$LGSN(SN)=p$
$LFRONT(SN)=q$
$ADRESS(SN+1)-ADRESS(SN)=p+q$
$GLOBAL=[i1, i2, ...ip, e1, e2, ...eq]$, to the addresses varying enters $ADRESS(SN)+1$ and $ADRESS(SN+1)$,
$LOCAL=[0,0, .., 0, l1, l2, ... lq]$

With the same addresses that above, $l1, l2, lq$ are the local numbers in the frontal matrix of $PAREND(SN)$. (values understood enters 1 and $NBLIGN(PAREND(SN))$).

$NBASS$, meter used also for the assembly, is defined as follows: $NBASS(FSN1)$ is the number of unknowns INC such as $INC<SUPND(SN+1)$, where $PAREND(FSN1)=SN$. It is thus the number of unknowns of $FSN1$, assembled in the matrix mother SN and who will be eliminated during elimination of SN.
$DEBFAC$ and $DEBFSN$, these 2 tables give the same values, first is subscripted by unknown, the second by super-node, they provide, for $DEBFAC$, the addresses of the diagonal coefficients of the unknowns in the factorized matrix. For $DEBFSN$, it is the address of the diagonal coefficient of the first unknown of the super-node.

One saw on Figure 2, that the columns corresponding to the unknowns of the eliminated super-node, (in grayed), constituted the columns of the factorized matrix which one calls $FACTOR$. The addresses of the diagonal coefficients provided by DEBFAC are addresses in a virtual table $FACTOR$ containing the factorized matrix. In fact a set of blocks JEVEUX will contain the factorized matrix, and one will handle an additional pointer for each block.

N.B. Programming
One sees on the figures preceding that one stores the columns of SN, all whole, (grayed rectangle), without taking into account the symmetry of the diagonal block. One consumes thus a little more memory, but one deals with a regular storage necessary to the use of the routines BLAS which require storages in tables FORTRAN of 2 dimensions.

2.6.2 MLTPOS

One recalls that the frontal matrixes resulting from eliminations are stored in a stack. All the matrixes girls of the same super node SN are stored (piled up), consecutively. Once read (depilated), they are not re-used any more, and the frontal matrix resulting from elimination from SN is stored with their core. The length of this stack decreases or increases with the wire of eliminations, It reaches a maximum which it is necessary to know.

MLTPOS traverses the tree structure, calculates $ESTIM$, maximum length of the stack for its later assignment, built a table $SEQ(1:NBSN)$ which provides the order of elimination of the super-nodes by traversing the tree structure upwards. It provides $ADPILE$ which contains the address in the stack of the frontal matrixes Des. SN
MLTPOS contains an algorithm of renumbering about elimination of the super-nodes, intended to minimize the length of the stack of frontal matrixes ([AS87])

2.6.3 MLTBLC

This routine builds the pointers of cutting in blocks of the factorized matrix. Each block will contain the columns of an integer of super-node. One will never meet the configuration where the various columns of the same super-node would belong to 2 blocks.

Data :
$MAXBLOC$: maximum length of the blocks. Each block will contain the columns of a maximum of super nodes. $MAXBLOC$ is calculated before the call to MLTBLC, it is in fact the length (in columns) of largest of the super-nodes, and the latter (in general highest in the tree structure) will only occupy a block with him.

Results :
$NBLOC$: Many blocks.
$LGBLOC(1:NBLOC)$: lengths of each block.
$NCBLOC(1:NBLOC)$: definition of the blocks, as follows the block IB is made up by the columns of the super-nodes $SEQ(NCBLOC(IB-1)+1)$, with $SEQ(NCBLOC(IB))$.
$DECAL(1:NBSN)$ table of shift which gives access the first diagonal term of each super-node in the factorized matrix. One will illustrate that by the following diagram:

```
ISN=0
For IB = 1, NBLOC                                                    !
Buckle on the blocks of factorized
      JEVEUO (JEXNUM (FACTOL, IB), "It, IFACL)
                          ! Block IB of collection FACTOL is charged in IFACL
     For NC = 1, NCBLOC (IB)              ! Buckle on the Super-nodes of block IB
           ISN = ISN +1
           SN = SEQ (ISN)
!          One follows the sequence of elimination
           ADFAC= IFACL + DECAL (SN) - 1
!          ADFAC is the address in ZR of the first coefficient of the super-NOEUD SN
```

2.6.4 MLTPAS

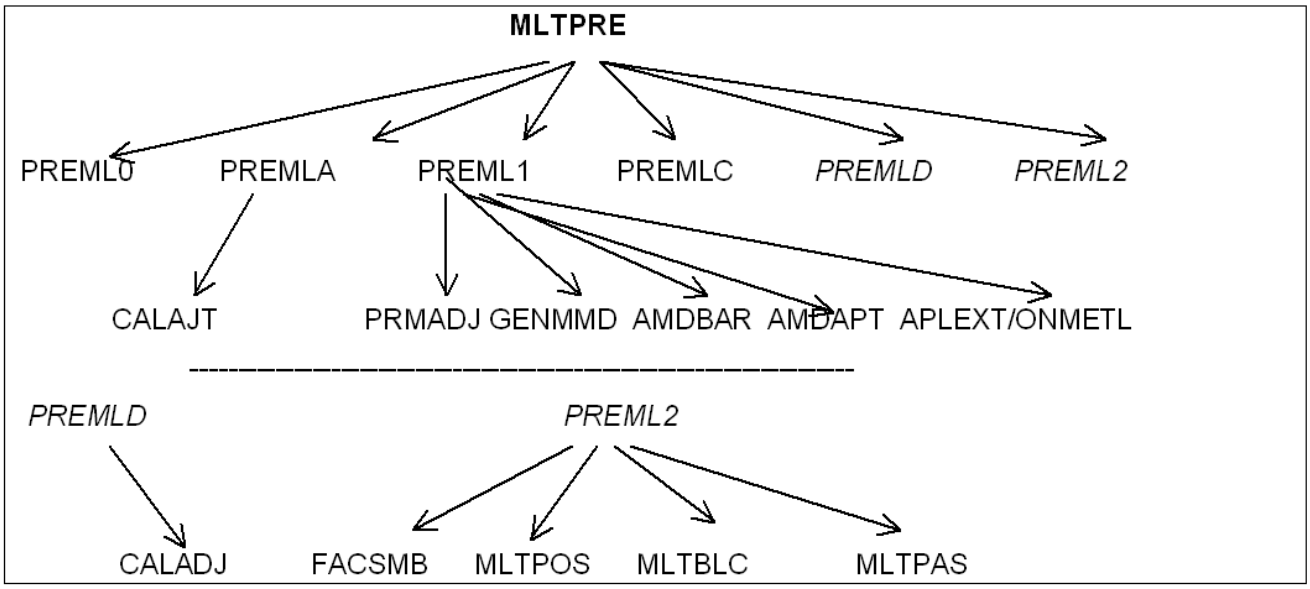
This routine calculates the addresses in the factorized matrix, of the coefficients of the initial matrix.
These addresses are stored in structure MLTF.ADNT, of name FORTRAN $ADINIT$ or COL length $LMAT$.

N.B. Characteristic of programming.

Certain addresses generated of ADINIT are negative. Indeed in the NON-symmetric case, there are 2 initial matrixes MATI and MATS which have same topology, (same neighbors, even hollow), factorization symbolic system is the same one.
However, it can happen that a coefficient of MATI (lower part of the initial matrix), has a destination in the upper part of the factorized matrix. (In an identical way enters MATS and the lower part of factorized). In this case the address of the initial coefficient is stored negative and the routine of injection of the coefficients of the initial matrix, MLTASA takes it into account and addresses the coefficients correctly.

```
IF (CODE.GT.0) THEN
                      ZR (IFACL+ADPROV-DEB) = ZR (MATI+I1-1): MATI injected into IFACL
(ower)
                   ZR (IFACU+ADPROV-DEB) = ZR (MATS+I1-1)
                ELSE
                   ZR (IFACL+ADPROV-DEB) = ZR (MATS+I1-1)
                   ZR (IFACU+ADPROV-DEB) = ZR (MATI+I1-1) MATI injected into IFACU (pper)
                ENDIF
```

2.7 Shaft of call of MLTPRE



3 Numerical factorization MULFR8

One deals with factorization itself, the routines called are:

1) MLTPRE
2) MLTASA
3) MLTFC1

MLTPRE, considering previously, is called if necessary. One checks that it was not already called upstream, in this case one leaves the routine.

3.1 MLTASA

This routine carries out the injection of the initial terms of the matrix in the factorized matrix. The table ADINIT calculated previously by MLTPRE provides the addresses.

Data :
Record .VALM of structure NOMMAT of the type sd_matr_asse provided.
$ADINIT$ and $LGBLOC(1:NBLOC)$ calculated by MLTPRE.

Results :
MLTASA creates a dispersed collection of name $FACTOL$ not $NBLOC$ being blocks lengths given $LGBLOC(1:NBLOC)$

par. In the case – symmetric, the routine reads 2 " .VALM " of respective names $MATI$ and $MATS$, left lower and higher the initial matrix, and creates 2 collections $FACTOL(ower)$ and $FACTOU(pper)$.

3.2 MLTFC1

One is if the stack of the frontal matrixes is arranged in a table FORTRAN named $PILE$ and allocated by WKVECT in the appealing MULFR8, this table is destroyed at the end of the routine.

A version with the frontal matrixes in dispersed collection was written (MLTFCB), but is not used.
MLTFC1 has following structure:

In an external loop on the blocks of factorized,
Loading of the memory stack
Buckles on the nodes of the block
SEQ provides the order of elimination
One thus eliminates the super-node SNI in various phases:
Assemblies of the matrixes "girls" by call to MLTAFF and MLTAFF
Elimination of the columns of SNI which are the columns of factorized: Up to date
Put MLTFLM of the remaining unknowns in the frontal matrix (complement of Schur): Fine
MLTFMJ of loop
End of loop

```
For IB = 1, NBLOC                                                              !
Buckle on the blocks of factorized
      JEVEUO (JEXNUM (FACTOL, IB), "It, IFACL)
      ! Block IB of collection FACTOL is charged in IFACL
     For NC = 1, NCBLOC (IB)  ! Buckle on the Super-nodes of block IB
           ISN = ISN +1
           SNI= SEQ (ISN)
           For all SN  the wires of SNI! assembly of the matrixes girls
            mltafp
              mltaff
           ! end of the assembly of the matrixes girls

            mltflm  ! elimination of SN: factorization on the columns of SN
            the mltfmj ! contribution of the columns eliminated on the other degrees of
freedom from the front, update of the frontal matrix
                     !        end of loop on the super nodes
!        end of loop on the blocks
```

Before describing the routines called, it is necessary to specify the way in which the matrix is arranged. The following diagram is looked at:

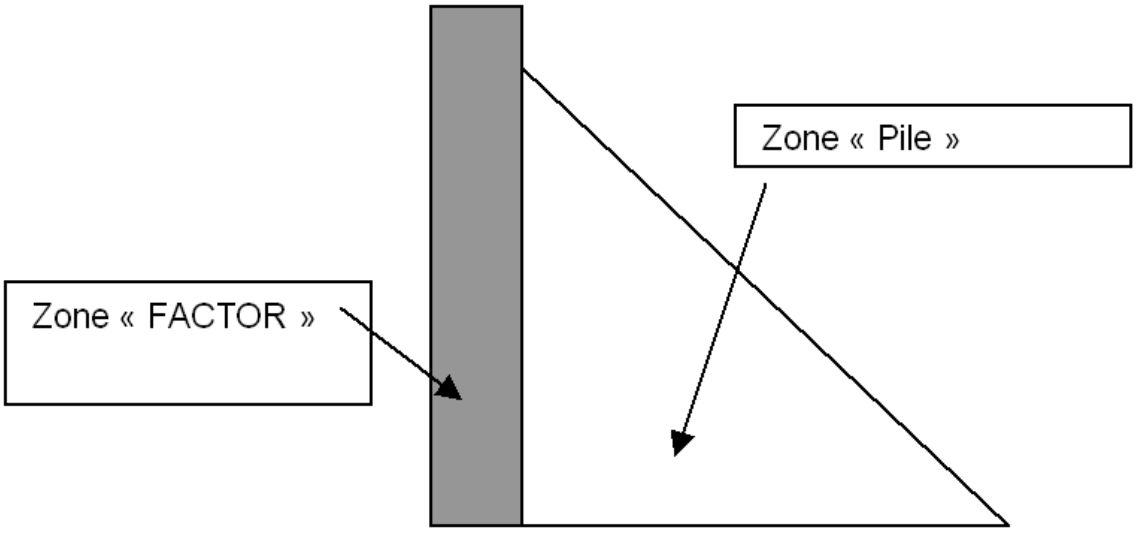


Figure 3 Decomposition of the frontal matrix in 2 storage sections

the grayed rectangular part represents active zone the "of the frontal matrix", in fact the columns of SN will be eliminated, and will constitute the columns of the factorized matrix $FACTOR$. To avoid a copy of memory between the frontal matrix and $FACTOR$, one stores directly the coefficients in $FACTOR$, one will say that it is the part " $FACTOR$ " frontal matrix. A with dimensions, there is the "passive" zone of the frontal matrix, (complement of Schur in fact), which will be stored in the stack, in the same way, to avoid a copy of memory, one directly stores this part of the matrix in the stack.

MLTAFP and MLTAFF are the routines which assemble the frontal matrixes "girls" in the frontal matrix "mother".

3.2.1 mltafp

This routine assembles the coefficients of the frontal matrix "girl", in the zone " $FACTOR$ " of the frontal matrix "mother".

3.2.2 mltaff

This routine copies the coefficients of the frontal matrix "girl", in the zone "crushes" frontal matrix "mother".

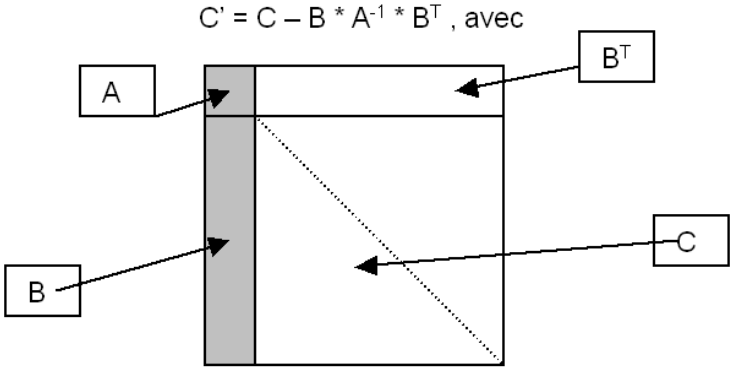
3.2.3 mltflm

Elimination of the super node SN, i.e factorization partial of the frontal matrix, work in the zone "". $FACTOR$ mltflm

CALLS : dgemv
: Blas routine which carries out the products matrice*vector mltfld
(CALL to DGEMV) mltflj
(CALL to DGEMM). mltfmj

3.2.4 Update

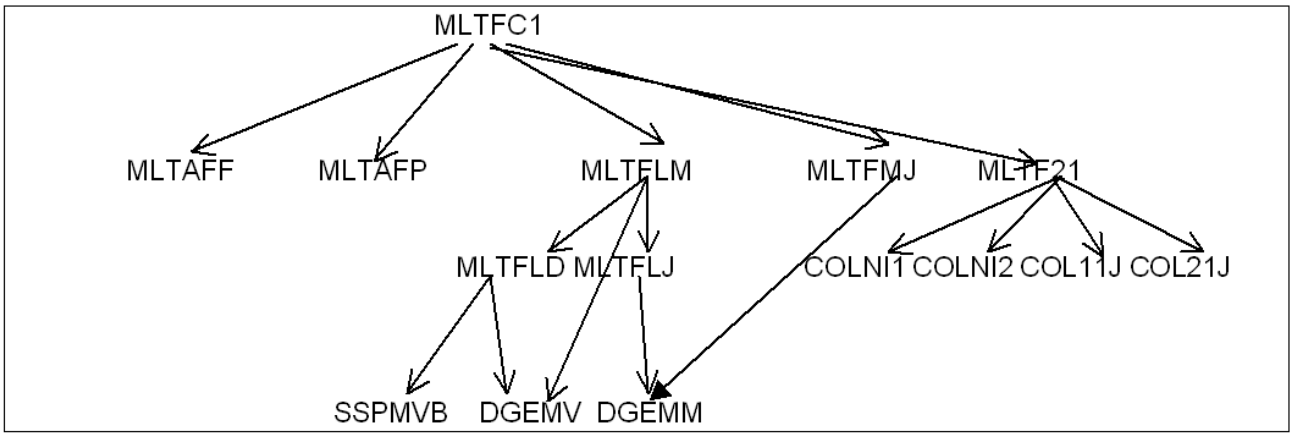
of the zone "" $PILE$ which is modified by the elimination of. SN mltfmj
CALLS : dgemm
: BLAS routine which carries out the products matrix-matrix. mltfmj
IS the routine most consuming computing time, it and the carries out the update of the frontal matrix on the lines columns of the degrees of freedom close to those eliminated, it is an operation which one can write: In order to



reduce the costs of computation, the matrixes virtually are divided, A and B under C blocks of order and NB the operation (1) above is carried out per blocks by calling the routine Blas DGEMM . This routine optimized by the manufacturer on each machine benefits owing to the fact that the small blocks of order thus NB multiplied hold in the primary mask, thus reducing the costs of access to the memory. is NB currently built-in to 96, this value generally about a few tens depends on the size of the mask, $L1$ nearest to the processor and the size of with the dealt problems. It could be D to estimate from time to time according to new acquisitions of machines, on a set of significant benchmarks. The tests carried out previously showed that the performances varied little when NB varied around 96. mltflm

USES also this division in blocks and uses DGEMM via mltflj . (If the number of columns to be eliminated is lower than a certain threshold (), $pmin=10$ the call to these 2 last routines is replaced by the call to MLFT 21). This was done by preoccupation with an optimization of the elimination of the "small" super-nodes, it would be appropriate to check that is always justified. Thus, by preoccupation with a simplification, after checking of the absence of degradation of the performances for the small cases, one could remove this threshold and thus eliminate a branch from subprogram call.

To illustrate this, the tree structure of the routines called in the symmetric case is the following: Figure



4 Factorization (symmetric real case). Increase

4 of the system: RLTFR 8 If

the number of second members to solve 4 simultaneously is higher than, one calls on a method per blocks implemented by routine RLBFR 8, if not MLTDRA is called for each second member. Data
: they are the pointers resulting from MLTPRE:

ADRESS
GLOBAL
SUPND
LGSN
ANC
NOUV
SEQ
LGBLOC
NCBLOC .
DECAL And

stamps it factorized resulting from MULFR 8:
FACTOL .VALF (and: *FACTOU* .WALF into asymmetric)

the second members: Results
$XSOL(1:\neq, 1:NBSOL)$

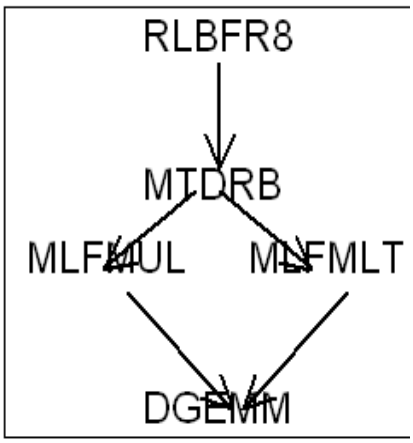
: They are found in the table which contained the second members: . *XSOL* MLTDRA

4.1 This

routine successively carries out, for only one second member, the descent, division by the diagonal term, and the increase. In the descent, one calls on the product matrix-vector of *DGEMV* the Blas libraries, beyond of a certain threshold. In lower part one optimizes "with the hand" in routine SSPMVB . (This optimization is a vectorization written for the CRAY, it could thus be re-examined even removed!) RLBFR

4.2 8 In the presence of

several second members, the calls to DGEMV quoted in the preceding paragraph, are replaced by calls to DGEMM , product matrice*matrice, on matric blocks of order. *NB* One thus aims the performance provided by these Blas of level 3, as in numerical factorization.
The routines called are: Figure

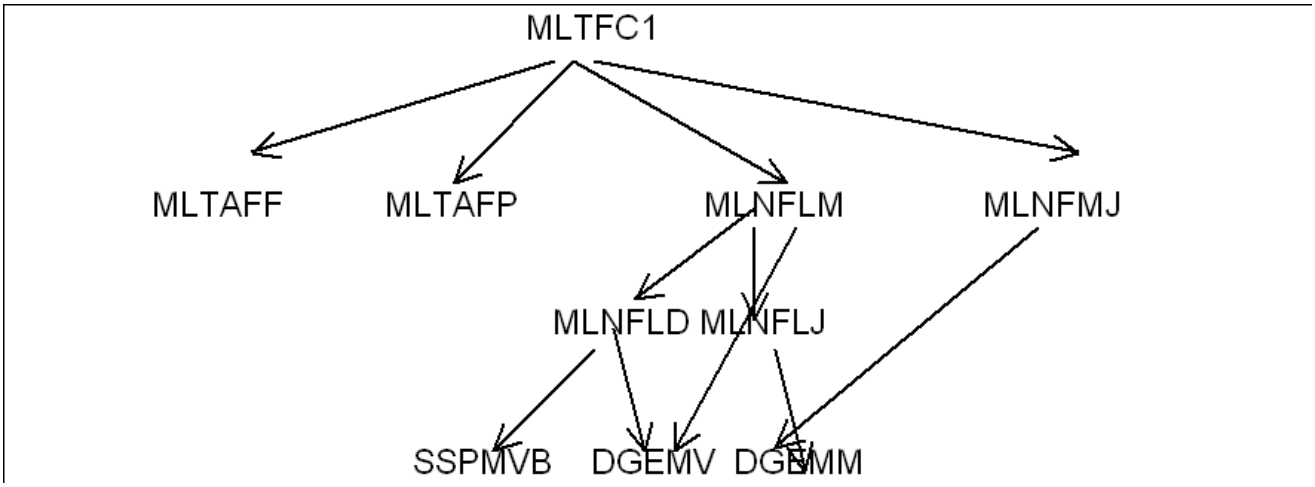


5 Descent-increase per blocks NON-symmetric

5 the divergence

between the symmetric versions and NON-symmetric Version is inside routine MLTFC 1, the tree structure of the routines called in the NON-symmetric case is the following. (MLNFLM

, MLNFMJ , MLNFLD , MLNFLJ respectively replace MLTFLM , MLTFMJ , MLTFLD , MLTFLJ). Figure



6 real Tree structure not – symmetric. Version

6 complexes symmetric

6.1 complex Factorization

symmetric complex factorization is represented by the following flow chart, the changes in the names of routines are marked in fat. MLFC 16 replaces MULFR 8 and MLTASC carries out the injection of the initial terms in a way similar to MLTASA . Complex

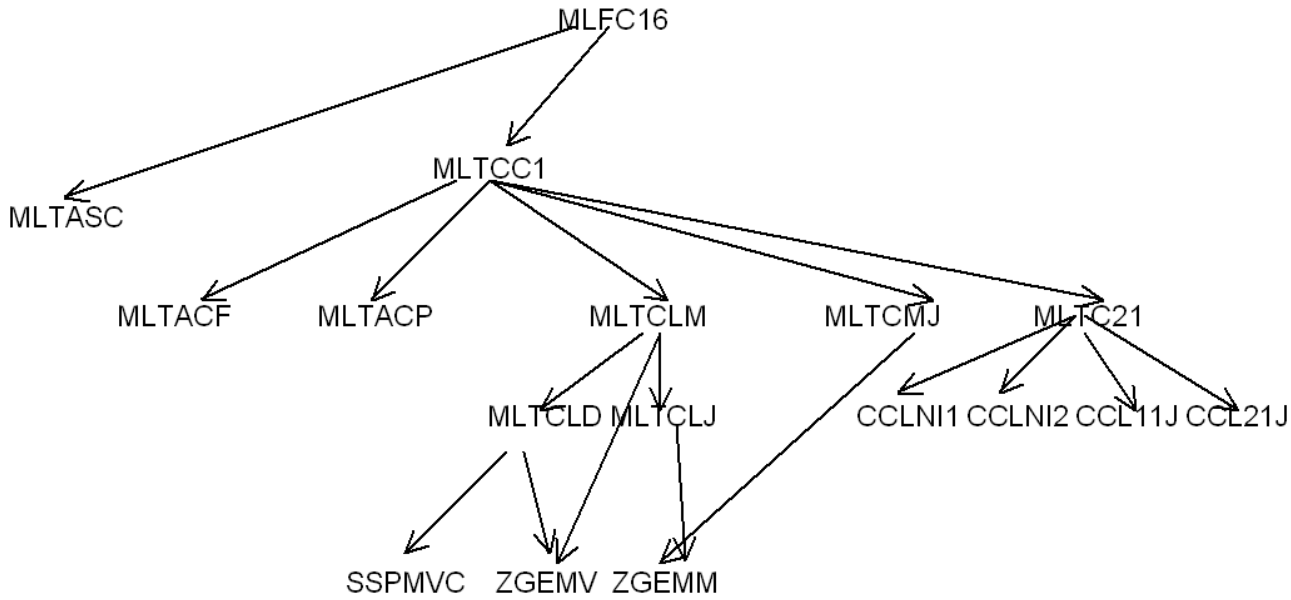


figure 7 Version symmetric NON-symmetric

6.2 complex Factorization

asymmetric complex factorization is represented by the following flow chart, the changes in the names of routines are marked in fat. Complex

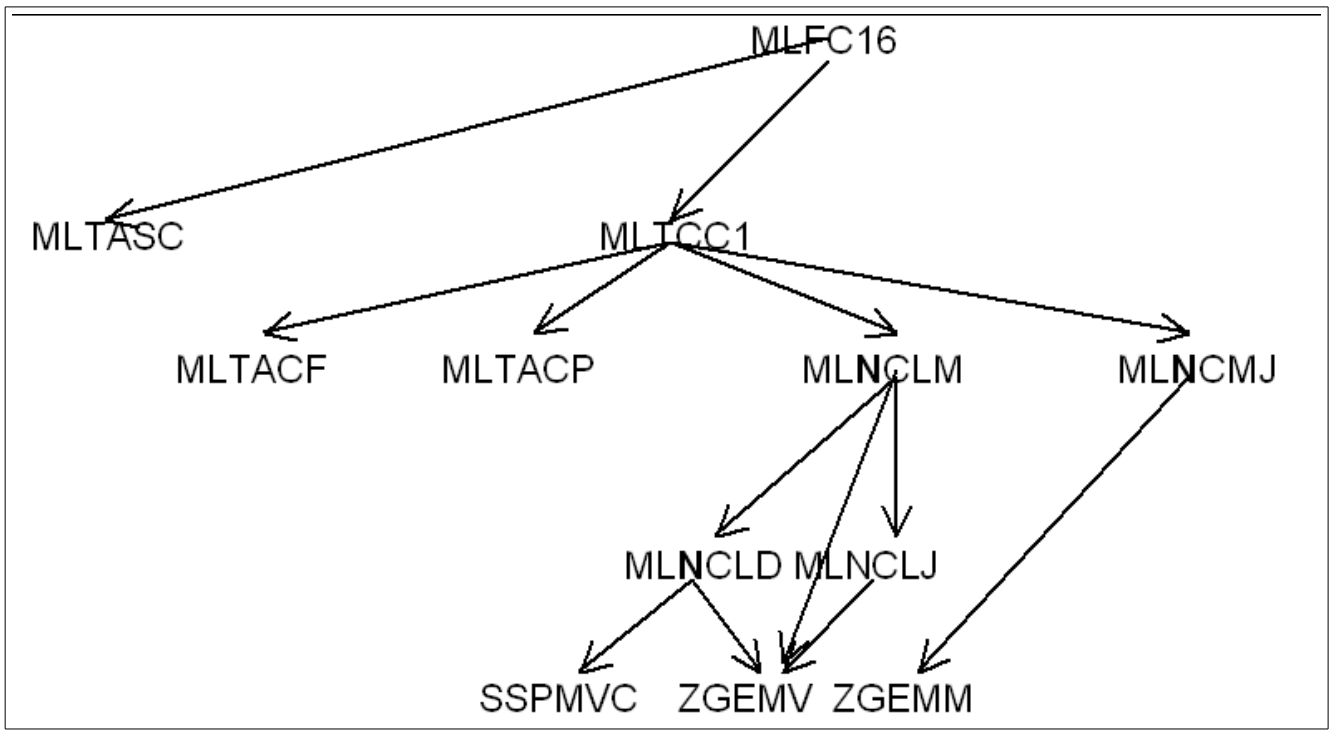


figure 8 Factorization asymmetric Descent

6.3 - increase complexes

routine RLFC 16 is the equivalent complex RLTFR 8, and MLTDCA, the equivalent of MLTDRA.
The version per blocks for several second members RLBFR 8 in realities does not exist in complex. MLTDCA

calls SSPMVC and ZGEMV, the latter, of the Blas library, are the complex version of DGEMV.
SSPMVC is the complex version of SSPMVB. Parallelization

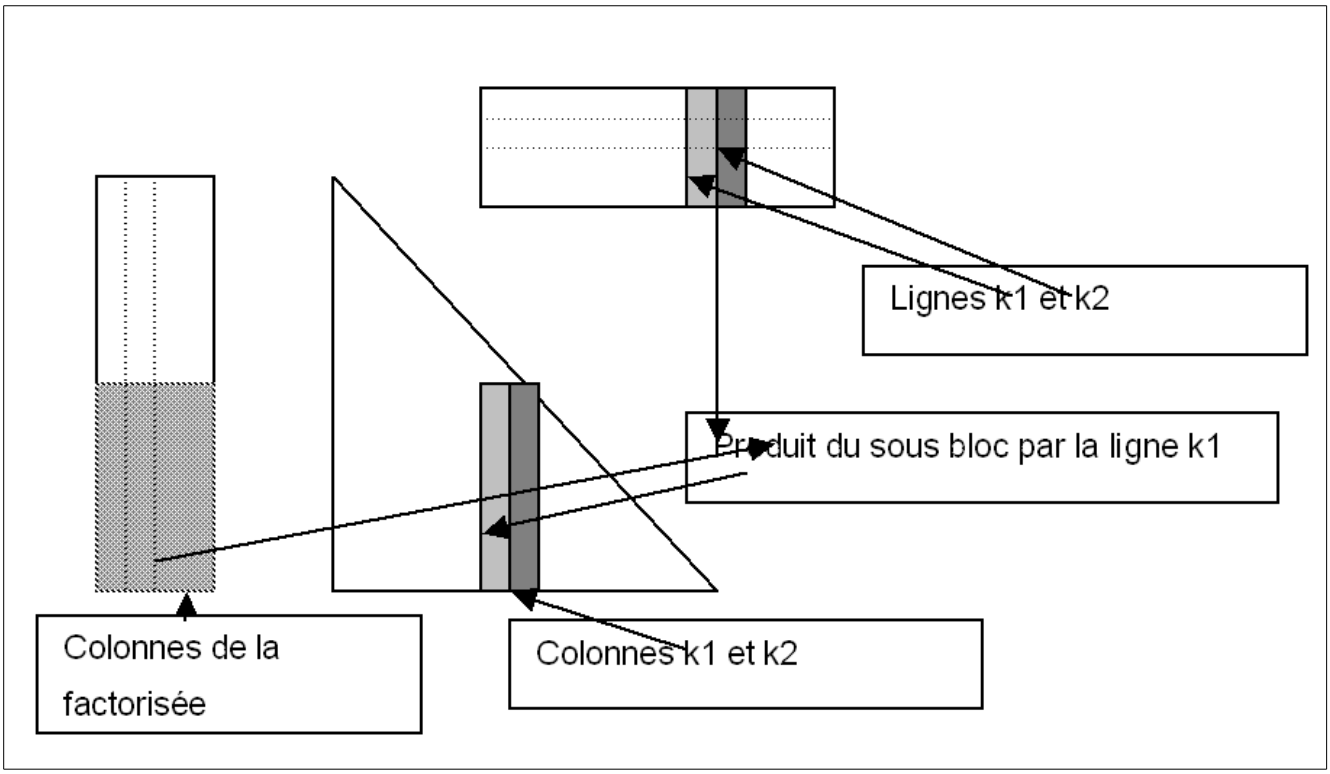
7

parallelization in MULT_FRONT is carried out by Openmp directives. These directives are placed in the following routines: Symmetric

real case: MLTFMJ, symmetric MLTFLJ
complex Case: MLTCMJ, asymmetric MLTCLJ
real Case : MLNFMJ, MLNFLJ asymmetric
complex Case: MLNCMJ, MLNCLJ

implemented parallelization is “known as” intern, it takes place inside the process of elimination of a super node. The elimination of the super nodes, known as “external” can also be paralleled. But it is not implemented for the following reason: Simultaneous elimination several super nodes requires an occupation of the memory higher than that of the sequential version. However the concern of the occupation of the memory always prevailed that of the saving of time of restitution at the time as of preceding developments of MULT_FRONT.

Internal parallelization, it, does not require any additional memory with that of the sequential version, it does not require either any development of particular code, only a simple addition of directives. One
will describe the parallelization of the routine MLTFMJ, that of MLTFLJ follows the same principles, as well as the other routines referred to above. Figure



9 Diagram of the update of the frontal matrix One

sees on the Figure above, a diagram of the update of the frontal matrix during the elimination of a node. The triangle represents the lower part of the frontal matrix, and the 2 rectangles represent the columns of the factorized matrix, columns corresponding only to the super eliminated node. Initially, one will reason by columns. It is known that one updates the column of $k1$ the frontal matrix by withdrawing to him the product of the under-block of columns (in grayed above) by line (multiplied $k1$ itself by the diagonal terms). (operation of the Blas2 type). This operation of update is paralleled without problem by a directive OpenMP, the columns of the frontal matrix are adjacent, it does not have no conflict of addresses there. All the variables are shared, except the indices of local loops and the variable. One saw above that by preoccupation with a performance, one works per block of columns, in order to use of Blas3, parallelization evoked above is thus done makes some on the blocks of columns and not on the columns themselves. Outline

of the code: C$

```
OMP PARALLEL C DEFAULT (PRIVATE) C$
OMP+SHARED (N, M, P, NMB, NB, RESTM, FRONT, ADPER, DECAL, FRN, WK., C) C$
OMP+SHARED (TRA, TRB, ALPHA, BETA) C$
OMP+SCHEDULE (STATIC, 1) C
     1000 KB = 1, NMB NUMPRO
     =MLNUMP () C
K    : INDEX OF COLUMN IN THE MATRICE FRONTAL (ABSOLU OF 1 A N) K
       = NB* (KB-1) + 1 +P C
       100 I=1, P S
         = FRONT (ADPER (I)) ADD
         = N* (I-1) + K C
         50 J=1, NB WK.
           (I, J, NUMPRO) = FRONT (ADD) *S! WK. contains the products: diagonal*ligne term ADD
                  = ADD + 1 50
 CONTINUE          100
 CONTINUE      C
```

```
          500 IB = KB, NMB IA
              = K + NB* (IB-KB) IT
              =1 CAL
              DGEMM (TRA, TRB, NB, NB, P, ALPHA, FRONT (IA), N, &
     WK.                    (IT, 1, NUMPRO), P, BETA, C (1,1, NUMPRO), NB) C
RECOPY     C

C
              501 I=1, NB I1
                 =I-1 IF
                 (IB.EQ.KB) THEN J1
                    = I IND
                    = ADPER (K + I1) - DECAL ELSE
                 J1
                    =1 IND
                    = ADPER (K + I1) - DECAL + NB* (IB-KB) -  I1 ENDIF
                 C
                 502 J=J1, NB FRN
                        (IND) = FRN (IND) +C (J, I, NUMPRO)! Recopy in the frontal
matrix frn IND
                    = IND +1 502
 CONTINUE           501
 CONTINUE         500
 CONTINUE      1000

 CONTINUE C$
OMP END PARALLEL C N.
```

B. Parallelization.

The sequential version requires one working table, TRA written for each block, it is necessary to duplicate it for parallelization. In the parallel loop, one calls on the function MLNUMP which provides the number of thread treating the iteration of loop; NUMPRO , one works then in plane NUMPRO of the table. TRAV Various

8 remarks Some

parameters, threshold values, are used in MULT_FRONT . They are intended to optimize the code, in terms of computing time. It is: NB
: length of the blocks for the use of DGEMM . *NB* is provided by the function LLBLOC () which returns value 96. It would be convenient with each change of processor to check if this value is optimal. (fixed *PMIN* at 10 in MLTFC 1) . This value is related to the preceding one. The super nodes whose size (many degrees of freedom, given by) *LGSN* is lower than, *PMIN* are treated by MLTF 21 and not by MLMTFLM , MLTFMJ . That wants to say that the unknowns are treated column by column and not per block with call to SDGEMM) . This

threshold aims at simplifying the processing of the small benchmarks and not to activate the machinery per blocks for the small super nodes. :

NBSOL It is the number of second members treated at the time of the gone up descent/, if is *NBSOL* lower than 4, the gone up Descents/are carried out the ones after the others by MLTDRA , if not one works per BLOCK in RLBFR 8. : *SEUIN SEUIK* values used in MLTDRA : they determine the use of DGEMV

for the product matrix-vector, under these thresholds, one will call SSPMVB " optimized" with the hand. (Being given the little of weight of MLTDRA , these 2 thresholds could be removed). As

one already noticed above, it would from time to time be advisable to check if these thresholds are adequate. Possible

9 conclusions, developments.

Report [RB12] was diffused. It serves as detailed conclusion. It offers an inventory of fixtures and more detailed prospects on maintenance and the possible developments for MULT_FRONT , in the context of the availability in Code_Aster , *of* another solver, MUMPS. One summarizes however in the 2 following paragraphs, the perimeter of execution and the assessment of the performances of MULT_FRONT . Perimeter

9.1 of execution

the perimeter of the multi-frontal method is almost complete since the developments of 2011 which make it possible to factorize the "generalized" matrixes known as. Only the numerically unstable systems, requiring a method of pivot (X-FEM for example) are to be excluded from the choice of solver MULT_FRONT . A less recent development (renumbering of the nodes of interpolation and either of the degrees of freedom), makes it possible to preserve the order of these degrees of freedom inside a node and makes it possible to treat the incompressible elements. The recourse to MUMPS is the solution for the systems requiring a method with pivot. However a development of MULT_FRONT is possible: it is possible to carry out, inside each super node, i.e. among the unknowns eliminated with each stage, a search (obviously partial) for pivot. A more complete search, would then imply the fusion of several super nodes (fusion of matrixes girl and mother) and appears not easily possible. This partial swivelling requires a considerable quantity of work and would constitute a risk for the stability of the code. Performance

9.2

the sequential performances (mono-processor mode) are comparable to those of MUMPS in much of case. Only the cases presenting many linear relations between the degrees of freedom can be very unfavourable with MULT_FRONT which creates matric filling in these cases. Sometimes it was enough to reorder the data of these boundary conditions to solve the problem. With regard to

parallelism (localised as one saw higher, inside the elimination of each super node), it is used little and to little offer a factor of acceleration between 2 and 3 for an execution on four processors (or hearts of processors). This parallelism is interesting for the large case requiring much memory and which must practically only be carried out out of machine. That makes it possible to notably reduce their period of residence out of machine. The arrival of processors equipped more and more with hearts should provide the occasion of new benchmarks for such large cases. However this parallelization in shared memory does not offer gain in memory. What allows parallelization in memory distributed (MUMPS). Often this problem of memory is a point blocking for the large linear systems.
The multi-frontal method gives the opportunity of another more elaborate parallelization on the various branches of the shaft of elimination. It is not possible to program it in MULT_FRONT , it would be "to remake" what is made in MUMPS. The code was not conceived for parallelization by sending of message. References

10 . [OF

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5 12] Pink C., Boiteau O., native multi-frontal Method in Code_Aster: prospect and inventory of fixtures, CR-I23-2012-001